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$((\lambda_1\lambda_2) \vdash n)$ [CT00]. $((\lambda_1\lambda_2, \cdots, \lambda_{m\leq(n/2)}) \vdash n)$ [CT00]. $(1 \leq I_i \leq 3)$ [Tem02a]. $(1 \leq n \leq 12)$ [GW06a]. $(2 \leq n \leq 30)$ [FBBB06]. $(2 \leq n \leq 7)$ [FTB04]. (2×2) [YT03]. $(m + n = 2--5)$ [GW06b]. $(m, n \leq 4)$ [PC09]. (n) [Tem02a]. $(n, m \leq 4)$ [FPC05]. $(n = 0, 1, 2, 3, 4)$ [TCS+08]. $(n = 0--2)$ [LWL+08]. $(n = 1--10)$ [SLW+07]. $(n = 1--26)$ [BFB08]. $(n = 1 - -3)$ [DZTZ05]. $(n = 1--4)$ [LLX+03]. $(n = 1--5)$ [ZLL+09a]. $(n = 1--7)$ [LCRB01, RBL04]. $(n = 1--8)$ [RBL08]. $(n = 2, 3)$ [FRT+00]. $(n = 2, 6)$ [WSC+05]. $(N = 2--10)$ [YKT+02]. $(n = 2--12)$ [AÖG07]. $(n = 2--4)$ [QMB+06]. $(n = 2--8)$ [FF09, JHLC09b]. $(n = 24, 25, 27, 28, 29, 30)$ [GI07]. $(n = 3--10)$ [QZ07]. $(n = 3--14)$ [LLYJ09]. $(n = 3--5)$ [MBOA09]. $(n = 3--8)$ [XL08]. $(n = 5--21)$ [BES08]. $(n = 5--8)$ [SSSK07]. $(N = 50)$ [YKT+02]. $(n = 7, 9, 11, 13, 15)$ [WSC+05]. $(n = 7--14, 19)$ [BGÖ+01]. $(nleq29)$ [WSBV05]. $(S = 3/2)$ [CC05b]. $(v', j' = 1)$ [BGG08]. $(v'' = 0, j'' = 1)$

[BGG08]. $(x + y = 6)$ [GP03]. $(x + y \leq 30)$ [LGBJ03]. $(x = 1, 2)$ [DR08]. $(x = 1, 2, 3)$ [BLM08]. + [CSG06, Cos06, GB06a, Gög06, LP00a, LWCF08, TKY00, TFBM02, XYS+03, YYZ+05c, YLZ07]. − [Buc02a]. $0, +1, -1$ [FRNM08]. 1 [BG02b, DFH02b, FA00, KG09, QLD05]. $1/r_{12}$ [AS04c]. 10.5 [PRM02]. $1s$ [GFMT08, PCT+04, Sah03]. 2 [Dei06, ITY+09, LQC+08, RI03]. 28 [VNP00]. $2'$ [RVP06]. 3 [BKM+02a, BG02b]. 3.6 [PRM02]. $4d$ [BC03]. $4f^{114}$ [Bec02]. $4n$ [Buc02a]. $4n + 2$ [Buc02a]. $4n\pi$ [Buc02b]. $4p$ [SK01a]. 5 [AGM02, BG02b, FS00, RLB02]. $5'$ [ZLSL06]. 6 [BNHB+02, FS00]. 9 [XXY00]. = [AZD06, Ano07g, Ano07e, BK04a, BDBG09, BB05d, CZPJ01, CMY06, DLTW04, DETA02, FRNM08, GR07a, GR07c, GR07b, GYF+09, HZJ+07, HGRL01, HS05, JLAR07, LTV02, LDXW04, LZJ+06, LLW+07, LDR+08, LAQ+09, LL04, Liu08, MMV05a, MOAM07, SYL05, SCHW07, SZJ+04, TLYW06, VK08, VGMN03, XD03, YST+05, YS05, YWC07, ZLHL02, ZL04, ZWSJ01]. $[2 \times 2]$ [RWW+06]. $^{+}$ [ASL06, AV04, AV05b, AL09, BTL+02, BG00c, Buc05a, CT05, CSDCCMZT03, CMY03, CMY06, DF07, Dei04, Dei06, DETA02, EBB06, GD00b, Gög06, HGS03, IAMY02, IN09, KYA03, KY05, KB08, LY09, LCRB01, LTLS05, LTL05a, MMS+09, MOA07, Met05, MTWN09, MHP04, NWSC08, SK01a, SK05a, SSSK07, SKA05, SZL+09, SdACAG03, Str00, UMDM06, WF04, XYS+03, Ye01, YW05, YCS09, ZLL+09a, ZJZ00, ZL04, ZFD00b, ZNZS00]. $^{++}$ [CCR09]. $^{+4}$ [BPM01]. $^{-}$ [Ano07g, Ano07e, ARBD05, BL02b, BBD07c, CK03, Dav04, DETA02, GR07a, GR07c, JLAR07, KZS07, LCRB01, LZJ+06, LAQ+09, LCL+09b, LČM01, Mar06b, MB07b, MD04, MBD05, MJ06, SYL05, TWZ03, YBS05, ZJZ00]. $^{-1}$ [XFLX+06]. $^{0/n+}$ [SCHW07]. ^{1} [BAG+08, DL06, GBA05, KM06, PGNT02, Pen00a, QCFJ05, TM05, YYZ+05c, Ye01, YW05, ZH06]. ^{1,3} [BBPG08, YAŞ00]. ^{10} [JNSF04, MOAM07]. $^{10-}$ [SCW09]. ^{11} [CT00]. $^{1}2$ [Tem02c, Tem04, Tem02c, Tem04]. ^{13} [BAG+08, PGNT02, RCF02, RNVTP09, Seb05, dLCRF+08]. ^{14} [Tem02c, Tem04]. ^{15} [PGP+07]. ^{17} [LV01b]. $^{18+}$ [SI09]. ^{19} [Sch05]. ^{1}D [HAL+02]. $^{1}\Delta$ [KPČM05]. $^{1}\Sigma$ [BMMC09a, RV05, YYZ+05c]. $^{1}\Sigma^{+}$ [KPČM05, KCS02, XYS+03]. ^{2} [BMŁT07, BMMC09a, BMMC09b, CDB02, FGR+07, GB06a, HH05, IV02, KCS02, LV01b, MB06, SI09, SCTK+09, TKY00, Tem02c, Tem04, WF04, YHC05, ZLH+08]. $^{2+}$ [ASL06, BMŁT07, BFAM03, CNC+06, GdRPLP08, MBD09, RSTG02, SGP+07, ŠUKŽŠ07, VRA+02, XL08, YCS09]. ^{2,3} [Str00]. ^{2,5} [DQZ04]. $^{2}-$ [ARBD05, AGLBM03, DETA02, GL00, VIGL+05]. ^{235} [Sch05]. ^{27} [LV01b]. $^{2}\Pi$ [TM05]. ^{3} [AGLBM03, DL06, FN04, GW05, IAMY02, KM06, Met05, SYLE07, STW+05, TM05, YHC05, YYZ+05c, ZCFD02]. $^{3}+$ [VSD+02, BMŁT07, Bec02, BSBS06, BSB07, CNC+06, JSvDA06, KNO09b, LMSB00, MMZ02, NF02, TFBM02, YWC07]. ^{31} [SKNN09]. $^{3}\_\_$ [CL07b]. $^{3}n \to \pi*$ [DW00]. $^{3}\Pi_u$ [SSZ+07, TBML06]. $^{3}\Sigma$ [PCBA08, TBML06]. $^{3}\Sigma^{-}$ [KPČM05, SYZ+09, SZL+09]. ^{4} [Bec02, GW05, LB06, SYLE07, SI09]. $^{4+}$ [CNC+06, SBM00, TFBM02]. $^{4-}$ [YST+05]. $^{4}\Sigma^{-}$ [TM05]. $^{5+}$ [EMM+02a]. $^{6+}$

[Sah03]. $^{6-}$ [BK04a]. ^{7} [PRM02, SSZ$^+$07]. ^{8} [MOAM07]. $^{\cdot}$
[BEM02, MB06, VG02]. ^{II} [ZSL$^+$09]. ^{III} [BPM01, ZLY05]. $^{n+1}$ [JHLC09a].
$^{n-}$ [YST$^+$05]. $^{\prime}$
[CN03, DBFP05, DDD03, KKMS04, RVP06, SBB05, WF04, ZLL$^+$05]. $^{\prime\prime}$
[BMMC09a]. ^{V} [YST$^+$05]. ^{VI} [YST$^+$05]. ^{y} [FRNM08]. $_{(1-x)/2}$ [Oni09]. $_{(10-n)}$
[BLC$^+$00]. $_{0}$ [Els05, PGP$^+$07]. $_{1}$ [BE07, BES08, DBFP05, DGLM09, GV06,
HH05, MLSG04, TM05, ZMAL04, ZLH$^+$08]. $_{1-x}$ [SZSP02, ZSPS03]. $_{10}$
[RWW$^+$01]. $_{11}$ [SNN$^+$09]. $_{12}$
[LDP05, MGAS09, SCW09, TI05, TOB02, YZY$^+$01]. $_{120}$ [TNO09, TRF$^+$00].
$_{14}$ [LDG$^+$06]. $_{15/2}$ [Bec02]. $_{19}$ [ZDQF08]. $_{2}$
[AM07, AGBY00, AC04, AC05, AC06, AC07, AWZD05a, AWZD05b, AZD06,
ANM03, AL09, ACB$^+$02, BB05a, BM01b, BGG08, Baň05a, BML01, BPM01,
BEM02, BDA$^+$02, BJ00, BT05, BCD$^+$05, BES04, BDBG09, BFBB06, BFB08,
BB01, BB04, BB05d, BGJJ01, BCS01, BZR02, BSK$^+$02, BMMC09a,
BMMC09b, CGL$^+$05, CB04, CSG06, CNPA04, CBMRN08, CZPJ01, CT05,
CCH05, CCH06, CC00c, CSTB08, CMY03, Cos06, CCB07, DCO$^+$08, DP06,
Dav04, DKS05, DW00, DLTW04, DS03, DGQT09, DMG09, DLM$^+$02,
DLM$^+$04a, DLM$^+$05, DZTZ05, DBLM06, DZ06a, DSW08, EMM$^+$02a, Eva04,
EP02, EB04a, ESU05, FL04, FFLZ02, FGC04a, FGC04b, FM02a, FBBB06,
FSLL04, FS08, GEB$^+$00, GSC00, GV06, GW02, GB06a, GBMMSA00,
GGS09a, Gre09, HZJ$^+$07, HL05, HGRL01, HSN$^+$09, HKMM04, HW02,
HDL00, HLMH07, HR05b, HH05, IAMY02]. $_{2}$
[ILB$^+$08, Irg04, Irg06, IN09, Jal02, JCTA08, JJ02, JFS$^+$09, JXW$^+$04,
JWM00, JG09, KM02, KNN$^+$04, KSI$^+$07, KSN$^+$09, KCS02, KSS00, KN08,
KTN02, KM06, LJL09a, LP00a, LLX$^+$03, LDXW04, LLW$^+$05a, LLW$^+$05b,
LZJ$^+$06, LZZ$^+$06a, LWL$^+$08, LC05, LN03, LLL$^+$07, Liu08, LJL09b, LXY00,
LWCF08, LNPL06, LH07c, MY08a, MKLP02, MA05, Mar09, MVdCD00,
MMCC02, MS05, MO06, MH09, MNJP05, MP00, MOA07, MZD01, MLZS06,
Met05, MJ00, MLL01, MCZWD06, MTO$^+$03, MJ06, NRS$^+$02, NF02, OM04,
POAVdlM08, PILD07, PR09, Pen00a, Pen06, Pet00, PM09, QTT07, QGW02,
RD00, RV05, RdTdLC$^+$07, RNS04, Sad02, SL07, SYLE07, SMAL01, SAM08,
SGP$^+$07, SBM00, SSZ$^+$07, SCRR02, SAE08, SdACAG03, SLCW04a,
SLCW04b, SSK09b, ŠPNU08, STW$^+$05, SHH$^+$06, SLW$^+$07, SZJ$^+$04, SNN$^+$09,
TI05, TLYW06, TSP$^+$07b, TSP$^+$07a, TBML06, TFBM02, TWZW09]. $_{2}$
[TIGD09, Tor04a, Tor04b, TM05, USM01, VRS01, VRA$^+$02, VBML01,
VHM$^+$04, VK08, VG06, VPS$^+$04, WQ00, WFS$^+$01, WGLX02, WSC$^+$05,
WZWC06, WML08, Woo02, WZWC07, XD03, XXJG04, XV00, XV01,
XXMJ06, XCC$^+$08, YST$^+$05, YMZH04, YYZ$^+$05c, YLS$^+$04, Ye01, YW05,
YHD$^+$07, Yur06, ZZFL00, ZLZ05, ZLL$^+$05, ZH06, ZD06, ZD07a, ZMAL04,
ZJZ00, ZHS06, ZD07b, ZD08, ZQF$^+$02, ZZW$^+$06, ZLY$^+$09, ZLH$^+$08, dD04,
dlPCLG$^+$00]. $_{2,3}$ [OCWY09]. $_{2-x}$ [CB04]. $_{20}$
[Tem02c, Tem04, KR07, LZXD05, Tem02c, Tem04, ZWMZ04, ZDQF08]. $_{21}$
[YST$^+$05]. $_{22}$ [LDG$^+$06]. $_{23}$ [YST$^+$05]. $_{2}4$
[LTL05a, CZS$^+$05, LDPP05, SRS$^+$04, YZY$^+$01]. $_{28}$

[MLL01, TCS+08, TNET03]. $^{+}_{2}$ [Jal02, PT00]. $^{-}_{2}$ [BG00c]. $^{2+}_{2}$ [Jal02]. $^{3}_{2}$ [GW05]. $^{4}_{2}$ [GW05]. $_{2A}$ [VED+02]. $_{2\mu}$ [MVdCD00]. $_{2n}$ [XL08, ZCWZ04, ZLL+09a]. $_{2n+1}$ [ZCWZ04, SSSK07]. $_{2v}$ [Buc00a, Gre09, QV01]. $_{3}$ [AWZD05a, AWZD05b, AL09, ACB+02, Ano07g, Ano07e, Ano07f, AGLBM03, BVG05a, BRL02, BT05, BCD+05, BKAT00, CIP+03, CA07, CK03, CGL+05, CSX+01, CBMRN08, CC00c, CSTB08, CMY06, CBC00, DETA02, DR08, DBG04, DBPG04b, DLM+02, DLM+04a, DLM+05, EBB06, ES02, EF03, EP02, EKZ06, ETBA06, FWZ09, FF01, FGC04a, FGC04b, FN04, FDLK02, GR07a, GR07c, GR07b, GSRL06, GJB02, GJ03, GB05, GDFT01, GMS+05, GMS01a, HGS03, HGRL01, HW02, HH05, Irg04, IN09, JCTA08, JJ02, JSvDA06, JFS+09, Kak03, LLW+05a, LLW+05b, LH07a, LLW+07, LP08, LDR+08, LC05, LMSB00, LH00, LWCF08, LH07c, MY08a, Mar09, MB06, MMV05a, MMCC02, MS05, MO06, MOAM07, MBOA09, Met05, MMZ02, MG08, MS00, MCZWD06, Mor04, MGAS09, NRS+02, NF02, Oni07, Oni08, Oni09, PILD07, PNBV07, Pet00, PTS03]. $_{3}$ [REHH07, RSFRB03, RD00, RNS04, SYLE07, SASS03, SGP+07, SdACAG03, SHC00, SP00, SZSP02, SVT06, SR07, SV08, SUH+01, SSK09b, SLWS07, TLYW06, TSP+07b, TCS+08, TW05a, TKS+05, TWZW09, UES04, VRA+02, VK08, WML08, Woo02, WCP+00, WZWC07, XXJG04, XV00, YST+05, YZG06, YLZ07, YLS+04, YKS+06, YW05, YYY+00, Yur06, ZSPS03, ZLHL02, ZD07a, ZLML05, ZCZF02, ZZW+06, dD04]. $_{3+8n}$ [COMA03]. $_{3-n}$ [SASS03]. $_{3-x}$ [DR08]. $_{3/2}$ [Bec02]. $_{30}$ [LZXD05]. $_{3}2$ [SCHW07]. $_{38}$ [MLW+09]. $^{+}_{3}$ [Hag01, RLGB01]. $^{2-}_{3}$ [CG09]. $_{3h}$ [GJ03, OBM06]. $_{3v}$ [GJ03]. $_{4}$ [AWZD05a, AWZD05b, Apo06, ARBD05, BB05a, BP03, BCD+05, CL05d, CXZ09a, CSTB08, COMA03, CT00, CMY03, DLM+02, DLM+04a, DLM+05, DBLM06, Eva04, GSRL06, GYF+09, Kak03, KZS07, LL04, LNSE02, LWCF08, LH07c, MMS+09, MST04, MST08, MVdCD00, MOA07, MS00, MTO+03, MC06b, PSN08, PBS02, PMLC09, PGP+07, RGP07, SNH00, TKY00, UML00, VRA+02, VIGL+05, VPS+04, WQ00, WNW05, WT06, XCC+08, YLZ07, YW05, ZCZF02, dD04]. $_{4-n}$ [LWL+08, TCS+08]. $_{4}0$ [Tem02c, Tem04, LPZW05, MLW+09]. $_{42}$ [MLW+09]. $_{44}$ [SCW09]. $^{-}_{4}$ [QV01]. $_{5}$ [BT05, CBMRN08, CC00c, FF01, GDFT01, GL00, IN09, LH07c, MVdCD00, MAS09, MGAS09, TSP+07a, VRA+02, VK07, YST+05, ZL04]. $_{50}$ [LPZW05, XXY+05]. $_{551}$ [STN+06]. $_{5}9$ [SYL05, RFS+00, SYL05, ZFD05]. $^{+}_{5}$ [CSM02]. $_{5d}$ [DGQT09]. $_{6}$ [BK04a, BC03, CC00c, DETA02, HDL00, ITY+09, LJL+03, LLYJ09, LH00, LLP05, Mar09, MVdCD00, MMZ02, MLL00, RSFRB03, RD00, SBM00, SCW09, SST00, SNN+09, ZLXL07, ZFD00b]. $_{6-n}$ [Sch05]. $_{60}$ [ASH08, BZR02, DM00, FFFR01, FFFR02, FRT+00, FRGF04, HNKiS01, JV05, MS03, Pau04, PDS04, RHH+02, SNZG02, She04a, She07d, SLA+05, SRS+04, VM07b, YLS+04, ZWMZ04, ZKRS07]. $_{69}$ [RFS+00]. $^{+}_{6}$ [CSM02, LJL+03]. $^{-}_{6}$ [LJL+03]. $^{2+}_{6}$ [MKLP02]. $^{2+/3+}_{6}$ [ZLHL02]. $_{6d}$ [LTL05a]. $_{7}$ [GDFT01]. $_{7-\delta}$ [Yur06]. $_{70}$ [CZS+05, VM07b]. $_{72}$ [MLL00, SUA+04]. $_{74}$ [LH07b, SUL+07, SUL+08]. $_{75}$ [TWZ03]. $_{78}$

[MLL00, SUA+04, TW05a, WT06]. $_{8}$ [BK04a, CGL+05, CXZ09a, CT00, DKS05, GEB+00, KSWR00, LZXL05, TOB02]. $_{80}$ [DGQT09, SLU+06, YKS+06, ZDQF08]. $_{81}$ [ZDQF08]. $_{84}$ [KLK08, RGP07]. $_{9}$ [MHP04]. $_{A}$ [FH02b, GS00b, GS01, GSH02, HSH02, HP07, KS09, Sey08]. $_{A1}$ [SKA05]. $_{A2}$ [SKA05]. $_{b}$ [JZZ+08]. $_{c}$ [DB04b, FPJR03, KKM+01, SM04, YYK+03, YNN+06]. $_{d}$ [TCS+08]. $_{g}$ [DL06]. $_{k}$ [SČL00]. $_{lab}$ [MMS+09]. $_{m}$ [FPC05, GWJ05, GW06b, JXW+04, KTK+04, PC09]. $_{\mu}$ [DZ01]. $_{N}$ [Ano07g, Ano07f, GR07c, GR07b, LB06, ONA05, SRW+06, YKT+02, ZRRC05, ASO+06, AÖG07, BE07, BES08, BLC+00, BFB08, BGÖ+01, CT00, DP06, DZTZ05, FRT+00, FTB04, FBBB06, FF09, FPC05, GGPS06, GWJ05, GW06a, GW06b, HEJ+00, Har04a, JHLC09b, JG09, KTK+04, LCRB01, LLX+03, LWL+08, LLYJ09, MOA02, MDJ01, MRT00, PC09, PBI+01, QMB+06, QZ07, RBL04, RBL08, RPB00, RBLS04, RNS04, Sad02, SASS03, Sch05, SLW+07, TCS+08, Tem00, TRF+00, USM01, WSBV05, WSC+05, XXJG04, ZMZ+09]. $_{n-1}$ [JHLC09a]. $^{+}_{n}$ [LTV02]. $^{-}_{n}$ [WFS+01]. $^{q}_{n}$ [MGCD01]. $_{n\leq 20}$ [Tem02b]. $_{QQ}$ [LV01b]. $_{x}$ [BLM08, DR08, GH03, GP03, LGBJ03, Oni09, SZSP02, ZSPS03]. $_{y}$ [GH03, GP03, LGBJ03]. $_{z}$ [WE01]. $^{\cdot}_{z}$ [WE01]. α [Bou03, CVPGH+06, CJZZ06, CC05a, CTLZ01, CHC05, CR08b, DFT+07, GYS+06, HOC00, JNF+09, JTC+03, LDM09, MCZWD06, NRS+02, PK01a, PVW03a, PVV+04, PVB+02, SSK09b, TA07, YF07, Yur08]. B [PH09, SHE+00]. β [AG08, CQN+03, CTLZ01, DH04a, ERC+02, HY04, HQL09, JTC+03, JFJMR08a, JFJMR08b, LSM+06, LWZ+09, MAFR08, NRK+05, PIGN02, Yur08]. $\mathcal{C}^{\lambda\vdash(n=20):(M)}$ [Tem02c, Tem04]. $\mathcal{S}_{20}$ [Tem02c, Tem04]. $\mathcal{S}_n$ [Tem02b, Tem02a]. $\cdot$ [JXZ+05, KSI+07, KS03a, ZLX+07, ZLML05]. $\chi(\mathcal{C}_i(\mathcal{S}_n \downarrow \mathcal{G}))$ [Tem00]. : [Mar09]. D [CCLK04, Mar06a, MAS07, CL07b, DB04b, HDL00, Mar87b, TOK+00, Whi03]. $D+1$ [DSLC05]. d^8 [MZMZ09]. D_{4h} [SNH00]. δ [AD01, Hog09b, KAE03, SSSS09]. $\downarrow$ [CT00]. $\downarrow \mathcal{G}$ [Tem00]. e [PA04a]. $E = [\rho_A, \rho_B]$ [DW05]. $E \otimes \epsilon$ [ADK02, FMBM05]. $\equiv$ [Sok02]. η^2 [MVdCD00, YLS+04]. η^3 [LH07c]. η^5 [LH07c]. η^6 [HDL00, LH00]. F [EKZ06, HDL00]. G [AVTPR09, CFP00, VATPR09, BG00b, BG00c, BG02b, Nee01, NGRR02]. $G^q_{-nn'}$ [GM02a, GM08]. γ [HR05b, JTC+03, KB00, Mal05b, XCS+03]. $G \supset T \supset D_2 \supset C_2$ [CFP00]. $\hbar\omega$ [KG02]. i [Tem00]. $I^{\text{outer}}M(i_1 \cdots i_n)$ [Tem02a]. J [YYT+04, Orl07]. K [SMDG09, Kut03]. κ [Mar09, RRGP05a, RRGP05b]. $\leftrightarrow$ [ZCZF02]. m [CT00, TOK+00]. μ [GA08, Ghe09, GARB08, JHR+00, KSN+04, MBOA09, NSS09, VGMN03]. N [HEJ+00, AD06, Ban02, Ban05b, FYSS09, Gál07, HQL09, JLPA09, LM02b, PGNT02, VX04, YYK+03, YNN+06, ABC+06, ABM02, BE07, CA01, CC00a, GTSK07, Gri08, GM03, HvLJ01, Kut03, LS01b, MMCC02, Tem02a]. $n + \ell, n$ [AK02]. $n = 0, 1, 2, 3$ [SASS03]. $n = 1, 2$ [TRF+00]. $n = 1, 2, 4,$ and6 [MGCD01]. $n = 1--12$ [USM01]. $n = 1--6$ [WFS+01]. $n = 2--9$ [MRT00].

$n = 2 - 6, 8$ [MDJ01]. $n = 3--8, 10$ [RPB00]. $n = 6--10$ [BLC+00]. $n = 7--12$ [BE07]. N' [HEJ+00]. $n \leq 3$ [PBI+01]. $O\dagger \supset C$ [Fan03]. ω [NMNB06, THP08]. $O \supset T \supset C_3$ [Fan01]. p [BF07, BA01, BA02a, Boe04, GCG05, HHGSRS02, MGG05, NFFA04, RFF05]. Π [DL06, PS03b, BBPG08, Buc00a, Buc00b, Buc02a, Buc02b, Buc05c, CC00a, DMV00, DGSD07, FRK+05, FS00, HBW+08, IA06, JWZ+08, KVF+08, LSPS01, LLW+05a, LLW+05b, LAL+08, LWL+08, LZWY07, MKLP02, MMZ02, Mor02, Mor03, NKN+05, PGB09, PREM05, RFRF05, SSSS09, SS09d, TOK+00, VDF+06, YS09]. pK_a [LS01b]. $\prime$ [BMMC09b, Moh00, YYXC01]. q [BKM+02a]. $q = -1, 0, +1, \text{and} + 2$ [MGCD01]. $Q^q_{nn'}$ [GM02a, GM08]. r_{12} [ANM03, FHK06]. r_{12}^{-2} [Har04b]. $\rightarrow$ [BEM02, Bec02, CSG06, Cos06, Eva04, FGC04a, GSRL06, Gög06, KS03a, LP00a, LWCF08, PREM05, SASS03, Sha07, SL09, VGMN03, WGLX02, XYS+03, YYZ+05c, YLZ07]. S [AV05a, AV06, AE02, RE06, GW02, MNA+99, MBR07]. S_{N2} [HSW+00]. sech^2 [HMMT04]. σ [KVF+08, MLP08, PML07, SSSS09, SMVMC07]. sp [BZG+02]. sp^3 [TT04a, TT04b]. spd [BZG+02]. $\text{su}(1, 1)$ [FDM09]. $SU(3 \leq m) \times \mathcal{S}_n \supset \cdots \supset \mathcal{S}_n$ [Tem02a]. su_q [BKRT03]. T [SEY07]. T_d [SNH00]. $\tilde{A}(^1A'')$ [SSB00]. $\tilde{a}(^3A'')$ [SSB00]. $\tilde{X}(^1A')$ [SSB00]. $\times$ [CT00, Tem00, WL00]. $\times\mathcal{S}_{20}$ [Tem02c, Tem04]. $U^{(r)}(2) \otimes U^{(v)}(4)$ [MYGD01]. φ [KVF+08]. X [BG02b]. $x = 0.5, 0.375$ [ZSPS03]. X_{14} [DETA02]. X_α [KNO09a, SMDG09, SSK09b, TNO09, YPS05, Yur06, Yur07, Yur08]. z [Por03]. $Z = N/3(N = 1--5)$ [SMS+02]. $\zeta(3)/\pi^3$ [BČ02].

***** [BBPG08, CC00a, MST08, PREM05, Ghe09].

-1 [Ess07, ML08]. **-1-benzoic** [HJT07]. **-2** [YYXC01]. **-A** [YS09]. **-acceptor** [SMVMC07]. **-acetyl-** [HEJ+00]. **-acryloyl-formamide** [QCFJ05]. **-Al** [MCZWD06, NRS+02]. **-alanine** [PVW03a]. **-amino** [JTC+03]. **-Aminoacrolein** [JFJMR08a, JFJMR08b]. **-AMP** [ZLL+05, ZLSL06]. **-argon** [PA04a]. **-auxiliary** [Tem02b]. **-band** [YYK+03, YNN+06]. **-based** [RFF05, BP03, She04a]. **-basis** [BZG+02]. **-benzene** [HDL00]. **-benzenesulfonic** [NFFA04]. **-benzylideneaniline** [JLPA09]. **-bipyridine** [CN03, DBFP05]. **-bis** [SBB05]. **-bithiazole** [Moh00]. **-bithiophene** [DDD03]. **-bromoacetyl** [NMNB06]. **-butane** [GTSK07]. **-butyl** [ABM02]. **-C** [LH00, LH07c, ZFD00b, YLS+04]. **-carbons** [CR08b]. **-catalyzed** [LTL06, MLZS06, ZSL+09]. **-chloro** [JNF+09]. **-chromous** [DFT+07]. **-CO** [MBOA09]. **-complexes** [MZMZ09, MWL08]. **-conjugated** [IA06, NKN+05]. **-COOH** [CTLZ01]. **-coupled** [Ban05b]. **-cyclic** [Buc00a]. **-cyclodextrin** [DH04a, HQL09]. **-cyclodextrins** [HY04]. **-D** [RI03, MOAM07, PGP+07, BKM+02a, DFH02b, QLD05]. **-D-glucose** [PVV+04]. **-decomposition** [SSSS09]. **-deformed** [BKM+02a]. **-delocalization** [Buc02a]. **-demethylation** [CVPGH+06].

-deoxyribonucleosides [KKMS04]. **-diimine** [CC05a]. **-diketonate** [NRK+05]. **-diketones** [AG08, AD01]. **-dimensional** [LM02b, MAS07]. **-dimethyl-2** [Moh00]. **-diphenylmethane** [SBB05]. **-DVM** [Yur06, Yur07, Yur08]. **-edge** [OCWY09]. **-electron** [ABC+06, CA01, FRK+05, Mor03, Whi03, Kut03, Mor02]. **-Electronic** [PGB09]. **-encoded** [Tem00]. **-ethylene** [CBC00]. **-ethylenediamine** [CLSD+01]. **-factors** [BG00c]. **-Fe** [SSK09b, KB00]. **-fluorouracil** [AGM02]. **-fold** [Tem02a, VX04]. **-formylnucleosides** [RVP06]. **-Fragmentation** [LSM+06]. **-functionalized** [THP08]. **-furylcinnamic** [PK01a]. **-helicenes** [DCW03]. **-helices** [HOC00]. **-helix** [CHC05]. **-heptane** [MMCC02]. **-Hole** [PML07, MLP08]. **-hydrogenase** [DMG09]. **-hydroxycarboxylate** [CJZZ06]. **-hydroxynitriles** [CQN+03]. **-ion** [SBK+09]. **-Keggin** [GYS+06]. **-lactam** [PIGN02]. **-lactamases** [ERC+02]. **-like** [DLM+02]. **-limit** [Ban05b]. **-matrix** [AE02, RE06, SEY07]. **-membered** [FS00]. **-methacryloyl-aminophenylarsonic** [HHGSRS02]. **-methyl** [PGNT02]. [**?**]methyl-NQiao:2005:TSO. **-methyl-salsolinol** [HQL09]. **-methylacetamide** [FYSS09]. **-methyladenine** [XXY00]. **-methylamide** [HEJ+00]. **-methylchrysene** [RLB02]. **-migration** [LWZ+09]. **-model** [YYT+04]. **-neopentane** [HH05]. **-nitroaniline** [BF07]. **-O** [CNPA04]. **-O-bridged** [NSS09]. **-O-Ru** [BPM01]. **-opioid** [JHR+00]. **-orbital** [CL07b]. **-oxo** [GARB08]. **-oxo-bridged** [KSN+04]. **-particle** [Kut03, Gál07]. **-particle-hole** [AVTPR09, VATPR09]. **-particles** [BA01, BA02a]. **-partitional** [Tem02a]. **-phenylene** [GCG05, RFF05]. **-phenylene-type** [TOK+00]. **-pinene** [Bou03]. **-polyamides** [PVB+02]. **-potentials** [KAE03]. **-proline** [CMR05, FWT08]. **-pyran** [YYXC01]. **-pyridyl-** [PK01a]. **-quartz** [LDM09]. **-representability** [AV06, AV05a, AD06]. **-ring** [Buc02a, Buc02b, PIGN02]. **-sigmatropic** [FBC+06]. **-silylalcohols** [YF07]. **-spin** [Gri08]. **-substituted** [MGG05]. **-subunits** [Yur08]. **-surface** [EB04a]. **-systems** [Buc02b]. **-tensor** [BG00b]. **-tensors** [NGRR02]. **-tetrahydroquinoxaline** [CSDCCMZT03]. **-tetrathia-** [DCW03]. **-thiophene-vinyl** [YYXC01]. **-transitions** [Mal05b]. **-type** [Boe04, GW02, LLW+05a, LLW+05b]. **-uranium** [HR05b]. **-wave** [DB04b, MNA+99, MBR07].

/Al [MMCC02]. **/b3LYP** [GBP05]. **/benzodiazepine** [FH02b]. **/Cl** [LLX+03]. **/ECP** [Mor06]. **/molecular** [BNS05]. **/Si** [LLYJ09]. **/V** [SMAL01].

1 [SCHW07, XXJG04, BMMC09b, CSDCCMZT03, DZ01, GMPIP01, NPLV05, RSFRB03, TGG01, ZZ05]. **1-** [Ess07]. **1-benzyl-tetrahydroisoquinoline** [HQL09]. **1-d** [SSB+07, RSFRB03]. **1-Density** [Pan07]. **1-diazo-2** [SBHF06]. **1-dimethylstannacyclohexane** [FFHT05]. **1-dioxide** [FB07]. **1-halogen-3-methoxy-1-propynes** [Iva05]. **1-hexyne** [ABM01]. **1-methylstannacyclohexane** [FFHT05].

1-methyluracil [PSK02]. **1-octanol** [DGD+05, FGdA00, FGdA02]. **1-oxide** [FS05]. **1-oxides** [SL09]. **1-phenyl-3-methyl-4-benzal-5-pyrazolone** [WJLL09]. **1-phenyl-3-methyl-5-pyrazolone** [DCO+08]. **1-propanol** [ZH05]. **1-substituted** [WT07]. **1/2** [CCEÖ06]. **10-** [DLZ+03]. **10-CH** [CSDCCMZT03]. **10-dimethylene** [OA02]. **10-perylene** [ZNF05]. **10-phenanthroline** [IABS08, MGMR04]. **100** [SWL04, AC05, BB05d]. **104** [Roy05a]. **106** [Ano06g, Ano07a]. **10A** [SWST04]. **1178** [BB05d]. **14-electron** [NJC02]. **141** [Yam05]. **16-valence** [DLZ+03]. **180** [Tem04]. **1999** [Cas00]. **1D** [DFH02a, FD09, MPKB06, OMNN04]. **1D-periodicity** [DFH02a]. **1H** [LCBC03]. **1H-benzotriazole** [LCBC03]. **1s** [Dei04, Dei06, JJWH04, MB07b, PCT+05, KVF+08].

2 [CSG06, DPS04, GR07c, GR07b, HJT07]. **2-** [HE05, MRST01, SŚRL07]. **2-2** [AS04c]. **2-aminopurine** [BSAL+06, HT07]. **2-aminothiazole** [ZR07]. **2-aryl-1** [AA09b]. **2-benzoquinone** [AEI00]. **2-butene-1** [FSLL02]. **2-butenenitrile** [OCK07]. **2-butyne** [Met05]. **2-D** [HGB08, RI05, SPN03, SBT+03, SPL03]. **2-di** [ML05, MLD06, ML08]. **2-dichlorobenzene** [FGFF06]. **2-difluoroethylene** [CGMT03]. **2-dihydroxybenzene** [VPSH00]. **2-dioxacycloheptane** [FHJ+08]. **2-hydroxybenzaldehyde** [EHN09]. **2-imidazoline** [CMASC01]. **2-indolinone** [LQM+09]. **2-matrix** [Zie02]. **2-methyl-2-propenyl** [HJT07]. **2-methyl-4-nitroaniline** [GBC+02]. **2-methyl-8-quinolinolato** [GSQ+04]. **2-methylol** [ZYC09]. **2-nitrimino-1-nitroimidazolidine** [ZXZ+09]. **2-nitroaniline** [CC01b]. **2-nitrophenol** [CC01b]. **2-nitrotoluene** [CC01b]. **2-O-hydroxypropyl** [HY04]. **2-pentoxy** [LH03]. **2-pyridylcarbonyl** [BT05]. **2-pyridylmethyl** [CLSD+01]. **2-pyridylpyrazolate-based** [BZL+09]. **2-rearrangement** [ZFFX05]. **2-Se-** [HJT07]. **2-silylethyl** [JFS+09]. **2-thienyl** [ML05, MLD06, ML08]. **2-thiosubstituted** [FDL03]. **2-thiouracil** [METSH02]. **2-trifluoroethanol** [dA08]. **2002** [Ano04f]. **2544** [Ano07a]. **2CH** [FGC04a]. **2ClF** [WGLX02]. **2D** [EB04a, CHC05, LLLZ06, LLZH09, Sun06]. **2Fe** [SKT+07]. **2Fe2S** [SKK+07]. **2MOLCAS** [VWSA+04]. **2N** [Eva04]. **2p** [CSTB08, MB07b]. **2PU** [LMDW09]. **2S** [SKT+07].

3 [DKS05, DPS04, PIGN02, SCHW07]. **3-** [NMNB06, SŚRL07]. **3-amino-N-methylphthalimide** [SBB06]. **3-amino-propenethial** [RJF+09b]. **3-aminobenzonitrile** [PRM+06]. **3-anilino-1-propanol** [ZTW+09]. **3-butadiene** [AZD06, BL02c, ML08]. **3-cycloheptadienes** [Hes02]. **3-cyclopentadiene** [DQZ04]. **3-dihalocyclobutanes** [LA06]. **3-dioxacycloheptane** [FHJ+08]. **3-dipolar** [KV05, LSCC01]. **3-disubstituted** [BBVS+06]. **3-hexyne** [CWBM06]. **3-hydroxy-propenethial** [RJN+08]. **3-imino-propenylamine** [RJF+09a]. **3-methylaniline** [KB08]. **3-methylfuran** [ZDMF08]. **3-nitro-1** [FXHL05]. **3-propenyl** [FBC+06]. **3-trithiacyclohexane** [FC04]. **3-trithiane** [FC04].

31G [MM07]. **31G*** [MM09]. **33rd** [Ano08c]. **3C** [YI04]. **3C-SiC** [YI04]. **3D** [EB04a, CL07a, JNSF04, Yur07, CLL08, LQC+08, PCKC08, PBTP06, RJP08, Sun06]. **3d-metal** [CL07a, Yur07]. **3D-QSAR** [LQC+08]. **3D-quantitative** [PCKC08]. **3p** [BMŁT07]. **3s** [BMŁT07].

4 [PIGN02, SSB+07, XXJG04]. **4-** [MSMS03, YYXC01]. **4-amino-N-methylphthalimide** [SBB06]. **4-aminobenzenesulfonamide** [PGP+07]. **4-aminophenyl** [HE05]. **4-bromo-** [FS05]. **4-butanediol** [FSLL02, FSLL04]. **4-dialkyl-benzonitriles** [PK01b]. **4-diaza-1** [AZD06]. **4-dibromo-4-silathiacyclohexane** [FS05]. **4-dichloromaleimides** [ZMB+03]. **4-difluoro-4-silathiacyclohexane** [FAE+05a, FAE+05b]. **4-difluorobutadiene** [CGMT03, HGTW03]. **4-diol** [FSLL02]. **4-dioxacycloheptane** [FHJ+08]. **4-fluoro-4-bromo-4-silathiacyclohexane** [Sha07]. **4-fluoro-4-chloro-** [Sha07]. **4-fluoro-4-silathiacyclohexane** [FAE+05a, FAE+05b]. **4-hydroxycoumarin** [MGB+06]. **4-hydroxycoumarins** [SJM08]. **4-imino-4H-pyrazolo** [SSB+07]. **4-methylamino-3-penten-2-one** [RMJ+07]. **4-methylpyridine** [CC00b]. **4-nitrobenzoic** [SŚRL07]. **4-nitroquinoline-1-oxide** [LLZ04]. **4-oxadiazole** [AA09b]. **4-pentadiene** [SBHF06]. **4-phosphasilacyclohexane** [SL09]. **4-pyridyl** [BVS+09]. **4-pyridylethene** [LTL06]. **4-silathiacyclohexane** [FAE+05a, FAE+05b]. **4-silatriafulvene** [TSK01]. **4-thiouracil** [MRST01]. **4-triazine** [LH07a]. **4-triazole-5-one** [FXHL05]. **450** [Pud02]. **496** [SCRSRE06]. **4d** [KDC09]. **4Fe** [KSS+08]. **4Fe-4S** [KSS+08]. **4H** [SSB+07]. **4N** [GEB+00]. **4S** [KSS+08].

5 [KZS07, MMCC02, SAE08, SZK07, SZ08, VED+02, ZMMS+00, ZLL+05, ZSKV04]. **5-** [MSMS03]. **5-azacytosine** [PRL01]. **5-azorhodanine** [EGEDH03]. **5-di-tert-butyl-semiquinonato** [BT05]. **5-dihydro-1** [LY09]. **5-dimethyl-1** [FC04]. **5-fluorouracil** [AGM01, FS08]. **5-hexadiene** [Sak00]. **5-hexatriene** [BL02c]. **5-hexynenitrile** [ABM02]. **5-HT** [VED+02]. **5-hydrogen** [Hes02]. **5-hydroxytryptophan** [ALI03]. **5-methyl-5** [BVS+09]. **5-methylcytosine** [SLL06, TX02]. **5-tetramethoxybenzene** [VBT+07]. **5-triazine** [BABL09, LH07a]. **5-trimethylbenzene** [DDA07]. **5-trinitro-1** [BABL09]. **594** [MCN+05]. **5A** [SWST04]. **5e-MRD-CI** [IMT+02].

6 [MM07, MM09, SBFV05]. **6-** [MSMS03]. **6-31G** [MM07]. **6-31G*** [MM09]. **6-bis-** [YYXC01]. **6-dibromocarbazole** [ZSWL07]. **6-pyrimidinetrione** [DB06]. **6-tetrafluoroanisole** [KCOV07]. **644** [AV06].

7-aminocoumarin [SKN09b]. **7-azaindole** [Cat05, SAMBS01]. **7-azaindole-water** [TYG05]. **7-Cyclization** [SBHF06]. **7-member** [MSMS03]. **784** [AWZD05b]. **7S** [SKK+06].

8-dimethylisoxanthopterin [SRO02]. **8-hydroxyquinoline** [SPS06]. **8-naphthalimide** [dlPOPP03]. **8-oxoguanine** [MSS05, SM05b]. **8-reference** [PČH02]. **85** [ND03]. **857** [AC05]. **85th** [AGL04a]. **870** [Roy05a]. **8Fe** [SKK+06].

9 [Kry08a]. **9-hydroxyphenalenone** [DKP+06]. **9-methylated** [JZZ+09]. **978** [Kry08a]. **978-0-470-86332-9** [Kry08a].

=
[Ano07f, ASO+06, ARBD05, BVG05a, BT05, BBD08, BB04, BG00c, CL07b, DLK00, FRNM08, GT07, HGS03, HDL00, KM02, LSC01, LC05, MGCD01, MMS+09, PSN08, PT00, Pet00, SCTK+09, SCHW07, Var07, WML08, WZJ04, XXJG04, XYS+03, YST+05, YCS09, ZZFL00, ZZHL08, ZJZ00].

A-I [PKT05]. **Ab-initio** [Cor04, PHNN09a, FFFR01, FFFR02]. **ability** [DPS04]. **absence** [LAS+07, OR07]. **absolute** [VV05, VRE+04, WRRF03]. **absorbing** [HV03]. **Absorption** [MP06, AEI00, BKAT00, CC05a, DYD00, DI05, IBB08, IOA+04, JNKMS03, KWWQ04, MVdCD00, NSS09, NFL+02, Noo03, OCWY09, RA03b, RBLS04, RSRMBFR00, SBM00, SL05d, SIT+06, WSC+05, WPB+06, YSS08, ZCZ+07, dVHB03]. **abstraction** [MBRS05]. **absurdum** [Kry05, Kry06, SDW07]. **ABT** [MCN+05]. **ABT-594** [MCN+05]. **AC** [VH00]. **Academy** [Ano00d]. **Accelerating** [YKGC09]. **acceleration** [BRZ09, GM09, Sal09]. **acceptance** [dAMM08]. **accepting** [HD03]. **acceptor** [DD05, GBB06, LC02, Lu06, New00, OOD+05, She04a, She07d, SMVMC07, TDS+02, Ver05, ZVVT07]. **acceptors** [Buc05a]. **account** [FBBB06]. **accounts** [Kry07b]. **Accuracy** [MNV07, RLER04, CS08, Goo03, JR02, RS08]. **Accurate** [AWZD05a, AWZD05b, ACFR05, CA09, GBP05, PCBA08, PSH00, VTP09, AVTPR09, ACM07, BSH04, DBd05, DSL06, DSW08, Fer01, GHT09, GSD+03, HT05a, JNSF04, JZZ+08, KS03b, LJ03, LSM05, Liu06, NN09, NJC02, PCS09, SH00, SH01, Saf04, TC05, ZW07, LSM05]. **acenaphthylene** [YLYD03]. **acetaldehydes** [BDA+02]. **acetate** [JFS+09]. **acetic** [CI06, Dre05, KF03a]. **acetone** [BF07, CCB07, DNC07, LYWX07]. **acetonitrile** [ČAV+09, CL05c, FG01, Pej02, WWTHF09]. **acetonitrile-exchange** [WWTHF09]. **acetyl** [HEJ+00, RKR+06]. **acetylacetaldehyde** [NJR+09]. **acetylacetone** [JNF+09, MD06]. **acetylcholine** [MCN+05]. **acetylene** [BVHS05, LLYL06, MZD+05, QC00, SO04a]. **acetylenes** [KPC05]. **acetylenic** [YLS+04]. **achiral** [ZWMZ04]. **acid** [ASL04, ASRL06, AMC07, AKK05a, CJ09, CS00a, CME07, CTI09, CI06, DDP+07, DFT+07, Dre05, DFZ04, HJT07, HHGSRS02, HSH02, HDWH09, IN09, JZL+08, KK08, KVSG02, KF03a, MRMR02, NFFA04, NRS+02, NSLR04, OMMWL02, OGJdlV03, PNG02, PK01a, PVW03a, PKS+00, QBTS05, RST08, RSTG02, SAR08, SSC+07, SSJ09, SLB+08, SGHL00, SLS+05, SS09c, SCHH01,

SCHH02, SFR08, ŠK03b, VRC04, XXJG03, ZMZ+00]. **acid-catalyzed** [IN09]. **acid-dissociation** [SAR08]. **acidic** [TC07]. **acidities** [AWZD05a, AWZD05b, JTC+07, KSBK08]. **Acidity** [AGM06, SCHH01, MRTT01, ZSKV04, ZMZ+00]. **acids** [AE07, CSL+02, CTLZ01, CHMIHS+05, DSL06, IK00a, JTC+03, KM00c, LLW+07, LDR+08, LS01b, RMB00, SŚRL07, Sta00, YHF+08, YWZ+09, YZ07]. **acp** [PFSFH06]. **ACPF** [CSG06, Gda01a]. **acridine** [ZDO00]. **acrolein** [BBPG08]. **across** [MRG02]. **acrylate** [TA07]. **acrylates** [GST+05]. **acryloyl** [QCFJ05]. **actinide** [BR02]. **action** [DDW+06, KVSG02, OB02, PS03c]. **Activation** [MBRS05, CX00, CPR06, FH02b, GCCM03, HSRP09, HGS03, KL00, Lad00, LVSG06, VED+02, ZCFD02]. **active** [BNHB+02, BSCB04, CZWZ05, CDDM05, GPW06, Han07, HKMM04, KSI+07, Kra00, LMRT08, LAS+07, MP06, Mic00, NOHN02, PHK+06, PSEP05, RP00, SMY07, SIT+07, SSS+05, Whi02a, WRK03, XXC08, YKGC09, Yur07, Yur08]. **active-space** [GPW06, PHK+06]. **activities** [GMPIP01]. **activity** [ATF03, Bou01, BMMA06, BAG+08, CBRBT03, GLF04, GBMMSA00, GKSL01, HH05, JNKMS03, KM04, Lav03a, LQC06, MEN+08b, MBA+08, NVA+03, PCKC08, PRS+09, PR05, RAdS05, SKSS09a, SHM09a, TTM01a, VAS06, WHD+05, XZGZ06, YLS+04, eSPM+08]. **actuation** [LLSY05]. **acyl** [AEMAO06, RVP06]. **acylation** [LFZ07, PNBV07, ŠFW00, ZLF+07]. **ad** [Kry05, Kry06, SDW07]. **adamantane** [KS02b]. **Adams** [Har09, Ver09]. **Adapted** [DHCD06, DEN02, DMH+05, KH01, MW06b, Muk00]. **adaptive** [PW07]. **Adaptively** [BKM+09]. **adatoms** [TBB09]. **adcluster** [NH00]. **addimers** [ZCZ00]. **Addition** [Wen00, Wen02, AG02a, ASM+03, BCK04, Buc01, Buc07, BZR02, KVZ+02, KVZT04, KWC09, MGG05, Sok02, TVK01]. **addition-substitution** [Buc01]. **Additional** [WF04]. **additions** [ETM00]. **Additive** [MGC00, FZ09]. **additives** [MARK08]. **additivity** [Šat03]. **AddRemove** [Swa03]. **adduct** [DGP08, LZHT03, LC02, VRFS05]. **adducts** [LXTT00, LXHT00, LZYT01, ZKRS07]. **adenine** [DZO00, EKN04, MHGR07, SM05b, TSZW08, XC07a]. **adenines** [SST00, SST00]. **adenosine** [MESH02]. **adhesion** [FYT09]. **Adiabatic** [AS04a, Lor08, SCP03, BJS09, Bro07, HGB08, KCS02, OYB+00, PCL+03, SCSWF04]. **adjustment** [PPP00]. **ADMA** [SEM05]. **adsorbate** [Mic06a]. **adsorbates** [DND06]. **adsorbed** [AML+01, IPPL05, LTV03, RKM09, Wal04a, WL00, ZW09a]. **Adsorption** [DBHT01, QCC05, ZH05, Bol04, CAHl08, DAD+03, EMV05, FGFF06, FFF07, Guo07, Hea00, HR05b, HR05a, KL03, LL04, MGZL04, MJG+05, NAE06, POAVdlM08, PC09, PR09, PLO02, SK05b, SZK07, SVT06, SLW+07, NRS+02]. **advanced** [Del03]. **affinities** [GW06b, HZJ+07, HKE05, JTC+07, KD05, KSBK08, LLX+03, LLYJ09, LZZ+06b, Mor08, STL+09, XXC08]. **affinity** [BSM+07, CNT+09, DSL06, GRC09, Mor06, METSH02, RS06, ŠPNU08]. **after** [BGGS08, LFZ07, ZLF+07]. **Ag** [MOAM07, SZJ+04, ZJZ00, CN03, JHLC09a, LC05, RKM09]. **AG18051**

[MAFR08]. **again** [Les03]. **against** [CBRBT03, LWZ+09, SKSS09b]. **AgBr** [SKA05]. **AgCl** [SKA05]. **agent** [PNBV07]. **agents** [CSL+07, SM05b, SUAL04, VBS+04]. **aggregate** [PD05, TNYY03]. **aggregates** [NFT+01]. **aggregation** [MMR+08]. **Agonist** [BNHB+02, XCS+03]. **AHMA** [CSL+07]. **AICA** [QCFJ05]. **aid** [RB07]. **aided** [SLS+05]. **AIM** [JFJMR08b, GMTM02, JFJMR08a]. **air** [CAHl08]. **Al** [CZPJ01, CMY06, Liu08, MCZWD06, MGAS09, NRS+02, SYL05, SCHW07, YS05, AML+01, DEN02, FDLK02, GGPS06, GWJ05, GW06a, LV01b, MMCC02, MTO+03, SLW+07, VTS04, VPS+04]. **Ala** [HEJ+00]. **alaninamide** [ZZWM07]. **alanine** [CL05d, PVW03a, JNKMS03]. **alanine-** [CL05d]. **Alanyl** [JNKMS03]. **album** [Ano09g]. **AlC** [RLGB01, RBL04]. **alcohol** [BK04c, MAFR08, SKSS09b, URBM04]. **alcohols** [VR01, YLS+04]. **Alder** [ARD03, SZML07]. **aldol** [AD01, FWT08]. **AlF** [MJ06]. **algebra** [BKRT03, BRZ09, Muk00, WK06]. **Algebraic** [CFP00, EFM06, Fan01, Fan03, MYRNYSB07, MVP00, Sch00, UP03, YM05, BCF03, ÇKB02, Fri06, GYM+02, LLP05, MZD01, Nég03a, Pan05, Pan07, QGW02, QGW04, RGMP06, YHD00, YYHD01, ZGY+03, ZYG00, ZD07b, ZD08]. **algebras** [Tem02c, Tem02b, Tem04]. **algorithm** [ACD02, ACDV01, BKL+02, BFF04, CB00, CR08a, DNMM06, DCA03, DS07, FRGM06, GMK+09, JG09, KN09a, LCN05, LSD02, LGBJ03, MGdS+08, NCB02, Özd04, PCT+04, QLD05, SBT+03, SSMG08, ŠK01c, TA06, TCM01, WC04, YINH00, dAMM05]. **algorithm-based** [CB00, NCB02]. **Algorithms** [ES06, RR00, CDF00, CL08, EFM06, GM09, KM00a, MT03, Mak07, ONK+00, ONK+05, ZDO00]. **AlH** [SHC00]. **AlHHO** [SS08a]. **alignment** [MP09, SK01a, SLCW04a]. **aliphatic** [AMO+01, CSPS05, Irg06, Sey08, WB05]. **alkali** [ABL03, BG00c, DLM+05, Elr09, FF09, GSA+09, HL05, KBV05, KL03, LTV02, OG00, Pyy01, RSRMBFR00, RF01, Sad00, SM05c, SVC+05, ZRRC05]. **alkali-doped** [SM05c]. **alkali-exchanged** [KL03]. **alkali-halide** [Sad00]. **alkaline** [BKLB06, Irg06, KK04, Pej02, PNBV07, Pyy01]. **alkane** [TKY00]. **alkanenitriles** [LMGM02]. **alkanes** [MBRS05, RS08]. **alkenes** [VDF+06]. **alkoxyborane** [LXHT00, LZHT03]. **alkoxyl** [LSM+06]. **Alkyl** [MBRA07, BNHB+02, FBC+06, PK01b, ZRRC05]. **alkylammonium** [ZS04b]. **alkylated** [HY04]. **alkylating** [CCA+06]. **Alkylation** [EPSC06]. **alkynals** [ZSL+09]. **alkynes** [REHH07, RVD03, VDF+06]. **alkynylaluminum** [SBF03]. **alkynylation** [MWL08]. **alkynylberyllium** [SBF03]. **All-electron** [BR00, MST08, HCTC07, MCZWD06, RIVB03]. **all-trans** [ZWJ02b]. **all-virtual** [MST08]. **allelochemical** [SPS02]. **Allen** [Ano03a, BH03]. **allowance** [Gin08]. **Allowed** [SMDM03, YCN+07]. **allowing** [BFF04, POM+08b, SB04]. **alloxan** [KS02a]. **alloy** [ZDQF08]. **alloys** [GKL+09]. **allyl** [Sha06, YKT+02]. **allyloxy** [TA07]. **almost** [HMB+04]. **almost-spherical** [HMB+04]. **AlO** [KZS07]. **alone** [MNA+99]. **along** [CM02a, CCR09, GGS09a, IKS08, IKS10, PCL+03, RA02]. **Alq** [TKS+05]. **AlSO** [Bu02]. **alternant** [Gin05a, Gin05b, Gin06, Man05, Tor02, WSK03]. **alternating**

[Buc05c, WWW+07]. **alternation** [BE07, MRT00, SC02b]. **Alternative** [CCL03, Glu04, KMN05, Ret06, ACC03, CZWZ05, KVSG02, PGW08]. **Alternatives** [Wil04a, XLX+09a]. **aluminium** [LHL+00]. **aluminophosphate** [LV01a, LPV05, LHTV05]. **aluminosilicate** [LV01a, XVRL04]. **aluminosilicates** [LV01b]. **Aluminum** [MML+02, AP00, EBR07, GSQ+04, Guo07, KWWQ04, MMR+04, MBRS05, MGAS09, PHNN09a, PHNN09b, TBJA03, VD00]. **aluminum-based** [TBJA03]. **always** [RFRF05]. **AM1** [FSLL04, HD03, HY04, SS08a]. **Amadori** [JRSA08]. **amazonensis** [CBRBT03]. **AMBER** [CWW09]. **Amide** [CHC05, DSW00, DSW02]. **amides** [KKK09, VVBT07]. **amidinate** [LWZ+09]. **amine** [BT05, DDT+03]. **amines** [BBD08, CSPS05, CCH05, JZZ+08, KKK09, LY09, PMLC09, RS06, Sey08]. **amino** [AG01a, CSL+02, CHMIHS+05, DSL06, JTC+03, KM00c, MGMR04, PVW03a, RJF+09b, RMB00, SBB06, SLB+08, SFR08, ŠK03b, YWZ+09]. **aminoacids** [MML+02]. **Aminoacrolein** [JFJMR08a, JFJMR08b]. **aminobenzenes** [WGX09]. **aminobenzenesulfonamide** [PGP+07]. **aminobenzonitrile** [PRM+06]. **aminocoumarin** [SKN09b]. **aminocyanocarbenes** [FG06]. **aminomethylphosphonic** [RST08]. **aminopeptidase** [GSK01]. **aminophenols** [GR05]. **aminophenyl** [HE05]. **aminophenylarsonic** [HHGSRS02]. **aminopurine** [BSAL+06, HT07]. **aminopyrimidine** [ZB08]. **aminothiazole** [ZR07]. **Amlan** [Roy05a]. **ammine** [TSH03]. **ammineaqua** [PBSC04]. **ammines** [Bou01]. **ammonia** [BVHS04, CZWZ05, Dou07, EZY00, FXHL05, GJB00, XCW07, ZHA01]. **Ammoniated** [Jal08a]. **AmO** [SNN+09]. **among** [ACC03, HGTW03, PS04, Pyy01, XXMJ06]. **amorphous** [ZDQF08]. **AMP** [ZLL+05, ZLSL06]. **Amsterdam** [Wol05]. **amyloid** [MAFR08, MMR+08]. **amyloid-** [MAFR08]. **analog** [CSDCCMZT03]. **analogous** [Tem02c, Tem04]. **analogs** [ATF03, AD01, GSK01, JHR+00, LQC+08, SDFM02, TKS+05]. **analogue** [CMS04, KRR08, QFC04]. **analogues** [GMTM02, SCRE08, ZZC09]. **analogy** [MSJ04]. **analyses** [CD03b, DMG09, KIN09, Sun06]. **Analysis** [CMY06, IN07, ITN06, KS08, MCN+05, OYB+00, PDS04, PRM02, Sey08, SZJ+04, YNY01, AS04a, AM09a, AZD06, AA09a, ASO+01, ASO+04, AT00, AA09b, BF08a, BES08, BL02b, BA06, BS00, BMR+07, BDMC06, BF09, CC00a, CDH05, CFV02, CC07, CTI09, CP09, CM09, DNN+06, DNC07, Ess07, ETBA06, FDL03, FBBB06, FGM05, FB07, FFDD07, FHJ+08, Fuk09, Goo03, GSK01, Hea00, HLH05, HMW02, IYSS07, IBN08, IOA+04, JNKMS03, JP01, KSBK08, KYT+04, KVZ+02, KO03, LA06, LSM+06, LAQ+09, LBAB02, LP05b, MB05a, MCF09, MHT+08, MS05, MH05, MPKB06, MEN+08b, MZ09, NP01, NKN+05, NŚM02, OC08, Ols04, OA02, OA03, ONA05, PRSLA08, PI02, PCKC08, PRS+09, PPP+08, PSB+05, PTLB00, PC04b, Ras02, RA02, RAA05, RSFRDNA04, RLNA02, SRA09, Sak00, Sak02, SMAL01, SFK09]. **analysis** [Sch02, SY05, She07a, SMDG09, SKT+07, SIS+08a, SCG07, SSSS09, SFR08, SNN+09, SCMS07, TYG05, TS07, TT04b, VAS06, VCF+00, Var08,

VSI$^+$07, WGD01, YW09, Yil06, ZZHL08, ZZW$^+$06, ZLY$^+$09, dA08, BGJJ01, GSCRO08, MPBM07]. **Analytic** [Har02b, VHM$^+$04, XVB05, HTN07, JTB09, LGKN04, MSC03, NF03]. **analytic-continuation** [MSC03]. **Analytical** [AH06, CA01, CW00, CC01a, DSH01, HSB$^+$00, ITN08, JLAR07, QS00a, RDK97, Wol05, YKT$^+$02, AS04c, BBC07, Gus02b, Gus04, KAE07, Man05, Özd04, Qui05, SO09a, SSZ$^+$07, TA02, vLvL06, RDK02, SNM$^+$04]. **analyzed** [Seb05, dLCPLD$^+$07]. **Analyzing** [RE06, LLLZ07]. **Anatomy** [CP09]. **and/or** [SLB$^+$08]. **Anderson** [SJE03]. **androgen** [BSKFT07]. **anesthetics** [BGP$^+$07]. **angle** [JC01, PA04a]. **angles** [CCLK05, GJ03, LH05]. **angular** [DGR$^+$00, DS06, HSB$^+$00, LL01, MY08c, SBMM03, LH05]. **Anharmonic** [IROW09, MD06, ADK02, BS05a, BKM05, CMS04, MSJ04, RdLJ$^+$02, RGMP06, SSDM05, Sch02, SCRR02, GW07]. **Anharmonic-model** [GW07]. **Anharmonicities** [TYG05]. **Anharmonicity** [KO04]. **anhydride** [CI06, XFLX$^+$06]. **aniline** [ĆMTS08, GS00b, KB08, dAMdG05, MGV00, PGN$^+$05]. **anilines** [GSH02]. **anilino** [ZTW$^+$09]. **anion** [BGGS08, Buc05b, Che00, GS05, KVZT04, LAK09, MSS05, NGRR02, PILD07, PFSP05, SGS00a, XFLX$^+$06]. **anionic** [CL07b, DKC00, Guo07, HBW$^+$08, KP02, KP05, LDPP05, XC07a, SASS03]. **anions** [AMC07, BS02, BBD07c, CS00a, DB06, GBS02, GV06, GT07, GW06b, KVZ$^+$02, LAQ$^+$09, LCL$^+$09b, MB00, Mon05, Mon08, NK05b, Ort05, SASS03, SM07a, WLZY08a, YST$^+$05, ZŠ05]. **anisole** [VBT$^+$07]. **anisotropic** [CCEÖ06]. **anisotropy** [MABB06, OB02]. **annealing** [CB03, DNM$^+$08, FCD08, dRPFCP08, RSM$^+$04b, SKMW00, dAMM08]. **annelation** [YCS09]. **annihilation** [DC05, MAS09, VNB$^+$03]. **Announcement** [Ano01a]. **Announcements** [Ano05a]. **annulenes** [HvLJ01]. **Anomalous** [BVSM04, KPP01, Por01, Dat04, VM06c]. **anomaly** [ABCS02, WSNB00]. **anomeric** [WT07]. **anomeric-like** [WT07]. **Ansatz** [MKCB05, ANM03, Kon09]. **ansatz-based** [Kon09]. **answer** [ERC$^+$02]. **antagonists** [BMR$^+$07, MESH02]. **anthracene** [OA02, ZDO00]. **anthracene-9** [OA02]. **anti** [ATF03, BMMA06, Duf07, GMPIP01, VBS$^+$04]. **anti-aromaticity** [Duf07]. **anti-HIV** [ATF03]. **anti-HIV-1** [GMPIP01]. **anti-inflammatory** [VBS$^+$04]. **anti-ulcer** [BMMA06]. **antiaromatic** [Buc01]. **antiaromaticity** [Buc00a, IS02]. **antibacterial** [MEN$^+$08b]. **antibody** [Chu09, MFR07]. **anticancer** [Bou01, CSL$^+$07]. **antiferroelectrics** [DLM$^+$04a]. **Antiferromagnetic** [RI05, FPJR03, NF02, Yar00]. **antiferromagnetically** [Mar09]. **antiferromagnetism** [Dro04]. **antifreeze** [CBWM09]. **antileishmanial** [MBA$^+$08]. **antimicrobial** [NVA$^+$03, TS01b]. **antimutagenic** [SM05b]. **antineoplastic** [AMOR07, SWST04]. **antioncogene** [Lad00]. **Antioxidant** [GLF04, ASL04, BKM$^+$02b, Lav03a, WHD$^+$05]. **antiparasitic** [SCRE08]. **antipocket** [RGP07]. **antiproliferative** [LQC$^+$08]. **antisymmeterized** [WO04]. **antisymmetrized** [TTM01b]. **antitumor** [HE05]. **antiulcerogenic** [BAG$^+$08]. **ANTO** [LCH05a]. **any** [GAR08b, Sce09]. **any-particle**

[GAR08b]. **AO** [DLM+04a]. **aparisthman** [BMMA06]. **apatite** [LADD00]. **apatites** [MTE09]. **APNO** [DPS04]. **apolipoprotein** [PKT05]. **apoptotic** [SWST04]. **appearance** [KG02]. **Applicability** [GR04]. **applicable** [Tem02b]. **Application** [BB07, CK06, Fri06, GQ00, Han07, HYC+00, JNSF04, Kan00a, KFTBS07, LLP05, MTRD04, MMV04, MHB05, MF03, Mor08, MC06b, ND03, PR09, PVW03a, ASM+03, BKL+02, Bar08, BKM+02a, Buc04, CL05a, CDG05, CMNH07, DWF+03, DLM+04b, EBS+09, FTM06, Gus02a, HS02, KSI+07, KOT09, LLZH09, MR00, ONA05, PGW08, Shi05, TN03, TT04b, YLS+04, YM05, ZLJ+09, AT00, CR06, Dei04, Dei06, DDD03, GGS09a, GMS01a, HKR09, HRDM+08, IKS08, IKS10, KKYT04, KCGB02, Kra00, LFADSF07, Liv02, LK02, Man05, MNMV02, MP00, MDSW07, MFR07, NF03, ND02, Obe00, PRCEM06, SSA07, SS01, SDZ+07, SS03b, ZB05]. **Applications** [Ano02m, CD03a, RRC03, ZWMZ04, BLA00, BRZ09, BCF02, CW00, Eye00, GBL06, IG06, JR02, LDR+05, MK01, Son04, SM06c, SEM05, ARBD05, DFMZO08, FS00, GD00a, GDV05, KM03a, PW07, SC02a, TG05, Tou09, VCHC07, XVB05]. **applicative** [VATPR09]. **Applied** [RDK97, Ada02, Ada05, ASDC08, CJ03, CBRBT03, CL08, DM08a, DKS05, DNMM06, DD05, DVM06, HMB+04, HMW05, NJD02, OR09, OCAMOHL07, PSCLGN07, PJdC00, RGMP06, RDK02, SK03a, SČL00, Tal03a, dAMM05]. **Applying** [Pea08]. **Approach** [FDM09, AGM06, AYD00, ÁBL06, ACG00, AT07, ART08a, BDG01, Bar08, BB02b, BGN+05, BG00a, BG02a, BKMHP04, Buc00a, Buc01, BMP+04, BCF03, Cab05, CL00a, CCM+05, CB00, CHMIHS+05, CSA09, DGR+00, DNM+08, DDT06, DC06a, DDD03, ESU04, EBR07, Fer09, FMBM05, FS00, Fri06, GC05, Gin03, GCG05, GAIK04, GAL+05, GBP05, GG00, GYM+02, GGDL07, GFDK09, HSRP09, HSN+09, HT04, IK00a, IK00b, IYO+04, JJC+06, JZL+08, JXC05, JTB09, KH05, KK02b, Kis04, KKS09, KSS00, KMS02, LFADSF07, Lav03b, LLR+00, LBSB08, LP08, LGBJ03, Mar08, MMV04, MYRNYSB07, MVP00, MO06, MNR07, MKZ04a, May06, May02a, MMV05b, MZD01, MYH03, MY00, MMB03, NY03, NCB02, NF06, Nég03a, ND02, ND03, NYU+08, NS02, PLC04, PMHW07, PMO04, Pir06, PTLB00, PGP+07]. **approach** [Put05, QGM+00, QCC05, RMJ+07, RRNG05, SN02, SKSB08, SA09, SAM08, SD08, SCP03, SL05b, She07c, SY09, SL00, SK03a, SSN01, SBF+04, ŠPNU08, TA02, TYY06, TDF09, Tap04b, TTM01a, TTM01b, TT06, VRFS05, VHM+04, Wal04a, WK03, WAJ04a, WAJ04b, XCS+03, XXY00, YNN+09, YHD00, Yar00, YSS08, ZKB03, ZD08, dD04]. **approaches** [BF07, CF05, DK03, Dat04, DVM06, DLK00, DM02b, EP02, GKL+09, GPW06, KC09, Noo06, PGW09, PPP00, PJP08, RP09, SEY07, TYY05b, TYSY07, YTK+03]. **Approaching** [SGP+07]. **approximants** [Goo03, ISS00, PCF05]. **Approximate** [ANM03, LMGM02, MY08a, MB07a, Pan01, PM04b, TYY04, AM09b, GGLS02, Kir08, KSI+07, LMJ00, Liu02, MB04, PSM07, Pea02, PGB00, PPP00, TGG01, Wei03, KKMS04]. **approximated** [EEJ04]. **Approximately** [KSN+09]. **approximation**

[AFC03, ASDC08, AGB06, Bou03, BČ02, DZ01, FCS03, GTR+05, GGDL07, GFDK09, HT05a, IYO+04, KN09a, KZvL09, LPV05, LZC04a, LN03, Mas02, MDJ01, Nak02, Nak07, PH09, QGW02, QGW04, SLE05, Sch05, SM03, SČL00, TW02, WW08, YŞ02, vLvL06]. **approximations** [CDG05, Cor05, Har02c, HM05a, Koc00, LV01a, Ort03, HNKiS01]. **aprotic** [LLW+07, LDR+08]. **aqueous** [AGM02, CME07, CTI09, HDWH09, IYSS07, JNKMS03, KM06, LHL+00, SAR08, TMS08, USM01, YSS08, dAGD08]. **aquifer** [Har01, Kry00, PHH08, Tem09]. **arbitrariness** [SS04b, SS06]. **Arbitrary** [SHZGP09, Alc04, CCR09, GMS01b, GMS01a, GM00, GM01, GM02a, GM02b, GM08, HSB+00, JJ00, Kat00, Orl07, Özd03, PJ09]. **Arbitrary-order** [SHZGP09]. **arc** [Mon09]. **architecture** [GBL06, NFT+01]. **area** [MB01b]. **arginine** [VED+02]. **argon** [Cab05, Jal08c, PCS09, PA02, PA04a, VD00]. **ArHCl** [ZNZS00]. **arid** [LTL04]. **arithmetic** [JJ00]. **armchair** [XZ07]. **Arnold** [CMS04]. **aromatic** [BCdP03, Buc01, DKD+07, DAD+03, DFMZO08, DSW00, FRK+05, JTH02, LXH+00, LXTT00, LXHT00, MML+02, MMZ02, PCML08, PGPA09, RLB02, RFRF05, RM07, RRD06, Sok04, TCM09, TSH03, TBCG05, VTS04, VTS05, WW08, ZCZC09]. **Aromaticity** [FCLH+06, IS02, BS00, CL07b, DP06, Duf07, HvLJ01, MSSM00, VHWM04, WW07, YS05, YWC07, ZMZ+00]. **Aromaticity-induced** [FCLH+06]. **Aromaticity/antiaromaticity** [IS02]. **arrays** [RL04]. **Arrhenius** [SSC+07]. **artemisinin** [ADTD05, DDT06]. **Artificial** [JBPZ02, ASM+03, Tap04a, YL02]. **aryl** [AA09b, BF09, DGLM09]. **arylazacrown** [FBGA04]. **arylmethyl** [Buc01]. **arylmethylene** [Ess07]. **ASA** [ACD02]. **ascorbate** [ASL06]. **ascorbic** [ASRL06, MRMR02]. **asFP595** [Sun06]. **aspartic** [CTLZ01, SAR08]. **Aspects** [SM07b, AGL04a, BM02, CDK01, CHR+06, FVPM05, FFHD00, KM03a, Mic00, Sok04, TFS+02]. **assembled** [THP08, TBB09]. **assemblies** [Mar00c, PK01a]. **assembling** [DMM+02]. **assembly** [SMVMC07, TQC05, VRC04]. **Assessing** [dGS06]. **Assessment** [BKM05, FP02, WPB+06, AYD00, MLSG04, SFD09, SE02a, AKN09, JPA05, KIN09, RS06]. **assignment** [ELY09, JNF+09, JLZY09, TIGD09]. **assisted** [NWSC08, SBKSS05, SLB+08, UKAM04, VAS06, WZWC06, WLZY08a]. **assisting** [YYQ+06]. **associate** [MROA06]. **Associated** [Vik07, FDM09, PC07, TKJ09]. **Association** [KOH03, BTL+02, CM05a, CRL+02, Mon09, MMF00]. **associative** [Pan06]. **astrochemical** [ABBS08]. **astrophysical** [Woo02]. **Asymmetric** [DBFP05, Buc02a, LTLS05, LTL05b, MVP00, MLZS06]. **asymmetrical** [SBF03]. **asymmetries** [MB05b]. **asymmetry** [BS05c, Kon04, Lat03a, Nic02, YHC05]. **asymptotic** [AD07, BB07, BBC07, CHS09, GSB00, KFD09, NFG05, TB03, MKZ04b]. **atmosphere** [GWSZ08, LLL+07]. **atmospheric** [DV00, HZW+08]. **atmospherically** [OM04, VBML01]. **atom** [AH06, ANM03, ACFR05, ACM07, BN04, BZH+07, Buc08, CR06, CSP04, CCLK05, CCLK07, CHS09, CTS08, Cou05, CCR09, DM02a, Dat04, DGG09,

DGC08, FTM06, GHT09, HR02, IG06, KWWQ04, KH06, KH07, Kis04, LKG09, LSM05, LH07b, LM02b, LGKN04, Mal05b, Mar04a, MYRNYSB07, MT02, MSMS03, MS09, MTB+02, NN09, NFP05, NF06, OMNN04, Pai00, PV09, RJ08, SBT+03, SMS+02, SH07, TKY00, TT04a, TT04b, TFBM02, XBHL04, YAŞ00, YF07, YSP06, YSP08, ZSW+00, ZY04]. **atom/molecule** [TFBM02]. **Atomic** [BBM+00, DNM+08, ERVR06, FM02b, HR07, KWG06, MH05, PLC02, SBM07, SSSS09, SPS05, ANM03, AR06, ACHB08, BB02b, BLRT02, ÇAK07, CSL+02, CC08, CMRMR00, CDGC05, DD05, Deb08, DES03, ESU04, FF09, Gra08b, GSH02, HdMB+05, HS02, Hog04, JÅM01, Kar04, KK07, Koh01, KG02, KDY+02, LV01a, LPV05, LTV07, LHG00, LM02b, MSB00, MGC00, MMV05b, OMC04, PRM+06, PVW03b, PS03b, PM04b, Put06, RBA07, RCJF00, RCD00, RdSH08, SJE03, SM07a, SEU02, VPSH00, VD04, XVB05, YŞ02, Yal04, ZWMZ02, ZLH+08]. **Atomic-orbital-symmetry** [SSSS09]. **atomically** [BNA03]. **atomistic** [Kan00b]. **atomization** [MST08, Vyb08]. **Atoms** [CCP00, Ada05, ASH07, AMGN00, AM09b, ARH00, ASDC08, AS00, BM01a, BBG00, BC06b, CBMRN08, CS03, CF05, CC02, CRTP05, CMNH07, DMH+05, DHCD06, DKM+04, Elr09, ER05, FGM05, GBS02, GBS04, GAIK04, Gui01, Gui06, GE09, HSS09, HSP+09, HMB+04, JNSF04, KDŁL07, KTK+04, KK07, Koz04, Kry07b, KS03b, Kut08, LK00a, LV01b, LWW+02, LJ03, Liu06, MGK+09, MKCB05, MB07b, MY08c, MM07, MM09, NR09, NB05, NS08, NS09, Nes04b, NJD02, NRJD03, NJR+09, OdSC05, PUH+08b, PUH+08a, PUH+09, PRG+04, Pea05, PJ03, PCL+03, QS00b, RdSH08, Rui05a, Rui05b, SK00a, Sap06, SL05b, SK03a, TN03, Yur07, ZSM+01, LKE03]. **Atoms-in-molecules** [CCP00, NB05]. **ATP** [YZX+08]. **attached** [BLC+00, PGW09, YF07]. **attaching** [KSS+08]. **attachment** [BGGS08, RA03a, RA04, SBKSS05, XC07a]. **attack** [SPS02]. **Attaining** [ZR03]. **attempt** [SR05]. **attempts** [Sce09]. **Attosecond** [BCN04, GLHH09]. **Attraction** [Gus03, BSH04, DS07, JJWH04, MROA06, ÖO02, ÖÖOY02, SH02a, Saf04, SS09b]. **attractive** [MSC03]. **Au/ZSM** [SAE08]. **Au/ZSM-5** [SAE08]. **AuCl** [REHH07]. **Auger** [MV02]. **augmented** [Eye00, LFK06, ND02, ND03, SYZ+09, SZL+09, VD00]. **AuPH** [FWZ09]. **Aurasperone** [dLCRF+08]. **aurophilic** [FWZ09]. **Automated** [PHK+06, RT06]. **Auxiliary** [ELF+08, FLE+06a, FS97, GM08, Bar00, FS09, Har04a, Tem02b, GM02a]. **AVB** [TGG01]. **Average** [GKR00, GSB00, HWPIM01, PMC02, RNVTP09]. **averaged** [AC07, ANM03, CP09, Gda01a, KFD09, TS01a, TGGV+04]. **averages** [CDG09, PCT+05]. **averaging** [BP04, LCK00]. **avian** [HPC+08, PCML08]. **avoided** [Apo06, PSCLGN07]. **Avoiding** [NFG05]. **axes** [Oku01, TPGD02]. **axis** [CCR09]. **aza** [BCdP03, CJ03, WW07]. **aza-substituted** [BCdP03]. **azacytosine** [PRL01]. **azaindole** [Cat05, SAMBS01, TYG05]. **azanions** [PGP+07]. **azapentalene** [GEB+00]. **azide** [ABI07, BF09]. **azides** [AEMAO06, AMO+01, KZG09]. **azines** [RRD06]. **aziridines** [KVPS05, KV07]. **azo** [DDD+00]. **azoalkenes**

[ARD03]. **azocarbenium** [LW08]. **azorhodanine** [EGEDH03]. **AZT** [CFR07]. **azulenes** [BBVS+06]. **azurin** [CDDM05, SSS+05, STN+06].

B [CZPJ01, CT00, CMY06, Deb08, FRNM08, GB05, Liu08, SYL05, SCHW07, TWZ03, TM05, WRK03, YS05, YZY+01, ZDQF08, AÖG07, BVG05b, Buc05c, DL06, GP03, Har04a, LDPP05, LDP05, LJL+03, LZXL05, MY08b, Mar04a, MG08, RPB00, SH00, SH02a, SKSB08, SDS04, SČL00, TFBM02, Wen02, Wen09, KPČM05, SSZ+07, TBML06]. **B-DNA** [SKSB08]. **B/F/H/N** [BVG05b]. **B2** [FSK05]. **B3LYP** [Mar06b, BEM02, BL04d, Dkh08, GSQ+04, LBP04, MBD05, MCN+05, PGP+07, SCB+06, SBL05b, SBBL05, TX02, TNJL05, WE01, WGLX02, ZXX02, GBP05]. **B3LYP/experimental** [PGP+07]. **B6** [SDFM02]. **Ba** [MGCD01, Oni09, ZL04, MB07b, TNET03]. **BAB** [DLZ+03]. **back** [Les03]. **backbone** [BBL09, DSW00, DSW02, JZZ+09, SSJ09, VDF+06]. **backdoor** [FHHC00]. **background** [PI02]. **BaCoO** [CIP+03]. **bacterial** [RHHH00, SN02, SZZ01]. **bacteriorhodopsin** [CM09]. **bacteriorhodopsins** [RSL+03]. **bacteriostatic** [SCES03]. **Baeyer** [LJL09b]. **balance** [AMGN00, HMB+04]. **Band** [GCG05, ZCZC09, AIG02, BBL09, BCWS09, Boe07, BL04d, FFHD00, HOC00, KSG03, LBP04, MBOL04, Nag04a, NK05a, NKS+09, Obe00, SDB03, SÖ04b, SBL05b, TDF09, YYK+03, YNN+06, ZKYA04, ZOK+05]. **band-structure** [TDF09]. **bandgap** [Oni08]. **bands** [ACF04, ACF05, Gin01, TOH+00, TIGD09, YYYM01, YYI+08]. **Bare** [AR06, LNPL06, PB09]. **barium** [DMH+05]. **Barkas** [Por02]. **Barkas-effect** [Por02]. **Barnett** [BS06]. **barrier** [BF08b, GPW02, KCOV07, Lef07, LP00a, PSML04, SS03a, SS04a, SS05a, ZCFD02, ZLH+08]. **barrier-free** [ZLH+08]. **barriers** [CC00b, CC01b, KL00, LH03, Moh00, MPBM07, RA03a, RA04, SSN03, SPS06, WKF+06]. **BAs** [HCRHM03]. **Base** [DW00, EKN04, HFGL02, KVSG02, KV01, Kry02, KS03a, KES03, LY02, MHGR07, MWXL05, SKSB08, SM05b, SSN01, SS09c, SBL05b, YYYM01, YL04, ZZZ+08]. **base-pair** [SKSB08]. **based** [AE04, AS04c, BZL+09, BDG01, BK04a, BN04, BP03, BKRT03, CLL08, CDF06, CB00, CB03, CSL+07, CIT+03, CF04, CP06, CL08, DYD03, DNN+06, DGQT09, DM02b, Fis00, FVPM05, FPJR03, GMTM02, Har02c, HM01c, HOIK09, HNR06, HMW02, IYSS07, IBN08, JG09, KTH+05, KK07, KSG03, Kir08, KSI+07, Kon09, KV08, KANK00, LLR+00, LCT00, LWZ+09, LD05, LLZH09, MK00, MB05a, MMM06, MGC00, MC06a, NM01, NKS+09, NCB02, NRK+05, OOK03, Ols04, ONA05, PSS05, Pau04, PH09, PRCEM06, Pog05, Pud02, RFF05, Roy08, RB07, SSA07, SKSS09a, SG03, SAM08, She04a, SY06, SY09, SSSS09, SPS05, Tak08, TYY05b, TBJA03, TB09, Tem02c, Tem04, TT02, TT06, THPN03, TŠPJ01, VLJ08, XCW07, YSY+00, YLS+04, dGS06]. **Baseline** [LS08]. **bases** [AG01a, ACC03, CJ09, CW00, DKC00, FCLH+06, KY00, MTRG04, MMT+07, MPIP+01, RSTG02, SGHL00, TOC06, VM06c, WKS03, XC07a, ZVVT07].

Basic [Eye00, GSD+03, GM02b, VTA+02]. **Basis** [BEM02, CJ09, DPS04, KS07, ACCC03, ANJ09, BML01, BZG+02, BBM+00, BKM05, Čár07, Čár09, CC01a, CJdC01, CKM09, DNM+08, DCA03, DBd05, DMH+05, DHCD06, DG04, DSW08, DDD03, DW05, ET09, FTW03, GSfLV08, GW02, GW04, GW07, HdMB+05, HW02, ITN06, JC00, JCP+08, JLZY09, KCOV07, KV02, KW03, KOT09, KANK00, KWC09, LFK06, LS08, LW05, LPV05, LTV05, LTV07, LJ03, LS01b, MG05, MST08, MDSW07, MM07, MM09, MW05, MW06b, NJC02, NJD02, NRJD03, PJdC00, PJ03, PLU08, PJS+09a, QGW02, QGW04, RLER04, SFD09, SJE03, Sch02, Sha04, SYZ+09, SZL+09, SGS00a, SEM05, Tal03a, TPGD02, VD00, WC04, XV00, ZŠ05, ZB05, ZT04a, dA08, ABLL02, HMK06]. **Basis-set** [KS07]. **batch** [CP06]. **bathochromic** [SB03]. **BaTiO** [Mor04, PTS03, SP00, SV08, UES04]. **Baylis** [FYH09]. **BC** [JWM00, YHD00, YYHD01]. **bcc** [WSNB00]. **BCS** [SM07b]. **Be** [SCHW07, YCS09, ZL04, CRL+02, DHCD06, MZN+03, Nes01a, PPP+08, SK09, Squ05, ASL06, BES04, CG09, GE09, HMB+04, RV05, SUL+07, ZLXL07, ZW03]. **Be-like** [ZW03]. **bearing** [BD07, MLW+09, ZPW+04]. **BeB** [PRNM03]. **BEC** [SM07b, TKT+05]. **become** [NN09]. **BEDT** [Mar09]. **BEDT-TTF** [Mar09]. **BeH** [CNC+06, GW04, Pen06, QGW04]. **Behavior** [BB06, AMOR07, AP00, BVS+09, BBVS+06, BF08b, CPH04, DMV00, DLM+02, FFFR01, FFFR02, FHHC00, GJ03, GWK+05, GSB00, IS03, LK00a, ONK+00, SBL05a, SFR08, SJM08, TB03, ZL06]. **BeII** [WBLQ00]. **Belgium** [GDV05]. **benchmark** [RP09, ZLJ+09, CL05e]. **benchmarks** [Flo08]. **bending** [Sad02]. **benefit** [Kai09]. **benzal** [WJLL09]. **benzaldoxime** [MCC08]. **benzamidine** [HNR06]. **benzamidine-based** [HNR06]. **benzazole** [ICRS08]. **benzazoles** [HE05, HKE05]. **benzazols** [IBB08]. **Benzene** [LH00, ABBS08, ACHB08, BSR02, DKD+07, DGLM09, DVHJ03, EZY00, GKC06, HVC08, HDL00, Kry07a, KB08, MMZ02, MABB06, Ras02, Ras04, SHE+02, VCHC07, VBT+07, VSS04, WGX09, ZMMS+00, JTC+07, Kry07a, MZD+05, Pal00]. **benzene-ammonia** [EZY00]. **benzenes** [ABCS02, TC05, ZGY+03]. **benzenesulfonic** [NFFA04]. **benzenoids** [BR08, BR12, RB08, RB11]. **benzil** [TUA06]. **benzimidazole** [JZL+08]. **Benzinger** [Chu02, Chu04, Chu06, Chu07, Chu09]. **Benzo** [KES03]. **Benzocyclobutadiene** [JTH02]. **benzodiazepine** [FH02b]. **benzoheterocycles** [ZZKS07]. **benzoic** [HSH02, PNG02, HJT07]. **benzoin** [TUA06]. **Benzonitriles** [PRM03, PK01b]. **benzophenone** [UC00]. **benzoquinone** [AEI00]. **benzotriazole** [LCBC03]. **benzotrifuroxan** [JXC05]. **benzyl** [HQL09, URBM04]. **benzylideneaniline** [JLPA09]. **BeO** [SE00]. **berberine** [HLH05]. **Bergman** [GCCM03]. **Berkeley** [Tay09]. **beryllium** [BN04, CC07, HI06, KD05, MBA+04]. **Bessel** [BS06, HF09, SB06a]. **Bethe** [Por03, Por04]. **between** [ARBC+05, Ada05, AG01a, AL09, ACF04, ACF05, BVHS05, Boh01, CZPJ01, CIT+03, CMY03, CR08b, DS03, DC03, DSW00, DWM+07, DM04, EEJ04, FXHL05, FYT09, GP08, Gra08b, HVC08, HDWH09, HN09, IYSS07, KC09, KF02, Koh02,

Kon09, KS09, Kry09, KS03b, LY09, LTV02, Lav03a, LZZ+07, LAL+08, LW08, LLZ04, LYWX07, LXXC08, LYCX08, Mar09, MTRG04, May04, MOAM07, MP09, MFR07, NY01, OA03, PYZ09, dRPFCP08, PB09, QCFJ05, QCC02, RSTG02, RRD06, SR05, SKN+09a, SLB+05, SSN03, SBM00, SBB05, SS08a, SEY07, SCHH02, SDZ+07, TQC05, TDS+02, TW02, TWSK09, VCHC07, VDF+06, XLX+09b, YNY01, ZZL04, ZDMF08, ZFD00b, ZQF+02, dBM05].
Beyond [CL05e, Chu02, AFC03, DFH02b, HM05c, SOLI04]. **BH** [GJ03, SASS03, GW02, PNBV07, QGW02, ZLZ05]. **Bi** [HS05, Men08a, OA02]. **bi-** [Men08a]. **biased** [BKM+09]. **biases** [LPV02]. **Bibliography** [Ano00a, Ano06a, Ano03a]. **bichromatic** [FGM05, KK04, Mon05, SS05a, SSA07]. **Bickelhaupt** [Ano07a]. **bicyclo** [CWY05, KCU09, QD04]. **Bicyclopropylidene** [NLD+04]. **bidentate** [CJZZ06, HCL03]. **bielectronic** [PCT+04, PCT+05, SH00]. **bifunctional** [DW05]. **bifurcation** [CVVA08, PFC02, PC07]. **bilayer** [FCD08, PFdP08]. **Bill** [Har09, Ver09]. **bimetallic** [BC03, FPC05, MB01a, POAVdlM08, PC09]. **bimolecular** [GMS01b, GMS01a, ZCZF02]. **Binary** [COMA03, PUH+08b, ŠK03b, WB05, ZZUO05]. **Binding** [KM05b, KM06, BML01, Bau09, BDMS01, BSKFT07, BCFR08, BBSS00, Cam04, CL05d, CC00c, Chu09, DCP01, DKM+04, DZO02, DC06b, EF03, FV04, GCG05, HKMM04, JJC+06, JHR+00, JWZ+08, JZW+09, KUS+03, LSWT05, LMRT08, MAFR08, MLSG04, NGTB06, NSZZ04, NSG+06, NPLV05, Ort05, OMMB07, Pud02, RACD00, RH03, SGLF01, SDS04, SM07a, SCG07, SGS00b, SSK+05, TC05, TOC06, Tak08, TY07, TS01b, Tor04a, Tor04b, YPS05, ZDO09, ZKB03, ZZ05, KF07]. **Binomial** [BD00]. **binuclear** [BL04c, MOA05, XLX+09b, ZLY05]. **bioactive** [FP02]. **bioactivity** [KM05a]. **biochemical** [CC05c, Yil06]. **biochemistry** [PBB+02]. **biodegradation** [DKD+07]. **biologic** [HT04]. **biological** [Chu00, Chu04, Chu07, EFM06, GHG04, Mal07, MVLM05, PMPI01, Stu00, XZGZ06]. **biologically** [PPP+08, vdVM00]. **Biology** [Har06, Chu02, Hyd06, Nég03b, Bar06]. **biomembrane** [ESKB04]. **biomolecules** [HD03, IKS08, IKS10, JJC+06, MFA00]. **bionanotechnology** [RSL+03]. **Biophysics** [ERU07, RRUE08]. **biopolymers** [MWHZ06]. **Biorthogonal** [PGW08]. **bipolarons** [DM03]. **bipyridine** [CN03, DBFP05]. **biradicals** [TYY06]. **birthday** [AGL04a]. **Bis** [BT05, Buc02b, CN03, HDL00, HCL03, IABS08, LC02, SBB05, YYXC01, GSQ+04]. **bis-** [HDL00]. **bis-adduct** [LC02]. **bis-bidentate** [HCL03]. **BisP*** [LTLS05]. **bistability** [BBD04]. **bithiazole** [Moh00]. **bithiophene** [DDD03]. **biurets** [AB08]. **Blind** [LLR+00]. **Blind-test** [LLR+00]. **Bloch** [KP00a, MP00, Por03, Por04]. **Block** [Gin05a]. **Block-diagonalization** [Gin05a]. **blood** [EBR07, KPP01]. **Blue** [RM07, YZG06, GSQ+04, Hob02, LLYL06, LLL+07, QCC02, RO01, SC02b, TS07, Yan09, FPC+08]. **Blue-shifted** [RM07, YZG06, LLYL06, LLL+07, TS07, Yan09]. **blue-shifting** [Hob02]. **Blundell** [OR09]. **BLYP** [LBP04, SBL05b]. **BN** [AdBM06]. **BNH** [MG08]. **BNN** [XL08]. **BO** [MS05, RSFRB03]. **boat**

[FAE+05a, FFHT05, FAE+05b, QD04, Sha07]. **bodies** [MVKN06, RBA07]. **Body** [FS97, ABGS00, BA01, BA02a, BG02a, BSK+02, CL05d, DFM+02, EWCT+05, FS09, HFS04, Har05c, HFS06, HN09, IZ04, KIN09, Kut09, LHL+00, LH07a, Lin06, LSH08, MRG02, NF03, PMHW07, RFCG09, RAA05, SL05a, SK01b, SH09, SKHY09, TYY04, UC06, YŞ02, Yal04, ZT02, Zot06]. **Bogoliubov** [YONY04]. **Bohm** [Koh02]. **Bohmian** [GR04]. **Bond** [CWZ03, DT02b, LWC01, Mar00a, AA04a, AS04b, ARE02, AL09, ASO+06, ADSTS06, Buc04, CGCS02, Cam04, CC00a, CP09, CNDÖ00, DD05, DLZ+03, DVHJ03, ENGY+07, GGLS02, Gin05b, HGS03, HEBS00, Hob02, HKR09, HS05, HWY+07, IBN08, JWZ+08, KC09, KCU09, KSBK08, KKK09, KUS+03, KNS+09, KVT04, LSM+06, LM02a, LLW+05a, LLW+05b, LAL+08, LWL+08, LZA+09, LTY09, LSC02, Lia08, MBRA07, MG08, Nal09a, Nal09b, OA02, OA03, ONA05, PSB+05, PMLTL07, QV01, QCC02, RMJ+07, RD00, RM07, SS09a, SL07, SBKSS05, SK06, SC02b, SPS06, SS08a, SSSS09, Sok02, SBL05a, SCLL07, SDB03, Tac04, TS07, TDS+02, TGG01, VDF+06, WZL+07, WSK03, XLX+09a, Yan09, ZMAL04, ZOK+05, dSNBG08, Nal09b, HvL09]. **bond-charge** [Cam04]. **bond-length** [SC02b]. **bonded** [ABBS08, AE07, AKK05a, CL05c, DS03, DLM+04b, Dre05, DZ06b, EHH09, EZY00, FC05b, FC05a, FG01, HEJ+00, IKS08, IKS10, Iye09, JZL+08, KKYT04, KS03a, NK05b, PSK02, TSZW08, VPSH00, VDF+06, YZC09, ZYC09]. **Bonding** [Dav04, FSK05, OA05, ZZHL08, ZLY+09, Bu02, CZ03, CSL05b, CS00a, CVVA08, CMY06, Dro04, DFZ05, EHN09, ESU04, ESU05, ETBA06, FTB04, FSGB05, GZD+05, HT04, JZK02, KK02a, KS08, KS04a, KK08, KSS00, KM00c, LTV03, LH07a, LCL+09a, LLZ04, Liu08, Mat00, MWHZ06, MROA06, MJ00, MLP08, NSS09, NGRR02, NJR+09, OG00, OHT03, PML09a, PML07, PTLB00, PC04b, RJN+08, RJF+09b, RJF+09a, RC05, SKN+09a, SBB05, She04b, SEU02, UES04, Var07, VK05, VMA03, WLZY08a, YKK+05, YL02, YI04, ZQF+02]. **bonds** [AG02a, AVBč06, BVHS05, BL02b, BRR04, BTL+02, BN01, Buc05c, CVPGH+06, CC07, DVHJ03, GT07, GBB06, HKR09, ISK+01, IROW09, KS06, KSS+08, KM01, LWC+09, LLYL06, LLL+07, LJL09b, MGB+06, MJ00, OA02, PM09, RWW+01, RG08, RS00, RRD06, SNM+04, SKK+05, SKK+06, SIT+07, SKT+07, SKK+07, SIS+08b, SIS+08a, TKY00, TQC05, VM06c, XLX+09b, YYI+09, YTS+05, YZG06, GSCRO08]. **Book** [Ano01b, Brä04b, Brä04c, Cal02a, Cal02b, CC09, Deu00, Deu06, DR04, Kar01, Kry08a, Lar01, Lin01, LM04, Lun04, Ort04a, Sul00a, Sul00b, Sut00, Tri04, Wil04b, Wil06]. **Books** [Ano00b, Ano01c]. **borane** [LXTT00, LZYT01, LZHT03, LZT03]. **Borderline** [FKR04]. **boriranes** [KV07]. **Born** [OMNN04, CA07, HT05a, IYO+04, Nak02, Nak07, OMN+03, PCBA08, SA09, Tak09, YOM+01]. **boron** [GJ03, JMP05, JWM00, Lia08, LČM01, MKCS05, RPB00, XL08, ZW04, ZRF+09]. **boron-like** [ZW04]. **Bose** [NNNY01, Pom04]. **boson** [PF06, YNN+06, SMB09, YNN+06]. **Bosons** [Wyb02]. **both** [RLB02]. **Bound** [Aze02, BPŠB00, KH06, KH07, MB02b, PE04, RJP08, Yal04, AV04, Bau09, CJZZ06, CCH05, CCH06, CF05, CW08, GW05, HN09, JZZ+09,

LCN05, MZF05, MSB00, Mar07b, OC08, PFSFH06, SASS03, SSSK07, SGS00a, SKT05, SB04, ZSW+00, ZWM+04]. **boundary** [BE07, BB06, DFM+02, ER05, PW07, Pla01, VNB+03]. **bounded** [Koh01]. **Bounding** [ISS00]. **Bounds** [Mor02, Whi02b, AC02a, MSB00, Mar05c, MB07a, Mor03, VATPR01, Zho07]. **bowl** [JPA03]. **bowl-shaped** [JPA03]. **box** [DGC08, TA06]. **boxes** [CMRMR00, CMNH07, MCLKC02]. **BP** [QMB+06, QMB+06]. **bpca** [BT05]. **bpy** [BPM01]. **Br** [Ano07g, Ano07e, Ano07f, ARBD05, BL02b, DETA02, GR07a, GR07c, GR07b, KTK+04, MMV05a, RdTdLC+07, Var07, WZJ04, ZJZ00, FL04, GMS+05, HLMH07, KM02, LWL+08, QTT07]. **Br-bond** [LWL+08]. **brackets** [CCLK04]. **branch** [LCN05]. **branch-and-bound** [LCN05]. **branched** [Pet00]. **branching** [ERVR06]. **Brazil** [SD03]. **Brazilian** [BCC05, CA06, CB08, SD03]. **BrCl** [WZWC07]. **breaking** [CNDÖ00, IDM+09, JPMM08, LP08, LP09b, MC00]. **Breathing** [SPL03]. **Breit** [DBd05]. **BrF** [LWL+08]. **bridge** [BA07, DD05, KWWQ04, LY09, Mai08a, Mai08b, SR05, SDZ+07, TOK+00]. **bridged** [BL04c, HCL03, KSN+04, KFS00, MOAB01, MOA02, SS08a, ZLY05, ZL06, NSS09]. **bridges** [CMM+07, PV09]. **bridging** [ERC+02, HC02, SBF03, YYQ+06]. **Brillouin** [HMW02, HMW05, PMHW07, PČH02, SH09, TKT+05]. **Brillouin-zone** [SH09]. **BrOClO** [Li09]. **broken** [HPR09, KSN+09, MYGD01, MJG+05, NYU+08, TYY06, ZLY05]. **broken-symmetry** [HPR09, TYY06, ZLY05]. **bromide** [KTK+04, SMS07]. **brominated** [EGE08]. **bromine** [BZH+07]. **bromo** [DKP+06, FS05, Sha07]. **bromoacetyl** [NMNB06]. **bromocarbons** [WLZY08a]. **bromoform** [VKIJ06]. **Brönsted** [SCHH01, SCHH02, TC07]. **Brownian** [OK04]. **Brueckner** [LS02, Ort04b]. **Brussels** [GDV05]. **BS** [KNS+09]. **BSSE** [ADSTS06, BVHS01, BKMS03, BVHS04, BS05a, HVSM02, May04]. **BSSE-corrected** [BS05a]. **BSSE-free** [ADSTS06, BVHS01, BKMS03, BVHS04, HVSM02]. **BTO** [RFE+00]. **buckminsterfullerene** [ASH07, Pau04, PDS04]. **buffer** [MGK+09]. **building** [AE04, Gui06, SEY07, SEY09]. **built** [TS01a]. **bulk** [CC00a, TMS08, USM01]. **bundles** [CAHl08]. **BuOO** [VG02]. **butadiene** [AZD06, BL02c, KP02, ML08]. **butan** [YZC09]. **butan-2-ol** [YZC09]. **butane** [GTSK07]. **butanediol** [FSLL02, FSLL04]. **butene** [FSLL02]. **butenenitrile** [OCK07]. **butyl** [ABM02, BT05, CDS06, MGZL04, MJG+05]. **butylphosphonates** [CDS06]. **butyltetrahedrane** [DAD05]. **butyne** [Met05]. **BWCC** [HMW05]. **BX** [BVG05a]. **byproduct** [PMBM09].

C [ASH08, Ano00a, Ano00k, Ano02c, BM01b, BE07, BES08, BK04b, BT05, CXZ09a, COMA03, CMY03, Cos06, FFFR02, FFLZ02, FRNM08, GV06, GJ03, HZJ+07, HDL00, KM02, LTV02, LLW+07, LH00, LH07c, MVdCD00, MOA07, PT00, PDS04, RCF02, RGP07, RD00, RÖ00, RSTG02, SYL05, SUA+04, SLA+05, SUL+07, SUL+08, SCHW07, TCS+08, Tem02c, Tem04,

VRA+02, YST+05, YKS+06, ZMAL04, ZFD00b, KMVR05, STN+06, YLS+04, YT03, ZMS05, ASRL06, AL09, BIP+07, BAG+08, BG00c, Buc00a, Buc05c, BZR02, CBMRN08, CZS+05, CC00c, Cos06, DS06, DGQT09, DM00, DBLM06, EBB06, FFFR01, FRT+00, FF01, FRGF04, GDFT01, GBA05, Gre09, GBB06, HNKiS01, HGS03, JV05, JXW+04, Kak03, KLK08, KES03, LCRB01, LV01b, LWL+08, LTY09, LTL05a, LZXD05, LPZW05, LDG+06, LH07b, LFR+08, LLP05, MLW+09, MS03, Mar04a, MNJP05, Met05, MLL00].
C [MLL01, OA02, PIGN02, PGNT02, Pau04, QV01, RNVTP09, RFS+00, RHH+02, Sah03, Seb05, She04a, She07d, SMDG09, SYL05, SUA+04, SLU+06, SRS+04, Sok02, TNO09, TSP+07a, TCS+08, TWZ03, TW05a, TR00, TRF+00, TOB02, VM07b, VHM+04, VK07, WSBV05, WSC+05, WT06, XXY+05, YZY+01, ZFD05, ZWMZ04, ZLL+09a, ZMAL04, ZFD00b, ZKRS07, dLCRF+08, PCBA08, TBML06]. **C-3** [PIGN02]. **C-4** [PIGN02]. **C-C** [OA02]. **C-NMR** [PGNT02]. **C-Si** [TR00]. **C1** [RS08]. **C3** [RS08]. **C60** [FRF02]. **Ca** [SCHW07, YCS09, ZL04, ASL06, AML+01, MTE09]. **CaB** [PRNM03]. **cadmium** [Boe07, LSK+06]. **cadmium-oxide** [Boe07]. **caespitate** [MK08]. **cage** [LTL05a, LZXD05, Sad02, VED+02]. **cages** [CZS+05, LZXD05, LPZW05, MSSM00, MSMS03]. **calcium** [CMM+07, FBGA04, PFSP05, SKNN08]. **calculate** [Bar09a, HN03, VHM+04, WC04]. **Calculated** [ABI07, Buc02a, Buc02b, FC05b, AGN04, AS00, BSR02, ÇAK07, DCTC03, IPPL05, JV05, KNO09b, LV01b, LPV05, LFR+08, OR07, TNJL05, WRRF03, YPS05]. **Calculating** [AG01b, BDG01, HPC+08, Kir08, LN03, MGK+09, Ort05, PGPA09, UB05, YSS08]. **Calculation** [ARBD05, Bou03, BKAT00, Col08, CS01, DPW00, ER05, FN04, Gos01, GM03, Har06, ILVMSB+02, KS00, Kýv09, LCK00, Mor06, NF02, OMY+01, ÖÖOY02, PJS+09a, RSM+04b, SSK09a, SNN+09, VB04, ZW04, AKN09, BBHQ04, BCG09, Bar00, BCvzGG04, BC06a, Bar06, Bar08, BKM05, BM07a, Bra08, CC00c, CSTB08, DD05, DBFP05, DETA02, EZ05, ESKB04, FSLL02, FD09, GY04, GMCS04, GAL+05, GBA05, Gög06, GM00, GM01, GM02a, GM02b, GM08, GE09, HAL+02, HW02, IMT+02, JÅM01, Khe09, KFS00, KF09, KNO09a, LTV07, MR00, Mal05b, MMV05a, MTE09, MWHZ06, MNV07, MBR07, MYS+09, Mor04, MC06b, MW06b, NKS+09, Nee01, NPLV05, OCWY09, PR05, PVZV00, PVB+02, PJ09, QTT07, RT06, Rom08a, Rom08b, RM07, SBM00, SC01, SNY01, SLCW04a, SCLL07, TC05].
calculation [TOC06, TYSY07, TMPI05, TB03, UT03, VBML04, WS00, WK06, WW08, XZGZ06, ZWMZ02, ZCFD02, vLvL06, HM01c, ILVMSB+03, MOL03, PMO04].
calculational [EYBM03, OM03]. **Calculations** [PKS+00, SCSWF04, Tor06, ARBC+05, AWZD05a, AWZD05b, AM09a, ACD02, ARH00, AK05, ASP+05, ANJ09, AÖG07, BF07, Bar09a, BKGF02, BDMS01, BZG+02, BZG+04, BLC+00, BR00, BR02, Boe03, Boe04, BR05, BSCB04, BKM+02b, BB01, BB02c, BB04, BB05d, BBG00, Buc05b, BLKJ00, BSK+02, CA07, CJ09, CL00a, CCGF07, Čár09, CS08, CL05e, CN05, CMY03,

DBd05, DFH02b, DCP06, DHZ06, DZO00, DFMZO08, DKW09, EB04b, EB04a, ESTU05, ETBA06, FS00, FG01, Fra06a, FVPM05, FFHD00, FSR02, Fuk09, GBS02, GSfLV08, GDB03, GT07, GGLS02, Gün06, HSS09, HBKG03, HT05b, HM05a, Hea00, Hea03, HH03, IBB08, IVK00, IZ04, JFC02, Jal02, JLAR07, JJ02, JKU02, KP02, KP05, KPČM05, KCOV07, KB00, KCS02, Koz04, KZvL09, KANK00, LFK06, LTV05, LHG00, LJL09a]. **calculations** [LSH08, LS01b, LZZ+06b, LE01, LSE05, MGCD01, MK00, MKCS05, MST04, MST08, MARK08, Mic06a, ML01, MAS09, Moh00, MBK01, MW05, MCZWD06, MMF00, MCC08, MBA+08, MTO+03, MTWN09, MTB+02, MJ06, NRS+02, NKP+02, Nic05b, NFL+02, NSZZ04, NSG+06, Obe00, OMNN04, Pat06, PCBA08, PF06, PJZ+09, PBMA03, PM04b, Pud02, QMB+06, QGW02, QGW04, QCK04, RLBK03, RA03b, RP09, RPPO00, RPB00, RBLS04, RLA+01, RSRMBFR00, RIVB03, RKR+06, RdTdLC+07, Roy08, SPN03, SFPA03, SLE05, Sch05, Seb05, SN06a, SFZO01, SH09, SMM06, SMEA08, SH02b, SK05b, SLCW04b, SHE+02, SHE+00, Stu00, ŠPNU08, STS+00, TI05, TKY00, TYY03, Tal03a, Tal03b, TDF09, TOB02, TMAB01, TR09, THPN03, VRA+02, VD00, VPSH00, VGMN03, VRE+04, WRRF03, WSBV05, WLZY08b, WTWT09, WSNB00, WL00, Yal04]. **calculations** [YYYM01, Yam09, YSY+01, YKGC09, ZT02, ZB05, ZLC04, ZS04a, ZFD+00a, ZLHL02, ZLY05, ZZM09, ZY04, ZT04b, dOEG+08, HNKiS01]. **Calibration** [ZMMK09]. **calliactine** [VRE+04]. **calorimetric** [MYS+09]. **cAMP** [ZLL+05]. **Can** [CL00a, CRL+02, MHGR07, Nes01a, Squ05, BBSS00, CBA+06, HR02, Mat00, PPP+08, SK09]. **Cancellation** [TPRVC01]. **cancer** [Lad00, SLS+05]. **cancerous** [Lad06]. **candidates** [GdA01b]. **cannabinoid** [BNHB+02, eSPM+08]. **canonical** [Fer02, FMBM05, KKMS04, NS04, PILD07, WO04]. **cap** [HPC+08]. **capable** [GGACT03]. **capacitance** [HKR09, JÅM01, STAO00]. **capacitance-polarizability** [JÅM01]. **Capillary** [DH04a]. **capping** [MLL00]. **caps** [SWSH09]. **capture** [TBM04]. **Car** [YZX+08, KOH03]. **carb** [Tem02c, Tem04]. **carbanion** [Bro05]. **carbazolyl** [WWW+07]. **carbene** [LYWX07, WML08]. **carbenelike** [VMRA04]. **carbide** [SMDG09, SM03]. **carbides** [FYT09]. **carbocation** [RJB+06]. **carbocations** [Vrc07]. **carbocyclic** [GMTM02]. **Carbohydrate** [BCFR08]. **Carbohydrate-binding** [BCFR08]. **carbohydrazide** [ZFZ+08]. **Carbon** [CVVA08, CPR06, JP08, AS04a, ALM05, AM09a, BBO04, BJAV08, Buc07, CMW03, CWZ03, CAHl08, CIT+03, CSDCCMZT03, COMA03, Col08, DDT+03, Den09, DGSD07, EMV05, FGFF06, GDFT01, Guo07, GWSZ08, JLM08, JLC+09, JWM00, KDŁL07, KVZ+02, KVZT04, KG08, KG09, LMMB03, LZC04a, LZC04b, LPC04, LTW09, PML09a, QFC04, QCFJ05, SL05a, SL05d, SHM+09b, SÖ04b, SS09d, TOH+00, TT04a, Tor06, VM06a, VML05, VM07b, WSBV05, WSC+05, ZLC04, ZCWZ04, ZLL+09a, ZA09]. **carbon-based** [CIT+03]. **carbon-containing** [AS04a]. **Carbon-donated** [CVVA08]. **carbonate** [ZFZ+08]. **carbonates** [WB05]. **carbonic** [QBTS05].

carbons [CR08b]. **carbonyl** [LML02, Mal02, WPB+06, XLX+09b]. **carbonylation** [DR08]. **carbonyls** [BDBG09, VR01]. **carboxylation** [TFS+02]. **carboxylic** [LS01b, YWZ+09]. **carboxypeptidase** [KVSG02]. **carboxypeptidase-A** [KVSG02]. **carbynes** [DM00]. **Carcinogenic** [TBCG05]. **carcinogens** [KES03, Lad00]. **Cardinalities** [MBM04, Tem02c, Tem04]. **Carl** [And05]. **Carlo** [AC05, NY03, AMOR07, AC02a, AC02b, AC04, AC06, AC07, AC09, AM09b, ASDC08, FGH09, GBS02, HI06, HKY07, KBV05, MGdS+08, NKP+02, SNY01, UT03, UC00, Vrb08, YYY+00, YOGR09]. **Carlo-quantum** [UC00]. **carotenoid** [MDS+09]. **carrier** [Tem02b]. **carriers** [HOIK09, SK00b]. **carrying** [OdSC05]. **cartesian** [KKS09, KOT09, RFE+00]. **CAS** [TYY04, TYY05b]. **CAS-DFT** [TYY04]. **Cascade** [SY07]. **CASCCSD** [IAL06]. **Case** [CTSÖD03, BM01b, BEM02, CC01a, FOM+03, GGS09b, LČM01, Noo06, Oni07, PW09, PLU08, SCM00, TTFP04, YTS+05, FCLH+06, IYY03, ZH06, ZNZS00]. **cases** [FKR04, MMB03, SBT+03]. **CASP3** [LLR+00]. **CASPT2** [AZD06, DGLM09, SB03]. **CASSCF** [AZD06, CY04, NUY+06, NYU+08, SB03, Sha06]. **CASSCF-DFT** [NYU+08]. **CASSCF/CASPT2** [AZD06, SB03]. **cast** [Now01]. **Catacondensed** [RB08, RB11]. **catalogs** [Tem02a]. **catalysis** [FTGH04, HP07, LZZ+07, MM02, TFS+02, YYQ+06]. **catalyst** [AGFM03, BPM01, GARB08, LXTT00, LXHT00, LZYT01, LZHT03, LTLS05, SAE08, YLS+04]. **catalyst-alkoxyborane** [LXHT00, LZHT03]. **catalyst-borane-keto** [LZYT01]. **catalyst-borane-ketone** [LXTT00]. **catalysts** [CC05a, CCA+06, LXH+00, MH09, NAE06, RS08, TBJA03]. **catalytic** [AG01a, CZWZ05, CCV+07, DCP01, GKL+09, GBMMSA00, HSN+09, HP07, KNRR05, KVSG02, LSWT05, RSM+04a, SWST04, Sch04, SUAL04, TTM01a, YLS+04, ZHA01]. **catalyzation** [ZL00]. **catalyzed** [BZBT01, CCV+07, DKD+07, EMV05, FWT08, IN09, LXH+00, LXTT00, LXHT00, LZYT01, LZHT03, LZT03, LYP+06, LTL05b, MLZS06, MWL08, REHH07, SPS02, SZML07, TGG01, VTS05, WML08, XFLX+06, YWZ+09, ZSL+09, LTL06]. **Categorization** [BM02, Kle03]. **CaTiO** [ES02]. **cation** [ABL03, BHK09, ELO+07, GTSK07, Kry07a, KB08, LSBDL02, MdlV03, MMZ02, NLD+04, PNBV07, RHHH00, RSTG02, SBL05a, SQZ+02, SKNN08, SZML07, XCW07, YWC07, JWZ+08]. **cation-** [MMZ02, JWZ+08]. **cationic** [DKC00, Guo07, IDM+09, LDPP05, LDP05, TW05b, ZNZS00]. **cations** [ASL06, BKLB06, BBD07b, Buc01, ČAV+09, CSM02, CMY03, DKWP04, DKM+04, Elr09, GBS02, GDB03, KWC09, MMR+04, PT00, Pej02, PMCOSC00, SM07a, VSS04, WWTHF09, YCS09, ZŠ05]. **CATIVIC** [MBA+04, RSM+04a]. **caused** [LWZ+05]. **causes** [Yam04, Yam05, LCH05a]. **causing** [OM03]. **cautionary** [Bau09]. **cavities** [BES04]. **cavity** [CSP04, FBGA04, Gri08, YSP06, YSP08]. **Caxambu** [SD03]. **Cayleyan** [Tem00]. **CB1** [BNHB+02]. **CC** [CGS01, ISK+01, MVdCD00, CC02]. **CC-SCE** [CGS01]. **CCSD** [FHK06, GBP05, HMW05, JKU02, Li09, Mor06, Mor08, PGF+06, ŠPNU08].

CD [WRRF03]. **CD26** [GI07]. **CD26-derived** [GI07]. **CDA** [VRFS05]. **CdCl** [VRA+02]. **CDK2** [LMDW09]. **CDK4** [LMDW09]. **CDn** [GI07]. **Ce** [TIGD09]. **cell** [GKR00, Lad00, Lad06]. **cells** [SMM02]. **cellular** [Nes03a]. **cellulose** [KFTBS07]. **Center** [Gus03, Har03, AGMK02, AS04c, Ave04, BSH04, Buc08, Bud04, CCV+07, CS01, CGS01, DRS00, DS07, EKZ06, Gin06, GM00, GM01, GM02b, Har02b, Hog09b, JJWH04, KS04a, KOT09, LPV07, MR00, ÖO02, Özd04, ÖKAY03, PC04b, Pri05, RFE+00, RFE+01, RLER08, RP00, RSM+04b, SH02a, Saf04, SB06a, SZZ01, SS09b, Sme02, VSD+02]. **center-expansion** [CGS01]. **centers** [BSCB04, HYC+00, NRS+02, SKA05, ZKEE07]. **Central** [SHG08, Gus02b, Gus04, MNA+99, TPGD02]. **centroid** [OOK03]. **ceramics** [KS00]. **ceria** [FVPM05]. **ceria-based** [FVPM05]. **cerium** [RSDNSB00]. **cerium-doped** [RSDNSB00]. **certain** [ASO+01, ASO+04]. **Cetraro** [RRUE08]. **CF** [MB06, TCS+08, DBPG04b, GMS+05, MY08b, MMS+09, MB06, MMV05a, XD03, ZD07a]. **CFC** [MMV04]. **CFCl** [SSB00]. **CFHO** [ZD07a]. **CFL** [Esc08]. **CFL-like** [Esc08]. **CH** [Ano07g, Ano07e, Ano07f, CSDCCMZT03, DBG04, FGC04a, FGC04b, GR07a, HGS03, JCTA08, JFS+09, LWCF08, TLYW06, TM05, VK08, YST+05, YLZ07, YW05, ZLML05, ZCZF02, Buc02a, Buc05a, CBMRN08, DLTW04, FGC04a, FGC04b, GR07c, GR07b, GSRL06, GMS01a, Irg04, KSI+07, LDXW04, LLW+05a, LLW+05b, LZZ+06a, LLW+07, LDR+08, LC05, PSN08, Pet00, RGP07, STW+05, SHH+06, TKY00, TSP+07b, TWZW09, TM05, VK08, WZWC06, Woo02, XD03, YMZH04, YZG06, YLZ07, ZD06, ZCZF02, ZZW+06, DGP08]. **Chain** [dFGM08a, BLC09, BFRB07, BBL09, Boh01, CVPGH+06, CFP00, Fan01, Fan03, IA06, IKS08, IKS10, KRR08, LLSY05, MPKB06, PK01b, Spr00, ST01, SDB03, dBC06, HBW+08]. **chains** [ASO+06, CWZ03, CK09, EYY06, GM05b, GM05a, JMP05, JWM00, KTK+04, KCGB02, Man05, MD08, MML+02, MBK01, MSC05, RZ07, SD09, VM06a, YZ08, ZCWZ04, ZLL+09a]. **chair** [FFHT05, QD04]. **chalcogenoacetylenes** [RME+03]. **chalcogenol** [RME+03]. **challenge** [AK02, Gre09]. **CHAMBER** [CWW09]. **Chang** [AWZD05b]. **change** [KPP01, LLSY05, SSC+07]. **changed** [Kut09]. **changes** [FCLH+06, HSW+00, Oni07, Pen00a, TX02, VSI+07, ZSM+01]. **Changing** [SM06c, SK00a]. **Channel** [Sad00, RE06, SEY09, TSP+07b, TBML06, TRMM04]. **channels** [BGJJ01, CCH05, CCH06, Nal09a, Nal09b, NSLR04, OCK07, She07a, TS01b]. **chaos** [ACG04, DH04b]. **chaotic** [MD02]. **character** [Bu02, HD03, Hua04b, JTH02, SBL05a, YKT+02]. **characteristic** [Ban05b, CD04, MBM05]. **characteristics** [ESTU05, KFD09, SBK+09, ZŠ05]. **Characterization** [HRDM+08, RP03, RG08, SNH00, SCRE08, YTD05, Bro00, CZWZ05, LW07, Liu08, MRMR02, MPIP+01, RMB00, Ran02, ZZW+06]. **characterized** [ABM01, MNA+99]. **Charge** [Buc05a, DNN+06, JdL08, MSC05, Nal00a, RWW+06, Sah03, SD00a, TFBM02,

TWSK09, vdVM00, ATN09, AZD06, BMŁT07, BL02a, BSN05, Bor08, Buc02a, Cam04, CFV02, CTP$^+$08, CM09, Dei04, Dei06, Del03, DFRS07, DLHP04, ELC08, EMM$^+$02a, Gin05b, GSH02, GBB06, HKR09, IPPL05, JCTD08a, Jal08c, KP05, KM00a, KM03a, Kor05, Laz02, LGJP05, LP05b, MO06, MESH02, RA02, RHH$^+$02, SN02, SASS03, SL05b, SK00b, SMS07, SHC00, SCHH02, SCTK$^+$09, TBM04, TC07, VLJ08, Von00, WLZY08a, YLYD03].
charge-assisted [WLZY08a]. **charge-dependent** [VLJ08]. **charge-dipolar** [ELC08]. **Charge-induced** [RWW$^+$06]. **charge-transfer** [ATN09, KP05, Kor05]. **charged** [Buc05c, FSGB05, För00, GB09, GT07, GMCS04, LDMR01, Mar00c, Mar06a, MSC05, SW02]. **charges** [Ess07, KK07, PRM$^+$06, SM07a]. **Charles** [ÖS00c]. **CHARMM** [CWW09]. **CHCH** [HGS03]. **CHCHCHX** [DLTW04]. **CHCl** [SSB00]. **check** [TOH$^+$00]. **Chelate** [DST$^+$04, CJZZ06, YPD$^+$07]. **chelates** [KWWQ04]. **chelators** [GP08]. **Chemical** [AA04a, AS04b, Bar09a, ESU04, Har06, Lar02, Mic09, Nal09a, OG00, OHT03, She07c, SSK$^+$05, YKK$^+$05, AMC07, AM09a, AKK05b, ASP$^+$05, ASO$^+$01, ASO$^+$04, AAB05, BFRB07, BF08a, BC06a, Bar06, BZ06, BZG$^+$02, BZG$^+$04, BBPG08, BBD04, Bou03, Buc05c, BM02, Cas00, ÇKB02, CC08, CBRBT03, DKD$^+$07, DDT$^+$03, DDW$^+$06, DFT$^+$07, Dro04, Dun01, Esc08, ESKB04, ESU05, ETBA06, FB01, FSLL02, Fra06b, GTSK07, GJB00, Gin03, GKL$^+$09, GQ00, GSK01, HSW$^+$00, Hog04, HKR09, Hyd06, Irg04, ISK$^+$01, IYY03, INS$^+$08, KK02a, KS08, KP05, KDC09, KF03b, KSS00, KMS02, Koz01, KS04b, KS09, KS03a, Lad00, LZC04a, LXH$^+$00, LXTT00, LXHT00, LZYT01, LWW$^+$02, LZHT03, LZT03, LFZ07, LVSG06, Mat00, May02a, MME09, MBK01, MEN$^+$08b, NOM00, Nal09b, Now01, Ou06, PIGN02, PNG02, PFC02].
chemical [PCKC08, PJZ$^+$09, PLO02, PSB$^+$05, RCF02, RVR00, RNVTP09, RVP06, RAdS05, RS00, STAO00, SRA09, SKN$^+$09a, SMOE02, SLRS02, Sch05, Sch00, Seb05, SSB00, SRK01, Sey08, SSK09a, SSJ09, SMM06, SNM$^+$04, SKK$^+$05, SKK$^+$06, SIT$^+$07, SKT$^+$07, SKK$^+$07, SIS$^+$08b, SIS$^+$08a, SYL05, SEU02, Sta00, SZSP02, SV08, SM09, ŠFW00, SQZ$^+$02, SKNN09, SCMS07, Tac04, TVK$^+$02, TOB02, UES04, Var07, VRE$^+$04, VG06, WHD$^+$05, Woo02, XR05, YYS$^+$09, YYI$^+$09, YL02, YKS$^+$06, YZ07, YPS05, ZVVT07, ZSPS03, ZS04a, ZD06, ZD07a, ZTSZ07, ZKEE07, dBC06, dAGD08, dVHB03].
chemically [MVL02, YY04]. **chemicals** [Bar09a]. **chemielectron** [TIGD09]. **chemiionization** [TIGD09]. **chemisorptions** [KDŁL07]. **chemist** [Mon00]. **chemistries** [DPS04]. **Chemistry** [AV06, AC05, AWZD05b, Ano07a, Ano07g, Ano07e, Ano07f, BB05d, DT02a, FAE$^+$05b, Har06, ND03, Roy05a, SD03, SCRSRE06, Tem04, Yam05, ABB$^+$07, BL04b, BCvzGG04, Bar06, BKGF02, BDL03, BD07, Brä06, CC05c, CMNH07, DCDW00, DKS05, DL03, DV00, DLM$^+$02, DLM$^+$04b, DKP$^+$06, EFM06, Fri06, GD00a, GMK$^+$09, GSPT$^+$07, GSD$^+$03, HM05a, Hyd06, Kai09, Kar09, Kar10, Kut09, Mat00, MVG$^+$04, Nal08, OSW07, OY01, PGF$^+$06, PL09, QG04, QW05, RT06, RSN$^+$07, RdTdLC$^+$07, RSM$^+$04a, RB06, She07b, SZZ01, SHG08, Sok02, SEM05, Tak09, TL05, VWSA$^+$04, XL08, YI04, ZFLL00, dLCPLD$^+$07,

Ano06f, Ano06g, BCC05, CA06, CB08, GDV05, Nag03c, PČ04a, VM07a]. **chemistry-like** [RdTdLC+07]. **Chemists** [Ano08c, Bau09, Wen09, Ano08a]. **Chemometric** [FA00, KF03a, WHD+05, eSPM+08]. **Chemometrical** [VNP00]. **chemotherapy** [SLS+05]. **CHF** [BDA+02]. **CHFCl** [ZCFD02]. **Chichester** [Kry08a]. **Chiral** [CL05b, DZ06b, YZC09, ZYC09, BBHQ04, DFZ05, GP01, JLM08, Kon04, LXH+00, LXTT00, LXHT00, MWL08, VM06a]. **chirality** [LWZ+05]. **CHIRAPHOS** [LTL05b]. **CHIRAPHOS-type** [LTL05b]. **chiroptical** [Pol06, WRRF03]. **Chirped** [Mal07]. **chloride** [IYSS07, KVPS05, LHL+00, Sch05, SMS07, SMSM02]. **chlorides** [PSH00]. **chlorine** [LWW+02, LDZ+05, ZDAZ03]. **chloro** [DK04, ET01, JNF+09, Sha07]. **chloro-** [ET01]. **chloroaniline** [MGV00]. **chlorofluoromethyl** [ET05]. **chloromethyl** [ET05]. **chloroperoxidase** [BSCB04]. **chlorophenol** [CJB08]. **chlorosilylenoid** [FFLZ02]. **chlorosulfonate** [SSN03]. **chlorotoluene** [CC00b]. **CHO** [GMS01a, BDA+02, LAL+08]. **CHOHNO** [YZG06]. **Choice** [Hog04, JR02, PJdC00]. **choices** [SMY07]. **choose** [SGS00a]. **chorismate** [SCMS07, WRK03]. **chromium** [KFS00, LH00]. **chromodomain** [JZZ+09]. **chromophore** [BL02c, May06, Sun06]. **chromophores** [BFRB07, BF08a, Kel05, KWT06, MW06a, PJP08, SR05, YS09]. **chromoprotein** [Sun06]. **chromous** [DFT+07]. **CHX** [LDXW04]. **CI** [GG00, BL02a, Ben05, DCDW00, FS00, GGDL07, GFDK09, Har05b, IMT+02, KH01, KH05, LZ05, MK00, MMM06, MTB+02, NYU+08, ONA05, PRCEM06, RLBK03, SCM00, SH02b, SNdAM08, TYSY07, TMAB01, YNN+09]. **CI/MP** [ONA05]. **circadian** [GHG04]. **circles** [CCLK05]. **circuits** [MSK+05]. **circulant** [ZY07]. **Circular** [JSvDA06, CMR05, CCLK05, JNKMS03, KBV05, Noo06, OCWY09, Ols04]. **circulenes** [MZ09]. **cis** [CGMT03, Bou01, CGMT03, HGRL01, HGTW03, SD08, BL02c, HFGL02]. **cis}-** [HGRL01]. **cis-Diamminedichloropalladium** [HFGL02]. **cis}-platinum** [Bou01, SD08]. **cis-trans}** [BL02c]. **CISD** [Mei08]. **cisplatin** [CHR+06, DCD08]. **CISTCP** [Cas00]. **citrate** [Cor06]. **City** [Cas00]. **Cl** [AZD06, Ano07g, Ano07e, Ano07f, ARBD05, BL02b, BBD07c, BBD08, BDBG09, DLTW04, DETA02, FBBB06, GR07a, GR07c, GR07b, HZJ+07, LSC01, LCRB01, LLX+03, LDXW04, Mar09, Sch05, SRS+04, Var07, VK08, WGLX02, WZJ04, dD04, DLK00, FWZ09, GSRL06, KM02, LCRB01, LLX+03, Mar09, MC06b, NWSC08, Pet00, SLCW04a, SLCW04b, YMZH04, ZCZF02]. **class** [BB06, JLZY09, LSWT05, SPS02, TDST07]. **classes** [SN06b]. **Classic** [Mar03a, KF03b, MDS04]. **Classical** [DM02b, BMP+04, CF04, CTP+08, DC03, DAA+06, Fer02, FYSS09, HM05a, HAL+02, IS03, KA05, Nég03b, Noo06, NU09, PA04b, SGGBB02, SdACAG03, VGB05, Zak04a, Zak04b, ZH06, BFBB06]. **classically** [QS05]. **classification** [FA00, TBCG05]. **clay** [MJG+05]. **ClB** [MJ06]. **ClCCCl** [GHH03]. **cleavage** [DGP08, SBKSS05, ZMAL04]. **Clebsch** [Fan03]. **Clemenger** [BKM+02a].

Clifford [Muk00]. **ClO** [YBS05]. **ClO/ClO** [YBS05]. **ClOBrO** [Li09]. **close** [CGS01, HK06]. **close-coupling-single** [CGS01]. **Closed** [JJWH04, LM02b, Pal01a, DMH+05, DHCD06, HdMB+05, JNSF04, MB00, Mon05, Ort05, PVW03b, TG05, AEI00]. **closed-** [PVW03b]. **Closed-form** [LM02b, Pal01a]. **Closed-open** [AEI00]. **closed-shell** [HdMB+05, JNSF04, MB00, Mon05, Ort05, TG05]. **closer** [SFR08]. **closes** [SÖ04b]. **closing** [JPA07, ZLL+05]. **closure** [CSWD06]. **Cluster** [KN08, ACB+02, BK09, BC03, BZR02, CZ03, DEN02, DM08a, DMM+02, EBS+09, FHK06, FD01, GT07, GBL06, GPW06, GWK+05, Hea00, HMW05, IBN08, ISK+01, JR02, KS00, KPČM05, KNO09a, KV08, KSWR00, KR07, LPC04, LP00a, LP00b, LP04a, LP08, LP09a, LMSB00, LZW+07, Luz08, MST04, MST08, MB06, Mei08, NRS+02, NS02, NBS04, OY01, PILD07, PBS02, PVW03a, Pej02, PHK+06, PGW08, PGW09, PČH02, PPP00, PJS09b, QCK04, QV01, RVP09, RNCM05, RNS04, SBM00, SYZ+09, SZL+09, Shi02, SKT+07, SKHY09, SM03, SSS02, SS08b, SMK08, TI05, TB06, TKT+05, TOB02, WZW+09, WF04, YKT+02, YNN+09, MDG07]. **cluster-configuration** [DEN02]. **clustering** [GHK05, KM00b, KM03a, KM03b]. **clusters** [AYD00, ACG00, ACF04, ACF05, AÖG07, BF08a, BCG09, BK04a, BT05, BDMS01, BCD+05, BLC+00, BŠM01, BKHPvD01, BKM+02a, BLRT02, BFB08, BGÖ+01, CGCS02, CNPA04, CGG05, CC07, CXZ+09b, CLL04, CL07b, Cou05, DP06, DRD+05, DKS05, DAD+03, Die00, DFRS07, Dkh08, DZTZ05, DPS04, FTB04, FSGB05, FBBB06, FF09, FV04, FPC05, GDFT01, GGPS06, GP03, GBC+02, GWJ05, GW06a, Guo07, Gur05, HZJ+07, HRDM+08, JAP+05, JCP+08, JXW+04, JHLC09a, JHLC09b, JG09, JZK02, KUS+03, KSS+08, KSK00, KG02, LDMR01, LCRB01, LDPP05, LDP05, LAK09, LP00b, LJL+03, LZXL05, LLYJ09, LB06, LGBJ03, LNPL06, Mar04a, MDJ01, MRT00, MMF00, NWZ+07a, NK05b, Nov07, ONK+00, ONK+05, OKY+08, POAVdlM08, PC09, PJZ+09, PBI+01, PHNN09b, QMB+06, QZ07, RKM09, RBL04, RBL08, RPPO00, RPB00, RWW+01, RAA05, RF01]. **clusters** [RdTdLC+07, Sad02, SKK+05, SKK+07, SBL05a, SS02a, SLW+07, TB03, TNET03, TL05, USM01, WFS+01, WNW05, WSBV05, WSC+05, XXJG03, XXJG04, XBHL04, YKT+02, YSV05, YWC07, YPD+07, ZLXL07, ZS04b, dLCPLD+07, dlPCLG+00]. **CM2** [LCT00]. **CM2/INDO/S2** [LCT00]. **CN** [BK04a, GL00, Mar09, Pet00, Tor04a, DZ06a, MD04, MJ06, Pet00, SUAL04, SHH+06, Tor04b, XXMJ06, ZD06, BEM02]. **CNDO** [HNKiS01]. **CNDO/S** [HNKiS01]. **CNMe** [TLC06]. **CNO** [PM09]. **CO** [AWZD05a, AWZD05b, AZD06, DR08, JG09, LH00, MP05, MBOA09, RD00, Tor04a, WML08, XYS+03, YYZ+05c, ZLML05, JSvDA06, MVdCD00, MMZ02, ZLHL02, CCA+06, Apo06, BLC+00, BDBG09, BZBT01, CCH05, CCH06, DW00, DS03, DND06, FD09, FS08, HW02, Jal02, LTV02, LXY00, MY08a, MZD01, MBD09, NRS+02, NAE06, OM04, POAVdlM08, QCC05, ŠUKŽŠ07, STW+05, SHH+06, TLC06, Tor04b, VRS01, XCC+08, ZD06, ZLY+09, AVBč06, BP03, DSW08, GBMMSA00, PBI+01, SGP+07, WZW+09].

co-catalysts [CCA+06]. **coalescence** [VU02]. **coarse** [DJNH02]. **coarse-grained** [DJNH02]. **cobalt** [CJ03, LWZ+09, PBI+01]. **cobalt-** [LWZ+09]. **CoC** [RBL08]. **COCH** [JCTA08, VK08]. **code** [GAR08b, GBL06, Nég03a, SST+03]. **codes** [ABB+07, BZG+02, BZG+04, Liv02, ZS04a]. **coding** [ŠK03b]. **coefficient** [BCG09, Boe07, JB07]. **coefficients** [ACC03, DGD+05, DWF+03, Fan03, Gus01, ILB+08, ÖÖOY02, PH07, WO04]. **coexistence** [WAJ04c]. **cofactor** [KFQ+02]. **COHe** [SPH+03]. **coherence** [MC00]. **Coherent** [PA08, RdLJ+02, AG02b, FDM09, HQM04, Mal05a, NY01, Pöt01]. **cohesive** [DWD+05]. **COHN** [BBL09]. **coinage** [PSH00]. **coincidence** [DKC00, Gin06]. **coke** [VVW+03]. **cold** [Boh03]. **collective** [RCJF00, Sch04]. **Collectivity** [LZ05]. **collision** [AE04, BGJJ01, Dei04, Dei06, GAL+05, NWSC08, PM06b, SI09, SCTK+09]. **collisions** [ASH08, BFBB06, BLM08, EMM+02a, LIBM03, OMC04, QDÖ09, RLBK03, RHH+02, SK00a, SK01a, Sah03, SL05d, TFBM02]. **color** [Bec05, GLHH09, Pöt01, SKA05]. **combination** [DSW08, MEN+08b, SYZ+09, SZL+09, TT06, Cor05]. **combinational** [FZ09]. **combinations** [Boe03, HJSS09]. **combinatorial** [Tem00]. **combinatoric** [DM08a]. **Combinatorical** [Ols04]. **combinatorics** [Tem02c, Tem02a, Tem04]. **Combined** [GP01, KF03a, dLCRF+08, BNS05, Buc08, GGS09a, GE09, JJC+06, JZL+08, KF03b, Koc00, KMS02, LSH08, LS01b, PRRMLB05, New00, PGP+07]. **combining** [PT06]. **comets** [PSC+07]. **CoMFA** [RACD00]. **Comment** [AKB06, Duf07, Gus03, Har03, Mar08, Mar06b, Sto08, SDW07, Zot06, HFS06]. **Comments** [CC05c]. **Common** [CCLK04, CCLK07, LKG09, Now01, ABB+07, Gin05a]. **Common-sense** [Now01]. **communication** [Nal09b, PGB09]. **Commutator** [MVK00]. **compact** [CHW04, DM08a]. **Comparative** [AMC07, CCE+07, FBBB06, GXT02, KFQ+02, KD05, LCL+09a, SKSS09b, TS07, VHV+05, ZBPD08, BCD+05, BLM08, FOM+03, KDF00, PKZN08, SSK09a, TKT+05, UML00, HGS03, NH00]. **compared** [För04, FB07, SM04]. **Comparing** [BG00b]. **Comparison** [BMŁT07, BL02b, ÇAK07, DLHP04, ET09, Gra08a, GSH02, HV03, HH02, KC09, KCOV07, LBP04, LS05, MLW+09, Pat06, CLSD+01, CN05, Dat04, Dkh08, FPC05, GL00, OM02, PGW09, RACD00, WRRF03, WF04, vdVM00, BF07, CRRL01, CW08, CMY03, DDP+07, EB04a, FA05, HMW05, NYU+08, PLA+07, QGW02, SSN03, SEY07, VR01, YNN+09]. **comparisons** [SEM05, AM09b, YYI+08]. **Compartmental** [BA06]. **compartments** [AG01b]. **compensated** [AM05]. **competing** [SMB09]. **Competitive** [GP08, AGM01, PML07]. **complement** [NN09]. **Complementary** [CM05c, PMC02]. **complements** [YYZ05b]. **Complete** [HNKiS01, JCP+08, KP00a, BM07a, CCLK04, CCLK07, CDGC05, DCLC05, Gus01, Gus02a, LKG09, LS01b, MP06, Pog05, SMY07, YKGC09, ZŠ05, ZQF+02, DPS04].

completely [PGW09]. **completeness** [Tem02c, Tem02b, Tem04]. **Complex** [Ras02, ABI07, AE02, AGLBM03, ASP+05, Bar09b, BLZ02, BKMHP04, Brä04d, Brä09b, CL05c, CL05d, CSL05b, CT05, CCH05, CCH06, CC05b, CPR06, DKR04, ELY09, EZY00, FRGF04, GSQ+04, GMK+09, GdRPLP08, HV03, ILB+08, JJ02, KAE03, KAE07, KCS02, KOT09, KBMM08, LZA+09, LH07c, MKCB05, MOAB01, MOA02, MFR07, Nic02, PRSLA08, PIGN02, RT06, RWW+06, SAM08, SOLI04, SS08a, SMS07, SMB09, STN+06, TYG05, WF04, Yam04, Yam05, YKS+06, YM05, YLYD03]. **complex-valued** [KOT09]. **complexation** [ELO+07, Elr09, JPA03, PMB08, Pud02]. **complexed** [FJK+01, FJK+02, KES03]. **Complexes** [FRF02, MROA06, ABBS08, ASH07, AE07, AZD06, AVBč06, BZL+09, BVS+09, BES08, BML01, BT05, BL02b, CLA+02, CG09, CSSB02, CMY06, DRPT02, DTT06, DH04a, DS03, DFZ05, DZ06b, EHH09, EGEDH03, FC05b, FC05a, FBGA04, GY04, GT07, GZD+05, GL00, HGRL01, HDL00, HY04, HQL09, IABS08, ITY+09, KP02, KP05, KM01, KFS00, KWT06, LTV02, LH07a, LWL+08, LWZ+09, LSK+06, Liu08, LK02, MBA+04, Mas04, May06, MOA05, MOA07, MOAM07, Men08a, MBOA09, MZMZ09, MRMR02, NSS09, Nee01, NRK+05, NFL+02, NSZZ04, NSG+06, OD03, OMMWL02, PGB09, PKT05, PML09a, PFSP05, PSB+05, PMLC09, Pye00, QBTS05, RVR00, RFRF05, RC05, SFD09, SD08, SSSK07, She04a, SM07a, SCHH02, STL+09, TS07, TSZW08, TDS+02, TTM01a, TW05b, TSH03, VDF+06, VMA03, WML08, WLZY08a, WZJ04, YZG06, YZC09, ZVVT07]. **complexes** [ZLY05, ZL06, ZYC09, ZLL+09b, ZOK+05, ZFD00b, ZRF+09, ZNZS00, MWL08]. **Complexity** [AA09a, AGL04a, LZ05, RP03]. **complicated** [Man05]. **component** [CDH05, CK09, Dya00, ITN08, KSN05, LJL09a, LCT00, MNA+99, MHT+08, MTWN09, YHN+07]. **components** [JMP06, MH03, PFA08, ZZUO05]. **composed** [BA01, BA02a]. **composition** [Krü06]. **compositions** [LGBJ03]. **compound** [FDLK02, JZL+08, KNN+04, LCH05a, RD00, Sch00]. **compounds** [BL04b, BL02a, BKGF02, BB09, BSKFT07, CX00, COMA03, DAD+03, DR08, FH02a, FJT+05, FTB04, För04, FPJR03, GBJM01, Hua04a, Koz01, Lat03b, LPV02, MYS+09, PBSC04, PMBM09, Pet00, PJS+09a, RAdS05, Spr00, SUH+01, Tch07a, TKS+05, TVK+02, VTP09, WHD+05, XXMJ06, dVHB03]. **Comprehensive** [DSL06, SRW+06, CWW09]. **comprising** [JZL+08]. **Compton** [ACA02]. **Computable** [NU09]. **Computation** [GB05, HZPY03, Har03, KMS06, LMMB03, ÖKAY03, WKS03, AS04c, DFH02a, Her06, New00, Nic02, SR05, SSK09b, TS01a, VAS06, Vrb08, Yil06, Ano06g]. **Computational** [BZL+09, BBVS+06, CBB01, CI06, DB06, EBR07, FC04, FAE+05a, FFHD00, GV06, GSD+03, GdRPLP08, HNR06, HQL09, JBMP03, JMP06, KWT06, Kry08a, Lia08, LCCH09a, LTL05b, MAFR08, MW05, MPIP+01, PFSP05, PMLC05, PML09c, Sha07, TUA06, TSH03, YS05, ZCZF02, BKL+02, Bau09, BGP+07, BDL03, BD07, CDK01, CLSD+01, CTI09, CCV+07, CC05c, DKWP04, FP02, FS05, FBC+06, FG06, GP01, Gre09, JRSA08, JZL+08, KRR08, Kap06, KF03a, LLW+07, LDR+08, MK08,

MHGR07, Mic00, MFR07, PNBV07, PDR+00, PL09, PBB+02, RS06, RR02, SL05a, SSN03, SPS06, SCG07, ŠK01c, TBJA03, AE07, CJZZ06, CN03, ELC08, FAE+05b, JAP+05, Pet00, Sok04, VM07a]. **Computations** [SUAL04, SUL+08, CRRL01, DC06a, DES03, MRTT01, MWL08, PRM+06, WML08, ZA09, LZ05]. **Computed** [GMPIP01, HWPIM01, MPIP00, PM09, SLA+05, SUL+07, CSL+02, CTS08, PMAA00]. **Computer** [BZR02, DMM+02, RB07, SLS+05, TRMM04, BDE+07, FFFR01, FFFR02, Fri06, KSK+04, KMM+06, Liv02, MSK+05, PHK+06, SP00, TMM+03]. **Computer-aided** [SLS+05]. **computer-algebraic** [Fri06]. **computers** [Kai09, SST+03]. **Computing** [AC02a, DAD05, Iye09, SZU+04, Tor02, BB02b, Ben05, GKC06, Gui06, LSD02, MMB03, PJP08, RR00, SS09b]. **CoMSIA** [RACD00]. **concept** [Buc04, CSPS05, NOM00, ZW03]. **concepts** [Brä04d, Pea02, Pea08, PGW09]. **concerning** [BBVS+06]. **concerted** [LSCC01, ZSWL07]. **Conclusive** [FZ09]. **condensates** [DB04b]. **condensation** [Chu06]. **condensed** [Chu08, JV05, Mar00b, Mic09, MC06b, Shi04, TGGV+04]. **condensed-phase** [TGGV+04]. **condition** [AP03, TOH+00, VTPRA08]. **Conditions** [KSN05, Liu06, TKJ09, AD06, Bau09, ER05, LPV07, MM02, NN09, NS08, Pla01, SM06b, SS08b]. **Condon** [HN03, MP05, Noo06, PSC+07, RR00, VRSF02]. **conductance** [BN03, EZ05, UKAM04]. **conducting** [TWSK09]. **conduction** [ACF04, ACF05, IKS08, IKS10, SY06, SY09]. **conductive** [IA06, Oni09]. **conductivity** [BBL09, KPP01, LY02, LK00b, SNT+00]. **conductometric** [EGEDH03]. **conductors** [CIT+03, KNO09a, TA02]. **cone** [XV00]. **cones** [Kle03]. **conference** [Ano02m, GDV05, VM07a]. **Configuration** [Nee01, CSG06, DEN02, DG04, HMW02, KPČM05, LMJ00, LMX+05, Luz08, MA05, Pan04, Pej02, PPP00, SY07, SČL00, TYY07, TKT+05, VRE+04, WRRF03]. **configurational** [Nic05b]. **configurations** [AK02, CIP+03, GKR00, KKM+01, PA08, Pen00b, SSR02, SNH00, SSS+05]. **Confined** [MB05c, ACFR05, ACM07, BC06b, CCLK05, CHS09, CTS08, CMRMR00, CS01, CDGC05, MAS07, MS09, PB04, SMS+02, Sin00]. **confinement** [CCR09, DGC08, HOIK09, RPHG04]. **confinements** [SBM07]. **confining** [HM03, KJW08, Win04]. **confirmation** [DSW08]. **Conformation** [WJLL09, BNHB+02, DSW02, FP02, GS05, LLSY05, MGV00, SDS04, VBT+07]. **Conformational** [AMOR07, AKB06, BMR+07, CdMCS05, CDS06, CWBM06, FDL03, FGML06, FHJ+08, OGJdlV03, QD04, RKR+06, SCG07, SST00, URBM04, ZMB+03, CFV02, FFDD07, FC04, FFS04, IKL04, KSBK08, KKMS04, LAS+07, MLD06, MCN+05, RRNG05, RRPJ07, Šat03, SBFV05, VSI+07, WT07, YNDJ06, ZZWM07, SCMS07]. **Conformations** [Bor08, CSM02, Moh00, AKK05a, AKK05b, FAE+05a, FFHT05, FAE+05b, FS05, FBGA04, GBJM01, GLX+00, GI07, LAS+07, LQC06, MP09, PLO02, RGP07, SK05a, TNJL05, YKS+06]. **conformeric** [DK04]. **Conformers** [CS00a, ABM01, ABM02, BP03, JPA05, RMJ+07, Sha07, SHC00, WF04]. **Congress** [Ano08c, Ano08a]. **conical**

[Apo06, AdBM06, EYBM03, HCZ05, LHV+09]. **conjugate** [MWXL05, MGG05]. **Conjugated** [Ou06, BN06, BRR04, DM03, IS02, IA06, KM01, NKN+05, PM06a, PM06b, PRCEM06, TOK+00, VVBT07, VGM05, VB04, WSK03, dBM05, dFGM08b]. **conjugation** [HBW+08]. **connected** [Bar08, Fer09, Mar08, Mei08, SLWS07]. **connected-moments** [Bar08, Fer09, Mar08]. **Connection** [Kon09, ZZL04, PCL+03, SCP03, VTPRA08]. **connections** [Kry09]. **connotations** [KM05a]. **conquer** [AKN09, KN09b]. **consequences** [EYBM03, SH07]. **conservation** [Her06, KF07, RS09, RS11]. **consideration** [Liv02, OYYY02]. **considerations** [ANJ09, Lad00, MB05c, PGW08, VED+02]. **consistency** [Del03]. **Consistent** [GAL+05, AKN09, CDG09, CL05e, DKW09, ET09, FTM06, GAIK04, MP06, MDSW07, Pea05, PVW03b, SRA09, SYZ+09, SZL+09, UT03, UC06, VD00, YKGC09, YM05]. **consisting** [Kan00b]. **Constant** [SS02b, BAZ05, OM05, OB02]. **constants** [AC04, AC05, Ben05, BKMS03, BBD07a, BBD07b, BG02b, GBA05, Gög06, JLAR07, KVF+08, LV01b, MMV04, MD04, MBD09, OD03, Ras04, SAR08, TT05, TC05, TG01, UB05, Ver05, YLZ07]. **Constrained** [GG07, CW04, CMNH07]. **constraint** [Esc08, Nal00b]. **construct** [WLWZ06]. **constructing** [MHV03]. **Construction** [LSM05, MBM05, MDBM05, WO04, ÁBL06, CB00, EYB02, PML09b, CSG06]. **contact** [YBS05]. **containing** [AS04a, BSCB04, Buc02b, CLL04, Cou05, FH02a, FS00, GT07, HKR09, KBUV07, LXH+00, LXTT00, LXHT00, MSC05, MLP08, NGTB06, OOD+05, Pet00, PV09, PJ03, SLWS07, WZW+09, WSK03]. **contamination** [LP00a]. **context** [HR02]. **contingency** [SST+02]. **continuation** [MSC03]. **continued** [Noo06]. **Continuous** [SS00a, SSA07, SH07]. **Continuum** [QLD05, AGM02, CCM+05, FG03, HM05a, LW05, LS01b, Mat02a, OMC04, PLA+07, RW00, SSN01, SCSWF04, CRRL01]. **contracted** [ACT+05, AVTPR09, GS09, MST08, PJdC00, VAT03, VTPRA08, WC04]. **contraction** [YINH00]. **contrasted** [SM04]. **Contrasts** [CT00]. **contribution** [CL05d, CFM+06, RE06, SL05b]. **contributions** [DFH02a, JCP+08, LCK00, MKCB05, MB07b, MZ09, SO04a, UKAM04]. **Control** [TTFP04, BKMHP04, KM00b, KM03b, MT03, Mal05a, Mal07, NIS+05, Pöt01, SK00b, TSS+09]. **controllable** [FGZ07, TVK+02]. **controlled** [GM05b, KSK+04]. **controlled-not** [KSK+04]. **Controlling** [AV06, ITY+09, AV05a, VAT03]. **controls** [ZR03]. **Convenient** [OM05]. **Conventional** [BM04, QG04, KS06, KIN09, TS07]. **converge** [HH09]. **Convergence** [Ada05, Ada09, ACT+05, Bau09, BEL01, BM07b, ELY09, FHHC00, JFC02, MBR07, Sal09, dAMM08, AKN09, BRZ09, CJ09, DMMV00, GM09, KFD09, LTV07, SB06a, YKGC09]. **convergent** [BB02b, YM05]. **conversion** [AGFM03, KS03a, Mat02b, Mat10, QD04, RS08]. **COOH** [CTLZ01]. **cooling** [FCD08]. **Cooperative** [GMCS04, Mal05b, ASO+06, BLC09, Baň05a, YYK+03]. **Cooperativity**

[KS06, CRL+02, LAL+08, RAA05, TQC05, XXJG03]. **Coordinate** [CSA09, DMH+05, DDD03, HdMB+05, LPV05, LN03, Lor08, NJD02, PJdC00, RA02, Rui05b, SGP+07]. **Coordinates** [Har03, Ano07a, Bud04, HCZ05, HM06a, HM06b, JJWH04, KKS09, KOT09, LV01a, LCK00, Oku01, ÖKAY03, PS03b, RBA07, Rom08a, Rom08b, SB06c]. **coordination** [BL02a, BCT+02, FJT+05, GP08, KN08, PBSC04, Sha07, SL09, SKA05, TY07, Tch07a, WJLL09]. **cope** [IYY03, Sak00]. **copolymers** [GCG05, RCF02, WWW+07]. **copper** [AP00, BZBT01, BJAV08, DGP08, EMV05, Gur05, JZK02, KNRR05, KTK+04, MTRG04, PSN08, RO01, SKN+09a, CLA+02]. **corannulene** [SS09d]. **cordatin** [BAG+08]. **Core** [AS00, GSA+09, LA07, AA04b, BBM+00, BB04, BB05d, BB05e, CC00c, IN07, LFK06, LJL09a, LK02, MKCB05, MB07b, MC06b, SKK+06, SPSS07, TC05, TOC06, Tak08, TMPI05, WTWT09, WBLQ00, ZMMK09]. **core-electron** [CC00c, TC05, TOC06, Tak08]. **core-excited** [LA07, WBLQ00]. **Core-ionized** [LA07]. **core-modified** [SPSS07]. **cores** [SNM+04]. **Coriolis** [ACDV01, BFBB06]. **Corollary** [PS03a]. **coronene** [OSSG07]. **corral** [Wal04b]. **Correct** [GB06b, BSN05, NF06, TB03]. **corrected** [BS05a, BL04d, FHK06, Mei08, SWSH09, STS+00]. **correction** [DKM+04, FHK06, IN07, KMM+07, KKS09, May04, UB05, YYKY01, YTS+05]. **corrections** [HMW02, KV08, Kut08, LCK00, LE01, RS00, SO09a, YNU+06]. **correctly** [CRL+02]. **Correlated** [DZS+06, LFK06, SDZ+07, WO05, AGSH09, AM09b, BEL01, BCS01, CA01, EWCT+05, GBS02, GBS04, Har05c, HM06a, HM06b, IBN08, KS00, LMJ00, LSE05, MJ06, Nic05b, PJS09b, SJE03, SLE05, SCR01, SCRR02, VD00, Vik07, Wei08]. **Correlating** [Pri05]. **Correlation** [BL04d, BTK+05, BF09, EEJ04, KJW08, AS04b, AV05a, AV06, AVTPR09, AK05, BE07, BDG01, Bec02, BŠM01, Cho08, DS06, Dkh08, DLM+04b, DD00, ET09, EJ06, EP02, FA05, FZ09, Flo08, GB05, GG07, GGS09b, Gra08a, Gra08b, GSB00, GB06b, GGDL07, GFDK09, HKY07, IYO+04, ISS00, JPA05, KJH09, KM00b, KYT+04, KNS+09, KN09b, KP00b, LMJ00, LSE05, MST04, Mar00a, Mar03a, MNJP05, MDSW07, MCH02, MCZWD06, MTWN09, Muk00, Nes00, Nes04b, NFG05, OdSC05, Ort04b, PMHW07, Pau04, PJ07, PO03, PO05, PCL+03, POV+03, PJS+09a, PT06, QS00a, SBMM03, SFPA03, Sch05, Sei03, SL05b, SYZ+09, SZL+09, SK03a, SZJ+04, TPRVC01, TB03, TSF04, VTA+02, VATPR09, VD00, WZ06, WZJ04, Whi03, YYK+03, YTK+03, YNU+06, ZDO09, ZLY+09, ZWSJ01, ZTSP00, Buc08, CIT+03, GGAMB03]. **correlation-consistent** [SYZ+09, SZL+09]. **correlation-kinetic** [SL05b]. **Correlations** [KS09, BLZ02, DGR+00, DB04b, HLO04, SM06c]. **corresponding** [AV05a, AV06, BG00c, TPRVC01]. **corundum** [MCZWD06]. **cosine** [BB07]. **COSMO** [DDT06]. **cosolvation** [WB05]. **Coulomb** [Har03, SDW07, AR06, ACC03, Ave04, BB07, BSH04, Čár07, Čár09, DSLC05, FGR+07, HFS04, HFS06, HM01c, HN09, KH08a, Kry05, Kry06, Lin09, MZD+05, MSC03, OCAMOHL07, ÖKAY03, PSM07, Pöt01, RLER08,

SH01, SH02a, Saf04, SB06a, SLE05, SBKSS05, SK01b, SS09c, TA06, VCF+00, Yan06, Zot06]. **Coulomb-like** [FGR+07]. **Coulson** [BS06]. **Coulson/Löwdin** [BS06]. **coumarin** [KAN+09, NMNB06]. **count** [Tor02]. **counterions** [TTK02, ZS04b]. **counterparts** [DVHJ03]. **couple** [Buc05a]. **Coupled** [BK09, BCF03, KCGB02, KN08, LP08, MOL03, Mei08, RNCM05, SKHY09, WF04, Ban02, Ban05b, BCK04, CM02b, DM08a, DPW00, EBS+09, FHK06, Gda01a, GPW06, GM05b, GM05a, HMW05, IBN08, ISK+01, JR02, JCP+08, KC09, KPČM05, KDM00, KV08, LP00a, LP00b, LP04a, LP09a, Luz08, MB05b, MB05a, MST04, MST08, MB06, MB01b, OY01, Pej02, PHK+06, PGW08, PGW09, PČH02, PPP00, PJS09b, RVP09, SPN03, SC02a, SYZ+09, SZL+09, SNT+00, SM06b, SSS02, SS08b, SMK08, TB06, TKT+05, VED+02, YNN+09, ZSW+00]. **Coupled-cluster** [LP08, Mei08, RNCM05, SKHY09, WF04, FHK06, GPW06, IBN08, ISK+01, JR02, KPČM05, KV08, LP00a, LP00b, LP04a, LP09a, MST04, MST08, MB06, OY01, Pej02, PHK+06, PGW08, PGW09, PČH02, SYZ+09, SZL+09, SSS02, TB06, YNN+09]. **coupled-clusters** [JCP+08]. **coupled-pair** [Gda01a]. **Coupled-perturbed** [KCGB02, MOL03]. **Coupling** [PBB+02, ARBD05, ADK02, BM01b, BMB02a, BL04c, Boe04, BFBB06, BG02b, Chr01, CGS01, CPH04, DM03, DD05, HC02, KFS00, KY05, LV01b, MKHP09, Noo06, RLBK03, TT05, TYY05a, TBML06, VHM+04, YBS05, YHC05, ZL06, dFGM08b, dD04]. **couplings** [ACDV01, PS03b, TY07, TCM01]. **covalent** [Cam04, FG06, Kry02, RSN+07, She04b]. **covariant** [Luz08, NU09]. **covered** [PLO02]. **Cp** [WML08]. **CPCM** [LS01b]. **Cr** [BB05d, GT07, LH00, MBP03, ZZFL00, Mor06, BB01, BB04, DF07, FDLK02, FSK05, KNS+09, LMSB00, Mar09, MTO+03, NF02, PBS02, PBMA03, QCC05, VPS+04, ZL06]. **CR-CCSD** [Mor06]. **Cr/Al** [MTO+03]. **Cracking** [Nég03a]. **CrCO** [KLI07]. **created** [CCH05]. **Crick** [GBB06, KS03a, MHGR07]. **criteria** [CT00, Sch00]. **criterion** [GR04, JLC+09]. **Critical** [AYD00, Buc04, GCCM03, LK00a, PA04a, SMB09]. **criticality** [SK01b]. **CrN** [JKU02]. **cross** [AE04, ACA02, Buc00a, DI05, EMM+02a, GAL+05, GBA05, Gög06, HSP+09, LIBM03, LBSB08, MB07b, PUH+08a, PUH+09, SEY07, SEY09, SL05d, UBS04, VML05]. **cross-entropy** [ACA02]. **cross-linking** [Buc00a]. **cross-section** [LBSB08]. **cross-sections** [AE04, HSP+09, VML05]. **crossing** [DGLM09, MB02a, TOH+00, XV01]. **crossings** [PSCLGN07]. **Crossover** [SM07b, SGP+07]. **Crystal** [BAG+08, MBA+08, PB03, AM07, BBDS06, BHG+06, BFF04, CIT+03, DRPT02, ES02, FN04, IPPL05, JXC05, KPTŚ03, NF02, OBK00a, OBK00b, PI02, PM04a, QLJ+09, RI03, RI05, SDTM02, SV08, SBBL05, PDR+00]. **Crystalline** [Seb05, DKP+06, DFT+07, ESU04, ESKB04, KF03b, KIK09, MS05, NF02, Obe00, OR07, OR09, PVW03a, PVZV00, SRS+04, VPS+05, ZKEE07]. **crystallization** [Mar06a]. **crystallographic** [CN05, ES06]. **crystallography** [KA05, PBB+02]. **crystals** [BM01a, DMV00, DETA02, EP02, ETBA06, IKL04, KG08, KG09, LMX+05, LMSB00, Mar03a, MC03,

MVA02, MWW+00, MT04, NKK+01, PRSLA08, PLC04, PDR+00, Put03, QGM+00, RSRMBFR00, SWL04, SEU02, TA02, UES04, VIGL+05]. **Cs** [MGCD01, SKA05, Irg06, MZD01, XYS+03, FF09, SBM00]. **CsCaF** [LMSB00]. **Cu** [BT05, CMY06, FPC05, KTK+04, Mar09, MOAM07, PC09, SZJ+04, VRA+02, YWC07, Yur06, ZJZ00, BT05, BT05, ACHB08, Bau09, BCD+05, BLZ02, BTL+02, CN03, CS04, Dkh08, DND06, FPC05, Hea00, KN08, KTN02, LGBJ03, NH00, SKN+09a, VRA+02, YT03]. **Cu-doped** [Dkh08]. **Cubature** [RH05, HR07]. **Cubic** [SGB00, EKZ06, ETBA06, OB02, CFP00]. **cuboctahedral** [PHNN09a]. **cubylnitrates** [ZXX02]. **CuCr** [XCC+08]. **CuF** [dD04]. **CuH** [GD00b]. **Cullen** [Ano03a, BH03]. **Cumulant** [Har02c, Zie02, Pir06]. **Cumulant-based** [Har02c]. **cumulants** [Her07, Kut03]. **Cumulative** [DGSD07, LV01a, LPV05]. **CuO** [Mar06b, dD04, CSX+01, MBD05]. **cuprate** [SMB09]. **cuprates** [BSN05, DB04b, SM04, YYI+08]. **CuPt** [ACB+02]. **curcumin** [KVSS05]. **Cure** [Kry02]. **Curl** [BMB02a]. **current** [CC01a, Laz02, MZ09, OdSC05, ZS04a]. **current-carrying** [OdSC05]. **currents** [BA07, SY05, WS00]. **curriculum** [Ano02k]. **Curtius** [KZG09]. **curvature** [LCK00]. **curve** [DGLM09, GGS09a, MB02a]. **curved** [Mla02, SS09d]. **curves** [BES04, JTC+07, MA05, RLBK03]. **CuS** [Mar06b, MBD05]. **cusp** [NN09, SK03a]. **Cusps** [RH09]. **cutoff** [KGI+05]. **CuX** [FRNM08]. **CX** [KM02, LC05, LC05]. **cyanide** [AKK05b, ABM02, FG06, LML02, MOA02, Pet00]. **cyanide-containing** [Pet00]. **cyano** [BHG+06, SE02b, ZLY05, ZL06]. **cyano-bridged** [ZLY05, ZL06]. **cyano-substituted** [BHG+06]. **cyanospherands** [ELC08]. **cyanothiophene** [DDD02]. **cyclamenaldehydes** [IK00a]. **cycle** [BKGF02, SB03]. **cycles** [FCD08, LS01b, Man05, YYZ05a]. **cyclic** [AG08, ACPG01, BCS01, Buc00a, Buc00b, Buc05c, DP06, FRK+05, Gri08, IS02, LXH+00, LXTT00, LXHT00, OSW07, QXJG05, SL05a, Sak02, ZTSZ07]. **cyclin** [LMDW09]. **cyclin-dependant** [LMDW09]. **Cyclization** [SBHF06, GCCM03, VHWM04, ZSL+09]. **Cyclized** [DM00]. **cycloaddition** [ARD03, LW08, LSCC01, LYWX07, LXXC08, LYCX08, SSB+07]. **cycloadditions** [KV05]. **cycloalkenes** [ZSL+09]. **cyclobis** [RFF05]. **cyclobutadiene** [DVHJ03]. **cyclobutane** [LSL+08]. **cyclobutanone** [CY04]. **cyclodehydration** [CI06, FSLL02]. **cyclodextrin** [DH04a, HQL09]. **cyclodextrins** [GI07, HY04]. **cycloheptadienes** [Hes02]. **cycloheptane** [FHJ+08]. **cycloheptyne** [YNDJ06]. **cyclohexane** [MZD+05]. **cyclohexanone** [LJL09b]. **cyclohexanones** [FDL03]. **cyclohexenone** [MGG05]. **cyclohexyl** [SSJ09]. **cyclohexyne** [YNDJ06]. **cycloimmonium** [KS04a]. **cycloisomerization** [MLZS06]. **cyclononane** [FFDD07]. **cyclooctyne** [YNDJ06]. **cyclopentadiene** [DQZ04, SZML07]. **cyclopentanepentaone** [XC07b]. **cyclopentene** [GMTM02]. **cyclopentylheptenyl** [Vrc07]. **cyclopeptides** [TQC05]. **cyclopolymerization** [TA07]. **cyclopropanaphthalene** [Ess07]. **cyclopropanation** [WML08]. **cyclopropylsilylene** [FF01].

cyclopropylsilylenes [FF01]. **cylinder** [BES04]. **cylinder-like** [BES04]. **cylindrical** [YSP06, YSP08]. **cysteine** [DCD08, HDWH09, KSS+08, LWZ+05, ŠFW00]. **Cytochrome** [Har02a, DKD+07, KMVR05, Pud02, STN+06, ZMS05]. **cytosine** [HFGL02, KANK00, MKLP02, PRL01, SLL06, SBBL05, ZLX+07]. **cytoskeleton** [Wal04b]. **cytostatic** [YZ07]. **cytostatic-fluorouracil** [YZ07].

D [DGQT09, DLM+04a, DLM+05, GJ03, GBA05, GB06a, IROW09, LTL05a, LLP05, MLL01, RI03, TKY00, VGMN03, YYZ+05c, Ye01, YW05, ZH06, ZLH+08, ÇAK07, KVSG02, MOAM07, PGP+07, SSB+07, YHC05, YSS08, BSH04, BKM+02a, BGJJ01, Dei06, DFH02b, DFT+07, DS07, Els05, HGB08, ITY+09, KH07, KG09, KES03, KBMM08, LQC+08, Now01, OBM06, PVV+04, QLD05, RI05, RSFRB03, SPN03, SBT+03, SPL03, YS09, CT00]. **D-** [YS09]. **d-d** [YSS08]. **d-p** [ÇAK07]. **D-states** [KH07]. **D-U** [Now01]. **D.C.** [BBL09]. **DAB** [AZD06]. **damage** [ZFLL00]. **damaging** [BDE+07]. **damping** [Pet04]. **Dancoff** [WW08, YSY+00]. **Darboux** [PMZGGR04, SHZGP09]. **Data** [DSW02, ABB+07, DSW00, FSLL02, Irg04, LBSB08, LS05, PMBM09, VSBD06]. **database** [CSL+02]. **Davidson** [KOT09]. **Davies** [SN02]. **day** [SC01]. **DBSQ** [BT05]. **DC** [GAIK04]. **DCM** [KLB+05]. **DCS** [Pai00, PA04a]. **dd** [GA08]. **deactivation** [BDMS03]. **deamination** [KVPS05, SLL06, TX02]. **Deb** [Deb08]. **debromination** [EGE08]. **Debye** [BSM+07, KH07, SM05a]. **decay** [AP03, CCM08, Nic02, RNS04]. **decaying** [Wen02]. **decker** [CG09]. **Decoherence** [KMM+06, MY09, KMK+05, TTFP04, TMM+03]. **Decomposition** [PFA08, TW08, AEMAO06, Alc04, AMO+01, BNS05, BF08b, Fis00, KIN09, LCH05b, LCCC08, MH05, NSLR04, OCK07, RAA05, Rua09, SSSS09, SZK07, SZ08, SSK+05, TB09, WB05]. **decoupling** [BCF03, Lor08, TTFP04]. **Dedication** [Ott04]. **Deduction** [Sko02]. **Deductive** [TT04a, TT04b]. **deep** [SM03]. **deep-level** [SM03]. **default** [MCF08]. **defect** [AGLBM03, Aze02, CB03, MMV05a, MMV05b, MSC05, SKT05, Van06, VBML04]. **defected** [LTW09]. **defective** [JLC+09]. **defects** [CB04, Kle03, LJMM09, LRS05, LMSB00, MAS09, Mor04, PM06b, PBS02, SVC+05, TBJ05, VPS+05, ZSM+01]. **deficiency** [VG06]. **defined** [Tal03a]. **definition** [CDG09, NS09, NF02, Sut02]. **deformation** [PFA08]. **deformations** [MFA00]. **deformed** [BKM+02a, BLRT02, Put03, RMM05]. **degeneracies** [VX04]. **Degeneracy** [MAS07, KZB01, Lef05, LLLZ06, SS00a, SS00b]. **degenerate** [Kap07, MTWN09, OBM06, TYY03, YSO+01, YYS+01]. **degradable** [VWMS03]. **Degree** [Sjö00, Ném03a]. **degrees** [IKL04]. **dehydrogenase** [MAFR08, PSEP05]. **dehydrogenate** [Ye01]. **dehydrogenation** [FSLL04, MBRS05, XC07a]. **dehydroxidation** [LPV07]. **Delocalization** [HvL09, AB08, Buc02a, NOY+01, PDS04]. **deltons** [McK04]. **demethylation** [CVPGH+06]. **denaturation** [Boh03]. **dendrimers** [ELG05, TSN+05]. **dendritic** [NFT+01, TNYY03]. **denominator** [SS02b].

dense [Chr01, DCTC03, GN01, KH06, SSM05]. **densities** [AM09b, ACA02, ABGS00, CHW04, Deb08, HH02, LPV05, NŚM02, SD00a, TS01a, TGGS06, VD04]. **Density** [ABD06, ACG00, Ano07e, ASM+03, BHG+06, BP03, BLC+00, BDMS03, CSX+01, CB04, Čár09, CCA+06, CL05c, CSL05a, CL05d, CC05b, CC00c, CSTB08, CF04, DV00, Die00, DBL+03, DZTZ05, Dre05, DFZ04, DWM+07, EZY00, FXHL05, FWZ09, FPC+03, FVPM05, FFHT05, GR07a, GSC00, GBVD05, GJB02, GR05, GZD+05, GYS+06, GW06a, Guo07, HMB+04, HR05b, JLAR07, JRSA08, JHLC09a, KLI07, KMVR05, KANK00, LDMR01, LML+04, LSCC01, LL04, MLZS06, MWL08, MLSB06, Mic00, Mic06a, MDJ01, NRS+02, NMNB06, NK05b, NOHN02, OR07, Pan07, Pej03, PMCOSC00, PCM00, PS03c, QGM+00, RDK97, SPH+03, Sch05, Sei03, SZK07, STL+09, TOK+00, TN09, TSZW08, TB03, UP05, WML08, XXC08, XXY00, YUN+07, ZR07, ZNF05, ZOK+05, ZQF+02, ZPW+04, AZ08, AG01b, AFC03, ACD02, AMGN00, AM05, AGB06, APN02, AP03, BDG01]. **density** [Ban02, Ban05b, BAZ05, BCG09, BK04a, BJS09, BKGF02, BBD07a, BGN+05, BKM05, BR02, BTK+05, BKM+02b, Bu02, CK03, CL05a, CW04, CC01a, CC05a, CCP00, Col01, CRTP05, CSA09, DCDW00, Dav03, DGQT09, DLK00, Elr09, EZ05, FCS03, FWT08, FA05, FKR04, FDZ04, FSR02, FM02b, Gál07, GJ03, GS09, GXT02, GXGT02, GGAMB03, HSS09, Har02c, HT05b, HYC+00, HGS03, HH02, Her07, HDL00, HMMT04, HM05b, IBN08, IABS08, ISK+01, Jal02, Jal07a, JNF+09, JNSF04, JXZ+05, KZB01, KIN09, KSG03, KSS+01, KYT+04, KB00, KSS00, KMS02, KSWR00, KZvL09, KG08, Kut03, KDF00, Lam07, LDR+05, Lat03a, Lat03b, Laz02, LGJP05, LMRT08, LRS05, LS02, LS05, Liu02, Liu06, LNSE02, LE01, LP05b, MZN+03, Mai05, MP05, MP06, Mar87b, Mar03b, MHV03, Mar05a]. **density** [Mar05b, Mar07a, MRTT01, MRST01, MTRG04, Mar06b, Mat00, MT02, Mic09, MBD05, MNV07, ML01, Moh00, MZ09, MS09, MC08, MESH02, NP01, Nag03a, Nag06, NKN+05, NUY+06, Nal00b, Nes00, NGRR02, OYYY02, OMN+03, PFA08, PRM+06, PS08, Pat06, PRG+04, Pea02, Pea08, Pej02, PBI+01, PGB00, PO03, PSB+05, PCL+03, PBM03, PB09, Pri05, Put03, Put06, QS00a, QCV06, QCC05, RBL08, RA03b, RH09, RA02, RRC03, RD00, RDK02, Roy08, SS09a, SS04b, SS06, SG03, SFD09, SKSB08, SD08, SCP03, SOLI04, SL05b, SRK01, SC01, SIS+08b, SL05c, SK05b, SS01, SWSH09, SHE+02, SCLL07, STS+00, TC05, TY07, TYY03, TYY04, TYY05b, TN03, TTM07, TX02, TCM01, TGGS06, TKJ09, VATPR01, VAT03, VU02, Van06, VCHC07, Var08, VR01, VPSH00, WRRF03, WZ06, WWW+07, WGX09]. **density** [Wei08, Wol05, WJLL09, XD03, XXMJ06, XCW07, YYYM01, YKT+02, YNY01, YYS+00, YYKY01, YYS+01, YOYY03, YTK+03, YNU+06, YOM+01, YCS09, ZXX02, ZLY05, ZCZ+07, ZZZ+08, ZW09b, ZMAL04, ZKYA04, ZFD00b, ZCZF02, ZW07, ZWJ02a, ZTSP00, Zie02, ZT04b, ZBPD08, dBKS01, eSPM+08, CZWZ05, CDG05, GDV05, Gog05, Kak03, MWXL05, MY00, MD04, MDG07, PW09, XC07a, ZTW+09]. **Density-dependent** [PS03c]. **density-functional**

[APN02, LS02, MC08, TC05]. **density-matrix** [OYYY02, TCM01, PW09]. **deoxynucleosides** [XXC08]. **deoxyribonucleic** [YZ07]. **deoxyribonucleosides** [KKMS04]. **deoxyribonucleotides** [ZDZO07]. **Deoxyribosic** [BGGS08]. **dependant** [LMDW09]. **dependence** [För00, HW02, JC00, KWWQ04, LH05, MKHP09, MW05, NOY+01, Por03, SBL05a, SS05b, SEM05, Von00, YBS05, FL04, KK07]. **dependences** [Kar04, KIK09]. **dependency** [SNT+00]. **dependent** [AP00, ACPG01, ASTO02, AGB06, BKM+09, BAZ05, BCG09, BJS09, Bil01, CW04, CC05a, CXZ+09b, CEÖ02, DGR+00, Deb08, DFT+07, DND06, EJ06, FCS03, FZRD07, FFDD07, Fra03, Gra08a, HBKG03, ICRS08, KP09, KSG03, KDF00, Mai05, MP05, MBP03, MSS09, MYH03, MSJ04, MB02a, MOPdP09, Nag03a, NFG05, OMN+03, POM+07, POM+08b, PGB00, PS03c, PA04b, QS00c, QC01, QCV06, RA03b, RW00, RW04c, SG03, SKSB08, SAM08, SHZGP09, SL05c, SMT06, VWB+03, VLJ08, VD04, WRD03, WRRF03, WZ06, WWW+07, WZW+09, YYYM01, YNU+06, ZCZ+07, dBKS01]. **depletion** [DNC07]. **depollution** [BZBT01]. **deposition** [DFRS07]. **deprotonated** [DKC00, Mas04]. **deprotonation** [LS05, MBK01, PGF+06, SS09c, TX02]. **Derivation** [BKM+02a, HN03, Kan00b, RW04a, BMB02a, Ban05b, PHK+06, PGW08, UP03]. **derivative** [GTR+05, NIS+05, XXY+05]. **derivatives** [ABD06, AA09b, BWS+02, CJ03, Čár09, CSL+07, CMASC01, DKD+07, DDD02, DKP+06, EGEDH03, FRT+00, GL07, IDH06, IBB08, KLB+05, LQM+09, LTL06, MNR07, MWXL05, MGB+06, MS09, METSH02, NFFA04, dlPOPP03, OGJdlV03, OK05, PIGN02, PGN+05, PFSFH06, PMCOSC00, RJF+09b, RH09, SKN09b, SL09, SM05b, SKSS09b, TSK01, TCS+08, TUA06, VBS+04, VNP00, Vrb08, WGX09, Wol05, XC07a, XXMJ06, XC07b, YZW+08, YYXC01, ZPW+04]. **derive** [Sce09]. **derived** [AM09b, ADTD05, Bec05, BF09, DDT06, FJ00, GI07, PVW03a, RAdS05, SN06a, TNO09, ZFD+00a, ZS04b]. **Deriving** [Tch07a]. **describe** [GGLS02, MO06, SGS00a, TGG01]. **describing** [BL02a, Gar08a, GGACT03, HCL03, IN07, KH05, SMB09, SS03b]. **Description** [LP07, VMA03, BT05, BVHS01, BKMS03, Buc00a, Buc01, CHW04, CHR+06, Dkh08, DBPG04a, DBG04, DAA+06, GMS01b, HVSM02, KCU09, KF03b, KS03b, Liu06, MSSM00, MC08, Oku00, PLU08, TT02, YN04, Qui05]. **descriptions** [DVHJ03, VGM05]. **descriptors** [CJ03, CBRBT03, MEN+08b, MK01, Nal09a, Nal09b, PSS05, PS04, Sey08, TBCG05, WHD+05, eSPM+08]. **design** [CSL+07, HR02, IA06, RB07, SLS+05, RSL+03]. **Designer** [WRW02]. **designing** [AD01]. **designs** [Tem02c, Tem04]. **desorption** [HSN+09, Saa00]. **desulfurization** [MH09]. **detachment** [IZ04, ZDZO07]. **detailed** [HZW+08]. **details** [FZ09]. **determinacy** [CT00]. **determinant** [HI06]. **determinantal** [Ret06]. **determinants** [FH02b, HPR09]. **Determination** [BZ06, CNC+06, ENGY+07, Irg04, KF03b, LGBJ03, MPRGLL03, NFP05, Ras04, SAR08, VV05, VRE+04, YYY05, Buc00b, EFM06, HI06, JC01, JMP06, KAE03, MA05, Nak02, Nak07, PML09c, Put03, SCM00, BFF04, WRRF03].

determinations [JZZ+08]. **determinative** [Nég03a]. **determine** [VBT+07]. **determined** [MYS+09]. **determining** [Gin08, HBTW04, Mar87a, Chu07]. **deterministic** [Lav03b]. **detonation** [EEJ04, WGX09]. **Detuning** [NY04]. **deuterated** [BWS+02]. **deuteration** [DKR04]. **Deuteron** [DLM+04a]. **deuteronic** [ITN06, ITN08]. **Deutsch** [HSP+09]. **developed** [HLP07]. **developing** [LCCH09b]. **Development** [EHH09, FTW03, HTN07, ITN06, VWSA+04]. **Developments** [ABC+06, AdWKG00, CS07, VAT03]. **device** [Bro00]. **devices** [EZ05, Lu06, TJAS08]. **Dewar** [Gin00]. **dexanabinol** [Hua04b]. **DFT** [ISK+01, KSS00, PGP+07, SL05c, AG08, AE07, AKK05a, AGFM03, AGLBM03, ADTD05, AK05, BVS+09, BCdP03, BFAM03, BK04b, BT05, BČZ07, BCD+05, BB09, BCT+02, BJAV08, BCS01, BSBS06, BSB07, CJ09, CBMRN08, CFV02, CSPS05, CSL05b, CL07a, CSL+07, CN05, CMY03, CMASC01, DCW03, DRD+05, DDT06, DDD02, ET05, EP02, EB04b, EKZ06, FYH09, FFF07, FZ09, FGZ07, FTGH04, FPJR03, GDB03, GGLS02, GKC06, GL07, Gra08a, GSCRO08, HE05, HVC08, ICRS08, JXC05, KZG09, KVPS05, KV07, KWWQ04, Kap07, KAG08, KV05, KCOV07, KNS+09, KVSS05, KO03, KS03b, KZS07, KB08, KBMM08, LPV05, LTLS05, LC05, LDG+06, LJL09b, LZZ+06b, LNPL06, LTL06, LH07c, MW06a, MARK08, MH09, MLSG04, MdlV03, MCC08, MBRS05, NID+06, NYU+08, dlPOPP03, OKY+08, OMMWL02, Oni08, OK05, OOD+05, PBSC04]. **DFT** [PK01b, PVV+04, PKZN08, PLA+07, QLJ+09, RPB00, RSFRB03, RKR+06, RS08, Rua09, RH03, SFPA03, SAR08, SCM00, SN06a, SPS06, SS08a, SNM+04, SKK+05, SKK+06, SKK+07, SCW09, SBFV05, SPSS07, SJM08, SBHF06, SSB+07, SKNN08, SKNN09, STW+05, SBL05b, SEM05, TI05, TT05, TOC06, TYY04, TYSY07, TSP+07b, TSP+07a, TG05, THP08, UML00, VRFS05, VMA03, Vrc07, WS00, XXJG03, XXJG04, XCC+08, Yam09, YST+05, YSV05, ZMB+03, ZMMS+00, ZLZ05, ZSL+09, ZT04a, ZZKS07, ZS04b, ZKRS07, dAGD08, dLCRF+08]. **DFT-based** [CSL+07, FPJR03]. **DFT-D** [KBMM08]. **DFT-EPR** [PVV+04]. **DFT-PCM** [ICRS08]. **DFT/AM1** [SS08a]. **DFT/GIAO** [dLCRF+08]. **DFT/MRCI** [PK01b]. **DFT/PCM** [dAGD08]. **DFTB** [KES03, KKMS04, WKF+06, ZLJ+09]. **DFTB/molecular** [HEJ+00]. **di-** [FJK+01, FJK+02]. **di-aza-** [WW07]. **di-i-propylphosphonates** [CdMCS05]. **di-n-butyl** [CDS06]. **di-n-propyl** [CdMCS05]. **di-sec-butylphosphonates** [CDS06]. **Diabatic** [KY00, AT07, ART08a, ART08b, EYB02, KCS02, KV02, Tap04a, Tap04b]. **diagonal** [Mar07a]. **diagonalization** [Gin05a, NCB02, SNY01]. **Diagonalizing** [Tap04a]. **diagram** [SM05c, SMB09]. **diagrams** [Mat07]. **dialkyl** [PK01b]. **dialkylaminoethyl** [ZPW+04]. **dialkylzirconium** [DBB+06]. **diallyl** [TA07]. **diallylamine** [TVK+02]. **dialuminum** [SS08a]. **diamagnetic** [Sal00]. **diamagnetism** [OR09]. **diameter** [Ou06]. **diamines** [Irg06]. **Diamminedichloropalladium** [HFGL02]. **diamond** [GBJM01, LPC04, Seb05]. **diamond-lattice** [GBJM01]. **dianhydride**

[ZNF05]. **dianions** [CG09]. **diarylethenes** [PMBM09]. **diastereoisomeric** [ARBC+05]. **diastereoselective** [GP01]. **diatomic** [ASDC08, ASM+03, BBD07a, BBD07b, BB05e, CC05c, GB08, HCTC07, MVK00, MK02, NJC02, PJdC00, PB04, RdLJ+02, SINN05, SIT+06, TSS+09, WHKM04]. **diatomics** [BG02b, DLK00, GW07]. **diaza** [AZD06]. **diazene** [SMK08]. **diazides** [AEI00]. **diazo** [SBHF06]. **diazoazoles** [SSB+07]. **diazocyclopropanes** [Bor08]. **diazonium** [BF09]. **dibromo** [FS05]. **dibromocarbazole** [ZSWL07]. **dication** [FSR02, Kry07a, MZD+05]. **Dicationic** [Kry07a]. **dications** [Buc00a, Buc02b]. **dichlorine** [LLX+03]. **dichlorobenzene** [FGFF06]. **dichloromaleimides** [ZMB+03]. **dichroism** [CMR05, CCM+05, JNKMS03, JSvDA06, KBV05, Noo06, OCWY09]. **dickite** [MGZL04]. **Dicoordinate** [LČM01]. **dicoordinated** [CLA+02]. **dicyanomethylene** [XC07b, YYXC01, ZFD+00a]. **dicyanomethylene-derived** [ZFD+00a]. **didehydro** [LP09a]. **dielectric** [DAA+06, LCT00, PMO04, TIV+07, BM01a]. **dielectrics** [RRGP05a, RRGP05b]. **Diels** [ARD03, SZML07]. **diesel** [MARK08]. **diesters** [LYDK02]. **diethylimidazolium** [SZML07]. **difference** [GdA01b, Mar05b, NY01, YNY01]. **Differences** [LTV02]. **Different** [Buc05b, YYQ+06, BE07, BES08, ÇAK07, CMS04, CLSD+01, GSB00, GSH02, HGB08, HM03, LS01b, MMCC02, PM06b, PJZ+09, RMJ+07, SK05a, SBB05, SSK09a, VGMN03, VGB05, PRBGLL04]. **Differentiability** [Lam07]. **differential** [AMGN00, ÇKB02, CW08, CDGC05, Her06, Hyd06, LBSB08, PA02, QS00c, HM03]. **differential-algebraic** [ÇKB02]. **differentiating** [JTC+03]. **Differentiation** [CTLZ01]. **diffraction** [DDBF09, LTV05, Mar07a]. **diffuse** [SYZ+09, SZL+09]. **Diffusion** [HKY07, ASDC08, FVPM05, ILB+08, KSN05, Wal04a, WSNB00]. **difluoro** [FAE+05a, FAE+05b]. **difluorobenzonitriles** [RPS+07]. **difluorobutadiene** [CGMT03, HGTW03]. **difluoroethylene** [CGMT03]. **difluoromethylene** [LYWX07]. **digermane** [GPW02]. **dihalocarbenes** [BCK04]. **dihalocyclobutanes** [LA06]. **dihydro** [LY09]. **dihydrogen** [SS08a]. **dihydrosphingomyelin** [SKNN09]. **dihydroxybenzene** [VPSH00]. **diimine** [CC05a]. **diiron** [BB09, SNM+04, BB09]. **DIIS** [CL00a]. **diketonate** [NRK+05]. **diketones** [AG08, AD01]. **dilated** [MV02]. **dilation** [AE02]. **dilute** [Pom04]. **DIMBOA** [SPS02]. **dimension** [PRCEM06]. **dimensional** [Ano06g, ACFR05, ART08a, ART08b, CCLK05, CCLK07, DLM+02, Dre05, Gin01, GGAMB03, HT05a, HMMT04, JJ00, KMS06, KTK+04, KCS02, LKG09, LLZ+00, LSLD01, LM02b, Mar87a, MOL03, MHI+07, MD08, MKDM03, MB01b, MAS07, NOY+01, PKB+01, SW02, SK01b, SH09, SMT06, TA02, TOH+00, WRD03, Wen00, Wen02, Wyb02, Yam04, Yam05, Živ09, dD04]. **dimensionality** [OBK00a, OBK00b]. **dimensionally** [Yam09]. **dimensions** [CCLK04, DSLC05, Her06, Mar87b, Mar06a, ZTSP00]. **dimer** [ADSTS06, BVHS04, CLA+02, CS08, DFZ05, FG01, FDZ04, HI06, HLP07, JCP+08, KSN+04, Kry07a, KANK00, KM05b, LXD00, LWZ+05, MKZ04b, OSSG07, POAVdlM08, PCBA08, PSK02, PLU08, QDÖ09, RP09, SPH+03,

SAMBS01, SSZ+07, SQZ+02, SS09d, XCW07, YUN+07, ZZW+06]. **dimeric** [VTS04]. **dimerization** [FWZ09, Hua04b, She07d]. **dimers** [AGM01, AGM02, BVHS01, BKMS03, BS05a, CNPA04, Dre05, DSW08, FG01, FG06, GKC06, HL05, HT04, HCL03, KD05, LME03, LLW+05a, LLW+05b, LLYL06, LB02, MCF09, MGV00, NY01, PCM00, RFS+00, RG08, SBF03, SSN01, Var07, XD03, YYYM01, YHC05]. **dimetal** [XLX+09a]. **dimethyl** [FC04, Moh00, PFSP05, ZFZ+08]. **dimethylamino** [SBB05]. **dimethylaniline** [SQZ+02]. **dimethylene** [OA02]. **dimethylisoxanthopterin** [SRO02]. **dimethylmethylenesilylene** [LYCX08]. **dimethylnitramine** [PCM00, PM09]. **dimethyloxirane** [Noo06]. **dimethylstannacyclohexane** [FFHT05]. **dinitrogen** [CZWZ05]. **dinitrotoluene** [TW08]. **dinuclear** [NSS09]. **diodes** [BK03, ZRF+09]. **diol** [FSLL02]. **dioxacycloheptane** [FHJ+08]. **dioxide** [BR00, Boe09, CB04, FB07, KVZ+02, OMMWL02, PJZ+09]. **dioxo** [GARB08]. **dioxo-** [GARB08]. **dioxygen** [DGP08, NGTB06, TY07]. **dipeptide** [FWT08]. **dipeptides** [ARBC+05, ZTSZ07]. **diphenylboron** [TKS+05]. **diphenylmethane** [SBB05]. **diphenylmethanol** [SS08a]. **diphenylpolyenes** [YCN+07]. **dipolar** [ELC08, KV05, LSCC01]. **Dipole** [JKU02, Mon08, SASS03, CTS08, CPH04, GB05, JÅM01, LA06, LMX+05, LCBC03, MB00, RPB00, SMS+02, SC02b, SGS00a, SGS00b, SHE+02, SCB+06, YSV05, YCN+07]. **dipole-allowed** [YCN+07]. **Dipole-bound** [SASS03, SGS00a]. **dipositronium** [DM04]. **dipped** [NH00]. **diprotonated** [SST00]. **dipyrone** [DCO+08]. **Dirac** [QGW04, Dat04, DBd05, DMH+05, DSLC05, GMK+09, HdMB+05, KPSH06, KP09, Kat00, Mar07a, MNR07, PM04b, QGW02, QGW04, SB04, Tal04, WTWT09]. **diradical** [YYI+09, YYS+09]. **diradicals** [DC05, LP09a]. **Direct** [Dun01, MP00, SBT+03, TWZW09, CWY05, FWT08, IN09, ITN09, JFC02, Koh01, TI05, Tem02a]. **direct-space** [JFC02]. **directed** [KM00b]. **directional** [MLP07]. **directionality** [CVVA08]. **directions** [ZA09]. **Dirichlet** [BB06]. **disclination** [Aze05]. **discontinuity** [GGS09b]. **discontinuous** [GB08, SB04]. **discontinuously** [GB09]. **discrepancies** [SBM00]. **Discrete** [Mat02a, RFCG09, Bil01, DCA03, JV05, JSvDA06, KK05, PA04b, WRW02]. **discretization** [FGR+07, MT03]. **discriminant** [MEN+08b]. **Discrimination** [ARBC+05, DFZ05, DZ06b, IK00b, YZC09, ZYC09]. **Discussion** [CD04, Cas00]. **disilene** [TVK01]. **disiloxane** [DGRB08]. **disorder** [DFT+07]. **disorders** [WK03]. **Dispersion** [MC06a, Bel04, Ben05, Gos01, JCP+08, QC02, RFF05, Sal05]. **dispersions** [SKHY09, Tor06]. **displacement** [HSW+00, MNR07, UP03]. **disruption** [VED+02]. **disruptors** [KM03a, KM03b]. **dissipation** [Bel04, BMP+04, DAA+06, GC05, MB01b]. **Dissipative** [MT02, dHG04, KSN05, NY03, Vel04, LTL04]. **Dissociation** [GEB+00, GB08, IAL06, BBD08, CGCS02, DLZ+03, ENGY+07, EMV05, GMS+05, GGS09a, GB06b, HI06, Jal02, KSBK08, KKK09, KUS+03, LTY09, MBD09,

PMLTL07, SSA07, SAR08, SSSK07, SCLL07, SIT+06, WSBV05, dSNBG08]. **dissociation/formation** [PMLTL07]. **dissociative** [FM02a, LL04, RA03a, RA04, WZWC06, ZW09a]. **dissolution** [XVRL04]. **distance** [BKL+02, FM02b, GCCM03, MP09, NŚM02, Pal01b, Pen00a, Stu00, YBS05, ZY07, ZT08]. **distances** [CR08b, CR08a, GKR00]. **distorted** [OMC04]. **distorted-wave** [OMC04]. **distortion** [DI05, FJK+01, FJK+02]. **distortions** [Oni07]. **Distributed** [GW02, GW04, GW07, KK05, MG05, QGW04]. **Distribution** [PFdP08, AD06, Ban02, Ban05b, BK04a, BSN05, CFV02, GW07, SHC00, SCHH02, dAMM08]. **distributions** [Bor08, Buc02a, Gri06, MFA00, MSC05, MCN+05, MESH02, SOLI04, SD00b]. **disubstituted** [ABCS02, BBVS+06, LSCC01, dSNBG08]. **disulfide** [KVZ+02, KVZT04]. **disulfides** [ACG00]. **dithiobiurets** [AB08]. **dithizone** [SLRS02]. **divalent** [ABL03, WWTHF09]. **divergence** [NFG05]. **divergent** [Fer01]. **diverse** [KS09]. **divide** [AKN09, KN09b]. **divide-and-conquer** [AKN09, KN09b]. **DNA** [BBDS06, Buc05b, BDE+07, CLL08, CDF06, Chu09, FCLH+06, HT07, JJC+06, KTH+05, KV01, Kry02, KS03a, LS08, Lak08, LLZH09, MKLP02, MTRG04, MMT+07, MWXL05, NID+06, PKT05, RLB02, SKSB08, SDS04, SSN01, TWSK09, XC07a, Yak02, YL04, YJ00, ZFLL00, ZZZ+08, ZLS07]. **DNAs** [DNN+06]. **Do** [Pet00, CBA+06, Tap04a, Wen09]. **Docking** [STN+06, OMMB07, dRPFCP08, SWST04, XCS+03]. **dodecahedrane** [LZXD05, LPZW05, Tem02c, Tem04]. **dodecahedrane-type** [Tem02c, Tem04]. **dodecamer** [MKLP02]. **Does** [GPW02, HH09, ZMS05, NN09, RLB02, BSN05, TKY00]. **Dolastatin** [AMOR07]. **domain** [CP09, Sch04]. **domain-averaged** [CP09]. **domains** [MB02b]. **donated** [CVVA08]. **donating** [HD03]. **Donor** [She07d, ARE02, BVHS05, DD05, Elr09, FRF02, GBB06, Lu06, New00, OOD+05, She04a, SMVMC07, TDS+02, Ver05, XLX+09b, ZVVT07]. **donor-** [SMVMC07]. **donor/acceptor** [New00]. **donors** [LC02]. **dopants** [SHM+09b]. **Doped** [dLCPLD+07, AML+01, CB03, DBL+03, Dkh08, ES02, GWSZ08, KS00, Mar09, RSRMBFR00, RSDNSB00, RSFRDNA04, RdTdLC+07, Sme02, SM05c, SM06c, SR07, XBHL04, YYI+08, YHF+08]. **doping** [Oni09, SM09]. **dot** [Fra03, KJW08, MW06b, SPN03, Win04]. **dots** [ASM+03, BTK+05, DVM06, HGB08, LPC04, RL04, SPN03, SPL03]. **Double** [AGB06, RZ07, TBM04, ARBC+05, ASM+03, CVPGH+06, CW00, DNN+06, DN06, GB09, HT07, JLM08, KK02a, KKYT04, KVT04, KSN05, LSC02, MB07b, NID+06, PML09b, RWW+01, SS03a, SLWS07, WKF+06, YHN+07, YHC05, Yur08, ZS04b, SSDB06]. **double-** [HT07]. **double-component** [KSN05]. **double-core** [MB07b]. **Double-electron** [TBM04]. **double-ionic** [ZS04b]. **Double-pole** [AGB06]. **double-strand** [DNN+06]. **double-wall** [JLM08]. **double-well** [DN06, SS03a]. **doubles** [IBN08]. **doublet** [BMMC09b, PRNM03, RVP09]. **doublets** [DM08a]. **doubly** [DGR+00, EF03, SM05a]. **Douglas** [MNR07]. **downhill** [Muñ02].

downward [Har04a]. **Dressed** [OK04]. **Dressed-particle** [OK04]. **driven** [AA04a, FZRD07, Har05b, PMLC09]. **driving** [SS04a]. **droplet** [SKMW00]. **Drug** [SKSS09a, AGM01, HR02]. **drug-drug** [AGM01]. **drugs** [SWST04, ZZ05]. **DSP** [Ess07]. **dt** [Ghe09]. **Dual** [KN09b, OMN+03, CLL08, LLZH09, Sce09, Tem02a, Tem02b]. **Dual-level** [KN09b]. **due** [HOIK09, Noo06, OB02, OdSC05, RFRF05]. **dUMP** [QFC04]. **duplex** [Chu09, KKYT04, TWSK09]. **duplexes** [Buc05b]. **Dupré** [OR09]. **during** [Boe04, LZT03, PMB08]. **DV** [KNO09a, SMDG09, SSK09b, TNO09, YPS05]. **DV-** [KNO09a, SMDG09, SSK09b, TNO09]. **DVM** [Yur06, Yur07, Yur08]. **DVME** [KNO09b]. **DVR** [LN03]. **dyad** [JLI+01]. **dyads** [GL01]. **dye** [DNC07, DDD+00, KLB+05, KFTBS07, LNPL06, SMM02]. **dye-sensitized** [LNPL06, SMM02]. **dyes** [ICRS08, IDM+09, JLPA09, KM06, SMM02, ZFD+00a, BD01]. **Dynamic** [AR04, CTS08, PMB08, ZGY+03, dBM05, MMS+09, MOL03, MCH02, Sad00, SGLF01]. **Dynamical** [FGM05, YHD00, YYHD01, CS00b, CK04, GYM+02, MC00, Sco00, SC02a, SC04, TFS+02, VGB05, ZYG00, TTFP04, ZLS07]. **dynamicity** [RT09]. **Dynamics** [BGJJ01, Cor06, DM03, IKL04, JZZ+09, MMS+09, Nov07, SN02, dFGM08b, AGM02, AMOR07, AE07, AP00, AT00, BBDS06, BKM+09, BGGS08, BFRB07, BDA+02, BK03, BBPG08, BFB08, Buc00b, CR06, CNPA04, CAHl08, CRRL01, CS03, CM02b, CBWM09, DCTC03, DM02a, DGD+05, DBPG04a, DJNH02, DH04b, DC03, ESE04, FG03, FGdA00, FGdA02, FYSS09, FDME01, GR04, GB09, GBL06, GI07, Hag00, Hag01, Hag05, HK06, HYC+00, HAL+02, HLP07, IN09, Iye09, JP01, JZW+09, KOH03, KM00a, KUS+03, KAN+09, KDM00, KOT09, LBMVDL06, LFADSF07, LHL+00, LYP+06, LDM09, LH00, MB05b, MB05a, Mal07, MHI+07, May06, Mic00, MT02, Mic06a, Mic06b, MB02a, MB00, Mon05, Mon08, MD02, MDS04, MVKN06, NNNY01, NOM00, NY01, NY04, OOK03, PM06a, PRSLA08, PFSFH06, PLO02]. **dynamics** [PW07, PFdP08, PS02, PSA05, RBA07, RF01, RP00, Saa00, SS03a, SSA07, SKMW00, SWC03, SFR08, SSK+05, TNYY03, TSN+05, TWZW09, TS01b, TCM01, TŠPJ04, VPS+05, Vik07, XV01, YLZ07, YZX+08, ZMX+05, ZNZS00, Buc05a, MB02a]. **Dyson** [Ort04b, PVW03b]. **Dzyaloshinskii** [TYSY07].

e-argon [PA02]. **e-atom** [Pai00]. **e-H** [SAM08]. **E.** [BB05d]. **E2** [CM02a]. **EA** [GPW06]. **EA-EOMCCSDt** [GPW06]. **early** [SB03]. **earth** [ABL03, BKLB06, BD07, EGEDH03, Sme02, STS+00]. **earth-bearing** [BD07]. **earths** [Pyy01]. **ebtellur** [SHM09a]. **eclipsed** [EHH09]. **ECP** [Mor08, Mor06]. **edge** [Man05, OCWY09, dVHB03]. **editor** [Bad03]. **EDOT** [DBL+03]. **education** [BM02]. **Effect** [CMR05, GXGT02, HQM04, HC02, IMTG06, JPMM08, JPA03, KDŁL07, LP00a, LSK+06, MBOL04, Nic05a, OBK00a, OBK00b, PKT05, SC02b, SS08a, SM05a, SSM05, WL00, YHC05, YCS09, AL09, BN06, Baň05a, BS00, BRR04,

Dat04, DST+04, DGLM09, DW05, EHN09, Elr09, FMBM05, GAIK04, GMS+05, GBMMSA00, HSN+09, IYSS07, IPPL05, ITN09, KKK09, KKM+01, KBUV07, LAL+08, Lia08, MB06, MMV05b, MWXL05, MdlV03, MGB+06, NK06, OKY+08, Oku00, OB02, PLC04, PLU08, Por02, QC00, RJN+08, SFD09, SD08, SSN01, SWSH09, TTK02, TTFP04, TD09, TMS08, VWB+03, VX04, WT07, XV00, YYQ+06, ZCZC09, MBRA07, Sha07, SBM07, VWMS03].
Effective [KMM+07, KPTŚ03, Mar87a, SI09, SDTM02, TTM01a, ABGS00, BBM+00, CBA+06, DRPT02, FTM06, KSK+04, KSS+01, KYT+04, KZ09, LFK06, LSPS01, LJL09a, MSJ04, MSK+05, NK05a, NKS+09, PW09, PS03c, SG03, Shi05, TOK+00, TG05, YKT+02, AA04b, PM06a, SY06].
Effects [CPH04, DI05, EP02, GSfLV08, LFR+08, PM06a, SS05a, SDS04, SS09c, SRHÖ06, TJAS08, VDF+06, AS04b, AGN04, ASO+06, BL04a, BL04b, BML01, BEM02, BLA00, Bec02, BR05, BŠM01, BKM+02a, BB04, BB05d, CLA+02, CDH05, DDT06, DDT+03, DFRS07, DKR04, DDBF09, Ess07, FL04, FBBB06, FSR02, Gin06, GAR08b, GS00b, GS01, GSA+09, HEBS00, HKMM04, HSH02, HS05, IS03, IDM+09, IROW09, JC01, JPA05, JM07, JSC01, KK04, KSS+08, KNS+09, Kor05, KF09, KFD01, KBMM08, LZC04b, LTY09, LSC02, LZWY07, LSE05, MB01a, MP05, MST04, MVdCD00, MMV05a, MNJP05, MVLM05, MESH02, MRG02, Nag04a, NY04, NGRR02, Noo06, Oni09, ONA05, PJ07, PML09c, PM09, QC02, Sap06, SMOE02, SPS06, SLCW04a, SUAL04, SM09, SCMS07, TSK01, Tak08, TY07, TBML06].
effects [TPRVC01, TMS08, VRSF02, VMA03, Wal04b, WRK03, YYK+03, ZDO09, ZMZ+09, ZWJ02a, ZWJ02b, dBC06, FdONGM08, dBKS01, dFGM08a, dSNBG08, BCT+02, MB05b, MLD06, MB00, NFT+01, PJS+09a, SS03a, YF07].
efficiency [GSQ+04, Har05b, SMM02, CMNH07].
Efficient [Čár07, FD09, Har04a, KN09a, KM00a, MG05, PJ09, TR09, ZDO00, HN03, Ort05, PMHW07, BGN+05].
EFP [YSS08].
egg [MFR07].
EHF [ISK+01].
Ehrenfest [Sah04].
EHT [CD04].
eigen [AD07, QLD05].
eigen-energies [AD07].
eigen-functions [QLD05].
eigenfunctions [ACFR05, LL01, RJ08].
eigenspectra [Man05].
eigenstate [PGW09].
eigenstates [ELY09, TPRVC01].
eigenvalue [BBB02, Fis00].
Eigenvalues [JJ00, Ano06g, ACFR05, Bar08, KMS06, LD05, Nic02, POM+08b, ZT08].
either [CN03].
elaboration [Buc05b].
Elastic [LIBM03, SL05d, ALM05, BCWS09, BLM08, HCRHM03, YPS05].
elected [Ano00d].
Electric [AC08, BČZ07, BSN05, KM02, RLRE04, ANJ09, Aze05, AdBM06, CJ09, DN06, Dya00, GB08, GM03, KBMM08, LHTV05, LTV07, Lef00, Lu06, MBOL04, PSH00, PML09c, PM09, PJ09, UP05, VMRA04, Lat03a].
electrical [BN03, BS05c, KK07, MB05b, RL04, XC07b].
electrochemical [GKL+09, XC07b].
electrocyclic [DLTW04].
electrodes [TWSK09].
Electrodynamical [GKL+09, OYYY02].
electrodynamics [GQ00, Sal05].
electromagnetic [Laz02, RW04b, SS05a].
Electron [Áng09, BSM+07, BŠM01, DZO00, DZO02, GC05, JTC+07, Mar87b, Mar00b, MB07b, MS09, PUH+08a, PKB+01, RDK97, SFZO01, SD00b, ŠPNU08,

UBS04, Win04, XC07a, YS07, YL04, ZDZO07, AB08, AGM06, AMGN00, AM05, AM09b, ABC+06, AP03, BGGS08, BDG01, BK04a, BSH04, BL02b, Bli02, BR00, BLM08, BG00b, BG00c, BG02b, Buc08, Bud04, CA01, CCGF07, CW04, CSP04, CC07, CBB01, CEK01, CM02b, CHW04, CC00c, CMRMR00, CDDM05, CCR09, CGS01, DL06, DKWP04, DLZ+03, DPW00, DGC08, DS06, DZS+06, DFMZO08, Duf07, DD00, FRK+05, Fle06b, GDFT01, GMCS04, GAL+05, GRC09, GGAMB03, GW06b, Gus02b, Gus04, Hag00, Hag05, HZJ+07, HSP+09, Har02b, Har05a, HT05b, HH02, HH09, HCTC07, Hog09a, HD03, IZ04, JPA05, Jal07b, JdL08, Jal08b]. **electron** [JNSF04, JM07, JPMM08, KS00, KD05, KS04a, KJH09, KNS+09, KL00, Koh01, Koh02, Koh04, KWG06, KTN02, Kry05, KOT09, Kut08, LK00a, LPV05, LIBM03, LMJ00, LLX+03, LZA+09, LLYJ09, LLZ04, Liu06, LH07b, LZZ+06b, Lu06, LSE05, LP05b, MZF05, MY08a, MY08b, MR00, Mai08a, Mai08b, Mak07, MMM06, Mal05b, MST04, MST08, MKHP09, MNMV02, Mar03a, Mar07a, Mar09, MO06, MHGR07, MF03, Mer04, MNV07, MV02, MCZWD06, Mor02, Mor03, Mor08, Muk00, NP01, NŚM02, Nes01a, Nes01b, Nes03b, NJC02, ND02, ND03, NS02, OB02, OR07, Ort03, Ort05, PUH+08b, PUH+09, PRG+04, PKS+00, PJ07, PGW09, PPP+08, Pir06, PCL+03, PS03c, PC04b, PBM03, PB09, PJS+09a, Pri05, PS02, Put05, QS00b, RI03, RVR00, Ret06, RBLS04, RFE+00, RA02, RR02, RW04b, RW04c, RIVB03]. **electron** [RDK02, Roy08, Rui05a, Rui05b, SS09a, SH02a, Saf04, SMY07, SFD09, SJE03, SLE05, SI09, SCM00, Sap06, SSR02, SBKSS05, SY05, SBB05, SBB06, She04a, SNT+00, SK03a, Sjö00, SGS00a, SL05d, SNdAM08, SD00a, SDZ+07, Stu00, STL+09, SZJ+04, SDW07, TC05, TOC06, Tak08, TPRVC01, TBM04, TS01a, TSF04, Tri03, VU02, VBML01, WS00, WZL+07, WZJ04, WO05, Wei08, Whi03, XLX+09b, YKT+02, YYK+03, YYI+08, YNY01, YBS05, YINH00, YN04, YJ00, ZDO00, ZDO09, ZZFL00, ZW09a, ZSW+00, ZSM+01, ZWM+04, ZMS05, ZFD00b, ZWSJ01, ZTSP00, Zie02, Kut03, MNJP05, SOLI04, IYO+04]. **electron-** [YYI+08]. **electron-accepting** [HD03]. **electron-attached** [PGW09]. **electron-collision** [GAL+05]. **electron-correlated** [KS00]. **electron-coupled** [SNT+00]. **electron-donating** [HD03]. **electron-doped** [Mar09]. **electron-electron** [VU02]. **Electron-impact** [UBS04, SI09]. **electron-NH** [BLM08]. **electron-nuclear** [Sjö00]. **electron-pair** [Duf07]. **electron-spin** [BG00b, BG00c, BG02b]. **electron-transfer** [CBB01, CDDM05, SCM00, ZZFL00, ZFD00b]. **Electronegativity** [Put09, KPTŚ03, KO03, Put06]. **Electronic** [AM07, AKN09, AM09a, AV05b, Ano02m, BMMC09a, CLSD+01, CN00, Cos06, FRNM08, FPC05, GSQ+04, GT07, GBC+02, Gup00, KP02, KLB+05, KM03a, KY05, KS02b, LJMM09, LADD00, LCBC03, MS05, MWW+00, MS00, MGV00, MESH02, PGB09, PT00, Pan05, Pan06, Pen06, Put03, QMB+06, RL04, SPN03, SNY01, SUA+04, SCRSRE05, SCRRE07, Spr00, SSS+05, SÖ04b, TW05a, TCM01, WTWT09, WSNB00, YST+05, YHF+08, YJ00, YYXC01, YPS05, ZFD05, ZZKS07, AAKAF07, AH06, AEI00, AWZD05a, AWZD05b, AV04, ARH00, AT07, ART08a, ART08b, APN02,

BMB02a, BK04a, BDA+02, BBO04, BJ00, BB00, Boe04, Boe07, BDBG09, BBPG08, BSAL+06, BCT+02, BLKJ00, CNC+06, CL00a, CXZ+09b, CDDM05, CK06, DL06, DEN02, DNMM06, DDD02, DD05, Deb08, DG04, DFH02a, DFH02b, Den09, DGLM09, DBL+03, DBPG04a, DBG04].
electronic
[DBPG04b, DB04b, ESE04, ES02, EWCT+05, EZ05, EP02, EB04a, ESTU05, FDL03, FL04, FRT+00, FCLH+06, Fuk09, GSfLV08, GB03, GD00b, GB05, GG03, GBMMSA00, Gos01, GGPS06, GP03, GW06a, Guo09, Hag05, HJT07, HSH02, IDM+09, IBB08, IMT+02, JMP05, JXW+04, JHLC09a, JSC01, KS08, KCU09, KSH04, KH05, KVF+08, KSN+04, KYA03, KH08b, KF09, KKTMA09, KFD01, LDMR01, Lam07, LW05, LDPP05, Lav03a, LSK+06, LPV02, LXY00, Lu06, LSE05, MUL02, MLW+09, MLD06, ML08, Mar00a, Mar04a, MVdCD00, MTE09, MHV00, MOA05, Men08a, MBOA09, Mer04, MdlV03, MW05, MD02, MHP04, MGAS09, Nak02, Nak07, NID+06, Nee01, Nes04b, NGRR02, NOHN02, dlPOPP03, Pan02, Pan04, PRNM03, Pen00a, PS03b, PDR+00, PDS04, QS05, RPPO00, RBLS04, RA02, RKR+06, SO04a, SFPA03, SCP03].
electronic [SLRS02, SRO02, SIS+08b, SCW09, ŠŠU+02, SLU+06, SCRE08, SMM02, SR07, SUH+01, SSK09b, STN+06, SNN+09, TN09, TNO09, TCS+08, Tap04a, TBML06, TWZ03, TKS+05, TRF+00, TT02, THPN03, TL05, UT03, VCHC07, VX04, VBML04, VHM+04, VD04, VG06, VNP00, WNW05, WWW+07, Wil04a, WT06, XZGZ06, Yal04, YZW+08, YPD+07, ZT02, ZSPS03, ZMB+03, ZCWZ04, ZCZ+07, ZXZ+09, ZMZ+09, ZLL+09a, ZLL+09b, ZTI+07, ZDQF08, ZT04b, ZRF+09, dAMM05, dD04, AÖG07, DLM+02, HNKiS01, LSPS01, MCLKC02, MOAB01, MOA02, NSS09, SCRSRE06].
electronic-structure [ZT04b]. **electronically**
[ACDV01, BABL09, IA06, Mic06a]. **electronics** [XR05, ZKB03]. **electrons**
[BCN04, BG02b, EWCT+05, Jal08a, JCTD08a, Jal08c, Koz04, Les03, Nes04a, OR09, She04b, She07b, SGS00b]. **electronuclear** [Tap04b]. **electrooptical**
[Bro00]. **electrophilic** [Buc07, PMC02, Pri05, VTS04, VTS05, XXC08].
electrophilicity [EPSC06, Von00]. **electrophoretic** [DH04a].
electrophylic [Sok04]. **electropolymerization** [NFFA04]. **Electrostatic**
[GKSL01, Jal07a, RJB+06, RdSH08, CDH05, CCE+07, DLHP04, EB04b, GMPIP01, HLP07, HWPIM01, KM00a, KK07, KM00c, LCT00, LPL04, MPIP00, MPIP+01, OSSG07, PMPI01, PLC02, PMC02, RLER04, SGLF01, SM07a, SCMS07, Whi02b, IPPL05]. **Electrostatically** [PMLC09].
electrostatics [CTP+08, JG09, LGJP05, CVVA08]. **electrostatics-** [JG09].
element
[Flo08, Khe09, LB03, QGW02, SYLE07, SCM00, Sce09, VMA03, ZY04].
Elemental [SD09]. **Elementary**
[Buc01, HCZ05, Kat00, RMKS08, VVW+03]. **elements**
[DZ01, DNM+08, Har05c, HSB+00, ILVMSB+02, ILVMSB+03, Kan00b, KMN05, Kýv09, LS08, MST04, MST08, RLBK03, SSF02, SSDB06, Tch07a, TTM07, VATPR01, WWTHF09, ZVVT07, ZMMK09, ZWMZ02]. **Eliashberg**
[NK06]. **elimination**

[Buc07, ITN08, MCC08, OCK07, SSC+07, SCSWF04, TGSK09]. **ellipsoidal** [Har02b]. **elliptic** [ACC03, ACCC03]. **Elliptical** [Har03, Bud04, ÖKAY03, SPL03]. **Elongation** [KGI+05, KGA05, PGPA09]. **Elucidation** [FGC04a]. **Embed** [PDR+00]. **embedded** [KS00, LMSB00, MMCC02, NRS+02, PBS02, PGPA09, QCK04, SLRS02, SBM00, Shi02]. **embedded-cluster** [KS00, PBS02]. **embedding** [AA04b, CTP+08, DKW09, PW09, QGM+00, SBF+04]. **embeddings** [CT00, Tem00]. **emeraldine** [ZTI+07]. **Emergence** [GHG04]. **emission** [GN01, HOIK09, MHV00, MME09, RSRMBFR00]. **emitting** [BK03, KWWQ04, ZRF+09]. **Empirical** [OC08, PUH+09, DCP06, DC06b, Šat03, UB05, KW03]. **employed** [MCF08]. **employing** [Pen00b]. **employment** [DKP+06]. **enamides** [LTLS05]. **enantio** [LTL05b]. **enantio-** [LTL05b]. **enantiomers** [HQL09]. **enantioselective** [LXH+00, LXTT00, LXHT00, LZYT01, LZHT03, LZT03]. **enantioselectivity** [FWT08]. **encapsulated** [JJFdL08, KG08, KG09, YW09]. **encapsulating** [LH07b]. **encoded** [SY07, Tem00]. **encounter** [PUH+08b]. **end** [KN08, SWSH09]. **end-on** [KN08]. **ended** [XZ07]. **endo** [CVPGH+06]. **endocrine** [KM03a, KM03b]. **Endofullerenes** [Gur05]. **Endohedral** [JWM00, VM06a, ASH07, RGP07, SCHW07, YKS+06]. **ene** [CWY05, KCU09, QD04]. **enediynes** [GCCM03]. **energetic** [AÖG07, FGC04b, FG01, LCH05a, LCH05b, LCCC08, LCCH09b, MYS+09, PML09c, VED+02]. **Energetics** [LP09a, Nav09, RVR00, ASH07, BC03, KN08, PM04a, RH03, SE02a, Shi04, SLA+05, DLZ+03]. **Energies** [AKB06, CRTP05, Orl02, WBLQ00, ATN09, AD07, AC06, ABM02, AS00, BEM02, BFB08, BBSS00, CL05d, CC00c, CN03, DB06, Deb08, DKM+04, DZO00, DZO02, ENGY+07, EBB06, FGH09, FA05, Flo08, FFS04, FAE+05a, FFHT05, FAE+05b, FS05, FJK+01, FJK+02, Ful00, Ghe09, Gin00, GKC06, GL07, HdMB+05, HSP+09, HPC+08, HWPIM01, IZ04, Jal02, JR02, JNSF04, JSC01, KAE03, KAE07, KSBK08, KVF+08, KLI07, KV08, KM00c, LSC01, Lef05, LCT00, LTY09, LN03, MSB00, MKCB05, MB07b, Mas04, MABB06, MBK01, MYS+09, MPIP+01, Ort05, Pai00, PA02, PUH+08a, Pea02, PGB00, PMAA00, PLC02, PMC02, PCL+03, QBTS05, QDÖ09, RRPJ07, RSRMBFR00, SK01a, Sah03, SG03, SFPA03, Šat03, ŠŠU+02, SKHY09, SCLL07, SMK08, TOC06, TG01, Van06, VD04, WZJ04, WSK03, YYY05]. **energies** [ZDZO07, ZDO09, ZKRS07]. **Energy** [BNS05, BK03, CM05a, CEÖ02, CCEÖ06, IV02, KP09, NTB02, Nes03a, OdSC05, PSB+05, SSDM05, TB09, YSP06, AA04a, AG01a, AGN04, ACPG01, Ano06f, ACFR05, ART08a, ART08b, ASM+03, APN02, BBHQ04, BDG01, Baň05a, Bau09, Bec02, BJ00, BM04, BS02, BAKK06, Bli02, BG00a, BG02a, BFBB06, BLM08, BLKJ00, BMMC09b, CGCS02, CTSÖD03, CNC+06, CSG06, CNPA04, CL05d, CX00, CT05, Cho08, CCB07, CSA09, DVV05, DRS00, DRPT02, DST+04, DGD+05, DI05, DBG04, Don09, Dou07, DZ06a, DW05, EJ06, EF03, ER05, EB04b, FRGM06, FOM+03, FYSS09,

Fuk09, FCD08, GCCM03, GBS04, GSRL06, GY04, Gin01, GMS+05, GG07, GMK+09, Gog05, GGAMB03, Gos01, Gra08b, GWK+05, GB06b, GHK05, GYM+02, GdA01b, HI06, HSW04, HAL+02, HBTW04, HTN07]. **energy** [HM03, HMMT04, HMK05, HMK06, IBN08, IDM+09, ISS00, JLAR07, JTC+07, JCP+08, JMP04, KIN09, KZ08, KCS02, KDM00, KNO09a, KANK00, KP00b, KM00c, LFADSF07, Lav03b, LLR+00, LBSB08, LAS+07, LYP+06, LXY00, LWCF08, LKE03, LGKN04, MZF05, MGdS+08, MZN+03, MST08, MA05, Mar03b, MHV03, Mar05a, Mar09, Mar05c, Mar07b, MHT+08, MNR07, MH03, MH05, MHB05, MZD+05, MKDM03, MK02, MB01b, MMF00, Mor02, Mor03, MTO+03, Mor04, NM01, NP01, Nag03a, Nal00b, NF06, Nes00, NFG05, NPLV05, OMY+01, Oku01, OM02, OM03, OK05, OA03, Ort05, Ou06, PA04a, PRSLA08, PC07, PD05, Pej03, Por01, Por02, POV+03, PJ09, QS00a, QTT07, QCC02, RMJ+07, RA03a, RA04, RZ07, RBLS04, RAA05, RO01, SK00a, Sal05, SSMG08, SKSB08, SLE05, SBKSS05, SSB00, SSSK07, SSZ+07, ŠŠU+02, ŠFW00, TC05, Tak08]. **energy** [Tch07a, TDS+02, TT01, TR09, TSF04, TGGS06, TW02, TKJ09, TGG01, VLJ08, VCF+00, VGMN03, VGB05, Von00, Vrb08, Vyb08, VSS04, WKF+06, XXMJ06, YHD00, YT03, YHD+07, ZCWZ04, ZLZ05, ZWMZ02, ZD08, ZCFD02, ZW07, ZLY+09, ZT04a]. **energy-based** [LLR+00]. **Energy-dependent** [KP09, NFG05]. **energy-driven** [AA04a]. **Energy-linearized** [Nes03a]. **energy-optimized** [GBS04]. **engineering** [GCG05]. **engines** [VAS06]. **England** [Kry08a]. **Enhanced** [DD00, ASP+05]. **enhancement** [ACT+05, LKE03, NKN+05, Pöt01]. **enol** [AG08]. **enolate** [GRC09, VTP09]. **enolates** [EPSC06]. **enoyl** [PFSFH06]. **enoyl-acp** [PFSFH06]. **Ensemble** [DH04b, TGGV+04]. **Ensemble-averaged** [TGGV+04]. **Ensembles** [Zak04a, Han02, Kry06, Tem02c, Tem02b, Tem04]. **Ensuring** [GSB00]. **entangled** [KMK+05]. **Entanglement** [MY08c, AT00, MY09, Sjö00]. **enthalpies** [DLZ+03, KKK09, dSNBG08]. **enthalpy** [CNT+09, NSZZ04, NSG+06, Pud02, SZU+04, TX02, DV00]. **Entirely** [GSD+03]. **Entropy** [NB05, ACA02, BBB02, FM02b, Gra08b, HSW+00, KOPP04, MB05a, NR09, NY01, SZU+04, VSI+07, YKT+02]. **entropy-based** [MB05a]. **Entropy/information** [NB05]. **Environment** [SMOE02, BBDS06, CMR05, KK07, MMR+04, YZX+08]. **enynes** [MLZS06]. **Enzymatic** [CZWZ05, BBSS00, Buc07, HJJ09, LZZ+07, MPRGLL03]. **Enzyme** [TFS+02, CBB01, DCO+08, LYP+06, MAFR08, PKZN08, PBB+02, TGGV+04, XZGZ06]. **enzymes** [LSWT05, NGTB06, PRBGLL04]. **EOMCCSDt** [GPW06]. **epidermal** [PBTP06]. **epothilone** [KRR08]. **epoxide** [DDW+06, Sch04]. **epoxy** [BFRB07]. **epoxyethane** [LXD00]. **EPR** [AK05, BKM+02b, PVV+04, SVC+05]. **Equation** [MB06, AH06, ACT+05, AVTPR09, AMGN00, Ano06g, BG00a, CNC+06, CDB02, CW08, Dat04, Deb08, DSLC05, DM02b, FGF06, GMK+09, GBL06, GPW06, HMB+04, JTB09, KMS06, KPSH06, KP09, KN08, KP00a, KV08, LLZ+00, LSLD01, LSD02, LD05, McK04, MP00, MSJ04, MOPdP09, NFP05, NF06, ND02, ND03, PVW03b, Pet04, PGW09, QLD05, QGW02, QGW04,

RW00, SBT+03, SA09, Sko02, SMT06, SS03b, UC06, VWB+03, VAT03, VTPRA08, VAS05, VD04, WRW02, YAŞ00]. **Equation-of-motion** [MB06, GPW06, KV08, PGW09]. **equations** [BMB02a, CW04, ÇKB02, FD09, Her06, HM03, HM05b, HW06, Hyd06, JJ00, KAE07, KV08, Kry09, Mar05b, Nag06, POM+07, POM+08b, PGW08, SHZGP09, SS08b, SB04, YONY04, ZSW+00]. **equilibria** [MRST01, SS09c]. **Equilibrium** [CGMT03, GS00a, METSH02, Pom04, BE07, BA01, BA02a, CZ03, HK06, MKZ04a, RNCM05, WT06, ZZL05, MESH02]. **Equivalent** [MY08b, MC06b]. **equivalent-core** [MC06b]. **ErCl** [BKAT00]. **Ermakov** [Kry09]. **Erratum** [AV06, AC05, AWZD05b, Ano00c, Ano01d, Ano02a, Ano02b, Ano07a, ACF05, BR12, BA02a, BB05d, DAD08a, Deb08, FFFR02, FAE+05b, FJK+02, FS09, GM08, ILVMSB+03, IKS10, JFJMR08b, Kar10, Mai08a, Mat10, MM09, ND03, RB11, RA04, RRGP05a, RS11, RDK02, Roy05a, SCRSRE06, Tem04, Tor04a, WAJ04a, Yam05]. **Error** [MB04, KMM+07, KWC09, SFD09]. **ESIPT** [ICRS08]. **ESIPT-exhibiting** [ICRS08]. **especially** [Mar04a, NM01]. **ESR** [GD00b]. **Essential** [CHMIHS+05]. **established** [RPS+07]. **esters** [RME+03]. **estimate** [RMJ+07]. **estimates** [CWF09, GGDL07, GFDK09, ZT04a, ZŠ05]. **Estimation** [Bec05, NKS+09, TC05, ACA02, GRC09, Oni08]. **estrogen** [DC06b, LYP+06]. **estrogens** [DH04a, PSS05]. **ethane** [QC00, VSI+07]. **ethanimine** [MWL08]. **Ethanol** [SVT06, FFF07, Tou09]. **ethene** [BCK04, PXZ+09, WML08]. **ethenes** [ETM00]. **ether** [DH04a, FBGA04, LZYT01, LZHT03, LZT03, MGZL04, MJG+05, TA07]. **ethers** [FBGA04]. **Ethyl** [GS05]. **ethylene** [BSR02, BKAT00, CL05e, CBC00, KV05, KL03, ML05, MLD06, QC00, RLBK03, YYS+09, YTD05, RCF02]. **ethylenediamine** [CLSD+01]. **ethylenedioxythiophene** [DBL+03]. **ethylenes** [LSCC01, Sak02]. **Euclidean** [MP09]. **eukaryotic** [PKT05]. **European** [DT02a, PČ04a]. **europium** [FJT+05]. **eV** [MMS+09, SBKSS05]. **evaluate** [CFM+06, Hog04, LFK06, NF06, PCT+04]. **evaluated** [DLM+05, SH02a]. **Evaluating** [GdA01b, WPB+06, DGD+05]. **Evaluation** [Bar09b, BČ02, Bud04, Dkh08, GKC06, Gus01, Gus03, HPC+08, KOT09, LHTV05, ÖO02, PCT+05, VCHC07, WZL+00, AH06, BSH04, BS06, Buc04, Čár07, Dun01, DS07, ELG05, GS09, GSD+03, Har02b, Har04a, HF09, HSB+00, KM00c, LLR+00, Mak07, MVdCD00, MKCB05, Mei08, Özd03, Özd04, SH00, SH01, TA06, TŠPJ01, VRSF02, AG02b]. **even** [Buc05c, CKM09, KW03, MZN+03, MRT00, YYZ05a]. **even-membered** [Buc05c]. **even-tempered** [KW03]. **events** [JPMM08]. **evidence** [CJB08, CL07b, FZ09, OM03]. **evidenced** [DBFP05]. **Evolution** [CB03, Hag05, NWZ+07a, RCJF00, SZA07, SÖ04b, Wal04a]. **evolving** [BPM01]. **Exact** [BBC07, BC06b, FZRD07, FS97, LGKN04, MSJ04, Nag03a, QS05, RdTdLC+07, YAŞ00, Živ09, FTW03, KSG03, KZ09, Mar03b, MPKB06, NN09, Nes01a, PGB00, SG03, SJE03, SRK01, SS04c, FS09]. **exact-exchange** [KSG03]. **Exactly**

[PRRMLB05, POM+07, POM+08a, Ada02, GGS09b, SBT+03, SS01].
examination [HS05, LSC02, Oku00, YZ07]. **examinations** [JNSF04].
example [Hog04, LGJP05, LADD00, QW05, RdTdLC+07, ZMS05].
examples [BCvzGG04, CDG05, SCM00, Wei08, KSZČ04]. **Excess**
[YCN+07, Jal07b, Jal08a, JdL08, JCTD08a, Jal08c, MHGR07]. **Exchange**
[DFH02a, Nes00, PCL+03, POV+03, Áng09, AK05, ADSTS06, Buc08, Dkh08,
DDBF09, EZY00, FTW03, FA05, FZ09, FD09, GGS09b, GSB00, GB06b,
GGDL07, GFDK09, HM05c, JFC02, JCP+08, KSG03, KSS+01, KYT+04,
KFS00, KZ09, KP00b, LP04b, MH03, MCZWD06, MVKN06, NKS+09,
NFG05, OD03, OdSC05, Orl07, PT06, QS00a, RHH+02, Saf04, Sah03, SG03,
Sch05, SL05b, Sme02, SSDB06, TOK+00, TB03, TSF04, TW02, WZ06,
WWTHF09, Whi03, YKT+02, YHC05, ZZFL00, ZLY05, ZL06].
Exchange-correlation
[PCL+03, AK05, Dkh08, FA05, GGS09b, GSB00, GB06b, GGDL07, GFDK09,
KP00b, MCZWD06, NFG05, OdSC05, Sch05, TB03, TSF04, WZ06].
exchange-energy [TW02]. **exchanged** [BJAV08, KL03]. **Excitation**
[CEK01, DL06, DRS00, PGB00, SG03, ATN09, Bec05, GDFT01, GAL+05,
GMS+05, GL07, KP02, LIBM03, LCT00, Mal05a, Nes02a, Nov07, OM02,
OM03, PD05, PREM05, Por02, Sal05, SI09, SMK08, VV05, YCN+07,
YLYD03, ZCWZ04, dFGM08a]. **excitations**
[BABL09, GBC+02, KSG03, RPPO00, TBML06]. **Excited**
[BL04b, DEN02, Roh00, SLU+06, Sun06, BDA+02, BL02a, BDBG09,
BBPG08, BABL09, Bu02, BMMC09a, ÇAK07, CS03, CT05, CTS08, CN05,
DGR+00, DYD00, DBFP05, DW00, DD03, DBPG04a, DBPG04b, FGH09,
GSQ+04, GG07, Gre09, HS02, Hea03, HGRL01, IN07, Jal02, JR02, KS08,
KS02a, KAN+09, KV08, LSL+08, Li09, LA07, LCBC03, Mic06a, MYS+09,
Nag04b, NKP+02, NRJD03, dlPOPP03, PK01b, PCBA08, PGW09, PREM04,
PRCEM06, PGPA09, RSKC08, SKN09b, SFPA03, SBB05, SBB06, SL00,
SL05c, SM05a, SS01, SUA+04, TN03, TPGD02, WRD03, WW08, WBLQ00,
YTD05, YCN+07, YOM+01, ZW03, ZW04, ZD07b, ZLS07, ZD08].
excited-state [DYD00, KAN+09, LCBC03, dlPOPP03, PK01b, SL00, ZW04].
excited-states [CS03, HS02]. **exciton** [NY01, PD05, TNYY03]. **excitonic**
[SC02a]. **excitons** [PTS03, May06]. **exclusion** [FHHC00, Nes04a]. **exclusive**
[Kap02]. **exhibit** [GPW02]. **exhibiting** [ICRS08]. **exist** [Pet00]. **Existence**
[KV02, ASO+01, ASO+04, Mal02, Str00]. **exo** [CVPGH+06]. **exohedral**
[TCS+08]. **exotic** [BSM+07, ER05]. **expanded** [FCLH+06, RH09].
Expansion [Har04b, Ada09, ANM03, BEL01, BM07a, BM07b, CS01, CGS01,
DCA03, EJ06, FD01, GWK+05, GM00, GM01, Gus01, Har02b, JSC01,
Kut08, LD05, MK02, PHH08, SEY07, SEY09, TG01]. **expansions**
[AE02, Har05a, SMB07, Tal07, Wen00, Wen02]. **Expectation**
[CDG09, GL01]. **experiment**
[För04, FB07, HWR05, SR05, SSN03, SBM00, SBK+09]. **Experimental**
[AEI00, EYBM03, KMK+05, SŚRL07, BMMA06, Buc08, CNPA04, FJT+05,
GV06, GP01, GFMT08, JJC+06, JZL+08, KVSS05, LGJP05, NFFA04,

PSK02, SHM+09b, VWMS03, VSBD06, YKS+06, ZFD+00a, CGL+05, LGJP05, VRFS05, PGP+07]. **Experimentation** [LS01b]. **experiments** [DBFP05, Mar07a, MMR+08]. **explanation** [MG08, RSDNSB00]. **Explicit** [Kry00, NSG+06, Tem02b, Wei08, JC01]. **Explicitly** [SCR01, SCRR02, BCWS09, CA01, GBS02, GBS04, PJS09b]. **Exploiting** [BBB02]. **Exploration** [HSW04, BKHPvD01, FCC07]. **Exploratory** [TIV+07]. **Exploring** [GHK05, OMMB07, THP08, MMS+09]. **explosion** [MZD+05]. **explosive** [ZCZC09]. **explosives** [LCH05b]. **exponent** [ITN06, ITN08, KOT09]. **exponential** [BB07, Gus01, Gus02a, Hog09a, PH09, RFLR00, RFE+01, Sha04, AH06]. **exponential-type** [Gus01, Gus02a, RFLR00, Sha04, AH06]. **Exponentially** [HT05a, AGSH09, Wen02]. **expressed** [PBM03, TG05]. **Expressing** [Oku01]. **Expression** [Ano08c, Ano08a, BAZ05, Kry00, OM05]. **expressions** [Fan03, Man05, Nag03a, Sal05]. **Extended** [INS+08, YYS+09, CDK01, CDB02, CD03a, CEÖ02, DMV00, DKM+04, HCL03, Jal08b, KDY+02, MDSW07, ND02, ND03, SA09, SH09, Spr00, Squ05, SÖ04b, TB09, Var08]. **extended-chain** [Spr00]. **Extending** [HT04]. **Extension** [GPW06, Oku00, VBML04, BGN+05, PGW09, dHG04]. **extensions** [CDB02]. **extensivity** [LP04a, RS09, RS11]. **external** [ART08b, Kar04, SBM07, TG05, VMRA04]. **Externally** [SS00b, Nal00a]. **extra** [MBRS05]. **extra-framework** [MBRS05]. **extracted** [PBM03, Por02, Por04]. **Extracting** [LHG00]. **Extraction** [FTM06]. **Extraordinary** [SLWS07]. **extrapolated** [ISS00]. **Extrapolation** [DHZ06, HBTW04, SB06a, dA08]. **extrapolations** [JCP+08]. **extreme** [Sei03].

F [Ano07e, Ano07f, ARBD05, BVG05b, BL02b, BBD07c, BBD08, BDBG09, DLTW04, DBLM06, FRNM08, GR07a, GR07b, JLAR07, LSC01, LDXW04, LWL+08, LC05, MNJP05, SASS03, TLYW06, TCS+08, Var07, VK08, WZJ04, KVF+08, VMA03, BB05a, BG00c, CSG06, DLK00, GB05, GBB06, KM02, KSI+07, KSN+09, KCS02, LP00a, Pet00, Sch05, SKA05, WGLX02, ZKEE07]. **f-element** [VMA03]. **faces** [LR01]. **factor** [AR06, AA09b, Gin08, LKE03, PBTP06, dRPFCP08, Put03, RACD00, SSC+07, UC06]. **factorization** [MGMP01]. **factors** [BG00c, BG02b, DD05, HN03, Pal00, PGN+05, PSC+07, SMEA08, VRSF02, VBT+07]. **facts** [Mar05a]. **failed** [Str00]. **faithful** [PB09]. **families** [ELG05, LAS+07]. **family** [BCFR08]. **far** [HK06, SVDGFC05]. **Farewell** [Ant04]. **farnesyltransferase** [SFR08]. **Fast** [BB02b, BB05c, BSH04, Fer01, KSK+04, Özd04, Esc08, FCD08, NOM00, RR02]. **fast-transient** [NOM00]. **fatigue** [PMBM09]. **fatty** [IK00a]. **Faujasite** [IPPL05]. **fcc** [BCD+05, Boe03]. **FCCF** [GHH03]. **FDTI** [GdA01b]. **Fe** [Apo06, DMG09, GL00, SSK09b, ZZFL00, ZLHL02, AML+01, AGLBM03, BB05a, DSW08, FN04, FDLK02, GdRPLP08, KB00, MBP03, Mar09, MS05, PBMA03, SI09, VSD+02, VPS+04, Yur07]. **Fe/Cr/Fe** [MBP03]. **FeAl** [FSK05]. **Feasibility** [FGF06]. **feature**

[PMLTL07, ZCWZ04]. **Features**
[BDA+02, CCB07, AIG02, BE07, CVPGH+06, CWZ03, OG00]. **FeBO**
[FN04]. **FeC** [CZ03]. **FeCHR** [WML08]. **Feenberg** [FHHC00, SS05b].
Feinberg [AM09b]. **Femtosecond** [KDM00, BKMHP04, DNC07, WZWC06].
fentanyl [JHR+00]. **FeO** [GSC00, Gre09, KB08]. **Fermi**
[PM04b, CP09, GMK+09, Hea00, MKZ04a, MZD01, Nes02b, Nes04a, PSM07].
Fermi-model [GMK+09]. **Fermion**
[HM05b, SMB09, HM03, SS04b, SS06, Mat07, YNN+06]. **fermionic** [Gri06].
fermions [SLE05, Wyb02]. **ferredoxin** [SKT+07]. **ferredoxin-type**
[SKT+07]. **ferrocenophane** [Bro05]. **ferroelectric** [DLM+02].
ferroelectrics [DLM+04b]. **Ferromagnetic**
[BNA03, RI03, Gri06, NNS+00, PBMA03, SQZ+02, Yar00]. **ferromagnetism**
[Dro04, NNS+00]. **ferromagnets** [Mar09, MKDM03]. **ferrous** [CCV+07].
Few [AGSH09, FS97, Kry09, AG01a, FS09, GHT09, HFS04, Har05c, HFS06,
Kon09, Koz04, Sap06, Zot06]. **Few-Body**
[FS97, FS09, HFS04, Har05c, HFS06, Zot06]. **few-electron** [Sap06].
Few-parameter [AGSH09, GHT09]. **Feynman**
[AM06, BSR02, Mat07, Pup02, SE00, SE02b]. **FF** [BR05]. **FH**
[CSG06, BPŠB00]. **FHF** [Dav04]. **fibroblast** [dRPFCP08]. **Field**
[WZWC06, AKN09, AM06, AR06, Aze05, AdBM06, BS08, BSN05, BS05c,
CC01a, CL05e, DRPT02, DM02a, DVM06, DLM+04b, DN06, FFF07, GB08,
GMCS04, GAIK04, Gri08, GLHH09, HJJ09, ITY+09, JP08, JV05, JSvDA06,
Kar04, KK04, KKM+01, Kry08b, LHTV05, LTV07, Lat03a, LS01a, Lu06,
LCK00, MK00, MP06, MNA+99, MBOL04, MHV00, MYH03, Mon05,
NKK+01, NNNY01, NY01, NY03, NY04, NF02, OB02, OR07, PSH00, PJ09,
RRPJ07, RLRE04, RW04b, Saa00, SS04a, SS05a, SSA07, SDTM02, Son04,
SE07, TYG05, UP05, UC06, VM07b, Wal04b, WAJ04b, XXY00, YKGC09,
YL02, YM05, Zak04a, dGS06, WAJ04a]. **Field-assisted** [WZWC06].
field-induced [Lu06, LCK00, NKK+01, Saa00]. **fields**
[ART08b, BL04a, BG00a, BG02a, BKM05, CTP+08, CWW09, Deb08,
DLHP04, HCTC07, KH05, KKS09, KSU04, KSU05, Lef00, OMNN04,
PML09c, PM09, SPN03, SPL03, SCSWF04, VD04, VMRA04, Zak04b]. **filling**
[AK02]. **films** [ASH08, BR05, CCM+05]. **final** [ZDO00]. **finally** [NN09]. **fine**
[Lin06, SAM08, WBLQ00]. **fingerprints** [Mar06a]. **fingers** [BN01]. **Finite**
[FS97, SYLE07, SM03, ZY04, CWZ03, DHZ06, EYB02, Flo08, FS09, GdA01b,
LB03, MPKB06, MB02b, QGW02, Shi05, UP05, Živ09, BS05b].
Finite-cluster [SM03]. **finite-dimensional** [Živ09]. **Finite-element** [ZY04].
Finite-temperature [BS05b]. **finiteness** [QS00b]. **firmer** [FCS03]. **First**
[Boe07, BSCB04, FGFF06, FG03, GWJ05, HCRHM03, IOA+04, JMEM07,
JLM08, JXW+04, LZW+07, MW06a, MTO+03, Mor04, MGAS09, Noo03,
OCWY09, RPPO00, RP00, SL05b, VVBT07, YT03, ZXZ+09, ZDQF08, AZ08,
BS05b, BG00b, CJdC01, CT05, DNM+08, DBPG04a, DC03, FTB04, GBS02,
GSQ+04, GTR+05, GBC+02, IN09, JMP05, KS07, LCBC03, dAMdG05,
MMR+04, MAS09, MC08, PJ07, PJdC00, PJ03, POV+03, QC01, RRGP05a,

RRGP05b, SO04a, SÖ09b, Seb05, SDTM02, SSDB06, SSK+05, TCM09, TM05, VPS+05, WWTHF09, YCN+07, YYXC01, ZA09, MNR07, WL00]. **first-** [CJdC01, PJ03, MNR07]. **first-excited** [CT05]. **First-order** [SL05b, BS05b, YYXC01]. **First-principle** [BSCB04]. **First-principles** [FG03, GWJ05, HCRHM03, IOA+04, JMEM07, JLM08, Mor04, MGAS09, Noo03, OCWY09, RPPO00, RP00, YT03, DC03, IN09, KS07, MAS09, MC08, RRGP05a, RRGP05b, Seb05, SSDB06, SSK+05, TCM09, VPS+05, WL00]. **first-row** [BG00b, FTB04, GBS02, PJdC00]. **Fisher** [Nal08]. **Fitting** [FRGM06, BGN+05, Čár09, FOM+03, MNV07, Var08]. **five** [Ada05, CLL04, KMM+06, MLL00, RS06, XVRL04, XLX+09b]. **five-electron** [XLX+09b]. **five-membered** [CLL04, RS06, XVRL04]. **five-qubit** [KMM+06]. **flavonoid** [VNP00, WHD+05]. **flavonoids** [CHMIHS+05, Mey00]. **flavonols** [GLF04]. **flavors** [Mat02b, Mat10]. **flexibility** [JZZ+09, SSJ09]. **flexible** [AYD00, Apo06]. **flipping** [KS03a, SST00]. **floating** [CS01]. **Floquet** [Lef06, PSML04, SSA07]. **flow** [DM08b]. **flows** [KIK09]. **fluctuating** [SS04a, SS05a]. **Fluctuation** [Bel04, DJNH02, DAA+06, SS03a]. **fluctuations** [BSR02, KO03, SGLF01, ZTSP00]. **fluid** [DB04b, Vik07]. **fluids** [DCTC03, Mar00c]. **fluorene** [GL07]. **Fluorescence** [KNO09b, DKC00, DNC07, HT07]. **fluorescent** [DKWP04, SWZ01]. **fluoride** [ADSTS06, BKMS03, HLP07, Oni09, RAA05, RSFRDNA04, RRD06, SKHY09, URBM04, ZRRC05]. **fluorides** [Sch05]. **fluorinated** [LMX+05, VSS04]. **Fluorination** [LZC04a, DGLM09, LZC04b, Lia08]. **fluorine** [BDA+02, HR02, IAL06, LWW+02, TCS+08]. **fluorine-substituted** [BDA+02]. **fluoro** [ET01, FAE+05a, FAE+05b, Sha07]. **fluoro-substituted** [ET01]. **fluorobenzene** [BS02]. **fluorohalo** [VTP09]. **fluoromethyl** [ETEA04]. **fluorospherands** [ELO+07]. **fluorosulfonate** [SSN03]. **fluorotoluene** [CC00b]. **fluorouracil** [AGM01, AGM02, FS08, YZ07]. **flux** [BP04, NS08]. **FNgX** [LAQ+09]. **Fock** [DBd05, GE09, ND03, Sko02, SNdAM08, WTWT09, YONY04, dAMM05, Cor05, DMMV00, DMH+05, DFH02b, DGRB08, DVM06, DBL+03, DSH01, EB04a, FFHD00, GXT02, HdMB+05, INS+08, KC09, KCGB02, Koc00, KGA05, LV01b, LTV05, LCN05, LP09b, MMM06, MOL03, May02a, Nes05, NJD02, ND02, Pan02, Pan05, Pan06, Pat06, PJdC00, PRL01, QC01, QGW02, QGW04, RVP09, RP09, She07c, SGHL00, TOK+00, TYY07, TOH+00, TB09, WF04, YYS+09, YYY05, ZBPD08]. **folate** [KFQ+02]. **fold** [Tem02a, VX04]. **folded** [ACA02]. **folding** [AT00, BLC09, Han02, LW07, Muñ02, ŠK01c]. **folding-unfolding** [AT00]. **folds** [AV02]. **following** [Ano00d]. **Fondation** [Ano04f]. **Fonsecinone** [dLCRF+08]. **food** [BKM+02b]. **forbidden** [IAMY02, Pen00b, QS05, YYZ+05c]. **Force** [AMGN00, RRPJ07, ACHB08, BS08, BKMS03, BKM05, CTP+08, CWW09, FFF07, HJJ09, HMB+04, KKS09, Kry08b, Ras04, TYG05, XXY00]. **Force-balance** [AMGN00, HMB+04]. **forces** [Boh01, Boh03, BSK+02, DWD+05, OSSG07, Zak04b]. **Foreword**

[AGL04b, MP08, Riv01]. **form** [AR06, HBKG03, LV01b, LC05, LM02b, Pal01a, Sce09, Tri03, YZC09]. **formal** [XLX+09a]. **formaldehyde** [BČZ07, CC00a, CSL05a, CNT+09, LXXC08, LYCX08, MVL+01, ZB05]. **formalism** [AG01b, BDG01, CW04, FD01, MNR07, MH05, MHB05, Sin00]. **formamide** [BVHS01, BS05a, BČZ07, DFZ04, DWM+07, FDZ04, QCFJ05, STL+09, ZZZ+08]. **formamidic** [DFZ04]. **format** [ABB+07]. **formate** [LTL05b]. **Formation** [BK04c, JCTD08b, KS04b, MYS+09, ZŠ05, AWZD05a, AWZD05b, BDMS03, BHK09, CLA+02, ĆMTS08, CP09, CNT+09, DV00, JTC+03, KSN05, LWCF08, MSS05, MET00, MTO+03, Mor04, NBS04, POAVdlM08, PBSC04, PMBM09, PMLC05, PMLTL07, RME+03, RRNG05, SS09a, SKA05, SMS07, SWZ01, SCLL07, VVW+03, Wal04a, WE01, YMZH04, ZXX02, JRSA08]. **formed** [DKC00, MFR07]. **formohydroxamic** [KK08]. **formose** [JPA07]. **Forms** [EMV05, AG02a, AKK05b, EHH09, GD00a, MPIP00, Oku01, VTPRA08, VTS04]. **Formula** [Kry07b, BCEG08, BD07, Fle06b, Gin00, Har01, HN03, KOT09, Mar07b, RW04a]. **formulae** [JJWH04, KW03]. **formulas** [AS04c, Bra08, CC01a, CTP+08, Gar08a, Mai05, Pal01a, RFE+00]. **Formulation** [IYO+04, KDY+02, YONY04, BOW+01, CW04, KA05, KMN05, Kut03, OK04, PA04b, SA09, VWB+03, ZGY+03]. **formulations** [Put06]. **formvar** [PRM02]. **formylnucleosides** [RVP06]. **Förster** [OM02]. **forty** [Mon09]. **forty-four** [Mon09]. **found** [PSN08]. **Foundation** [CDG05, FCS03]. **foundations** [NS08, NS09]. **Four** [PČH02, RFE+01, VTPRA08, Buc08, Bud04, CPH04, LZHT03, Mon09, MTWN09, PCL+03, RBA07, WSK03, XLX+09b, YHN+07, ZZC09]. **Four-** [PČH02, Buc08]. **Four-center** [RFE+01]. **four-component** [MTWN09, YHN+07]. **four-electron** [Bud04, PCL+03, XLX+09b]. **four-membered** [LZHT03, WSK03]. **four-wave** [CPH04]. **Fourier** [AS04c, CTS08, DFH02b, FFHD00, FD09, KFD09, MB02a, Özt04, RR02, SSA07, TDF09]. **Fourier-transform** [Özt04]. **Fourier-transform-based** [AS04c]. **fourth** [CJdC01]. **fourth-row** [CJdC01]. **FQ** [KK07]. **fractal** [NFT+01]. **Fractional** [TYY03, TYY05b, BS00, DK03]. **fractionally** [Kry06]. **fragment** [BZL+09, Buc02b, DYD03, SFK09, SEM05, CDF06]. **Fragmentation** [LSM+06, QV01]. **fragmentations** [BGGS08]. **fragments** [BLC09, HPC+08, SSDB06]. **framework** [FTW03, MBRS05, XVRL04]. **frameworks** [LTV03]. **Franck** [Noo06, HN03, MP05, PSC+07, RR00, VRSF02]. **Frank** [Ano09a, Ano09g, MMS+09, Mon09, SÖ09b, Tay09]. **free** [AGN04, ADSTS06, Bar09b, BVHS01, BKMS03, BVHS04, BBSS00, CDGC05, CP06, DM08a, DHCD06, DGD+05, DKW09, GPW02, GdA01b, GST+05, HVSM02, HSW04, JZZ+09, KKMS04, NN09, PW09, PMAA00, RJ08, SSR02, SLRS02, SN06a, ŠFW00, VWB+03, VHV+05, VG02, YYYM01, ZLH+08, MOPdP09]. **free-base** [YYYM01]. **free-energy** [DGD+05, HSW04, ŠFW00]. **Free-particle** [MOPdP09]. **freedom** [IKL04]. **frequencies**

[BVHS04, BS05a, GW06b, HZJ+07, KSN+09, LFR+08, MCZWD06, PRM03, RNCM05, SSB00, ZCFD02]. **Frequency** [LBAB02, CVVA08, KKYT04, LS01a, QC01, QC02, SMEA08]. **frequency-dispersion** [QC02]. **fresh** [TS01a]. **Frontier** [GJ03, LGJP05, DMG09, TVK01]. **Frozen** [WTWT09]. **Frozen-core** [WTWT09]. **frustrated** [HSRP09, TYY05a, YSY+01, YSO+01, YYS+01]. **FSM** [Squ05]. **FTIR** [NAE06]. **fuel** [MARK08]. **fuels** [SGB00]. **Fues** [YAŞ00, YŞ02, Yal04]. **Fues-Kratzer-type** [YAŞ00]. **Fukui** [CDG09, CCGF07, FCC07, SRK01]. **Fulfilling** [May02a]. **Full** [DCDW00, KB00, MA05, XZGZ06, ZZ05, DAD05, LZ05, SKT+07, SIS+08a]. **Full-CI** [DCDW00]. **fullerene** [BIP+07, BZR02, CZS+05, FRT+00, FRF02, KLK08, LR01, LTL05a, RGP07, SNZG02, She07d, SYL05, SUAL04, TCS+08, TW05a, XXY+05, YW09, YLS+04, HNKiS01, MLL01]. **fullerene-based** [YLS+04]. **Fullerene-C** [HNKiS01]. **fullerene-like** [LR01]. **fullerenes** [JJFdL08, LTW09, MLW+09, MDBM05, SLB+05, She04b, She07c, SZU+04, SUA+04, SCHW07]. **Fulleride** [SM04, SM07b, SM08, Squ05]. **fullerides** [SM05c, SM06c]. **fulleropyrrolidines** [RSN+07]. **Fully** [BR02, Boe03, HM06a, HM06b, MST04, ZTI+07]. **Function** [NY03, ANM03, AM09b, AG02b, ART08b, Ban05b, BL02b, BCS01, Cam04, CDG05, CSG06, CCLK07, CC07, Chu02, Chu04, Chu06, Chu07, Chu09, DVV05, DD05, Del03, Dou07, ER05, FCC07, Gál07, GJ03, GS09, GMK+09, GHT09, Har01, Har04a, HF09, IYO+04, KS08, KF07, Kan00a, KK02b, KYT+04, KSS00, KMS02, Kry00, KOT09, LBSB08, LKG09, Loe00, LFR+08, Mal05a, MB07b, Mat07, MF03, MLZS06, MB04, NN09, PA08, Pau04, PBMA03, PHH08, PPP+08, POV+03, PBB+02, Roh00, SS06, SL05b, SRK01, SM06a, SMB07, SSZ+07, SEY07, SY06, SK05c, Tem09, TWSK09, WD01, Yam04, Yam05, YOM+01, ZLML05, ZCZF02, dGS06]. **function-based** [dGS06]. **Functional** [GDV05, MLSG04, PBM03, AFC03, ABD06, ACG00, Ano07e, AGB06, ASM+03, APN02, BAZ05, BCG09, BHG+06, BP03, BJS09, BKGF02, BBD07a, BLC+00, BR02, BTK+05, BSCB04, BKM+02b, Bu02, BDMS03, CK03, CSX+01, CZWZ05, CL05a, CB04, CC05a, CCA+06, CL05c, CSL05a, CL05d, CC05b, CC00c, CSTB08, CF04, CRTP05, CSA09, DV00, Die00, DGQT09, DBL+03, DLK00, DZTZ05, Dre05, DFZ04, DSW08, DWM+07, Elr09, EJ06, EZY00, EZ05, FCS03, FWT08, FXHL05, FWZ09, FPC+03, FZ09, FVPM05, FFHT05, FKR04, FDZ04, FSR02, GR07a, Gál07, GGACT03, GSC00, Gda01a, GBVD05, GJB02, GJ03, Gog05, GR05, GXT02, GXGT02, GZD+05, GYS+06, GW06a, Guo07, HSS09, HT05b, HGS03, HDL00, HM05b, HR05b, IABS08, ISK+01, Jal02, JLAR07, JRSA08, JNF+09, JXZ+05, JHLC09a, Kak03, KZB01, KSG03, KLI07, KSS+01, KYT+04]. **functional** [KSS00, KMS02, KSWR00, KZvL09, KG08, KMVR05, KANK00, KDF00, LDMR01, Lam07, LDR+05, LML+04, Lat03a, Lat03b, LP07, LMRT08, LSCC01, LRS05, LL04, LS02, LS05, Liu02, LKE03, LGKN04, LE01, MZN+03, Mai05, MP05, MP06, Mar05b, Mar07a, MRTT01, MRST01, MTRG04, Mar06b,

Mas02, Mat00, MWXL05, MWL08, MLSB06, MFA00, MDJ01, MD04, MBD05, ML01, Moh00, MCZWD06, MC08, MDG07, Nag03a, Nag06, NUY+06, Nal00b, NRS+02, NMNB06, Nes00, Nes02a, NGRR02, NK05b, NOHN02, OYYY02, OMN+03, PRM+06, PS08, Pat06, Pea02, Pea08, Pej02, Pej03, PBI+01, PMCOSC00, PW09, PGB00, PO03, PMO04, PO05, Pir06, PLU08, PSB+05, PCM00, PCL+03, PT06, PJS09b, Put06, QS00a, QCV06, QGM+00, QCC05, RBL08, RA03b, RRC03, RD00, Roy08, SS04b, SS06, SG03, SPH+03, SKSB08].
functional [SD08, SCP03, Sch05, Sei03, SL05b, SRK01, SC01, She07a, SIS+08b, SL05c, SK05b, SS01, SZK07, SWSH09, SHE+02, SCLL07, STL+09, TC05, TOK+00, TY07, TN09, TYY03, TSZW08, TN03, TX02, TB03, UP05, VU02, Van06, VCHC07, VCF+00, VR01, VPSH00, VED+02, WRRF03, WZ06, WWW+07, WML08, Wol05, WJLL09, XD03, XXC08, XC07a, XCW07, XXY00, YYYM01, YYS+00, YYKY01, YYS+01, YOYY03, YTK+03, YNU+06, YUN+07, YOM+01, YCS09, ZR07, ZXX02, ZLY05, ZCZ+07, ZZZ+08, ZMAL04, ZKYA04, ZNF05, ZOK+05, ZTW+09, ZFD00b, ZQF+02, ZPW+04, ZW07, ZWJ02a, Zie02, ZBPD08, eSPM+08, VSI+07].
functionalized [ELG05, THP08]. **functionals** [ATN09, BJS09, BKM05, DVV05, Dkh08, FA05, Gra08a, GSCRO08, HM03, JNSF04, Liu02, Mar03b, MHV03, Mar05a, NP01, NFG05, PT06, RMKS08, SC01, TGGS06, TW02, Wei08, dBKS01]. **Functions** [FS97, ACD02, AD06, BB06, Bar00, BS06, BSZ07, BD00, CDK01, CD03a, CDG09, CCGF07, CC01a, CCLK04, CCLK07, CT00, ELF+08, EYB02, ESU04, ESU05, FDM09, FLE+06a, FGR+07, FS09, Ful00, GBS02, GBS04, GW07, Gui01, Gus01, GM02a, GM08, HI06, Har05c, HGB08, HMK06, ITN06, ITN08, JLAR07, KA05, KH01, LLB01, Lav03b, Laz02, LKG09, LP09b, LH05, LM02b, LP05b, MK00, MHV00, Mer04, MJ06, Nak02, Nak07, NN09, Nic05b, NF02, PSM07, Pea02, POM+08a, PML09b, PH07, PH09, Pup05, Put05, QLD05, RH09, RFLR00, RFE+01, RLER08, RS00, Rui05b, SH00, SH02a, Saf04, SFPA03, Sch02, SWC03, SYZ+09, SZL+09, SMEA08, SEU02, SHE+00, Str00, SSS02, SB04, TYY04, Tal03a, Tap04b, TS01a, TT06, UES04, VSI+07, WC04, WO05]. **functions** [Wen02, Wen09, XVB05, YTK+03, YN04, ZSW+00, Zno00, dAMM08].
Fundamental [CDB02, CL05e, PS08]. **furan** [REHH07]. **Further** [FCC07, Por03, PGW08, GI07]. **furylcinnamic** [PK01a]. **fused** [FS00, Yam09, ZZKS07]. **fusion** [GA08, Ghe09, Mon00]. **future** [NU09, ZA09]. **Fuzzy** [SEM05].

G [DB04a, Kry08a, RRGP05a, RSTG02, KVF+08, Ano06a, BvL06a, KES03, SS09b, VED+02]. **G-protein-coupled** [VED+02]. **G2MP2** [DDP+07]. **G3B3** [DDP+07]. **G3X** [EBB06]. **Ga** [CMY06, Liu08, SYL05, YS05, GW06b, CCM08, KZS07, MM07, MM09, SZK07, SZ08, VTS04]. **Ga-like** [CCM08]. **Ga-ZSM-5** [SZK07, SZ08]. **Ga/ZSM** [KZS07]. **Ga/ZSM-5** [KZS07]. **GaAs** [KSK00]. **GABA** [FH02b]. **Gadolinium** [DLK00]. **Gai** [Ano07g, Ano07e, Ano07f]. **gain** [CTSÖD03]. **Gallium**

[GW06b, KZS07, PSCLGN07]. **Gamow** [GL01]. **GaN** [XXJG04]. **Gang** [Ano07g, Ano07e, Ano07f]. **GaO** [BCS01]. **gap** [ACPG01, Boe07, FPJR03, GCG05, HOC00, NK06, SR05, ZKYA04]. **gaps** [DB04b, FG06, ZCZC09]. **garnet** [MGAS09]. **Gas** [CN03, MRTT01, MTRG04, MMT+07, ZTW+09, ABL03, AGM01, ASH07, Ano07g, Ano07f, BBD07a, BBD07b, CQN+03, DF07, FGC04a, GR07c, GR07b, GGAMB03, GMS01b, GMS01a, GYM+02, HE05, HKE05, HDWH09, IAMY02, JTC+07, KBV05, KS03b, KM06, LME03, LDR+08, LAQ+09, LS05, LYDK02, MGK+09, Mar87b, MRST01, Mic09, MBK01, MCC08, Mor08, METSH02, NSLR04, PJZ+09, PGF+06, PMLC05, RJB+06, Rua09, RSTG02, SSC+07, SCB+06, TI05, TSF04, USM01, XYS+03, ZR07, ZLL+05, ZDMF08, ZFD00b, ZMZ+00, ZTSP00, Zie02, BCS01]. **Gas-phase** [CN03, MRTT01, MTRG04, ZTW+09, Ano07g, Ano07f, GR07c, GR07b, GMS01b, GMS01a, LS05, MBK01, Mor08, METSH02, NSLR04, PGF+06, SSC+07, ZDMF08, ZMZ+00]. **gas-surface** [GYM+02]. **gaseous** [CME07, GWSZ08, Mic06a, MG08]. **gases** [Pom04]. **gate** [GM05b]. **gated** [TRMM04]. **gates** [KSK+04, SY07]. **gathering** [Bar06]. **gauge** [BAZ05, VCF+00]. **gauge-origin** [BAZ05]. **Gaunt** [PH07]. **Gauss** [BS06, ELF+08]. **Gaussian** [ANJ09, Boe03, Čár07, Čár09, CC01a, CJdC01, CKM09, DKS05, DBd05, DMH+05, DHCD06, DPS04, Fuk09, GW02, GW04, GW07, HdMB+05, HSB+00, ITN06, ITN08, KK05, KOT09, LJ03, LS01b, MG05, Mak07, Mat02b, Mat10, NN09, NJC02, NJD02, NRJD03, PI02, PH09, PJdC00, PJ03, QGW04, RFLR00, RFE+01, RLER04, Sch02, TS01a, VD00, WS00, YHN+07, ZT04a]. **Gaussian-** [LS01b]. **Gaussian-2** [DPS04]. **Gaussian-3** [DKS05, DPS04]. **Gaussian-type** [Boe03, HSB+00, ITN06, ITN08, Mak07, TS01a, WS00, YHN+07]. **Gaussians** [CA01, CS01, HM06a, HM06b, Sha04]. **GC** [GBB06, MSS09]. **GCM** [Mor08]. **Gd** [RSFRB03, DLK00]. **GdX** [DLK00]. **Ge** [HZJ+07, JLAR07, SYL05, LL04, MS00, ZCZ00]. **GeC** [UMDM06]. **GeF** [SBM00]. **Gegenbauer** [Har05a, ÖÖOY02]. **Geminal** [PLC04, RS00, WO04]. **geminal-type** [RS00]. **geminals** [TTM01b, TT06]. **GeNaF** [TLYW06]. **genealogical** [KH01]. **General** [ÁBL06, Hog09a, RCD00, TBJA03, ACD02, FZRD07, HM01c, KVSG02, LP04a, Mar03b, MJ00, Oku01, Qui05, RW04a, TNO09, YINH00, MH05]. **general-acid** [KVSG02]. **general-base** [KVSG02]. **general-model-space** [LP04a]. **Generalization** [CW04, Gin00]. **generalizations** [CDB02]. **Generalized** [AT07, ART08a, EYY06, KA05, PC04b, Sal05, SPH00, Tap04a, YSY+01, YYS+00, YYKY01, YSO+01, YOYY03, ZZL05, ZKB03, ART08b, AS00, BG00a, Bou03, CSPS05, DNM+08, EE09, Gri06, Han02, KC09, KJH09, KP00a, MP00, MDJ01, MP09, MK02, Nag06, dRPFCP08, Tap04b, TW02, YSY+00, YTK+03, ZZL04, dAMM08, ARH00]. **generate** [NJD02]. **generated** [DMH+05, LN03, LGKN04, MLL00]. **generating** [AG02b, CCLK04, CCLK07, KW03, LKG09, Wei03]. **Generation**

[GLHH09, KW03, LB03, Met05, RCJF00, BL04a, FGM05, HQM04, HCTC07, Kon04, LPC04, LP05a, Liu02, MG05, Mar05a, QC01, RT06, SKA05, TR09]. **generator** [DMH+05, DDD03, HdMB+05, LN03, NJD02, PJdC00]. **Generic** [TT02]. **genetic** [BFF04, CB00, CDF00, CL08, FRGM06, LGBJ03, Luc02, MGdS+08, NCB02, Nég03a, ONK+00, ONK+05, SBT+03, SSMG08]. **Geometric** [CM02b, GB03, VX04, XV00, Bra08, Buc00b, DBL+03, MLW+09, SLRS02, MB01a]. **Geometrical** [RPS+07, SE07, AT00, Jal02, BSCB04, PNG02]. **Geometrically** [PB09]. **Geometries** [HZJ+07, WNW05, BEM02, Buc02a, Buc02b, CN03, DPS04, LTV05, MHT+08, MBK01, MESH02, PJ07, TLYW06, WT06]. **Geometry** [CZS+05, DSFS00, KSI+07, LA06, MKCS05, PRBGLL04, SBBL05, ART08b, BN06, BC06a, BFF04, BS05a, Buc07, JC00, JC01, KLK08, KSK00, LV01b, Mar04a, METSH02, NOHN02, PRM+06, RPHG04, RNCM05, SKSB08, SKT+07, SIS+08a, SH07, SS02a, TMS08]. **Gerais** [SD03]. **germanium** [FB01, IV02, SPI04]. **germaniumlike** [IV02]. **germylidene** [LXXC08]. **GeSi** [UMDM06]. **get** [NF03]. **Getting** [NS04]. **GGA** [PT06]. **GIAO** [dLCRF+08]. **Gilda** [Ano02d, Ano02c, Ano02l]. **Ginzburg** [ZZL04]. **give** [BSN05]. **glass** [FYT09]. **glassy** [Tou09]. **Global** [GH03, AV02, CT05, FCD08, GD00a, Lav03b, MRT00, UP03]. **Glória** [SD03]. **glucocorticoids** [PKT05]. **glucose** [BTL+02, JRSA08, JG00, PVV+04]. **glue** [KP00b]. **glutathione** [SPS02]. **glycinamide** [ZZDY06]. **glycine** [BS08, JRSA08, LRB04, MPIP00, PILD07, SK05a, SK06, SVDGFC05, TMS08, PILD07]. **glycylcarbonyl** [SST00]. **going** [MG08]. **gold** [ACG00, KR07, SRH02, TBB09, YS07, MOA05, PGB09]. **Gordon** [Fan03, Sko02]. **Gossamer** [SMB09]. **gradient** [Bou03, HTN07, Lat03a, MDJ01, TW02, YYKY01]. **gradients** [BSN05, CA01, DSH01, PSH00]. **Graduate** [Nag03c]. **grain** [DFM+02]. **grained** [DJNH02]. **Graph** [Man05, GKYY06, Pog05, Ran02]. **graph-based** [Pog05]. **graphene** [JM07, PR09, ZHS06]. **graphic** [JLZY09, ZWMZ04]. **graphical** [CLL08, LLLZ06, LLZH09, RVNP09, Ret06, SSR02, WLWZ06]. **graphically** [GS09]. **graphite** [CR06]. **graphitic** [ASH08]. **graphs** [MBM04, MBM05, MDBM05, Man05, Pal01b, PBM03, YYZ05a, YY04, ZY07, Zho07]. **Grassmann** [AG02b]. **Gray** [SST+03]. **GRECP** [IMT+02, MTB+02, TMAB01]. **GRECP/5e** [IMT+02]. **GRECP/5e-MRD-CI** [IMT+02]. **GRECP/MRD** [MTB+02, TMAB01]. **GRECP/MRD-CI** [MTB+02, TMAB01]. **green** [SWZ01, BD00, DVV05, DD05, Del03, GMK+09, IYO+04, KA05, KK02b, Mat07, MHV00, Mer04, Roh00, SEY07, SY06, TWSK09, WD01, YOM+01]. **Greenberger** [KMM+06]. **Grid** [Roy08, CTS08, MB02a, PSA05, RWW+06, SSA07, WS00, KIN09]. **Grid-** [KIN09]. **Grid-based** [Roy08]. **grids** [HR07, PW07, RH05]. **Grignard** [Iva05]. **groove** [BNHB+02]. **Gross** [GBL06]. **Ground** [BN04, CS03, CT05, Ful00, Gre09, Mar04a, SMK08, TKT+05, VD04, WRD03, AGSH09, AMGN00, AM05, AM09b, BJ00, BDBG09, BM07b, BMMC09b,

CA07, CTS08, DKM+04, DBG04, DBPG04b, ER05, FS00, GWK+05, GHT09, HS02, HGRL01, Jal02, KLI07, KB00, Li09, LXY00, MZF05, MA05, Mar07a, MBR07, MYS+09, NFP05, NSLR04, NKP+02, ONK+05, PBS02, QGW02, QGW04, SK00a, SYLE07, SI09, SH02b, ŠŠU+02, TMAB01, TPGD02, Vrb08, WTWT09, XYS+03, YCN+07, Deb08, IDM+09, LCBC03]. **Ground-** [CS03]. **Ground-state** [Ful00, Mar04a, VD04, AMGN00, AM09b, ER05, GWK+05, MA05, Mar07a, NSLR04, Vrb08, Deb08]. **ground-states** [HS02]. **Group** [TT06, YN04, ARE02, AL09, BB04, BB05d, CLL08, CBA+06, CFP00, CT00, DZ01, DAD05, DDA07, DAD08a, DAD08b, DCDW00, DWF+03, Fan01, Fan03, Fri06, HR02, HC02, JTC+03, JBMP03, Kan00a, LAL+08, LCL+09a, LZA+09, LADD00, LVSG06, MYGD01, MFA00, Muk00, OYYY02, PML09b, PV09, PSB+05, SWSH09, Sto08, Tem02b, VAS06, VTS05, WK03, YHN+07, Yar00, ZVVT07, ZMMK09, ZCZ+07, ZPW+04]. **groups** [Buc05a, CW00, CFP00, DDT+03, DLZ+03, DSW00, DSW02, ES06, Fan01, GMPIP01, GBB06, LL01, MBRA07, MWXL05, PBM03, VBT+07, XXMJ06, XLX+09b]. **Growth** [JZK02, LTL05a, LZW+07, MLL01, PBTP06, dRPFCP08]. **GSA** [DNMM06, dAMM05]. **GSO** [TYSY07]. **GSO-HF** [TYSY07]. **GTO** [RFE+00]. **guanine** [CHR+06, Els05, HFGL02, KM05b, MBOL04, MLSG04, MSS05, SMS07, XC07a, ZZZ+08]. **Guidelines** [Bar09b]. **guiding** [LCCH09b]. **Guo** [AWZD05b]. **GW** [OMY+01, Pat06, YSO+01]. **gyrase** [SDS04]. **gyrating** [OR09]. **Gyroscopic** [DETA02]. **GZT** [LCCC08].

H [AC05, AWZD05b, AL09, Ano02d, Ano02c, Ano02l, BVG05b, BPM01, BEM02, BT05, BDBG09, BFB08, BSK+02, CSG06, CBMRN08, CC00c, CT00, CMY03, Cos06, DP06, DKS05, DLTW04, DLM+02, DLM+05, DZTZ05, EBB06, FF01, GH03, GB06a, HDL00, HH05, JLAR07, Kak03, KTK+04, LSC01, LP00a, LDXW04, LWL+08, LLYJ09, LC05, LZXD05, LPZW05, LDG+06, LJL09b, LH00, LLP05, LWCF08, LH07c, MKLP02, MMS+09, MVdCD00, MNJP05, MOA07, Met05, MHP04, PILD07, RD00, RNS04, Sad02, SL07, SCRR02, SHC00, SCHW07, TI05, TSP+07a, Tem02c, Tem04, TOB02, USM01, VRA+02, VK07, XXJG04, YST+05, YW05, YWC07, YCS09, ZZFL00, ZLL+09a, ZFD00b, ZQF+02, AGBY00, AG02a, AC04, AC06, AC07, AWZD05a, ARE02, ANM03, AM06, AL09, ACB+02, BMLT07, BB05a, BM01b, BVG05a, BJ00, BCD+05, BFBB06, BAG+08, CGCS02, CA07]. **H** [CSG06, CBMRN08, CZPJ01, CT05, CSTB08, CNDÖ00, CCR09, DZ01, Dei04, Dei06, DW00, DLK00, DLM+04b, DFT+07, EMM+02a, Ess07, FFLZ02, FM02a, FOM+03, GW02, Gög06, GGS09a, GSCRO08, GBB06, Hag01, HEJ+00, HGS03, Hob02, HW02, IPPL05, IKS08, IKS10, IN09, IROW09, JFS+09, KKYT04, KM02, KKK09, KUS+03, KVF+08, KVSG02, KF03a, KSS00, LY09, LV01b, LP00a, LLYJ09, LJ03, LN03, LLL+07, LFR+08, MY08a, MGdS+08, Mar04a, MCR03, MJ00, MG08, MDG07, NF03, NWSC08, PGNT02, PR09, QTT07, QGW02, RKM09, RFRF05, RM07, SK01a, Sah03, SLB+05, SAM08, SASS03, SGP+07, SSSK07, SdACAG03, SLCW04a, SLCW04b, SST00, SHC00, SR07, SCTK+09, TLYW06, TBML06,

TFBM02, VDF+06, VHM+04, Woo02, WZWC07, Ye01, YYY+00, YPS05, ZCWZ04, ZLL+05, ZH06, ZLX+07, ZOK+05, ZWSJ01, dlPCLG+00, KCS02]. **H-** [PGNT02]. **H-bond** [Hob02, RM07, ZOK+05]. **H-bonded** [DLM+04b, HEJ+00, IKS08, IKS10, KKYT04]. **H-bonds** [GSCRO08, AG02a]. **H-cluster** [MDG07]. **H-cyclopropanaphthalene** [Ess07]. **H-doped** [SR07]. **H-Faujasite** [IPPL05]. **H-form** [LV01b]. **H-imidazole** [LY09]. **H-indole-3-acetic** [KF03a]. **H/D** [DLM+05, DFT+07]. **H3** [BMR+07, JZZ+09, JZW+09]. **H8** [HMW05]. **half** [CCV+07, JG00]. **half-reaction** [CCV+07, JG00]. **halide** [Mon08, NK05b, Pye00, RSRMBFR00, Sad00]. **halides** [DGLM09, ESU04, NK05b, Pog05, RF01, SVC+05, SRW+06, ZRRC05]. **Hall** [BS00]. **haloacids** [VDF+06]. **halogen** [Iva05, LZWY07, Nic05a, Sha07, VDF+06, WZL+07, WLZY08a]. **halogen/** [LZWY07]. **halogeno** [PBSC04]. **Hamilton** [CNC+06, NFP05, NF06, Yan06]. **Hamiltonian** [AM06, Ban02, Ban05b, Bar08, CD04, DLM+05, EBS+09, Gin05a, HN09, Irg04, Kir08, Lef06, MTRD04, MNMV02, May02a, MHB05, MB02a, MGMP01, NCB02, Oku01, Orl07, Rui05a, Sad06, SSA07, SJE03, Tap04a, TTM01a, TR09, TPGD02]. **Hamiltonian-based** [SSA07]. **Hamiltonians** [BKRT03, Dya00, FJ00, VGM05, YM05]. **Hammett** [Ess07, TC05]. **Hammond** [AT07]. **handling** [PS03b]. **hard** [CS01, GJ03]. **hardness** [ADSTS06, FCC07, JK00, KMS02, KO03, MH06, Put06, STAO00, SRK01, SSK09a, ZY06]. **hardnesses** [MRT00]. **Harmonic** [BL04a, BS08, Sch02, BVHS04, BS05a, BZG+04, BKM+02a, BLRT02, BCF03, CCLK04, DLCY+07, FGM05, GB09, HN03, HCTC07, MAS07, POM+08b, Ras04, RNCM05, SMEA08, Wyb02, YŞ02, Yam04, Yam05]. **harmonics** [ABLL02, ACCC03, HSB+00, WK06]. **Harris** [Ano09a, Ano09g, MMS+09, Mon09, SÖ09b, Tay09]. **Hartree** [ND03, QGW02, QGW04, CD03a, Cor05, DMMV00, DFH02b, DGRB08, DVM06, DBL+03, DSH01, EB04a, FFHD00, GXT02, GE09, INS+08, KC09, KCGB02, Koc00, KGA05, LV01b, LTV05, LCN05, LP09b, MMM06, MOL03, Nes05, NJD02, ND02, Pat06, PJdC00, PRL01, QC01, RP09, She07c, SGHL00, SNdAM08, TOK+00, TYY07, TOH+00, TB09, WF04, YYS+09, YONY04, YYY05, ZBPD08, dAMM05]. **HBC** [LCL+09b]. **HBCN** [LČM01]. **HBr** [HAL+02]. **HC** [MHP04, ZCWZ04]. **HCB** [LCL+09b]. **HCCF** [MNJP05]. **HCCH** [GHH03]. **HCl** [VDF+06, YW05, ZCZF02, Bol04, CSTB08, GSRL06, GSPP+06, HW02, ZL00]. **HCl.HCl** [RA04, RA03a]. **HCN** [ASO+06, AE07, BK04b, LWC+09, MY08a, SSA07, Woo02, BEM02]. **HCOOH** [PLO02, Woo02]. **HCOOH-covered** [PLO02]. **HD** [GBA05, XV00, XV01]. **HDFT** [KNS+09]. **He-H** [AGBY00]. **He-isoelectronic** [FGF06]. **He-sequence** [MZF05]. **He/H** [TFBM02]. **heating** [FCD08]. **heats** [AWZD05a, AWZD05b, EEJ04, PMLC05, SCLL07, ZXX02]. **Heavy**

[RDK97, BKLB06, GP08, Khe09, MGK+09, MST04, MST08, MKCB05, Nic05b, PMCOSC00, RDK02]. **heavy-element** [Khe09]. **heavy-metal** [GP08]. **HeH** [CNC+06, CCR09, GW04, QGW04]. **heights** [LP00a]. **Heisenberg** [CL05a, KF02, OD03, SK09, TR09]. **Heitler** [Cor05]. **HEL** [MFR07]. **helical** [JC01, LQC06, LWZ+05, SFK09]. **helicenes** [DCW03]. **helices** [HEJ+00, HOC00]. **Helium** [Lin06, AC08, CS08, CS03, DMH+05, DGG09, ER05, GBS04, GBO04, JCP+08, KH06, KH07, KH08a, LSM05, LB02, NN09, NFP05, PCBA08, PLU08, RdTdLC+07, SYLE07, SM06b, SH02b, SK03a, UBS04, Vik07, ZY04, dLCPLD+07]. **helium-like** [GBO04, SM06b, SH02b, SK03a]. **heliumlike** [SBMM03]. **helix** [BNHB+02, CHC05, HSW04]. **helixes** [KK02a, KKYT04]. **Hellmann** [Pup02]. **Helmholtz** [CD04]. **help** [PSS05]. **heme** [BML01, CCV+07, KMVR05, Loe00, NGTB06, PBB+02, SMOE02, TN09]. **hemocyanin** [TY07]. **hemoglobin** [Yur07, Yur08]. **hemoprotein** [Tor04a, Tor04b]. **Henry** [TG01]. **heparin** [dRPFCP08, SFK09]. **hepatoprotective** [PRS+09]. **hept** [CWY05, KCU09, QD04]. **hept-2-ene** [CWY05, KCU09]. **hept-6-ene** [QD04]. **heptagonal** [LR01]. **heptakis** [HY04]. **heptalenes** [FRK+05]. **heptane** [MMCC02]. **Herbert** [HW04]. **Hermite** [Fle06b]. **Hermitian** [Alc04, CDG09, May02a, Sal09, YM05]. **Herzberg** [Noo06]. **Hess** [MNR07]. **Hessian** [Bof03, KSN+09]. **Hessians** [vLvL06]. **hetero** [ARD03]. **heteroanalogues** [SBHF06]. **heteroaromatic** [DT02b, ZFD+00a]. **heteroatom** [CPR06]. **heterobimetallic** [GT07]. **heterobinuclear** [BLZ02, KFS00]. **heterocycles** [MLP08]. **heterocyclic** [KFTBS07, RS06]. **heterodimer** [Pej03]. **heterofullerenes** [RFS+00, TR00]. **heterogeneous** [MM02]. **heterojunction** [OKY+08]. **heteroleptic** [ZLL+09b]. **Heterolytic** [HGS03]. **heteromeric** [ASO+06]. **heteromolecular** [CNC+06, GKC06]. **heteronuclear** [HCTC07, Men08a]. **heterostructures** [KKS+03]. **heuristics** [RB07]. **hexaammineruthenium** [YSS08]. **hexaazaadamantane** [XXMJ06]. **hexacarbonyls** [XLX+09a]. **hexacoordinated** [IABS08]. **hexacoordination** [Pye00]. **hexacyanide** [DRD+05]. **hexadecapole** [KM02]. **hexadiene** [Sak00]. **hexagon** [KLK08]. **hexagon-bearing** [MLW+09]. **hexagonal** [EYY06, RZ07, YZ08]. **hexahydrated** [LAK09]. **hexahydro** [BABL09]. **hexahydro-1** [BABL09]. **hexasolvated** [WWTHF09]. **hexatriene** [BL02c]. **hexyne** [ABM01, CWBM06]. **hexynenitrile** [ABM02]. **HF** [Dav04, LP00a, SLWS07, VDF+06, YW05, HDL00, ASO+06, BČZ07, CJ09, CCH05, CCH06, CC02, Cor05, EP02, EB04b, FD09, HW02, Jal07b, KSS00, LBP04, LLW+05a, LLW+05b, MBOL04, MJ00, MJ06, Nak02, SL07, SEM05, TYSY07, VGB05, WZWC07, YSY+00, ZKRS07, Hob02]. **HF-LCAO-CO** [FD09]. **HF.HF** [RA04, RA03a]. **HFSO** [LLL+07]. **Hg** [ILB+08, MTB+02]. **HgH** [MTB+02]. **HgSe** [dBKS01]. **HH** [JJ02]. **HI** [SBFV05]. **HI-6** [SBFV05]. **Hidden** [DLCY+07]. **Hierarchical** [EYB02, LLR+00, GHK05, KN09b, Tem02c, Tem04]. **Hierarchy** [Nag06, CSL+02]. **High** [DMV00, GY04, HCTC07, IAMY02, Jal02, SNZG02,

SMDG09, SH02b, SSK09b, VRS01, ZH06, CS08, CC07, CMY03, CPR06, DGSD07, DLK00, DB04b, FPJR03, FYT09, GSQ+04, HLP07, JHLC09b, KKM+01, LV01a, LPV05, LS01a, LP07, LPL04, Liv02, LLP05, Luz08, MHB05, RLER04, RRGP05a, RRGP05b, SKMW00, SC02a, SC04, SM04, TSN+05, TPRVC01, TVK+02, Tou09, VATPR01, WZW+09, XXMJ06, YYK+03, Zie02, vdVM00, CS00b, YNN+06]. **high-** [RRGP05a, RRGP05b]. **high-density** [Zie02]. **high-efficiency** [GSQ+04]. **high-energy** [MHB05, XXMJ06]. **high-frequency** [LS01a]. **High-level** [GY04, IAMY02, VRS01, CMY03, vdVM00]. **high-molecular-weight** [TVK+02]. **High-order** [HCTC07, ZH06, LV01a, Luz08, TPRVC01, VATPR01]. **High-precision** [SH02b]. **high-quality** [RLER04]. **high-rank** [HLP07, LPL04]. **High-resolution** [SMDG09]. **High-spin** [DMV00, SNZG02, CC07, DLK00, JHLC09b, LP07, TSN+05, WZW+09]. **high-T** [FPJR03, YYK+03, YNN+06]. **high-temperature** [Liv02, SKMW00, SC04, Tou09, CS00b]. **high-valent** [CPR06]. **higher** [BG00b, Her07, LP00b]. **higher-order** [Her07]. **Highly** [ACM07, DBd05, LJ03, NJC02, Saf04, ZD07b, ELO+07, SM05a, XLX+09a, XLX+09b, ZD08]. **Hilbert** [CDB02, CKM09, EBS+09]. **Hilbert-Sobolev** [CDB02]. **Hiller** [AM09b]. **Hillman** [FYH09]. **hindered** [AGMK02]. **hindrance** [Lad00]. **Hiral** [LZC04b]. **Hirao** [Ano09c, Ano09d]. **Hirshfeld** [SRA09]. **histamine** [BMR+07, DKR04]. **histidine** [MPIP00, VR01]. **histone** [JZZ+09, JZW+09]. **historical** [Sti06]. **History** [Ano08a, Wen09]. **HIV** [ATF03, CFR07, FA00, GMPIP01, NPLV05, TGG01, ZZ05]. **HIV-** [FA00]. **HIV-1** [NPLV05, TGG01, ZZ05, CFR07]. **HL** [Cor05]. **HMB** [KBMM08]. **HMT** [VRFS05]. **HN** [HGS03]. **HNC** [MY08a, Woo02]. **HNCH** [BEM02]. **HNCO** [LZZ+06a]. **HNO** [LLL+07, SLB+08, Liu08]. **HNS** [YYQ+06]. **HNS/HSN** [YYQ+06]. **HOCl** [ZL00]. **HOD** [CNDÖ00]. **Hoff** [Buc08]. **Hohenberg** [SDW07, KSU04, KSU05, Kry05, Kry06, Mas02, PS03a, Pan07]. **Hole** [PML07, SP00, AVTPR09, Áng09, MLP08, OCAMOHL07, PSM07, VATPR09, YYI+08]. **hole-doped** [YYI+08]. **holes** [CP09, MB07b, PCL+03]. **homeomorphisms** [PB09]. **homo** [ASO+06, ACPG01]. **homo-** [ASO+06]. **HOMO-LUMO** [ACPG01]. **homocitrate** [CJZZ06]. **homocyclic** [CSM02]. **homogeneous** [Gál07]. **Homology** [SWST04, OMMB07]. **homomolecular** [GKC06]. **Homonuclear** [LME03]. **homopolypeptides** [BL04d, LBP04]. **HON** [SLB+08]. **HONO** [DS03]. **Honor** [AGL04a]. **Hoogsteen** [KS03a]. **hook** [DM00]. **hook-and-ladder** [DM00]. **Hooke** [LGKN04]. **Hookean** [ANM03]. **HOONO** [WF04]. **HOOO** [YLZ07]. **Hopping** [LY02, MPKB06, SSDB06, CEÖ02, KZS07, LSPS01]. **horizontal** [Mak07]. **horminone** [NVA+03]. **Horne** [KMM+06]. **horseradish** [VCHC07]. **Hosoya** [CXZ09a, XZ07]. **hosts** [ELO+07]. **Hot** [MFR07]. **Hotel** [SD03]. **HP1** [JZZ+09, JZW+09]. **HPCN** [LČM01]. **HRh** [DR08, RD00]. **HRPC** [SGLF01]. **HS** [BGG08]. **HSAB** [GD00a, MGG05]. **HSH** [VK08]. **HSN** [YYQ+06]. **HSO** [DV00]. **HT** [VED+02]. **HTSC** [SM05c, SMB09]. **Huang**

[Ano06f]. **Hubbard**
[CEK01, CEÖ02, FS00, SJE03, WK03, YYK+03, YNN+06, YYI+08, YYY05].
Hückel [Buc00a, Buc01, CD03a, Gin05a, Gin05b, Gin06, OYB+00].
Hückel-type [Gin05a]. **huge** [JMP05]. **Hulthén** [PS07]. **human**
[LYP+06, OMMB07]. **Humboldt** [VM07a]. **Hund** [MHT+08, YKK+05].
HXSiS [LSC01]. **Hy** [SH02b]. **Hybrid**
[DRPT02, HEJ+00, KZvL09, Shi04, SBF+04, TT05, TY07, YSS08, AYD00,
ATN09, ÁBL06, ALI03, AK05, BJS09, BSH04, BMP+04, CTP+08, DTT06,
EE09, FZ09, GDB03, GBP05, GSCRO08, GM02b, ISK+01, KSS+01, Oni08,
Pat06, SH02a, SNM+04, SRHR05, TT01, ZBPD08, SKK+05, SKK+06,
SKK+07, SIS+08b, TX02, NYU+08]. **hybrid-density** [ZBPD08, SIS+08b].
hybrid-DFT [Oni08, SNM+04, SKK+05, SKK+06, SKK+07, NYU+08].
Hybridization [QC00, GB05]. **hybrids** [HJSS09, RH02]. **hydantoin**
[BVS+09]. **hydratase** [NOHN02, PKZN08]. **hydrate** [TI05]. **Hydrated**
[NS02, AKK05b, JCTD08a, KKYT04, SN06a, TWSK09]. **hydration**
[AGN04, AKK05a, BSBS06, BSB07, FSR02, GdA01b, JJC+06, Pye00,
SBK+09]. **hydrazine** [DFZ05, ZFZ+08]. **hydrazoic** [XXJG03]. **hydride**
[Buc05a, Buc08, LAK09, LZT03, MBRS05]. **hydrides**
[ABBS08, OG00, OHT03, OA05, SCR01, SSF02]. **hydrocarbon** [RLB02].
hydrocarbons [AGFM03, BE07, DGSD07, DFMZO08, Gin05a, Gin05b,
Gin06, IS02, JPA03, LSPS01, TCM09, Tor02, TBCG05, WW08, WSK03].
hydrodynamic [BMB02b, BOW+01, VWB+03]. **hydrodynamical**
[Deb08, VD04]. **hydrodynamics** [BMP+04, MHI+07, MKZ04a, Mic06b].
hydroformylation [LTL05b, LTL06]. **Hydrogen**
[CSL05b, LH07a, Liu08, MCLKC02, NGRR02, NJR+09, PV09, RRD06, SL07,
SBL05a, VK05, ABBS08, Ada05, AE07, ARE02, AL09, AKK05a, ACFR05,
ACM07, AVBč06, ASO+06, ADSTS06, BK04b, BKMS03, BVHS05, BL02b,
BŠM01, BRR04, BTL+02, Bro07, Buc04, Buc05a, Buc08, BC06b, CR06,
CC00a, CS08, CK09, CCLK05, CCLK07, CC07, CS03, CL05c, CS00a, CF05,
CHS09, CTS08, CVVA08, CK06, CCR09, CPR06, Dat04, DS03, Dre05,
DFZ05, DZ06b, DM04, EHH09, EHN09, EZY00, FC05b, FC05a, FG01,
FBC+06, FG06, GZD+05, GBB06, Gup00, HSRP09, Hes02, HKY07, HT04,
HLP07, HWY+07, Iye09, JZL+08, JWZ+08, KK02a, KDŁL07, KS06, KK08,
KTK+04, KSS+08, KS03a, KM00c, LY09, LTV03, LS01a, LKG09, LLW+05a,
LLW+05b, LAL+08, LCL+09a, LZA+09, LWC+09, LLZ04, LLYL06, LLL+07,
LJL09b, MYRNYSB07, MWHZ06]. **hydrogen**
[MROA06, MGB+06, MH06, MJ00, MS09, MLP08, NN09, NF06, NK05b,
OMNN04, PSK02, PML07, QCC02, RMJ+07, RJN+08, RJF+09b, RJF+09a,
RAA05, RC05, SS09a, SBT+03, SK06, SMS+02, SBB05, SPS06, SKHY09,
SMSM02, TQC05, TS07, TSZW08, TBJ05, Var07, VPSH00, VDF+06,
VM06c, WL00, YKT+02, YZG06, Yan09, YZC09, YWC07, YSP06, YSP08,
ZYC09, ZQF+02, Sco00, TI05]. **Hydrogen-bond** [SL07, JWZ+08].
hydrogen-bonded [ABBS08, AE07, AKK05a, CL05c, DS03, Dre05, DZ06b,
EZY00, FC05b, FC05a, Iye09, JZL+08, KS03a, NK05b, PSK02, TSZW08,

VPSH00, VDF+06, YZC09, ZYC09]. **Hydrogen-bonding** [NGRR02]. **hydrogen-like** [BC06b, CF05, CHS09]. **hydrogenase** [MDG07, DMG09]. **hydrogenated** [GSfLV08, LLYJ09]. **hydrogenation** [EKN04, GP01, LZC04b, LTLS05, YLS+04, ZLC04]. **Hydrogenic** [ACC03, ACCC03, SSM05]. **hydrolase** [LVSG06, Sch04]. **hydrolysis** [BKLB06, LYDK02, ZLSL06]. **hydrolytic** [SLL06]. **hydroperoxide** [DZ06b]. **hydroperoxy** [QBTS05]. **hydrophobic** [Chu01, CRL+02, Hua04b]. **hydroxide** [GSQ+04, KVT04]. **hydroxo** [SNM+04]. **hydroxy** [RJN+08]. **hydroxyacetone** [JCTA08]. **hydroxybenzaldehyde** [EHN09]. **hydroxybenzoyl** [AKK05b]. **hydroxycarboxylate** [CJZZ06]. **hydroxycoumarin** [MGB+06]. **hydroxycoumarins** [SJM08]. **hydroxycyclohexadienyl** [HWY+07]. **hydroxyl** [DDT+03, ET01, HR02, KBUV07, ZQF+02]. **hydroxylated** [BR02, MLZS06]. **Hydroxylation** [INS+08]. **hydroxylations** [YYI+09]. **hydroxynitriles** [CQN+03]. **hydroxyphenalenone** [DKP+06]. **hydroxypropyl** [HY04]. **hydroxyquinoline** [SPS06]. **hydroxytryptophan** [ALI03]. **HyHEL** [MFR07]. **HyHEL-10** [MFR07]. **Hylleraas** [Rui05a, Rui05b, Str00]. **Hylleraas-type** [Str00]. **Hyper** [GKYY06, Kel05, QCV06, SCB+06]. **hyper-Raman** [Kel05, QCV06]. **Hyper-Wiener** [GKYY06]. **hyperbolic** [Don09]. **hyperbolic-type** [Don09]. **Hyperconjugation** [DDT+03, HvL09]. **hyperfine** [BG02b, GD00b, HEBS00, Khe09, MGK+09, TT05]. **hypericin** [EGE08]. **hyperpolarizabilities** [BB00, CK09, GG00, KCGB02, LCK00, dAMdG05, MW06a, PJ07, RPB00, Ver05, ZWJ02a]. **Hyperpolarizability** [NKN+05, GBC+02, JMP05, NOY+01, QC00, QC01, SO04a, SC02b, SHE+02, YYXC01]. **hyperquantization** [ACDV01, DCA03]. **Hyperspherical** [ABLL02, ACCC03, LB06, PRSLA08, WK06]. **hypersurface** [Pej03]. **hypersurfaces** [BBHQ04, MMF00]. **hypervirial** [AVTPR09, VTPRA08]. **hypoxanthine** [SL05c]. **hysteresis** [MB01b]. **HZSM** [MMCC02, ZMMS+00]. **HZSM-5** [MMCC02, ZMMS+00].

I-Cl [YMZH04]. **I6.46** [BNHB+02]. **IB** [ZWMZ02]. **ibuprofen** [VBS+04]. **ice** [Bol04, ZL00]. **ices** [Woo02]. **ICl** [ZT02]. **icosahedral** [CW00]. **idempotent** [Mar07a]. **identifiability** [BA06]. **identification** [MFR07, Pen00b, ZLS07, BZ06]. **identities** [Kat00]. **identity** [AM09b, Buc08, KN09a, MH05]. **idiosyncrasy** [BBD04]. **if** [Sce09]. **ignition** [MARK08]. **II** [BZL+09, BVS+09, BLZ02, BL04c, BB09, CC05a, DTT06, DRD+05, DKR04, GL00, LSK+06, MTRG04, MBA+04, MWL08, MMR+04, PBSC04, SKN+09a, SD08, TSH03, WML08, WZW+09, YSS08, YPD+07, dAGD08, ARH00, CLSD+01, DNMM06, DD05, ELF+08, GM01, HM01b, IYO+04, LSE05, NFL+02, PGN+05, Pye00, Rom08b, Rui05b, SKK+05, SBK+09, Wen02, YYK+03, YYKY01]. **II/III** [DRD+05]. **III** [AVBč06, BB09, CJB08, DRD+05, GSQ+04, GM08, KFS00, KWC09, LHL+00, MML+02, MMR+04, RVR00, ZL06, ZLL+09b, BFF04, Dav03, DDD+00, GM02a, JC00, KKS+03, SKT+07, YNN+06, ZZM09]. **illustrated**

[Ano06f, HMK05, SM07b]. **Ilya** [AGL04a, Kry08a, Ant04, Brä04a, Mar04b]. **image** [GGACT03, SKA05]. **images** [LMMB03]. **imaginary** [HV03]. **imaging** [ACHB08, DND06, Mal07]. **imidazole** [Gog05, KS06, LY09, SGP+07]. **imidazolidine** [QFC04]. **imidazoline** [CMASC01]. **imido** [CPR06]. **imino** [RJF+09a, SSB+07]. **Impact** [Boe04, CX00, LH07b, DL06, HSP+09, JR02, LK00a, PUH+08b, PUH+08a, PUH+09, SI09, UBS04, ZCZC09, WSNB00]. **imperfect** [KS04b, KSN05]. **implantation** [ZKYA04]. **Implementation** [GG00, MVKN06, TŠPJ01, ZLJ+09, BCWS09, HN03, OD03, PHK+06, YHN+07, POV+03]. **implemented** [ZT04a]. **implication** [CJZZ06]. **implications** [Del03, DAA+06, SC01, IS03, LW05]. **implicit** [Cor06, CRL+02, HM01c, NSG+06]. **implicit/explicit** [NSG+06]. **Importance** [TVK01, DST+04, EZY00, PCS09, PRM03, VTS04, DD05, DFH02a, RRPJ07, Sta00]. **Important** [Bec02, DJNH02, LLL+07, RFF05, VBML01, vdVM00]. **Imposing** [VATPR01]. **improper** [Hob02]. **Improved** [BL02a, LK02, NJD02, Shi02, CTP+08, MM07, MM09, PJdC00, Ras04, BCF03]. **Improvement** [HK09, KSS+01, LTV05, SMEA08, AKN09, YYY05]. **Improvements** [EE09, RMKS08]. **Improving** [Goo03, Har05b, Pea02, Sad06, WW08, YOGR09, SB06a, SSS02]. **impulse** [Wal04b]. **impurities** [FDME01, GM05a, LH07b, PM06a, QGM+00, SPI04, SM03, VIGL+05, VGM05, VPS+04]. **impurity** [AGMK02, BFAM03, GBMMSA00, HGB08, OBK00a, OBK00b, SV08, XBHL04]. **in-loop** [YYQ+06]. **in/photon** [Guo09]. **Inactivation** [DMG09, Lad00]. **include** [Noo06]. **included** [AS04b]. **including** [KSU04, KSU05, LJL09a, RACD00, SM05c, VMA03, LSE05]. **Inclusion** [FHK06, Hea03, DH04a, HK09, HY04, HQL09]. **incomplete** [HF09]. **Incorporation** [ZWJ02a, BLKJ00, FSR02]. **increase** [Baň05a]. **increasing** [ZWJ02b]. **increments** [PR09]. **independence** [LH05, NS04]. **independent** [BAZ05, BN04, CDI02, Col08, HT05a, JTB09, Kap02, LLZ+00, LSLD01, LSD02, Mar87a, Nes01a, Nes01b, Nes03b, QLD05, dAMM08]. **independent-electron** [Nes01a, Nes01b, Nes03b]. **independent-particle** [Mar87a]. **indeterminacies** [Dou07]. **index** [BCEG08, FM02b, FYT09, JV05, KM00b, KM03b, Pal01a, PH07, YZ08, ZY07, ZT09]. **indices** [EYY06, FCC07, IYY03, KS09, LZ05, NB05, Pog05, VHV+05, VPSH00, Zho07]. **individual** [Nag04b, RE06]. **INDO** [LCT00, BL02a, DZ01, HNKiS01, NFL+02, SRH02, BD01]. **INDO/1** [DZ01]. **INDO/S** [BL02a, HNKiS01, NFL+02, BD01, SRH02]. **INDO/S-CI** [BL02a]. **indole** [CDH05, KF03a, Pej03, VCHC07]. **indoles** [PCKC08]. **indolinone** [LQM+09]. **indolinospirobenzopyran** [Bro00]. **induced** [ABL03, BS05c, CN05, Eva04, FS05, FCLH+06, GB08, GN01, LA09, LLSY05, Lu06, LCK00, Mon08, NKK+01, PVV+04, RVR00, RPHG04, RHM05, RWW+06, Saa00, SM08, Vik07, WZWC06]. **induces** [BNHB+02]. **induction** [KK07]. **Inductive** [Tak08]. **industrial** [PKZN08]. **inelastic**

[AGBY00, BGJJ01, PSA05, ZYG00]. **inequalities** [Dav03]. **Inequivalent** [AM09b]. **inert** [MGK+09]. **Infinite** [PJS09b, BBL09, CWZ03, CEK01, DT00, IPPL05, Kan00a, KCGB02, Mar87b, MB02b, TOH+00]. **infinite-layer** [DT00]. **Infinite-order** [PJS09b]. **inflammatory** [VBS+04]. **inflection** [PC07]. **Influence** [Aze05, AdBM06, DFM+02, LTV03, MCZWD06, NWZ+07b, PK01b, PNBV07, RME+03, SAE08, TQC05, ACPG01, BSR02, CCH06, Kar04, KK07, KM04, MZMZ09, SSC+07, ZZZ+08, ZMS05, ASM+03, Sch05, YYKY01]. **Information** [NŚM02, Nal09b, AM05, Bar03, DAA+06, FM02b, JB07, KMM+07, MB05a, NY01, NB05, Nal08, Nal09a, PS07, SY07, YKT+02]. **information-entropy** [NY01]. **Infrared** [CCM+05, WSBV05, YW09, BWS+02, CMR05, Dre05, FC05b, GXT02, PGNT02, PSK02, PRL01, SVDGFC05, SKNN08, ZB05]. **InhA** [PFSFH06]. **inhibition** [DCO+08]. **inhibitor** [CFR07, GdA01b, LMDW09, MAFR08]. **inhibitors** [BBSS00, DGD+05, FA00, GMPIP01, HNR06, LSWT05, LMRT08, LQM+09, PBTP06, Pud02, RACD00]. **inhibitory** [GKSL01]. **inhomogeneous** [CL05a, Esc08, KS04b]. **initial** [LLR04, NN09, SK00a, SK01a]. **initialization** [SST+03]. **initiated** [HZW+08, XFLX+06]. **initiation** [Lad00]. **initio** [ARBC+05, AB08, AGM01, AG01a, AWZD05a, AWZD05b, AdWKG00, ASL06, ASRL06, AMC07, AV05b, AKK05a, ACB+02, ACHB08, BM01b, BN03, BBHQ04, BVHS04, BKGF02, BBD07a, BNS05, BDMS01, BZH+07, BSR02, BDBG09, BZBT01, BBG00, Bu02, Buc05b, BSK+02, BSBS06, BSB07, Čár09, CFV02, CGG05, CSL05b, CM09, CMY03, Cor04, CMASC01, DCD08, DYD03, DDD02, DBFP05, DDM00, DC06a, DBHT01, DGRB08, DETA02, DS03, DHZ06, DLK00, DZS+06, DBPG04a, DBG04, DBPG04b, DZ06a, DSW00, DSW02, ET01, ET05, ELO+07, Els05, ETBA06, FFFR01, FFFR02, FGC04a, FC05a, FG01, FFDD07, FDZ04, FYSS09, GSQ+04, GSfLV08, GH03, GY04, GXT02, Goo03, HT05b, Hea00, HAL+02, HVC08, HDL00, Hua04a, HR05a, HP07, IAMY02, Irg06, IBB08, Iva05, Iye09, JLPA09, Jal02, JJ02, JFJMR08a, JFJMR08b, JG09, KVPS05, KV07]. **initio** [KLI07, KAN+09, KCS02, KVZT04, KKS09, KFS00, KSK00, Kra00, KANK00, KS03b, LTV07, LME03, LZJ+06, LLW+07, LDR+08, LRS05, LLZ04, LTW09, LDM09, LMSB00, MGCD01, MCF09, MKCS05, MST04, MKHP09, Mar05a, MPS+02, MHT+08, MWHZ06, MC03, Mey00, MMR+08, Moh00, MRMR02, MCC08, MYS+09, NFFA04, Nak02, NAE06, NPLV05, OCK07, OA02, PRSLA08, PBS02, Pau04, PR05, PVB+03, PBMA03, PS03b, PJ07, PHNN09a, PDR+00, PRL01, Pye00, QC00, RCF02, RLBK03, RA03a, RA04, RSRMBFR00, RSFRDNA04, RM07, RRD06, Sad02, SWL04, SBF03, SBM00, SY05, SBB05, SBB06, SVDGFC05, SWC03, SGHL00, SL00, SYL05, SK05b, SHC00, SHE+02, SDZ+07, SVC+05, ŠFW00, Stu00, SKNN09, TI05, TSK01, TKY00, TYSY07, TTM07, TOB02, TNET03, UML00, USM01, VRS01, VWMS03, VVW+03, VV05, VGM05, VBS+04]. **initio** [VTS04, VTS05, VG06, VPS+04, WZL+07, WLZY08b, Woo02, XVRL04,

YKT+02, YTS+05, YZX+08, YKS+06, YNDJ06, YW05, ZT02, ZMB+03, ZB08, ZCZ00, ZD06, ZD07a, ZHA01, ZKYA04, ZJZ00, ZHS06, ZL00, ZZW+06, vdVM00, MUL02, PVB+02, LML02, YSS08]. **initio/EFP** [YSS08]. **initio/LD** [ŠFW00]. **initio/Rice** [LML02]. **Inner** [GFMT08, ZLHL02, BK04a]. **Inner-shell** [GFMT08]. **Inner-sphere** [ZLHL02]. **inorganic** [BLA00, MWW+00, SKK+06, YHF+08]. **insensitivity** [FZ09, LCH05a]. **inseparable** [McK04]. **insert** [TKY00]. **Insertion** [DR08, RD00, FG06, KB08, TLYW06, YW05]. **insertions** [NWZ+07b]. **insight** [ASL06, CDV08, MP05, SBL05a]. **insights** [Chu02, NJR+09, SHM09a, WLZY08b, CP09, PFdP08]. **insoluble** [ITR02, TIV+07]. **instabilities** [BNA03]. **instability** [DMMV00, TOH+00]. **instantaneous** [YW09]. **insulating** [Mar00c, SM06c]. **Insulator** [ML03, WK03]. **Insulator-to-metal** [ML03]. **Integer** [Gus03, GM03, JJ00, ÖO02, Özd04]. **Integral** [KAE07, Nal00b, AG02b, BSR02, Cab05, DN06, Dun01, Gri06, JJWH04, Koc00, KOT09, KFD09, Mak07, NKS+09, PCT+04, SB06b, dOEG+08]. **integral-ab** [BSR02]. **Integrals** [Gus03, Har03, HM06a, AH06, AS04c, Ave04, Bar00, Bar03, BSH04, Bud04, Čár07, Čár09, CS01, DZ01, DS07, ELF+08, FLE+06a, Fle06b, GSD+03, GM00, GM01, GM02a, GM02b, Gus02b, GM03, Gus04, GM08, Har02b, Har05a, Hog09a, JJWH04, Kir08, KSS+01, KYT+04, MR00, MNV07, ÖO02, Özd03, Özd04, ÖKAY03, ÖÖOY02, Özt04, PCT+04, PCT+05, RFE+00, RFLR00, RFE+01, RLRE04, RLER08, Rom08a, Rom08b, RSM+04b, RR00, SH00, SH01, SH02a, Saf04, SB06a, SS09b, Tal03a, Tal04, YINH00, Rui05b]. **integrated** [HT04, MK01]. **integration** [CHN09, CMNH07, GdA01b, JP01, ZH06]. **integrations** [SH09]. **integrators** [CW08]. **intense** [AM06, BL04a, HCTC07, KH05, LS01a, OMNN04, SCSWF04]. **intense-field** [LS01a]. **intensities** [MMV04, VBML04, WHKM04, ZB05]. **intensity** [IK00b, LA09]. **intensive** [BA01, BA02a]. **inter** [CR08a, YT03]. **inter-nitrogen** [YT03]. **inter-residue** [CR08a]. **interact** [RLB02, Wen09]. **interacting** [Chu07, CHMIHS+05, CN03, HVSM02, HRDM+08, Kar08, KCGB02, KT05, LME03, LSPS01, Mat07, NNNY01, NY01, NY03, NY04, Nal00a, Nes04a, SBT+03, SSDM05, WRD03]. **Interaction** [BS05c, ČAV+09, Gri08, KB08, LLL+07, MSS05, Pej02, RS00, XD03, XCC+08, Ada05, ASL06, ACB+02, BNHB+02, BGP+06, BCD+05, BL04c, BSZ07, CSL05b, CBC00, DCD08, DEN02, DG04, DGSD07, DSW00, DSW02, DWM+07, ELC08, FXHL05, FWZ09, FFFR01, FFFR02, GKC06, GZD+05, GGDL07, GFDK09, Gus04, HPC+08, HFGL02, Hog09b, HMW02, HN09, IYSS07, IN07, JCP+08, JHR+00, KPČM05, KTK+04, KK07, KS03b, LMJ00, LXD00, LZZ+07, LMDW09, Lin09, LLZ04, LE01, LP04b, Luz08, MA05, MTRG04, MMT+07, MMCC02, Mas04, MOAM07, MD02, MLP07, NKN+05, NMNB06, Nee01, NK05b, NPLV05, OM03, OA02, ONA05, Orl07, PCS09, Pan04, PPP00, QS00b, QCC02, RW04b, RFF05, RSTG02, Sad00, SKSS09a,

SLE05, SLB+05, SFK09, SASS03, SK05a, SNH00, She04a, STS+00, SČL00, TOK+00, TYY07, TKT+05]. **interaction** [TG01, TSF04, VG02, WGD01, Win04, WZWC07, YNN+06, YYKY01, YT03, YCS09, YZ07, ZMMS+00, dBM05, dlPCLG+00]. **interaction-based** [SKSS09a]. **Interaction-induced** [BS05c]. **Interactions** [AKB06, JJFdL08, Kry08a, RST08, AGM01, Bor00, BB05e, Chu01, Chu09, CHR+06, CFM+06, DFM+02, ET09, FDL03, FFS04, FD01, GSK01, GBB06, HVC08, HDWH09, HCL03, IMTG06, JWZ+08, Kap06, KFTBS07, LHL+00, LH07a, LZWY07, MKLP02, MK08, MML+02, MT04, MMZ02, NK05a, New00, OA03, PBSC04, PYZ09, PS04, PLU08, PMPI01, PML07, QCK04, RME+03, RFRF05, RWW+06, SL05a, SL07, Sal00, Sme02, SBM+05, SLWS07, TVK01, TM05, VCHC07, WLZY08a, WLZY08b, Whi02b, Whi03, XXJG03, XCS+03, YKT+02, YPS05, Yur08, ZLY05, ZZC09]. **Interatomic** [MH03, RV05, MGK+09, YI04]. **intercalated** [CWF09]. **intercalating** [KES03]. **intercalation** [HVC08, KNN+04]. **interchain** [DM03, dFGM08b]. **Interconversion** [AKB06, BF09, FC04, FFS04, Kak03, VR01]. **interdependence** [BBB02]. **interelectronic** [ANM03, Rui05b]. **interest** [ABBS08, Alc04]. **interesting** [YY04]. **Interface** [Guo09, KKS+03, DC03, MBP03, MVG+04, TT04b]. **interfaces** [MRG02, YS07]. **interference** [FL04]. **Interferometric** [Sad00]. **interfluorine** [WLZY08b]. **interlay** [LWC+09]. **interlayer** [RST08]. **Intermediate** [EBS+09, Pai00, PA02]. **intermediates** [AMO+01, BKGF02, EBB06, FGC04b, FTGH04, LZHT03, LZT03]. **intermetallic** [Mat00, MYS+09]. **Intermolecular** [Ada02, Kap06, Mas04, She04a, Zak04b, Ada05, Ada09, AG02a, BKMS03, BVHS04, Bro05, HBTW04, IMTG06, KKYT04, KK08, LXD00, MD08, NKN+05, OM03, PBSC04, PM04a, RP09, Sal00, SLWS07, Kry08a]. **Internal** [KZ08, MKDM03, NOM00, Buc00a, CSL+02, CC00b, CC01b, HQM04, KCOV07, LH07b, Mar09, Yak02, ZMS05]. **Internal-rotation** [KZ08]. **internally** [AKK05a, ACA02]. **International** [AV06, AC05, AWZD05b, Ano07a, Ano07g, Ano07e, Ano07f, BB05d, FAE+05b, GDV05, ND03, Roy05a, SCRSRE06, Tem04, Yam05, Ano02m, Ano00d, Ano06g, ERU07]. **Internationl** [Ano06f]. **internuclear** [Pen00a]. **interoperability** [ABB+07]. **interparticle** [HM06b]. **Interplay** [AG02a, OSSG07, Sap06, SZU+04, XLX+09b]. **Interplaying** [BLC09]. **Interpretation** [Gin01, CWZ03, MHT+08, NAE06]. **Interrelations** [May04]. **intersection** [Apo06]. **intersections** [EYBM03, HCZ05, LHV+09]. **Intersite** [SLE05]. **interstellar** [BEM02, BK04c, JCTD08b, LRB04]. **interval** [LCN05]. **intestinal** [FP02]. **Intra** [KK08, AG02a, KKYT04]. **intra-** [AG02a, KKYT04]. **intracule** [GBO04]. **intraline** [LHV+09]. **Intramolecular** [ABL03, ATN09, AVBč06, HWY+07, RJF+09b, RJF+09a, ZNZS00, ARD03, AD01, BRR04, BTL+02, CS00a, EHN09, HK09, Lu06, MD08, MGB+06, MY09, MDS04, OA03, RMJ+07, RJN+08, RNVTP09, RRPJ07, SBB06, Sha07, SL09, SPS06, ZZZ+08, ZZC09]. **Intrinsic**

[WT07, ZKYA04, CK04, LLSY05, RA02]. **introducing** [Oku01].
Introduction
[Ano02e, CL00b, CÖ05, Def00, Har06, Hyd06, JS08, Lag04, Nag03b, ÖS00a, ÖS00b, ÖS01a, ÖS01b, ÖS02, ÖS03, ÖS04, ÖS05a, ÖS06, ÖS07, ÖS08, ÖS09, PJM01, RÖ00, RRUE08, SW09, Tch02, Tch04a, Tch04b, Tch05, Tch06, Tch07b, Tch08, UE04, Zer00, Yam04, Yam05, Ano02a, Mic06b]. **intruder** [FHHC00, PCF05]. **intuition** [SRA09]. **invariance** [BDMC06, Tem00]. **invariant** [Alc04, BKRT03, Fra06b, HN09, MSJ04, WKS03]. **invariants** [Tem02b]. **Inverse** [Kar09, DLCY+07, LBSB08, VM06c, VSBD06, Kar10]. **Inversion** [VNB+03, GJB00, GJB02, Gri06, KZ08, TSK01, ZRRC05]. **investigated** [HH03, Muñ02]. **investigating** [JZL+08]. **Investigation** [ATF03, DCW03, DD03, DCP06, DGQT09, DDD03, FB01, FSLL04, KK07, LQC06, LPV02, MAS09, Noo06, QC02, SMVMC07, VSD+02, YI04, AEMAO06, BD07, BSR02, Bro05, BCS01, BHK09, CCA+06, CME07, DKS05, DKM+04, DV00, Den09, DR08, DDD+00, ETEA04, ET05, Elr09, GD00b, Gin03, GAR08b, GWJ05, HE05, HKE05, HZW+08, ICRS08, KMK+05, KT05, LZC04a, LW08, LDR+08, Liu08, LTL05b, ML05, MM02, MDS+09, MH09, NSS09, NGRR02, PC09, PVB+03, PJZ+09, PJ07, PLA+07, Pye00, QLJ+09, RFS+00, RRGP05a, RRGP05b, RC05, SYLE07, SOEW08, SLB+05, SAM08, SS00b, SRO02, SMM02, SM09, STW+05, TKS+05, TM05, Var07, VKIJ06, VG06, WGLX02, WLZY08a, WGX09, YLYD03, YCS09, Yur08, ZVVT07, ZDAZ03, ZRRC05, dBC06, dAGD08]. **Investigations** [CBWM09, SYZ+09, SL00, CM05c, FSLL02, GP01, Mat00, PML09a, RJF+09a, SSZ+07, SZL+09, ZFD+00a, ZZKS07]. **Involvement** [LSL+08, Sch04]. **involving** [DLM+04b, GBB06, KS06, LWC+09, MKCB05, MJ00, RT09, RFE+00, SK00a, Sal00, TOK+00, TW05b, VR01, VM06c, Woo02]. **inward** [CD03a]. **iodide** [Bro07, KG09]. **iodo** [DKP+06]. **ion** [AM07, Ano07f, BJAV08, BHK09, CT05, DCP01, FN04, FBGA04, GR07b, GMCS04, KVT04, KYA03, KY05, KNO09a, LRB04, MTRG04, MMT+07, MCLKC02, Met05, MT04, NF02, NYU+08, NBS04, Oni09, Orl02, Pye00, RHH+02, She07a, SZL+09, SBK+09, SRW+06, TFBM02, TNJL05, VIGL+05, WB05, YNN+09, YSS08, ZKYA04, ZRRC05]. **ion-C** [RHH+02]. **ion-exchanged** [BJAV08]. **ion-molecule** [LRB04]. **ion-radical** [NYU+08, YNN+09]. **ionic** [AL09, BZ06, BŠM01, CMM+07, Mar03a, MVA02, MPBM07, QCK04, SR05, SBF+04, VED+02, ZS04b]. **Ionization** [BRL02, Cou05, OMNN04, TTM01b, ZW03, AA09a, AS00, BCdP03, DZO00, FGM05, HSP+09, HWPIM01, Jal02, JMP04, LK00a, LSM05, LZZ+06b, MY08a, MY08b, MSB00, MKCB05, MB07b, MPIP+01, Nov07, PUH+08b, PUH+08a, PUH+09, PHNN09b, PMC02, SMY07, SSK09a, SC01, STL+09, SS03b, UBS04, UB05, Vik07, WZWC06, ZW04, HdMB+05]. **ionization-potential** [LSM05]. **ionized** [LA07, PGW09]. **ionizing** [Lad00]. **ionosphere** [MMV04]. **Ions** [RDK97, ANM03, AGMK02, AS00, BMŁT07, BIP+07, BCT+02, BF09, CNC+06, CJdC01, CCM08, CCR09, DEN02,

DLZ+03, DLM+05, GBO04, GAL+05, IYSS07, IOA+04, IVK00, IV02, IZ04, JNSF04, KNO09b, KBUV07, LW08, OC08, PM04b, PRM02, SMDM03, SBMM03, Sap06, SK05a, SN06a, SM05a, SSM05, SM06b, SH02b, SDTM02, TTFP04, UMDM06, VPS+04, WZW+09, ZSW+00, RDK02]. **IP** [GPW06]. **IP-EOMCCSDt** [GPW06]. **IPCM** [RKR+06]. **IPM** [FS00]. **IPR** [MDBM05, MLL00]. **Ir** [HGS03, ARBC+05, BAG+08, CWF09, CHC05, GV06, IROW09, PRM+06, PGP+07, PLA+07, SŚRL07, XXY00, ZNF05, ZOK+05, DSW08, ZLL+09b]. **iron** [CLSD+01, CC05b, NGTB06, Pud02, SE02a, SKK+05, SIS+08a, WML08, YYS+09, YYI+09]. **iron-binding** [Pud02]. **iron-containing** [NGTB06]. **iron-oxo** [SIS+08a, YYS+09, YYI+09]. **IrPt** [dlPCLG+00]. **Irreducible** [LP05b, BKRT03, CW00]. **irreps** [Tem02c, Tem02a, Tem04]. **ISBN** [Kry08a]. **ISBN-13** [Kry08a]. **Ising** [Gri06, ONK+05]. **iso** [DEN02, ZW03, YMZH04]. **iso-CH** [YMZH04]. **iso-electronic** [DEN02]. **iso-spectrum-level** [ZW03]. **isocyanate** [PXZ+09, SRW+06]. **isocyanogen** [RSKC08]. **isocytosine** [SL00]. **isodensity** [SSN01]. **isoelectronic** [AA09a, CM02a, FGF06, GE09, NJD02, SMDM03, UBS04]. **isolated** [BE07, GLHH09]. **isolation** [OMMWL02]. **isoleucine** [RKR+06]. **isomer** [CGMT03, JK00]. **isomeric** [DK04, FRT+00, FC05a, ML01, SZU+04]. **isomerism** [ZDZO07]. **Isomerization** [SLB+08, VK07, BL02c, CM09, DQZ04, FFLZ02, JCTA08, JAP+05, LSBDL02, LH03, LZW+07, ZPW+04]. **isomerizations** [SUAL04, YYQ+06]. **Isomers** [WCP+00, Bu02, CC00c, CGMT03, HGTW03, Kak03, KLK08, KSWR00, LSC01, LZXD05, LPZW05, LDG+06, MLW+09, MLL00, QXJG05, RBLS04, Rua09, SBF03, SLU+06, SUL+08, SPSS07, SMK08, TNO09, WQ00, ZDAZ03, ZLY+09, ZKRS07, SUA+04]. **isomorphous** [SAE08]. **isoniazid** [PFSFH06]. **isoorotic** [CME07]. **isopolyanions** [GYS+06]. **isoprene** [KP05]. **Isospectral** [MOPdP09, PMZGGR04, POMGM01, PRRMLB05]. **isostere** [MKCS05]. **isotherm** [Boe09]. **isothiocyanate** [ZRRC05]. **isothiocyanates** [SSB+07, ZRRC05]. **isotope** [CHC05, DFT+07, DKR04, GAR08b, IS03, WRK03]. **isotope-dependent** [DFT+07]. **isotope-labeled** [CHC05]. **isotopes** [Khe09, Mar04a]. **isotopic** [VGMN03]. **isotopomeric** [Tem02c, Tem04]. **isotopomers** [AC06, JNKMS03, XV00]. **isotypes** [RT09]. **isovalent** [MVL02]. **issues** [DL03, Del03]. **Istvan** [Ano09b]. **Italy** [RRUE08]. **iteration** [AD07, BB07, BBC07, CHS09]. **iterative** [ACT+05, JTB09, MP00, UP03, YKGC09]. **iterative-perturbative** [UP03]. **iteratively** [GH03]. **Itinerant** [Dro04]. **IV** [KWT06, GM02b, JC01, JR02, PSB+05, SKK+07, VSI+07, YYI+08, ZZM09]. **IVA** [ZCZ+07]. **IX** [GdRPLP08, Pud02, QGW04, SIT+07, YYS+09]. **IX-based** [Pud02].

Jaap [Ano06a, BvL06a]. **Jacek** [CJKK04]. **Jacobi** [CNC+06, NFP05, NF06, Yan06]. **Jahn** [PLC04, ADK02, BFAM03,

FMBM05, MP05, MB06, MdlV03, Pup05, Pup07, VX04, VIGL+05]. **Jankowski** [JS08]. **Jastrow** [UC06]. **Jerome** [Ano06f]. **Jeziorski** [Kon09]. **Jeziorski-Monkhorst** [Kon09]. **Jhon** [Ano05f]. **Jing** [Ano07g, Ano07e, Ano07f]. **Jing-Gang** [Ano07g, Ano07e, Ano07f]. **John** [Ano04e, Kry08a, ÖS05b]. **Jones** [BBD07a, HW04]. **Journal** [AV06, AC05, AWZD05b, Ano06g, Ano07a, Ano07g, Ano07e, Ano07f, BB05d, FAE+05b, ND03, Roy05a, SCRSRE06, Tem04, Yam05, Ano06f]. **Józef** [Ano02g, Ano02f, Szu02]. **Julocrotine** [MBA+08]. **July** [Ano04f, ERU07]. **jump** [Sko02]. **junction** [BP04]. **junctions** [BLA00]. **June** [ERU07, RRUE08]. **justification** [Šat03]. **JWKB** [SS04c].

K-edge [dVHB03]. **K-shell** [CS07, HSP+09, OM04, PUH+08b, PUH+08a, PUH+09]. **kagome** [YYT+04]. **Kalogiratou** [Ano06g]. **kaolinite** [CWF09, CM05b]. **Kaplan** [Kry08a]. **Karle** [Ano06f]. **Karol** [JS08]. **Kassel** [LML02]. **KCl** [VIGL+05]. **KCuF** [dD04]. **KDP** [SWL04]. **Keggin** [GYS+06]. **Kekulé** [Tor02, TDST07]. **Kellner** [GBO04]. **Kernel** [HMK05, HMK06, Ano06f]. **ketene** [Noo03]. **Keto** [AG08, LZYT01, LZHT03, LZT03, VTP09]. **Keto-enol** [AG08]. **keto-enolate** [VTP09]. **ketone** [LXTT00, RRNG05]. **ketones** [LXH+00, LXTT00, LXHT00, VKIJ06]. **keV** [QDÖ09]. **key** [FTGH04, KM00c, PGW09]. **Kick** [BvRSS07]. **kicked** [GB09]. **Kimihiko** [Ano09c, Ano09d]. **kinase** [YZX+08]. **kinases** [HH03, LMDW09]. **kinematic** [ABLL02]. **Kinetic** [WRK03, APN02, Baň05a, CTSÖD03, CSA09, GC05, HM03, HMMT04, IS03, LKE03, NM01, Nal00b, Oku01, Rom08a, Rom08b, SL05b, TW02, TKJ09, ZL04]. **kinetic-** [TW02]. **kinetic-energy** [Oku01]. **Kinetics** [CHR+06, LCCC08, Esc08, Fra06b, MPKB06, MCC08, Muñ02, RME+03, TWZW09, TGGV+04, VHV+05, ZFZ+08]. **kinks** [KG02]. **Kirchhoff** [BCEG08, Pal01a, YZ08, ZY07, ZT09]. **Klaus** [Ano00e, Zer00]. **Klein** [Sko02]. **KMgF** [AGLBM03, LMSB00]. **known** [LAS+07]. **Kohn** [MNR07, SDW07, AK05, BZ06, BGN+05, CW04, DKM+04, EJ06, FJ00, FCC07, GSB00, KSG03, KSU04, KSU05, Kry05, Kry06, KDY+02, LSM05, Mas02, MH06, Nal00b, Nes04a, PS03a, Pan07, PL00, QS00a, QS00b, RJ08, SG03, SL05b, SFZO01, TKJ09]. **Kolmogorov** [CMS04]. **Koopman** [ASDC08]. **Kr** [LZJ+06, LAQ+09, WZJ04, ZZHL08, MM07, MM09, NRJD03, PRSLA08]. **Kramers** [PML09b]. **Kratzer** [BBC07, Mat02a, SD06, YAŞ00, YŞ02, Yal04]. **Kratzer-type** [YŞ02, Yal04]. **KRb** [KYA03, KY05]. **Kringle** [DSFS00]. **Kroll** [MNR07]. **Kronig** [AC02b]. **Kryachko** [Har01]. **Kutta** [HW06]. **KvAP** [TRMM04]. **Kwiatkowski** [Ano02g, Ano02f, Szu02]. **KZnF** [LMSB00].

L [AC05, AWZD05b, JNKMS03, WML08, DCD08, FGR+07, HEJ+00, JNKMS03, MRMR02, OCWY09, PVW03a, RKR+06]. **L-** [PVW03a]. **L-Ala** [HEJ+00]. **L-Alanyl-L-Alanine** [JNKMS03]. **L-ascorbic** [MRMR02].

L-cysteine [DCD08]. **L-methionine** [DCD08]. **La-doped** [ES02]. **labeled** [CHC05]. **labels** [Tem02b]. **lactam** [PIGN02]. **lactamases** [ERC+02]. **lactones** [PRS+09]. **lactonitrile** [RC05]. **Ladder** [DL02, DLF02, Pla01, SD06, CEÖ02, CCEÖ06, DM00, MYRNYSB07]. **LaF** [MTWN09]. **Lagrangian** [GTR+05, SRHÖ06]. **Laguerre** [FDM09]. **Lamda** [Kar04]. **LaMnO** [UES04]. **Lanczos** [Fis00, WC04]. **Landau** [OR09, PSCLGN07, ZZL04]. **landscapes** [GHK05, LTL04]. **language** [Luc02, SB06b]. **languages** [HWR05]. **LaNi** [MAS09]. **lanosterol** [CVPGH+06]. **lanthanide** [BL02a, NRK+05, WTWT09]. **lanthanum** [SM09]. **LaOMPn** [YYI+08]. **Laplacian** [PBM03]. **Large** [GI07, dAMdG05, MVLM05, Ban02, Ban05b, BML01, BCWS09, BZG+02, BZG+04, CC05c, Col08, DJNH02, KCOV07, MWXL05, Nes03a, SK01b, SK05b, YKGC09, SBM00]. **large-** [Ban02]. **large-dimensional** [SK01b]. **Large-ring** [GI07]. **Large-scale** [MVLM05, BZG+04, SK05b, YKGC09]. **Laser** [NIS+05, TSS+09, UKAM04, BL04a, Bec02, FGM05, GMCS04, GLHH09, HCTC07, KK04, KLB+05, LA09, Mal05b, MYH03, NWSC08, OMNN04, Saa00, SSA07, SKA05, SCSWF04, Vik07, WZWC06]. **laser-** [Saa00]. **Laser-assisted** [UKAM04, NWSC08]. **laser-electron-nuclear** [GMCS04]. **laser-induced** [LA09, Vik07]. **laterally** [SPN03]. **Latin** [Ano08c, Ano08a]. **LaTiO** [Oni07]. **Lattice** [JM07, Baň05a, CT00, GBJM01, IPPL05, JFC02, KF03b, MAS09, OBK00a, OBK00b, PTS03, SPI04, Tem00, VRC04, WK03, YYT+04, ZZL04, ZZL05]. **lattice-point** [CT00, Tem00]. **lattices** [CEK01, Kan00b, OB02, TT05, TSN+05, Tem02c, Tem04, VPS+05]. **laws** [BK03, Her06]. **layer** [DT00]. **layered** [Mar09]. **layers** [RPHG04, Wal04a]. **laying** [AAKAF07]. **LCAO** [FD09, CS04, DC06a, ESTU05, Obe00, Tal03b]. **LCGTO** [BR00, BR05]. **LCGTO-FF** [BR05]. **LD** [ŠFW00]. **LDA** [BSN05, LBP04]. **lead** [GP08, KG09]. **leading** [HM01b, LRB04, Nov07, TBML06]. **leads** [SDZ+07]. **leaky** [Har01, Kry00, PHH08, Tem09]. **learnt** [PPP+08]. **leaving** [LVSG06]. **Leffler** [AE04, SEY07, SEY09]. **Left** [MCH02, PGW09]. **Left-eigenstate** [PGW09]. **leg** [CCEÖ06]. **Legendre** [CSA09, NM01]. **Leishmania** [CBRBT03]. **Leland** [Ano03a, BH03]. **Length** [MKHP09, BLC09, CWZ03, KDŁL07, KIK09, PK01b, SC02b, YYZ05a, dBC06, dFGM08a]. **Length-dependence** [MKHP09]. **Lennard** [BBD07a]. **Lennard-Jones** [BBD07a]. **Lenz** [OB02]. **less** [YKK+05]. **Letter** [Bad03]. **leucine** [GSK01]. **level** [Apo06, CMY03, DFH02b, GH03, GY04, Gri08, IAMY02, Jal02, KN09b, KGA05, LV01b, MC06b, SM03, VRS01, ZW03, vdVM00]. **levels** [BJ00, BCS01, CNC+06, IV02, Kar04, MZD01, NF06, SSDM05, YSP06, ZWMZ02, ZD07b]. **levulinic** [VRC04]. **Lewis** [HSRP09, NRS+02, ZVVT07, ZSKV04]. **LFDFT** [ARBD05]. **Li** [BMMC09a, FF09, QV01, SKA05, SSZ+07, SCHW07, YWC07, YCS09, ASL06, BE07, BES08, BPŠB00, BMMC09a, BMMC09b, CGL+05, FPC05, Gög06, Hag01, HL05, MA05, Mar04a, PC09, Pen00a, PRM02, RSFRB03,

SLB+05, SLWS07, WB05, WCP+00, ZWSJ01]. **library** [Bee09, TŠPJ04]. **LiCCH** [GS00a]. **lie** [ZYG00, GYM+02, MZD01, MYGD01, RGMP06, YHD00, YYHD01, ZGY+03]. **Lieb** [Lam07, OC08]. **life** [Chu08]. **lifetime** [VNB+03]. **lifetimes** [VBML04]. **Ligand** [CLA+02, BL02a, CJZZ06, CFM+06, ERC+02, ITY+09, KWWQ04, LTL05b, MMV05a, MOA02, MMZ02, NSZZ04, NSG+06, Pet00, SDS04, SLS+05, TY07, VMA03]. **ligands** [DC06b, JHR+00, KSS+08, MOAB01, SGP+07, TSH03, YPD+07]. **ligated** [KN08]. **Light** [HOIK09, BK03, CN05, Mar04a, MDS04, Por01, SKA05, SSF02, VSBD06, ZRF+09]. **light-emitting** [BK03, ZRF+09]. **light-induced** [CN05]. **light-scattering** [VSBD06]. **lignin** [Bar09b]. **LiH** [CNC+06, GW02, Gög06, MA05, QGW02]. **like** [BES04, BC06b, CCM08, CF05, CHS09, DLM+02, Esc08, FGR+07, GBO04, GAL+05, GKE01, HNR06, HMB+04, LR01, PNN08, RVNP09, RdTdLC+07, SI09, SM06b, SH02b, SK03a, SM06c, UES04, WT07, YYYM01, ZW03, ZW04]. **limit** [Ban02, Ban05b, GB06b, KL00, LFK06, SJE03, SK01b]. **limitations** [FS00]. **limited** [HMW02]. **limiting** [NTB02]. **limits** [LM02a, Sei03, JKU02]. **line** [IROW09, Tou09]. **Linear** [ACPG01, Dav03, JMP05, MNR07, ZCWZ04, AG08, ASO+01, ASO+04, Boe03, BRZ09, CWZ03, CZ03, CCM+05, DGSD07, DWF+03, DHZ06, FHK06, GDFT01, GWK+05, HJSS09, JC00, KN09b, KFS00, KGI+05, LP08, Man05, MARK08, MBK01, MEN+08b, MW05, MHP04, NS04, Nes02a, ND02, ND03, PS03b, TA06, VH00, Var07, VV05, VSBD06, WSBV05, WSC+05, YZ08, ZLL+09a, ZBPD08]. **linear-** [FHK06]. **linear-scaling** [KN09b]. **Linearized** [DKW09, Nes03a]. **lines** [MGK+09, ZD08]. **lineshapes** [Sad00]. **Link** [TW02, Swa03]. **linkage** [WQ00]. **linkages** [PML09c]. **linked** [Buc02a, YYYM01]. **Linking** [VGM05, Buc00a, KCU09]. **Liouville** [BG00a, DM02b]. **Liouvillian** [BG02a, Tem02b]. **lipid** [SKNN08, SKNN09]. **lipoproteins** [KPP01]. **liquid** [CHC05, DGD+05, FGdA00, FGdA02, IKL04, KS07, LPL04, LMX+05, MC03, PMLC05, TL05, ZDQF08]. **liquids** [HM05a]. **List** [Ano00f, Ano00g, Ano00h, Ano00i, Ano00j, Ano01e, Ano01f, Ano01g, Ano01h, Ano01i, Ano02h, Ano02j, Ano02i, Ano03b, Ano03c, Ano03d, Ano04a, Ano04b, Ano04c, Ano04d, Ano05b, Ano05c, Ano05e, Ano05d, Ano06b, Ano06c, Ano06d, Ano06e, Ano07b, Ano07c, Ano07d, Ano08b, Ano09a, Ano09e, Ano09f, Ano02d, Ano04f, Ano02b, Ano02f, Ano06a, Ano07i, Ano09b, Ano09d]. **Literate** [QW05]. **Lithium** [BES08, AGSH09, BNA03, BL02b, CGG05, CC07, FFLZ02, GHT09, KNO09a, LCL+09a, NWZ+07b, Oni09, PMB08, Pye00, SRW+06, ZSW+00, ZRRC05]. **lithium-chlorosilylenoid** [FFLZ02]. **lithiumlike** [ZSW+00]. **living** [Lad06]. **LiX** [Ano07f, GR07b]. **LMP2** [KKMS04, RFRF05]. **Ln** [KWC09]. **Loc.3** [FCS03]. **Local** [APN02, ESTU05, JMP04, Mat00, MKZ04a, MGG05, ML01, Nes01b, PREM05, VPSH00, YKS+06, AFC03, AIG02, BGP+07, EP02, FGZ07, GD00a, Gin01, HJSS09, HWPIM01, LKE03, LGKN04, Mar07b, MET00, MPIP+01, OD03, PRCEM06, PMC02, POV+03, SAM08, SPI04,

SGLF01, SS09c, STS+00, TT02, TT06, VRA+02, BTK+05]. **local-scaling** [LKE03, LGKN04]. **local-spin-density** [STS+00]. **localizability** [Koh04, KWG06]. **Localization** [LK00b, AA04a, Áng09, BCN04, BL02b, CC07, MC00, MF03, PPP+08, PS02, Put05, SS00b]. **localize** [MHGR07]. **Localized** [AK05, Gin05b, Jal08b, PREM04, Whi03, DVHJ03, OBK00a, OBK00b, PA08, SS00a, SS00b, SWC03, SBF+04, TTM01b]. **Locally** [HJSS09]. **lock** [KM00c, VED+02]. **Loew** [Ano02d, Ano02c, Ano02l]. **Logarithmic** [BB02a, BB05b]. **logic** [Nég03b]. **logical** [LS08, SY07]. **London** [Cor05]. **Long** [JC01, LLW+05a, LLW+05b, QCK04, Var08, HLO04, OA02, SWSH09, SBM+05, Stu00, TGGS06, YJ00]. **long-distance** [Stu00]. **Long-range** [JC01, LLW+05a, LLW+05b, QCK04, Var08, SWSH09, SBM+05, TGGS06, YJ00]. **long-time** [HLO04]. **Longitudinal** [MNJP05, ZWJ02b]. **look** [HH09, SFR08, TS01a]. **Looking** [XXMJ06]. **loop** [CSWD06, SDS04, YYQ+06, MB01b]. **loops** [MB01b]. **Lorentz** [Pet04]. **loss** [BF09, DAA+06]. **losses** [Por01]. **Lou** [Ano06f]. **Low** [DKP+06, KKYT04, KV05, RSKC08, SKN09b, SBKSS05, AAKAF07, AZD06, BDA+02, BLM08, Gre09, KYA03, LA09, LAS+07, LB02, NRJD03, PCBA08, SK00a, SK01a, Sah03, SKA05, TA02, WW08, dD04, RBLS04]. **low-dimensional** [TA02, dD04]. **Low-energy** [SBKSS05, BLM08, SK00a, RBLS04]. **Low-frequency** [KKYT04]. **low-intensity** [LA09]. **low-laying** [AAKAF07]. **Low-lying** [KV05, RSKC08, SKN09b, AZD06, BDA+02, Gre09, KYA03, NRJD03, PCBA08, WW08]. **low-Rydberg** [SK00a]. **Low-temperature** [DKP+06, LB02]. **Löwdin** [AK02, Ano02k, BS06, BDMC06, CD04, HM01a, HM01b, Kry02, May02a, May02b, NS04, ÖSB01, Sut02]. **Lower** [MSB00, Mar05c, AC02a, MB07a, Mar07b, PRNM03]. **lower-lying** [PRNM03]. **lowering** [OdSC05]. **lowest** [BDA+02, BDBG09, BBPG08, DBPG04b, HAL+02, LSM05]. **LSDA** [TN03]. **Ltd** [Kry08a]. **Lu** [HDL00]. **LuA** [JLAR07]. **Lulu** [Ano06f]. **luminescence** [FJT+05, RSDNSB00]. **Luminescent** [TKS+05]. **LUMO** [ACPG01]. **lying** [AZD06, BDA+02, Gre09, KV05, KYA03, NRJD03, PCBA08, PRNM03, RSKC08, SKN09b, WW08]. **lysine** [JZZ+09]. **lysozyme** [MFR07].

M

[BB05d, CZPJ01, Deb08, GT07, HGS03, HDL00, JLAR07, MOAM07, PSN08, PFSFH06, RRGP05a, SZJ+04, Tem02c, Tem04, VGMN03, XD03, XYS+03, YS05, YCS09, ZZFL00, ZLHL02, ZJZ00, ZL04, YZC09, BB04, BG00c, DCW03, DLM+04a, HDL00, MOAM07, POAVdlM08, PSN08, SZJ+04, Tem02c, Tem04, YI04, YPS05, ZZFL00, ZLHL02, ZJZ00, ZFD00b, ZWSJ01]. **M-C** [ZFD00b]. **m-form** [YZC09]. **M3** [OMMB07]. **MacM** [MOA02]. **MacMCN** [MOA02]. **macroconfiguration** [KH05]. **Macroconfigurations** [KSH04]. **Macromolecular** [VSBD06, SEM05]. **macromolecules** [LA07]. **macroscopic** [AGL04a]. **made** [GM05b]. **Madelung** [AK02, Sce09]. **magic** [BKM+02a, KR07]. **magnesium**

[CMM+07, KD05, MMR+04, OHT03, Pet00, PFSP05]. **magnet** [BP03]. **Magnetic** [AGMK02, MT04, MABB06, YL02, ZLY05, AM06, Aze02, BL04a, BB05c, BT05, BL04c, BG00c, BS05c, CC01a, CLSD+01, DM02a, DT00, Deb08, Den09, DVM06, Dya00, GM03, HC02, HCL03, HLH05, JP08, JTH02, Kar04, KKM+01, KTK+04, KBV05, KYT+04, KSU04, KSU05, KSN+04, KFS00, KZvL09, LDMR01, MKDM03, ONK+00, OCWY09, OB02, OR07, Oni07, PBMA03, PHNN09a, PGW08, RIVB03, RWW+06, SPN03, SPL03, TY07, VSD+02, VD04, WZW+09, YNY01, YHC05, ZL06, dGS06, dD04]. **Magnetic-field** [YL02]. **Magnetically** [OMC04]. **Magnetism** [BC03, CIP+03, KM01, KSU04, KSU05, MBP03, Mat00, MC08, Nag04a, She07b, YYS+00, YYKY01, YYT+04]. **Magnetizability** [RVP09]. **magnetization** [BJS09, LNSE02, Mar09]. **magneto** [KK04]. **magneto-optical** [KK04]. **Magnetoresistance** [OB02]. **magnetostructural** [BLZ02]. **Magnitude** [Her07]. **Magnus** [LD05]. **Maillard** [JRSA08]. **main** [BFRB07, LGBJ03, ZMMK09, DZ01]. **mainly** [SLWS07]. **major** [CCR09]. **maleamic** [CI06]. **maleic** [XFLX+06]. **maleimide** [HBW+08]. **malonaldehyde** [Shi04, WKF+06]. **malonic** [JZL+08]. **manganese** [ISK+01, KSN+04, NWZ+07b, Oni09, RSTG02, XLX+09a, YUN+07, dVHB03]. **manganese-oxo** [KSN+04]. **manganese-oxygen** [ISK+01]. **manganites** [SSDB06]. **manifestations** [Duf07, SGGBB02]. **manifestly** [NU09]. **manifold** [SI09]. **manifolds** [CS00b, Fra06b, Sco00, SC02a, SC04]. **manipulating** [BDE+07, SHM+09b, ZR03]. **manipulation** [YL02]. **Many** [Ave04, DGC08, EWCT+05, HM03, Kat00, PMHW07, RAA05, SL05a, AP03, BA01, BA02a, BG02a, CL05d, DFM+02, IAL06, IZ04, Kry05, Kut09, LH07a, Lin06, LSH08, LP05b, MNMV02, MT02, Muk00, Nag04a, NF03, RFCG09, Ret06, Roy08, Rui05a, Rui05b, SSR02, SH09, SKHY09, SDW07, YYK+03, ZT02, ZSM+01, MRG02]. **many-atom** [MT02]. **many-band** [Nag04a, YYK+03]. **Many-body** [EWCT+05, PMHW07, RAA05, SL05a, BA01, BA02a, BG02a, CL05d, DFM+02, IZ04, Kut09, LH07a, NF03, RFCG09, SH09, SKHY09, ZT02, MRG02]. **many-body-QED** [Lin06, LSH08]. **Many-center** [Ave04]. **Many-electron** [DGC08, AP03, Kry05, LP05b, MNMV02, Muk00, Ret06, Roy08, Rui05a, Rui05b, SSR02, SDW07]. **Many-fermion** [HM03]. **Many-particle** [Kat00, IAL06]. **many-valence** [ZSM+01]. **map** [LBAB02]. **Maple** [VAS06]. **Maple-assisted** [VAS06]. **mapped** [CTS08]. **mapping** [TG05]. **mappings** [Tem02b]. **maps** [Ran02]. **Marcel** [Ano07a]. **March** [Ano04e, NM01]. **March-Murray** [NM01]. **marching** [Esc08]. **Marcus** [LML02]. **marginally** [BLC09]. **Märk** [HSP+09]. **Markovian** [Put05, Sko02, Tou09]. **MaSK** [PL09]. **masked** [Pri05]. **mass** [ENGY+07, Ghe09, MB05b, MSJ04, MOPdP09, POM+07, POM+08b, SHZGP09, Sco00, SMT06]. **mass-nonsymmetric** [Ghe09]. **mass-spacetime** [Sco00]. **Massa** [Ano06f]. **Master** [RFE+00]. **matching** [YYZ05a, ZT09, Zno00]. **matchings** [YYZ05b]. **material** [GSQ+04, Mar09, Sta00]. **materials** [BD07, CN00,

DLM+02, DLM+05, FVPM05, Gup00, JMEM07, KTH+05, KNO09b, LCCH09b, PMBM09, Sme02, SBF+04, SM09, STS+00, Yar00, ZCZC09]. **math** [Bee09]. **Mathematical** [Bar06, Gar08a, Har06, NU09, VCF+00, Živ09]. **mathematicians** [Wen09]. **Mathieu** [EYB02]. **matrices** [Alc04, AV05a, AV06, Brä09b, CD00, CD04, Col01, Dav03, GS09, GTR+05, Har02c, HH02, LP05b, MHV00, PRG+04, TR09, VATPR01, VTA+02, VATPR09]. **Matrix** [Luz08, OMMWL02, AZ08, AG01b, AE02, BKL+02, BM01b, BDG01, Bof03, Cab05, CD03a, DCDW00, Gin05a, Gin05b, GKYY06, HZPY03, Har05c, HYC+00, Her07, HMB+04, HSB+00, ILVMSB+02, ILVMSB+03, Jal08c, KMN05, Kýv09, MKHP09, Mar07a, May02a, Mic00, MT02, Mic06a, OYYY02, PW09, PO03, RLBK03, RE06, RW04a, SCM00, SGLF01, SEY07, SRS+04, SSDB06, TT05, TTM07, TBJ05, TCM01, VAT03, Wei08, YNY01, ZT08, Zie02, ZT04b, QGW04]. **Matrix-covariant** [Luz08]. **matter** [Mic09]. **Matthias** [Ano07a]. **maxima** [Koh01]. **maximal** [RZ07]. **maximally** [KMK+05, SWC03]. **Maximum** [ZT08, BBB02, JK00, JHLC09a, YYZ05b, ZY06]. **maximum-spin** [JHLC09a]. **Maxwell** [GN01, HW06, Pet04]. **Maya** [FPC+08]. **Mayer** [Ano09b]. **MBPT** [Kut09]. **MCD** [FRK+05]. **MCDF** [CM05c]. **McMurchie** [KOT09]. **MCSCF** [DQZ04, GGDL07, GFDK09, MY08a, OY01, SFPA03]. **MCSTEP** [MY08a, MY08b]. **MCWF** [NY03]. **MD** [TI05, TŠPJ01, ZDQF08]. **Me** [AZD06, LH07c, WML08, HGRL01, LTV02, WML08]. **Me-DAB** [AZD06]. **Mean** [WAJ04b, DLM+04b, Por02, WAJ04a]. **Mean-field** [WAJ04b, WAJ04a]. **means** [BZ06, CCV+07, CTS08, Fis00, RdSH08, SFD09]. **measurable** [HH05]. **measure** [AT00, Koh04, RJB+06]. **measured** [WRRF03]. **measurement** [FT04, MYS+09]. **measurements** [DCP06, PRM02, Por02, Por04]. **measures** [CDG05, LZ05, PS07, RCD00, SFD09]. **meccanos** [Tap04a]. **mechanical** [BPM01, BDA+02, BNS05, BČ02, CCM+05, CW08, CTP+08, CHR+06, DDD+00, DK04, EEJ04, FPC+08, GB05, GAIK04, HEJ+00, HBKG03, Kap02, Mar00a, Mar00b, MHV00, MRMR02, Muñ02, NSG+06, PSK02, Pol06, RLB02, SRO02, Sta00, TT01, XXY00, Yam04, Yam05, ZZ05]. **mechanical/molecular** [CTP+08, TT01]. **mechanics** [Bad03, BOW+01, Buc05b, CSSB02, CK04, DK03, DRPT02, DCA03, DSW02, EGEDH03, Fer02, GYM+02, HM05a, ILVMSB+02, MTRD04, NU09, Roy05a, Roy05b, TT04a, TT04b, TTM07, TT02, UC00, WRD03, Zak04a, Zak04b, dHG04, ILVMSB+03]. **Mechanism** [HSRP09, HH03, KVSG02, KTN02, LTLS05, NH00, ZDMF08, Baň05a, BZH+07, Bro00, Bro05, CY04, CWY05, DDW+06, FYT09, Har02a, HBW+08, HZW+08, JFS+09, JHR+00, KCU09, KVT04, Kry02, KB08, LWW+02, LDXW04, LDZ+05, LZZ+06a, LQM+09, LLSY05, LTL05a, LXXC08, LYCX08, LWCF08, LTL06, MC00, MS03, MLL01, PXZ+09, PMBM09, RT06, Sha06, SWZ01, Sok04, STW+05, SHH+06, TSP+07a, TFBM02, TWZW09, VK08, VED+02, VLK+08, WGLX02, WGX09, XFLX+06, XCW07, YMZH04,

YYZ+05c, ZD06, ZZDY06, ZFD00b, ZRRC05, BDMS03]. **Mechanisms** [ZFZ+08, AG01a, HGS03, KV07, LCH05b, LYWX07, Sak02, TW08, TFS+02, VR01, YYK+03, YYS+09, YYI+09, ZTW+09, ZZW+06]. **Mechanistic** [SAM08, KZG09, SRW+06, Tch07a, ZLH+08, GSPP+06]. **MeCl** [HGRL01]. **MEDF** [KYT+04]. **media** [Chr01, KM06, TMS08, USM01]. **mediated** [JPA07, SLL06]. **medium** [Irg06, IROW09, JCTD08b, LRB04, Mic00, MY00]. **meet** [Mat00]. **megazol** [RAdS05]. **megazol-derived** [RAdS05]. **melamine** [VRC04]. **melting** [PCS09]. **member** [MSMS03]. **membered** [Buc00a, Buc02b, Buc05c, CLL04, FS00, LZHT03, RS06, RLNA02, WSK03, XVRL04]. **members** [Ano00d]. **membrane** [PD05, TS01b, Wal04b]. **memoir** [Tay09]. **Memorial** [Har09]. **Memory** [Mai05, And05, BvL06a, HW04, ÖS05b]. **MEP** [GSRL06]. **Mercury** [KG08]. **merocyanine** [MUL02, BD01]. **meshes** [LB03]. **meso** [Cor06]. **mesoionic** [FH02a]. **mesoscopic** [BS05c, JPMM08, XR05]. **meta** [JSC01, MGV00, PT06, RB07]. **meta-chloroaniline** [MGV00]. **meta-GGA** [PT06]. **meta-heuristics** [RB07]. **metabolic** [ABD06]. **Metabolism** [DKD+07]. **metabolites** [KES03, LZZ+07, eSPM+08]. **Metal** [WK03, ABL03, ASL06, ACF04, ACF05, BL04b, BT05, BKM+02a, BB04, BB05d, BB05e, BCT+02, BG00c, CJZZ06, CL07a, CL07b, DRPT02, DLM+05, DKR04, DSW08, EM05, ERC+02, FTB04, FSGB05, FF09, FV04, FBGA04, FPJR03, GKL+09, GP08, HSS09, HSN+09, HDL00, HRDM+08, IOA+04, ITY+09, JJFdL08, JKU02, JPA03, KK04, KBV05, KDC09, KM01, KSN+04, KBUV07, LTV02, LH07b, ML03, MSMS03, MMZ02, MABB06, NNS+00, Nee01, OD03, OCWY09, OKY+08, OG00, PML09a, Pej02, PMCOSC00, PSH00, QS05, RWW+06, RH03, Saa00, SK05a, SM07a, SH07, SSK09b, TTM01a, TB03, VMA03, XBHL04, XLX+09a, XLX+09b, YWC07, Yur07, ZL06, ZKEE07]. **metal-binding** [RH03]. **metal-bound** [CJZZ06]. **metal-encapsulated** [JJFdL08]. **metal-organic** [RWW+06]. **metal-oxo** [KSN+04]. **metal-substituted** [ERC+02, SSK09b]. **metal/rare** [KBV05]. **metallic** [FGFF06, GGACT03, KOH03, RL04, TOH+00]. **metalloenzyme** [Kra00, Whi02a]. **metalloenzymes** [SNM+04, SKK+05, SKK+06, SIT+07, SKT+07, SKK+07, SIS+08b, SIS+08a, YYI+09]. **metalloglutathione** [Kra00]. **metalloid** [FDME01]. **Metallomacrocycle** [MOA02]. **metallophilic** [MROA06]. **metallophthalocyanines** [ZCZ+07]. **metalloproteins** [RH03]. **metals** [AFC03, EGEDH03, FA05, FDME01, GKL+09, HKR09, KKM+01, MMR+08, Pyy01, WSNB00, ZW09a]. **Metastability** [AV02]. **Metastable** [BGGS08, GL00, BDMS03]. **metathesis** [Han07, ZCZF02]. **methacrolein** [SZML07]. **methacryloyl** [HHGSRS02]. **Methane** [TGSK09, HGS03, HKMM04, HMB+04, LWW+02]. **methane-like** [HMB+04]. **methanes** [ET01]. **methanol** [AGFM03, FYH09, FC05b, FC05a, FDZ04, NH00, SKT05, TL05, VSI+07, VLK+08]. **methionine** [DCD08]. **Method** [HW02, Obe00, AD07, ASDC08, Ano06f, AS00, BKM+09, BL02a, BB07, BBC07, BP04, Bol04, BKM+02a, BOW+01, CdMCS05, CDS06, CD03a,

CCL03, ÇKB02, CK09, CSL05b, CL07a, CB03, CF04, CHS09, CTS08, Cor05, CS04, DSFS00, DRPT02, DTT06, DNMM06, DMH+05, DNN+06, DKM+04, DFH02b, DES03, DDD03, EE09, EBS+09, EZ05, Esc08, Eye00, FDL03, Fer01, Fer09, FSLL04, Flo08, FFHD00, Fuk09, GH03, GS09, GGLS02, GG07, GMK+09, GMS01b, GMS01a, GdA01b, GM00, GM01, HdMB+05, HV03, Han07, HYC+00, HTN07, HMK05, HMK06, ITN09, IYO+04, IAL06, JKU02, JZZ+08, JJ00, KKYT04, KS00, KSK+04, KMM+07, KH01, Kir08, KSS+01, KYT+04, KSI+07, KSN+09, KGI+05, KGA05, KNO09b, KNO09a, KV08, KZ09, KDY+02, KFTBS07, LCN05, LMJ00, LP00b, LP04a, LP09a]. **method** [LLLZ07, LD05, LLP05, LE01, MY08a, MY08b, MR00, MMM06, MBA+04, MVK00, May02b, Mei08, MYGD01, MB02a, Mor06, MVKN06, MPBM07, NF03, Nes03a, NJD02, ND02, ND03, OD03, OMY+01, OOK03, OCAMOHL07, Özt04, PR09, PSH00, PW07, PGW08, PJdC00, PČH02, PGPA09, PRBGLL04, PA04b, QC01, RVP09, RGMP06, Rui05a, Rui05b, RB06, SH00, SSA07, SMY07, SAR08, SFK09, SGLF01, SS04c, SNY01, Shi05, SMDG09, SNdAM08, SSK09b, SČL00, SEM05, SBBL05, SMK08, TMPI05, TNJL05, TGG01, UT03, UP03, VAT03, WGLX02, WLWZ06, Wei03, YM05, YPS05, ZXX02, ZWMZ04, ZYG00, ZWMZ02, ZLJ+09, ZS04b, Zno00, dAMM05, dAMM08, dOEG+08, KN08]. **Method/basis** [HW02]. **methodologies** [CCV+07, UML00]. **methodology** [VBML04]. **Methods** [Har06, HF09, Kry08a, ZT04b, AGN04, AC02a, AC04, AC05, AC06, AC07, AC09, AZD06, Ano06g, Bar06, Bar09b, BNS05, Bof03, BDBG09, BBG00, BRZ09, CM05c, CLSD+01, CCE+07, CL05e, DCW03, DDP+07, DL03, DBG04, DBPG04b, DLHP04, EEJ04, ELF+08, FGH09, FB01, FLE+06a, FP02, FZ09, Fra06b, FDZ04, GSfLV08, GY04, GKC06, GXT02, Goo03, GPW06, Gre09, HJJ09, HFS04, HFS06, HPC+08, HSW04, HBTW04, HMK06, Hyd06, IBN08, ISK+01, JR02, KMS06, Kap06, KKMS04, Kon09, KFD09, LPV05, LS01b, MP06, Mal07, MPRGLL03, OY01, PCF05, PHK+06, PGW09, POV+03, PJS+09a, RRC03, RR02, RACD00, RSM+04b, RMKS08, RH03, SB06a, SE02a, SSN03, SSK09a, Tal03a, TT01, VCHC07, VAS05, VGM05, WHD+05, Wil04a, WZL+00, YSY+00, YI04, ZXX02, Zot06, dGS06, dLCPLD+07]. **methods** [eSPM+08, vdVM00]. **methoxy** [Hea00, Iva05, VBT+07]. **Methoxyphenols** [BKM+02b]. **methyl** [AL09, BVS+09, Buc08, DCO+08, DK04, DZ06b, ETM00, GSQ+04, GBC+02, HJT07, Hes02, HQL09, LAL+08, LCL+09a, LZA+09, MGZL04, MJG+05, PGNT02, QCFJ05, RRNG05, RNCM05, SSN03, SMS07, SRW+06, TT05, TS07, TKS+05, TNJL05, TA07, WJLL09, ZSWL07, ZRRC05]. **methyl-1** [Hes02]. **methyl-AICA** [QCFJ05]. **methyl-chloro-peroxide** [DK04]. **methyl-substituted** [ETM00]. **methylacetamide** [FYSS09, MKCS05]. **methyladenine** [XXY00]. **methylamide** [HEJ+00, RKR+06]. **methylamine** [AG01a, KZ08, LHV+09, PSEP05]. **methylamino** [RMJ+07]. **methylaniline** [KB08]. **methylated** [JZZ+09]. **methylation** [JZW+09, SMS07]. **methylchrysene** [RLB02]. **methylcytosine** [SLL06, TX02]. **methylene** [FFLZ02, MHT+08, QCC02]. **methylfuran**

[ZDMF08]. **methyllithium** [TLC06]. **methylol** [ZYC09]. **methylphosphine** [KZ08]. **methylphthalimide** [SBB06]. **methylpotassium** [GBP05]. **methylpyridine** [CC00b]. **methylstannacyclohexane** [FFHT05]. **methyluracil** [PSK02]. **MeV** [PRM02]. **Mexico** [Cas00]. **MFI** [NAE06]. **Mg** [SCHW07, YCS09, ZL04, ASL06, CG09, MKLP02, QZ07, SUA+04]. **MgAl** [VPS+04, MTO+03]. **MgB** [Baň05a, KNN+04, PRNM03]. **MgC** [BRL02, TKT+05]. **MgCr** [MTO+03]. **MgH** [HSN+09]. **MgO** [AML+01, CXZ+09b, Cou05, EB04b, ESTU05, ESU05, LRS05, QCC05]. **MH** [CZPJ01]. **MHP** [JK00]. **Michael** [Ano00a, Ano00k, ÖS00c, RÖ00]. **microcavities** [BLA00]. **Microdomain** [Wal04b]. **microdomains** [VED+02]. **Microdosimetric** [ZFLL00]. **microiterative** [PRBGLL04]. **Microscopic** [AGL04a, Brä09a, KOPP04, MS03, FVPM05, MB01b, Baň05a]. **microscopy** [ACHB08]. **microsolvated** [Oku00]. **microsolvation** [FBGA04]. **microtubule** [RT09]. **might** [Bar09a, MZN+03]. **migrating** [Buc05a]. **Migration** [ST01, KVT04, LWZ+09, RVP06, TNYY03, ZSWL07]. **MIKA** [THPN03]. **millimeter** [RRC03]. **millimeter-wave** [RRC03]. **Milne** [Kry09]. **mimic** [GBB06]. **Minas** [SD03]. **minerals** [LADD00, MJG+05]. **minima** [MMF00, YKS+06]. **minimal** [LW05, Ou06]. **minimal-basis-set** [LW05]. **minimization** [DW05, Lav03b, MB04, Pai00, PA02]. **Minimum** [ACA02, EF03, FCD08, LYP+06, LTY00]. **mining** [DSW00, DSW02]. **Mismatch** [SM05b, ASM+03]. **mispairs** [KS03a]. **Mittag** [AE04, SEY07, SEY09]. **Mittag-Leffler** [SEY07, SEY09]. **Mittag-Leffler-based** [AE04]. **Mixed** [MDS04, NSG+06, Čár07, Čár09, DRD+05, DDM00, KMK+05, MT04, Pet00, THP08, YHC05, BMP+04]. **mixed-ligand** [Pet00]. **mixed-valence** [YHC05]. **mixed-valent** [DRD+05]. **mixing** [CPH04, Nic05b]. **mixtures** [RT09, WB05]. **ML** [ITY+09]. **MLS** [BOW+01]. **MM** [CRRL01, ALI03, Bol04, CdMCS05, CDS06, CRRL01, FJK+01, FJK+02, KAN+09, MMCC02, MPRGLL03, NRK+05, SBB05, Shi04, SBF+04, SRHR05, Swa03, TT04b]. **MM-pol-vib** [AYD00]. **MM/QM** [CdMCS05, CDS06]. **Mn** [RSTG02, SBM00, ZZFL00, ZLHL02, ZL04, DRD+05, MO06, QGM+00, dAGD08, dVHB03]. **MNDO** [DTT06, KVSG02, LZC04a, ZLC04]. **MNDO/d/H** [KVSG02]. **MnF** [Oni09]. **MO** [BB05d, BK04a, DETA02, GT07, YST+05, ACD02, BE07, BB01, BB02c, BB04, CD03a, DC06a, DZ06a, HT04, KANK00, MC06a, Nak02, SBF03, TSK01, Tal03b, ZXX02, BK04a, GARB08, ZLY05, ZL06]. **MO-LCAO** [Tal03b, DC06a]. **MO/HF** [Nak02]. **MO/MO** [HT04]. **mobilities** [CT05]. **mobility** [BES08, För00, Yak02]. **Möbius** [ACPG01, HvLJ01]. **mode** [Boh01, BCFR08, Gri08, JP01, LMRT08, MBRA07, NY01, NY03, NY04, PRSLA08, RLNA02, ZZW+06]. **Model** [BGN+05, FJ00, GKE01, JR02, Kry08a, PBI+01, Pog05, WAJ04c, Ada02, AC02b, AM06, ART08b, BK04a, BN04, BL02a, BFF04, BBL09, BKGF02, BB09, BL02c, Buc07, Buc08, Cam04, CCM+05, CDF06, CRRL01, CEK01, CEÖ02, Cho08, Chr01, CC02, Col08, CGS01, CPH04, DYD00, DKS05, DHCD06, DD05, Dei04, Dei06, DPS04, DB04b, ELY09, ESKB04, ESU05,

FHK06, FS00, FPC+08, GCCM03, GGLS02, Gin05b, Gin06, GW07, GMK+09, GGS09a, Gri06, Gri08, GSB00, HSP+09, HM01c, HEBS00, HMW05, JMP05, JÅM01, JV05, Kap06, Kar08, KK07, Kis04, KL00, KM00c, Lar02, LSPS01, LPC04, LCT00, LP04a, LB06, LMSB00, LK02, MZF05, MCR03, MGC00, MMV04, MOL03, MHB05, MC03, MMR+04, MOPdP09, MCF08, Muñ02, NH00, Nes01a, NF02, NBS04, Now01, NOHN02]. **model** [OYB+00, OMNN04, OR09, PIGN02, PBS02, PUH+08b, PUH+09, PVZV00, PGF+06, PGW08, PM04b, Pud02, RVP06, RT09, RNS04, SS04b, SS06, SKMW00, SE02a, Sch02, SBM00, Shi02, SSN01, SS01, Sok02, Sok04, Squ05, SMB09, SDZ+07, SÖ04b, Swa03, TT05, Tch07a, VGM05, WKF+06, WK03, YYY05, YYT+04, ZZL04, ZZL05, ZMMK09, ZZZ+08, ZWM+04, ZD07b, ZS04b, Baň05a, FBGA04, LTLS05]. **Modeling** [BFRB07, BN01, GST+05, HJJ09, HVC08, JB07, LH07c, MD02, NGTB06, New00, TA07, Von00, Yak02, YLS+04, AA04a, AS04b, AGM01, ACHB08, BB05a, BLZ02, BWS+02, BA06, BZR02, BSK+02, CMM+07, CP06, DCO+08, DRPT02, DTT06, DL03, DFT+07, GMS+05, GKL+09, GSB00, HQL09, Irg06, JHR+00, KVPS05, KCS02, Koz01, LSWT05, LLW+07, MTRD04, MEN+08b, NRK+05, OMMB07, PK01a, RCF02, RRPJ07, RVD03, SK05b, SP00, TA02, TVK+02, TSH03, VAS06, VG02, Whi02a, XCS+03, YS06, ZKB03, CÖ05, TFS+02]. **modelling** [Yur06]. **Models** [DCP01, LB02, Bar09b, BKM+02a, BSCB04, Buc05b, CL05a, CD00, CT00, CDGC05, CRL+02, EB04b, EB04a, FDM09, GHG04, GKSL01, Gui06, IAL06, JWZ+08, KFQ+02, Kan00b, KF02, KN08, LTV07, LS01b, Mar05a, NY01, Nes01b, Nes03b, NSG+06, PLC04, Pan02, PVW03a, PLA+07, RP00, RO01, SWST04, SJE03, TIV+07, TY07, Tem00, Tor04b, VLJ08, YYK+03, YNN+06, YYI+08, ZKEE07, ZBPD08, Mar03b, ZLHL02, Tor04a]. **Modern** [KCU09]. **modes** [BMB02b, Jal02, KKYT04, Sad02, SPL03]. **Modification** [SMY07, CDH05, MSS05, MCF08, SSJ09]. **Modifications** [BBO04, LFR+08, YM05, Živ09]. **Modified** [BFF04, HSP+09, HS02, BZL+09, DL02, Don09, HEBS00, MB05c, ÖÖOY02, PS07, PM04b, Por03, SPSS07, SMB09, TSF04, ZKYA04]. **Modular** [BC06a, Nég03a]. **modulated** [HGB08]. **modulation** [RWW+06, SS03a, SS05a]. **modules** [BCFR08]. **modulo** [Tem00]. **modulo-** [Tem00]. **modulus** [PVZV00, PVB+02, PVB+03]. **MoFe** [SUH+01]. **MOH** [ZWSJ01]. **moieties** [Bar09b, OOD+05]. **moiety** [ELC08, KMVR05, MHGR07]. **Molecular** [AP00, AKK05a, Ano00d, AS01, BBDS06, Bar03, BDBG09, BKRT03, Bou01, CMM+07, CFV02, DCO+08, ESE04, EGEDH03, EMM+02a, FGdA00, FGdA02, FH02b, FYT09, GHH03, IA06, IK00a, IK00b, JNF+09, JZW+09, KM00b, KM03b, KM01, LHL+00, LSWT05, LLX+03, MMV05a, Mer04, MY00, MTWN09, PRSLA08, PFSFH06, PMPI01, RFLR00, RF01, RHH+02, STAO00, SNdAM08, SFR08, SHE+00, Tap04b, TS01b, VIGL+05, VKIJ06, Whi02a, dOEG+08, AH06, AGM02, AMOR07, AC09, AKK05b, ASTO02, AT00, BKM+09, BN03, BFRB07, Bar00, BFF04, BBD07a, BBD07b, BNS05, BKM05, BM07a, BFB08,

Bro00, Buc05b, BA02b, CR06, Cam04, CCL03, Cat05, CCP00, CAHl08, CRRL01, CC00b, CSL+07, CS07, CIT+03, CHW04, Cho08, Chu00, Chu01, Chu02, CTP+08, CC08, Col08, CS01, CCR09, DCTC03, DRPT02, DTT06].
molecular
[DMV00, DP06, DGD+05, DNN+06, DPW00, DETA02, DMG09, DES03, DZS+06, DC03, DSW02, ELF+08, EMV05, EZ05, EMM+02b, FL04, FG03, FGH09, FLE+06a, FBBB06, FGZ07, Fra06a, FDME01, GBJM01, GSQ+04, GJB02, Gin05b, GMPIP01, GAR08b, Gos01, GM00, GM01, GM02a, GM02b, GM03, GM08, HT05a, HR07, HJT07, HSRP09, HEJ+00, Har04a, HM05a, HPC+08, HQM04, HTN07, HLH05, HR05a, HWPIM01, IN09, ITN08, ITN09, IYO+04, Iye09, Jal07b, Jal08a, JdL08, Jal08b, JCTD08a, Jal08c, JP01, JÅM01, JMP06, JG09, KKM+01, KM00a, KSH04, KUS+03, KAN+09, Kle03, KIK09, Koc00, KKS09, KO03, KO04, KSK00, KYA03, KY05, KT05, KY00, Kry08b, KOT09, KM00c, LFK06, LW05, LFADSF07, LB03, Lav03b, LHG00, LWC01, LA09, LZZ+07, LMX+05, LCH05a, LDM09, LBAB02, Lu06, Mai08a, Mai08b].
molecular
[MKHP09, Mar00c, MHT+08, MCLKC02, MKZ04b, MD08, MYGD01, MLSB06, Mic06a, MD04, MVA02, MT04, ML01, MG08, MK01, MW05, MVKN06, MRG02, MJ06, MPIP00, NKK+01, Nak07, NFT+01, NY04, NŚM02, Nal09a, Nal09b, OMC04, OBM06, OMY+01, OOK03, OK05, Özd03, PRM+06, PK01a, PD05, PVW03a, PF06, PMCOSC00, PFdP08, PO03, dRPFCP08, PREM04, PMAA00, PLC02, PMC02, Pup07, QGW02, RCF02, RPHG04, RP03, RLA+01, RFF05, RP00, RB07, SB06b, SWST04, SFD09, SKMW00, SFK09, SS00b, SOLI04, SGGBB02, SY07, SPH00, SSC+07, SWC03, She07b, Shi02, SY06, SY09, SMDG09, SK05b, Sjö00, SCHH02, SS02a, SDZ+07, SSK+05, TA02, TNYY03, Tal03a, Tal03b, Tap04a, TT04a, TT04b, TTM07, TBJ05, TVK+02, TDS+02, TT01, TT02, TT06, TCM01, TJAS08, TŠPJ04].
molecular [TPGD02, TWSK09, UKAM04, VAS06, VD00, VPS+05, VG02, VBML04, Ver05, WKF+06, WS00, WZW+09, Wil04a, WZL+00, XXY00, YYS+09, YYS+00, YYKY01, YS06, YHN+07, YZX+08, YLS+04, YNDJ06, ZFD+00a, ZKB03, ZSKV04, ZWJ02a, ZWJ02b, ZBPD08, eSPM+08, AEMAO06, GI07, HLP07, JHR+00, MPIP+01, OCK07, TIV+07, XCS+03].
molecule
[AAKAF07, AG02a, ANM03, BM01b, BP03, BDA+02, BBD07a, BES04, BPŠB00, CS08, CZPJ01, CCH06, CBC00, DL06, DI05, DBPG04a, DBG04, DBPG04b, Dou07, DM04, EF03, FOM+03, GD00b, GA08, Ghe09, GJB00, GJB02, GB08, GGS09a, HKY07, HLMH07, IAL06, KPČM05, KTH+05, KK07, KH08b, KF09, KKTMA09, Krü06, LRB04, LCCC08, MGdS+08, MP05, MK08, MHT+08, MTB+02, NF03, Pal00, PGN+05, PRM+06, PJ09, PB04, RLBK03, RLNA02, SSA07, SKN+09a, SK05a, SBFV05, SRS+04, SIT+06, SKNN08, SKNN09, ŠPNU08, Sut02, TI05, TSS+09, TFBM02, UML00, VBML01, VHM+04, WQ00, XR05, YW09, Yak02, YWZ+09, Yur08, ZB05, ZMMS+00, ZNF05, ZYG00, ZD07b, ZQF+02, ZLH+08].
molecule-based [KTH+05]. **molecule-surface** [ZYG00]. **molecules**

[AS04a, AGN04, AMGN00, ASDC08, ASM+03, BBHQ04, BN06, BCN04, BL04a, BVG05b, Boh01, BRR04, BB01, BB04, BB05d, BB05e, BCS01, BA07, CCP00, CC02, CC05c, CRTP05, CMNH07, DVV05, DLZ+03, DD03, DV00, DWF+03, DNC07, DDD03, EYBM03, ERVR06, FTB04, FRF02, Gin00, GMS+05, GW05, GWSZ08, GN01, HK06, HN03, HCTC07, HVC08, Hog04, HMB+04, IK00a, Jal07a, Jal07b, JCTD08b, JBPZ02, KK07, KH05, KF03b, KSS00, KBUV07, LTV03, LR01, LP07, LMJ00, LP08, LAQ+09, Liu06, MGCD01, MG05, MST04, MST08, MMV04, MKCB05, MVK00, May06, MZD+05, MY08c, MY09, MK02, MD02, MDS04, NB05, NS08, NS09, Nes03a, Nes04b, NJR+09, OC08, OA03, OCAMOHL07, Ort05, OOD+05, PIGN02, PSC+07, Pea05, PRNM03, PS03b, PV09, PJdC00, PJ03, PMO04, PML09c]. **molecules** [PGPA09, PLA+07, RBA07, RdLJ+02, RdSH08, Roh00, Saa00, SPN03, SG03, Sal00, SOLI04, SLRS02, SBB05, SLB+08, SdACAG03, SYL05, SBM+05, SINN05, SRHR05, SMVMC07, SBBL05, TSN+05, TKY00, TSZW08, TG05, TMPI05, VAS06, VM07b, Ver05, VK07, VK08, WPB+06, WHKM04, YNY01, YSY+01, YL02, YJ00, ZŠ05, dGS06, vdVM00, CL05b]. **Moletronics** [YS06]. **Møller** [RS11, CK09, FHHC00, Fra06a, HH09, IBN08, IVK00, KN09a, MNMV02, RS09, TB09]. **molybdena** [Han07]. **molybdenum** [CZWZ05, Die00, YPD+07]. **moment** [Áng09, Aze02, GM03, HW02, KY05, LA06, LMX+05, MKDM03, MK01, SCB+06]. **momenta** [MY08c]. **Moments** [HT05b, AGMK02, Ban02, Bar08, BG00c, CPH04, Fer09, GHH03, HL05, JKU02, JÅM01, KM02, KV08, LV01a, LPV05, LCBC03, Mar08, OBM06, PRG+04, PGW08, RRPJ07, SHG08, WZL+00, YSV05]. **Momentum** [GBS04, ACCC03, Bar06, CP09, Dat04, EMM+02b, HT05b, HSB+00, KWG06, LL01, TS01a]. **Monkhorst** [Kon09]. **mono** [Buc00a, NFL+02, PGB09, WW07]. **mono-** [Buc00a, NFL+02, WW07]. **monoanion** [MP06]. **monoatomic** [Wal04a]. **monoborane** [GJ03]. **monoborides** [KDC09]. **monocarbides** [KDC09]. **monochalcogenocarboxylic** [LLW+07]. **monochalcogenosilanoic** [LDR+08]. **monochloroethylene** [SMM06]. **Monoclonal** [Chu09]. **monocyclic** [PIGN02, RBL04]. **monoethers** [MARK08]. **monofluorides** [KDC09, WTWT09]. **monohalo** [VTP09]. **monohydride** [ZFD05]. **monolayers** [ITR02, TIV+07, TBB09, THP08]. **monomer** [CS00a, SAMBS01, TL05]. **monomers** [MCF09, MOAB01, SSJ09]. **mononitrides** [CL07a, JKU02, KDC09]. **mononuclear** [DGP08]. **monooxide** [EMV05]. **monooxygenase** [HKMM04]. **monosubstituted** [GKC06, SO04a]. **monosulfide** [SL05d]. **monotonic** [AP03]. **monovalent** [ČAV+09, EMV05, ZS04b]. **Monovasilis** [Ano06g]. **monoxide** [BJAV08, EMV05, Guo07, PML09a, PYZ09, SL05a, VML05]. **monoxides** [KDC09, ML01]. **Monte** [AC05, HI06, AMOR07, AC02a, AC02b, AC04, AC06, AC07, AC09, AM09b, ASDC08, FGH09, GBS02, HKY07, KBV05, MGdS+08, NY03, NKP+02, SNY01, UT03, UC00, Vrb08, YYY+00, YOGR09]. **montmorillonite** [BJAV08, RST08]. **mordenite** [DBHT01]. **Morita** [FYH09]. **Moriya**

[TYSY07]. **Morse** [AD07, Ban02, Ban05b, BM07a, DLF02, MB05b, SD06, SK05c, VRSF02]. **MoS** [GBMMSA00, MH09]. **Moser** [And05, CMS04]. **motifs** [PK01a, VED+02]. **motion** [GPW06, HQM04, KV08, MB06, NIS+05, OK04, PGW09, SS03b, TSK01, KN08]. **motions** [ITN08, JZZ+09, Oku01]. **motivated** [AM06]. **Mott** [PTS03]. **move** [Tap04a]. **movement** [Sch04]. **moving** [PW07, PSA05, VNB+03]. **MP** [ONA05]. **MP2** [FRGF04, KN09a, Flo08, FGZ07, GDB03, JNSF04, KMN05, KCOV07, KBMM08, LBP04, MCN+05, MJ06, SY09, SZ08, YSY+00]. **MP2-R12** [KMN05]. **MPE** [GSRL06]. **MPH** [MOAM07]. **MPI** [TŠPJ01]. **MPI-based** [TŠPJ01]. **MQDO** [MMV05a, VML05]. **MR** [Gda01a, HMW05, CSG06, MK00, Mei08]. **MR-ACPF-2** [Gda01a, CSG06]. **MR-BWCC** [HMW05]. **MR-CI** [MK00]. **MR-CISD** [Mei08]. **MRCI** [Li09, PK01b, UMDM06, YTD05]. **MRD** [IMT+02]. **MRD-CI** [MTB+02, TMAB01]. **MRSDCI** [PRNM03]. **MS** [DGLM09, XYS+03, GT07]. **MS-CASPT2** [DGLM09]. **MSn** [XD03]. **MSP** [Ess07]. **MSubPc** [YS05]. **MTD** [BSKFT07, KFTBS07]. **MTD-PLS** [BSKFT07, KFTBS07]. **Mu** [Ano05f]. **Mu-Shik** [Ano05f]. **Mulliken** [Ess07, KIN09, SRA09]. **Mulliken-** [KIN09]. **Multi** [CG09, Fra06a, HI06, TBML06, GMCS04, Her06, ITN08, MTRD04, RVP09, TSP+07b]. **Multi-channel** [TBML06, TSP+07b]. **multi-charged** [GMCS04]. **multi-component** [ITN08]. **Multi-decker** [CG09]. **Multi-determinant** [HI06]. **multi-dimensions** [Her06]. **multi-reference** [Fra06a, RVP09]. **multi-scale** [MTRD04]. **Multi-state** [Fra06a]. **Multicenter** [PTLB00, CA01, GSD+03, Gus02b, Gus04, Özd03, SH00, SB06b, Tal03a]. **multicomponent** [ITN09, ZZL04, ZZL05]. **multiconfiguration** [LCL+09b]. **Multiconfigurational** [KK02b, LZ05, MY08a, MY08b, MTWN09, SMY07, YM05]. **multidimension** [Irg04]. **multidimensional** [PW07, SSA07, TGGV+04]. **multielectron** [Gui01, GM00, GM01, GM02a, GM02b, GM08, Özd03]. **multifunctional** [Bro00]. **Multigrid** [THPN03]. **Multigrid-based** [THPN03]. **multiharmonic** [GN01]. **multilevel** [OYB+00, SN02]. **multinuclear** [PGB09]. **Multiobjective** [RB06]. **Multipartitioning** [RS09, RS11]. **multiphoton** [GMS+05, SSA07, SINN05, SIT+06]. **Multiple** [MMF00, EYBM03, HS05, MMM06, YTS+05]. **multiplet** [WZ06]. **multiplicities** [DLK00]. **Multiplicity** [DMMV00, VMRA04]. **multipliers** [SRHÖ06]. **multiply** [GT07]. **multipolar** [Sal05]. **Multipole** [OBM06, Tal07, GM03, LV01a, LPV05, RRPJ07, TG01]. **multipoles** [PE04, RdSH08]. **Multireference** [HMW05, IZ04, KPČM05, YNU+06, CDI02, Gda01a, HMW02, IVK00, KJH09, LP00b, LP09a, PMHW07, PCF05, SNdAM08, SČL00, TKT+05, Wil04a, YTK+03, ZT02]. **Multiresolution** [NP01]. **Multiscale** [SK05b]. **Multisite** [SDB03]. **multistep** [HV03, VAS05]. **multiterminal** [JM07]. **muonic** [EF03, GA08, Yal04]. **Murray** [NM01]. **muscarinic** [OMMB07]. **musk** [IK00b]. **mutagen** [SM05b]. **mutagenic**

[LPV02, MSS05]. **mutase** [SCMS07, WRK03]. **mutations** [Kry02, MLSG04]. **Mutual** [Mat02b, Mat10, Zak04b]. **MX** [JLAR07]. **MX/MX** [JLAR07]. **My** [Mon09]. **myoglobin** [RP00].

N [CMY03, EBB06, FRNM08, GP03, GWJ05, JXW+04, Mar09, MS00, PT00, SASS03, SYL05, SST00, SCHW07, Tem02c, Tem04, VRS01, YKS+06, YZY+01, ASO+06, BBPG08, Buc05c, CdMCS05, CDS06, GE09, LP09a, Sad02, SCTK+09, TGSK09, XXJG04, AG02a, BVG05b, BVG05a, BK04b, BP04, BG00c, Buc05c, CNPA04, CTLZ01, DLK00, EMM+02a, Eva04, GEB+00, GB06a, GFMT08, GW06a, GYF+09, Hob02, HW02, IAMY02, ILB+08, IN09, IG06, JWM00, Kar08, KKK09, KTN02, LTV02, LP08, LLL+07, MKCS05, MP00, MG08, MJ06, Nes01a, PIGN02, PGP+07, QCFJ05, RFS+00, RWW+01, RKR+06, SBB06, SAE08, SUAL04, SST00, SQZ+02, TKY00, TFBM02, VAT03, VBML01, WQ00, YYI+08, YT03, ZMB+03, ZLZ05, ZSWL07, ZHS06, ZD07b, ZPW+04, ZLH+08].
N-acetyl-L-isoleucine-N-methylamide [RKR+06]. **N-atom** [IG06]. **N-bands** [YYI+08]. **N-derivatives** [PIGN02]. **N-dialkylaminoethyl** [ZPW+04]. **n-didehydro-polyene** [LP09a]. **N-dimethylaniline** [SQZ+02]. **N-electron** [Nes01a]. **N-glycylcarbonyl** [SST00]. **N-HF** [Hob02]. **N-methyl-N-nitrosobenzene-sulfonamide** [ZSWL07]. **N-methylacetamide** [MKCS05]. **n-pentane** [TGSK09]. **N-phenylalkyl-3** [ZMB+03]. **N-phosphorylation** [CTLZ01]. **N-protonated** [AG02a]. **N-representability** [VAT03]. **n-Slater** [GE09]. **N-terminal** [BP04]. **N/B** [Buc05c]. **N/C** [Buc05c]. **NaAr** [RBLS04]. **NaBr** [QGM+00]. **NAD** [Buc05a]. **NADH** [Buc05a]. **NADH-NAD** [Buc05a]. **NADPH** [VR01]. **NaF** [VGMN03]. **NaI** [MB02a]. **nano** [YS07]. **nano-Gold** [YS07]. **nanoalloy** [LGBJ03]. **nanobioelectronics** [Lak08]. **nanocarrier** [ELG05]. **nanoclusters** [MB01a, MH09, PCS09, PHNN09a, PNN08]. **nanocontacts** [GSfLV08]. **nanocrystals** [LNPL06]. **nanodevices** [JM07, JPMM08]. **nanofluidic** [KIK09]. **nanohorns** [AM09a]. **NANOPACK** [BZG+02]. **nanoparticles** [Guo09, Nav09]. **nanopore** [DM08b]. **nanorings** [KAG08]. **nanoscale** [SMVMC07]. **nanostructure** [Wal04a]. **nanostructures** [HOIK09]. **nanotechnologies** [GSPT+07]. **Nanotube** [VM07b, CAHl08, CXZ+09b, DGSD07, JP08, LZC04b, LPC04, TOH+00]. **nanotubes** [ALM05, BBO04, CMW03, CXZ09a, Col08, Den09, FGFF06, GWSZ08, JLM08, JLC+09, JWM00, KDŁL07, KG08, KG09, LMMB03, LZC04a, LTW09, SHM+09b, Tor06, VM06a, VM07b, XZ07, ZLC04, ZWMZ04, ZA09]. **NANOVIBR** [BZG+04]. **nanowires** [EM05, LJMM09]. **naphthalene** [WW07]. **naphthalimide** [dlPOPP03]. **NaRb** [KF09]. **narrow** [CMW03]. **nationality** [HWR05]. **native** [AV02, BLC09]. **Natta** [CCA+06, MM02]. **Natural** [IBN08, PMO04, PO05, PLU08, BMMA06, BAG+08, LP07, LP05a, MBA+08, NU09, PA08, Pir06, LSM+06]. **naturally** [DSL06]. **Nature** [RHHH00, Tor04b, NSS09, PBS02, WLZY08b, WZWC07, ISK+01, KP00b,

Tor04a]. **Nb** [SCW09]. **NBO** [JFJMR08b, JFJMR08a, ONA05]. **NBO-based** [ONA05]. **NC** [BEM02, XXMJ06]. **NCN** [Buc02b]. **NCO** [PXZ+09]. **ND** [SYZ+09]. **NDDO** [GG00, MGC00, MC06a]. **NDDO-based** [MGC00, MC06a]. **NDDO/CI/SOS** [GG00]. **NdO** [BB02c]. **Ne-like** [GAL+05]. **near** [MP06, OCWY09, Pup02, SJE03, dVHB03]. **near-edge** [OCWY09, dVHB03]. **near-resonance** [MP06]. **Necessary** [AD06]. **Neel** [SZA07]. **negation** [Nég03b]. **negative** [AM07, BLKJ00, CJdC01, IZ04, MZN+03, PM04b]. **negative-energy** [BLKJ00]. **NEGF** [SY09]. **NEGF-based** [SY09]. **neglect** [CDGC05]. **neglecting** [Boe04]. **NeICl** [ELY09]. **neighboring** [DDT+03, DSW02, MB00]. **nematic** [IKL04]. **NEMO** [HK09]. **neolignans** [CBRBT03]. **neon** [GBS04]. **neopentane** [HH05]. **Nephelauxetic** [TD09]. **Net** [PS07, TC07]. **network** [ASO+01, ASO+04, CP06, Koz01]. **network-based** [CP06]. **networks** [BBSS00, CBRBT03, CL08, FOM+03, FS00, HLP07, Kle03, LFADSF07, SS09d, Yil06]. **Neural** [CP06, Koz01, LFADSF07, Wal04b, BBSS00, CBRBT03, CL08, FOM+03, HLP07]. **neutral** [AG02a, CIT+03, DBL+03, FSGB05, För00, Guo07, JAP+05, LDMR01, LDPP05, LDP05, LVM01, LAQ+09, MP06, Mal05b, Mor04, PFdP08, SH02b, TW05b, WE01]. **Next** [Mar05a]. **NF** [GJB02, KPČM05]. **Ng** [LAQ+09, ZZHL08]. **NgAuOH** [ZZHL08]. **NH** [GB05, HGS03, Irg04, Liu08, MMZ02, TLYW06, TWZW09, VRA+02, YW05, ZLHL02, AE07, AV04, AV05b, BLM08, DZ06a, HGRL01, HW02, JJ02, Pet00, SGP+07, VK08, Woo02, WZWC07]. **NHN** [LY09]. **NHNOH** [RG08]. **NHNOH-bonds** [RG08]. **NHON** [RG08]. **Ni** [BLZ02, ZDQF08, BL04c, BGJJ01, BGÖ+01, CJB08, DSW08, FDLK02, GBMMSA00, KSWR00, Mar09, MDJ01, QCC05]. **nickel** [CJB08, CC05a, LWZ+09, MRMR02]. **nickel-based** [LWZ+09]. **nicotine** [MCN+05]. **nifurtimox** [SCRE08]. **Nile** [DCP06]. **Nilsson** [BKM+02a]. **NiO** [Pat06]. **nitramines** [QXJG05]. **nitrate** [ZDAZ03]. **nitration** [LCCH09a, Sok04]. **Nitrenes** [AMO+01]. **nitric** [Har02a, Rua09, SSC+07, ZHA01]. **nitride** [FTB04, Guo07, JWM00]. **nitrides** [XL08]. **nitrile** [LSCC01, NOHN02, PKZN08]. **nitriles** [GV06, LW08]. **nitrilotriacetamide** [SCG07]. **nitrimino** [ZXZ+09]. **Nitrite** [NBS04, KNRR05]. **nitro** [FXHL05, WGX09, ZCZC09]. **nitroalkanes** [SSC+07]. **nitroamines** [EEJ04]. **nitroaniline** [BF07, CC01b, GBC+02, SCB+06]. **nitroanilines** [GFMT08]. **nitrobenzene** [CC01b]. **nitrobenzoic** [SŚRL07]. **nitrofurans** [SCRSRE05, SCRSRE06]. **nitrogen** [BJAV08, BF09, ÇAK07, DL06, EMV05, FGH09, GJB02, Lia08, OMMWL02, TT04b, YT03]. **nitrogenase** [CJZZ06]. **nitroimidazolidine** [ZXZ+09]. **nitromethane** [PM09, SCLL07]. **nitrophenol** [CC01b]. **nitroprusside** [BDMS03]. **nitroquinoline** [LLZ04]. **nitrosamine** [RG08]. **nitrosobenzene** [ZSWL07]. **nitrosomethane** [DBPG04a, DBG04]. **nitrosothiol** [Rua09]. **nitrosyl** [CC05b, GL00, KVPS05, XLX+09b]. **nitrosyls** [XLX+09b]. **nitrotoluene** [CC01b]. **nitrous**

[LIBM03, MVL+01, OMMWL02, SZK07, SZ08]. **nitroxyl** [LLYL06]. **NiX** [ARBD05]. **NLO** [MVdCD00, DCW03, JPA05, MNJP05, SR05]. **NMCSCF** [XVB05]. **NMR** [AK05, BSR02, Bou03, BAG+08, FC05a, Gün06, Hog04, JJ02, KSK+04, KMM+06, MC03, MSK+05, PGNT02, PMB08, RCF02, SŚRL07, SST+03, Sch05, Seb05, SKNN09, TMM+03, Tem02b, TCM09, ZA09, dBC06, dLCRF+08]. **NMR-quantum** [KSK+04]. **NNO** [PM09]. **NO** [BT05, DBG04, GL00, MVdCD00, TSP+07b, ZLH+08, KLK08, BJ00, BZBT01, CC00c, DBPG04b, LTV02, LTY09, MY08b, Nak02, PRSLA08, SAE08, TSP+07a, VBML04, VK07, XCC+08, YHD+07, ZSWL07, ZLML05, ZD08]. **nobelium** [DHCD06]. **noble** [ASH07, FSGB05, FV04, LAQ+09]. **nodal** [Pup05, Pyy01, Yar00]. **noise** [Mai08a, Mai08b]. **Non** [CA07, YOM+01, CCV+07, FRK+05, Lef06, NGTB06, OMN+03, RW04c, Sal09, Sko02, Tou09, TDST07, VRSF02, YM05, OMNN04, Tak09]. **non-aromatic** [FRK+05]. **Non-Born** [CA07, YOM+01, OMN+03, Tak09]. **non-Condon** [VRSF02]. **non-Floquet** [Lef06]. **non-heme** [CCV+07, NGTB06]. **non-Hermitian** [Sal09, YM05]. **non-Kekulé** [TDST07]. **non-Markovian** [Sko02, Tou09]. **non-wavepacket** [RW04c]. **nonadditive** [Nal00b]. **Nonadditivity** [LZA+09, LCL+09a]. **Nonadiabatic** [Baň05a, Hag05, YYY+00, ZMX+05, ACDV01, BM01b, BMB02a, KTN02, OM02, OM03, OM05, RLBK03, TCM01, VHM+04]. **nonalternant** [MT04]. **nonanes** [RNVTP09]. **nonbonded** [RME+03]. **nonbonding** [LMDW09]. **noncentral** [DCLC05, Gus02b, Gus04, SHZGP09]. **nonclassical** [BMR+07]. **Noncollinear** [LNSE02, YYS+01, BJS09, WZ06, YYS+00, YYKY01]. **nonconjugated** [YS09]. **noncontact** [ACHB08]. **noncooperative** [BLC09]. **Noncovalent** [PM04a, ET09, LZWY07, MLP07, PMPI01]. **Nondynamical** [Cho08]. **Nonempirical** [BF07, YI04, KP02, NS02, NBS04, Nov07, RNS04]. **Nonequilibrium** [HK06, Oku00, Pom04, ZZL05]. **nonexponential** [Nic02]. **nonharmonic** [BCF02]. **nonhydrogenic** [GAIK04]. **Noninteger** [Gus03, GM03, GE09, ÖO02, Özd03, Özd04]. **nonintegral** [CCGF07]. **noninteracting** [LKE03, NM01, SS04b, SS06]. **nonionic** [MPIP00]. **nonisothermal** [CP06]. **Noniterative** [KV08, Mei08]. **Nonlinear** [Chr01, KK04, MKZ04b, MLL00, RMM05, SR05, SMB07, Ver05, ZFD+00a, BN06, BFRB07, BF07, BF08a, BSZ07, BS05c, CDB02, DHZ06, GB03, Her06, JV05, Kel05, KF03b, MB05a, MVdCD00, MOL03, NFT+01, PCL+03, PTLB00, PJS09b, SH02a, SM06a, SWSH09, VRFS05, WRD03, YS09, Zak04a, ZCWZ04, dFGM08a]. **nonlinearity** [ZGY+03]. **Nonlocal** [GGACT03, Mar03b, Nes03b, Nes04b, Bel04, HM05c, MHV03, ML01]. **nonmagnetic** [RI03]. **nonorthogonal** [Pen00b, SJE03]. **Nonperturbative** [SMT06, Gin05a]. **nonplanar** [RLB02]. **nonreactive** [LLR04]. **Nonrigid** [DDA07, BFB08, DAD05, DAD08a, DAD08b, Sto08]. **nonrigidity** [SGHL00]. **nonsingular** [Kýv09]. **nonspherical** [SK00a]. **nonsymmetric** [Ghe09]. **Nonsymmetrical** [SSS02]. **nontransition** [Tch07a]. **noradrenaline** [AG02a]. **norbornene** [KCU09, RCF02]. **Normal** [RLNA02, JP01, Lad06, PS03b, IK00a]. **Normalization** [PSM07].

normalized [MK01]. **Note** [PFC02, vLvL06, Ano04e, Mas02, Pyy01]. **noteworthy** [PMLTL07]. **Notice** [Ano07g, Ano07e, Ano07f]. **notions** [Eye00]. **Novel** [KAG08, LLLZ07, LW07, LE01, BDG01, DGD+05, JLI+01, LSWT05, LHV+09, SLS+05, Wei03, TA06]. **November** [Cas00, SD03]. **NQR** [Lat03a]. **NTO** [LCH05a]. **Nuclear** [CCGF07, GA08, Gus03, HLH05, Laz02, Nak07, PRG+04, XV01, BSH04, BSR02, CM02b, CCR09, DS07, GMCS04, GMK+09, Hag00, Hag05, HTN07, ITN09, JJWH04, KZvL09, Mal05b, MNR07, MD02, Nak02, ÖO02, ÖÖOY02, PB09, RCD00, SH02a, Saf04, Sap06, Sjö00, SS09b, Tem00]. **Nuclear-Attraction** [Gus03, ÖÖOY02]. **nuclei** [DDT+03, PLC02]. **Nucleic** [Sta00, CJ09, RSTG02, SSJ09, SGHL00]. **nucleobases** [DZO02, KKYT04]. **nucleoside** [ATF03, CFR07, LVSG06]. **nucleosides** [GMTM02]. **nucleotide** [KKYT04, LY02, MPIP+01, OSW07, SOEW08, ŠK03b, SBL05b]. **nucleotides** [CLL08, DZO02, LLZH09]. **nucleus** [DHCD06, Mal05b, MS09, QS00b, SLWS07, IYO+04]. **nudged** [BCWS09]. **Null** [POM+07]. **Number** [ND03, Tem04, CCGF07, ELY09, KG02, Kry07b, LTY00, MBM05, SBL05a, TYY05b, YYZ05a, YYZ05b, ZT09]. **numbering** [CSL+02]. **Numbers** [Gus03, BKM+02a, Koh01, ÖO02, Özd03, Özd04, Özt04, TYY03]. **numeric** [Yil06]. **Numerical** [ARH00, ÇKB02, Fis00, KAE03, LLZ+00, LSLD01, LD05, RW00, Rom08a, Rom08b, Tal03a, TDF09, CW08, CHN09, DL03, DS07, GMK+09, GSD+03, IYO+04, KSN05, KFD09, LSH08, Mer04, Saf04, SS00b, Tal03b, Tal07, VHM+04, VAS05, CHC05, PD05]. **Numerically** [LN03, Tal03a].

O [AL09, AGLBM03, BB05a, BPM01, BT05, BFBB06, BFB08, CK03, CGL+05, CNPA04, CT05, CC00c, DP06, DKS05, DGQT09, DZTZ05, EP02, FRT+00, FGC04a, FGC04b, FRNM08, GYF+09, HY04, IN09, JLAR07, KSI+07, KN08, KM06, LLX+03, LLW+05b, LLW+07, LDR+08, LAQ+09, LJL09b, LWCF08, MKLP02, Mar09, MB06, MMCC02, MS05, Met05, MCZWD06, MTO+03, MGAS09, NSS09, NRS+02, NF02, PT00, PILD07, QZ07, RNS04, Sad02, SL07, SCRR02, SCW09, SZSP02, SSK09b, SLW+07, SNN+09, TI05, TW05a, TRF+00, Tor04a, USM01, VPS+04, WQ00, WT06, XCC+08, YST+05, YYZ+05c, YLZ07, YW05, Yur06, ZSPS03, ZZFL00, ZZW+06, HZW+08, AKK05b, BGG08, BML01, BJ00, BG00c, BSK+02, CGCS02, CK03, CNPA04, DMG09, DLK00, HAL+02, HKMM04, HW02, HR05b, JJ02, KSI+07, KSN+09, KTN02, LV01b, LLX+03, LLW+05a, LLW+05b]. **O** [LN03, MY08a, Met05, MJ00, POAVdlM08, RNS04, SI09, SGP+07, SAE08, ŠPNU08, STW+05, SLW+07, TIGD09, Tor04b, VRS01, VBML01, VG06, Woo02, WZWC07, XXY+05, YYZ+05c, ZLL+05, ZH06, ZD07b, ZCFD02]. **O-H** [CGCS02]. **O-hydroxybenzoyl** [AKK05b]. **O-like** [SI09]. **o-xylene** [HZW+08]. **O.** [Sut02]. **O6** [SMS07]. **O6-methylation** [SMS07]. **Obituary** [Ano05f, CJKK04, DB04a, Mar04b]. **objects** [Sta00]. **OBO** [MO06].

observable [Put09]. **observations** [Por03, Sut02]. **Observed** [Por02, ABM01, PSC+07, Por04, TIGD09]. **obtain** [ACD02]. **obtained** [GGDL07, GFDK09, HdMB+05, Mar07a, PCT+04, Sal05, SSMG08, TWSK09]. **obtaining** [Man05]. **occasion** [AGL04a]. **occupancies** [POV+03]. **Occupation** [Koh01, FDLK02, TYY03, TYY05b]. **occupied** [Kry06]. **occur** [Hyd06]. **occurring** [DSL06, ŠFW00]. **occurs** [YZX+08]. **OCOCH** [JFS+09]. **octahedral** [ADK02, BFAM03, Fan01]. **octanol** [DGD+05, FGdA00, FGdA02, JB07]. **octanol/water** [DGD+05]. **October** [Ano04e]. **Odd** [Buc00a, MRT00, She04b, She07b, Buc02b, HM06b]. **Odd-even** [MRT00]. **Odd-membered** [Buc00a, Buc02b]. **odor** [IK00a, IK00b]. **Off** [SM07a, AGMK02, Gri08]. **Off-atomic** [SM07a]. **off-center** [AGMK02]. **off-resonant** [Gri08]. **OH** [JCTA08, LLW+05a, LLW+05b, Mar09, PT00, TLYW06, TM05, AE07, Cab05, CBMRN08, HEBS00, HZW+08, JXZ+05, Pet00, TWZW09, XFLX+06, ZDMF08, dSNBG08]. **OH-initiated** [HZW+08]. **OH**$\cdots$ [LAL+08]. **OHO** [ZQF+02, LAL+08]. **ol** [YZC09]. **old** [CBB01, HFS04, HFS06, MP05, Zot06]. **OLED** [GSQ+04]. **olefin** [GARB08, Han07]. **Oligo** [TNJL05, ML05, ML08]. **oligoaniline** [YHF+08]. **oligoelements** [GP08]. **oligomer** [DHZ06]. **oligomers** [BFRB07, CSL05a, DBL+03, IMTG06, dAMdG05, NKN+05, PJ07, SL05a, SNZG02, TTK02, ZTI+07, ZWJ02b, dBC06]. **oligonucleotide** [KKYT04]. **oligonucleotides** [KK02a]. **oligopeptides** [BS08]. **oligosaccharides** [FJK+01, FJK+02, SFK09]. **Oligothiophene** [GDB03]. **Olov** [Ano02k, ÖSB01]. **OMe** [WML08]. **omeprazole** [BF08b]. **on-top** [TYY04]. **ONCCNHX** [Var07]. **oncogene** [Lad00]. **One** [CSDCCMZT03, KIN09, MMM06, MO06, PO03, RBLS04, TNYY03, AM05, Ano06g, Bar08, CSP04, CC07, FXHL05, Gin01, Gin06, Gus02b, HT05a, HH02, HMMT04, JJ00, KDŁL07, KMS06, KTK+04, Koh01, Koh02, LLZ+00, Mar87a, MOL03, MD08, Mer04, NOY+01, NY01, PKB+01, QFC04, QCFJ05, RMJ+07, RFE+00, RSM+04b, Rui05b, SH09, SGS00a, SNdAM08, SMT06, TYY04, TOH+00, UC06, WRD03, WO05, Wei08, WD01, Wyb02, Yam04, Yam05, ZZUO05, ZTSP00, HWR05, Lef00]. **One-** [TNYY03, Gin06, NY01]. **One-body** [KIN09, TYY04, UC06]. **One-carbon** [CSDCCMZT03, QFC04, QCFJ05]. **one-center** [RSM+04b]. **one-dimensional** [Ano06g, HT05a, HMMT04, JJ00, KMS06, KTK+04, LLZ+00, Mar87a, MOL03, MD08, NOY+01, PKB+01, SH09, SMT06, TOH+00, WRD03, Wyb02, Yam04, Yam05]. **One-electron** [MMM06, MO06, RBLS04, AM05, CSP04, CC07, Gus02b, HH02, Koh01, Koh02, Mer04, RFE+00, SGS00a, SNdAM08, WO05, Wei08]. **One-particle** [PO03, Bar08, WD01]. **ones** [SK09]. **ONH** [LLW+05a, LLW+05b]. **ONIOM** [SS08a, FRGF04, Han07, HKMM04, HT04, LMDW09, OSW07, QFC04, SOEW08, ZLJ+09]. **only** [LR01]. **ONO** [XXMJ06]. **ONOONO** [WQ00]. **onto** [LL04]. **OO** [FGC04a, MBRA07]. **OOH** [GMS01a, WF04]. **Open** [May06, AEI00, Buc05c, CL05a, DM08a, Glu04, GW04, KRR08, KGA05, LP07, LP09b, Nal00a, OdSC05, PVW03b, PGW09, PTLB00, WF04, XZ07].

open-chain [KRR08]. **open-ended** [XZ07]. **open-shell** [DM08a, Glu04, GW04, KGA05, LP07, LP09b, OdSC05, PVW03b, PGW09, PTLB00, WF04]. **opening** [Bro00, CJZZ06, JPA03, KV07, NLD+04, SMM06]. **openness** [LZ05]. **operator** [BG02a, Gün06, LJL09a, MY00]. **operators** [ASO+01, ASO+04, BKRT03, BCF02, CDG09, CD03b, DL02, DLF02, Dya00, LP04b, MYRNYSB07, Mic09, NP01, Pan07, Pla01, RFLR00, SD06]. **opioid** [JHR+00]. **Oppenheimer** [OMNN04, CA07, HT05a, IYO+04, Nak02, Nak07, OMN+03, PCBA08, SA09, Tak09, YOM+01]. **opposite** [Buc02b]. **Optical** [KSG03, KDF00, RKM09, RSN+07, SRHR05, VRA+02, BN06, BFRB07, BF07, BF08a, BKAT00, FYT09, HH05, HRDM+08, IOA+04, IMTG06, JNKMS03, KK04, LQC06, ML05, MLD06, ML08, MVdCD00, MOL03, MLL00, NFT+01, PR05, SR05, SWSH09, VRFS05, Ver05, YS09, ZFD+00a, ZMZ+09, ZGY+03, ZZWM07, ZRF+09, dBKS01]. **optics** [GB03, Kel05]. **optimal** [BB05c, BKMHP04, SMY07, Sce09, SS02a, ZR03]. **Optimization** [Ano07a, CL08, SM06a, SB06c, Tal03b, DSFS00, DNM+08, GH03, HSW04, HPR09, ITN08, KSI+07, KS07, MY08a, Mak07, MAFR08, MHT+08, PRBGLL04, PJS09b, SKT+07, SIS+08a, SBBL05, TMS08]. **optimize** [DGP08]. **Optimized** [MGK+09, Shi05, SS03b, TNET03, GBS04, GW02, GW04, GG07, HP07, KZ09, ŠPNU08, TYY07, TGGV+04]. **Optimizing** [BD07, JC00, JC01]. **options** [PRBGLL04]. **OPTX** [PT06]. **orange** [ABI07]. **orbit** [ACDV01, ARBD05, Boe04, BSZ07, FTM06, KY05, KF09, LJL09a, MB07b, PS03b, TYY05a, TYSY07, TMAB01]. **Orbital** [EJ06, GBB06, LPC04, MH06, MC08, Nes02a, PW09, WZW+09, AA04a, AEMAO06, AK02, AS04c, BHG+06, BEL01, BBM+00, Bou01, CDF06, CL07b, Col08, DYD03, DNN+06, DKW09, EE09, FYT09, GSQ+04, GJB02, GJ03, GAR08b, Gra08a, GSB00, HSRP09, Hog09a, HTN07, IBN08, IK00a, IK00b, ITN08, ITN09, JR02, Koc00, KSK00, Kýv09, LSM+06, LHG00, LP07, LP05a, MKHP09, MMV05a, MO06, MG08, MZ09, Nak07, Nal09a, Nal09b, NFG05, OOK03, PFA08, PF06, PMO04, PO05, Pir06, PLU08, PB03, POV+03, SK01a, SFK09, SPH00, SMDG09, SSSS09, SBBL05, TA02, TVK01, Tal07, TDF09, VPSH00, VBML04, VKIJ06, Whi03, YSY+01, YSO+01, YTK+03, YNU+06, YNDJ06, ZFD+00a]. **orbital-** [NFG05]. **orbital-based** [CDF06, DYD03, IBN08]. **Orbital-dependent** [EJ06, WZW+09, Gra08a, YNU+06]. **Orbital-free** [PW09, DKW09]. **Orbital-polarization** [MC08]. **Orbital-stoichiometric** [LPC04]. **orbitally** [OBM06]. **Orbitals** [Gus03, Har03, AH06, ÁBL06, ACC03, ACCC03, Bad03, Bar00, BSH04, Boe03, Bud04, BLKJ00, CC08, DMG09, ELF+08, EWCT+05, EMM+02b, FLE+06a, Gin05b, GSD+03, GM00, GM01, Gus01, GM02a, GM02b, Gus02a, Gus02b, GM03, Gus04, GM08, GE09, Hea03, Hog04, HC02, KZvL09, LW05, LHG00, LWC01, LP05a, LH05, LS02, MY08b, Mat02b, Mat10, MH06, Ort04b, ÖO02, Özd03, Özd04, ÖKAY03, Özt04, Pen00b, PCT+04, PCT+05, PH09, PREM04, PREM05, PRCEM06, RH09, RLA+01, RLRE04, RJ08, SH01, SS00a, SS00b, ŠPNU08, Tal03b, Tal04, TT06, WS00]. **orbits** [OB02]. **order**

[AZ08, ACT+05, BS05b, Buc04, CK09, DPW00, DFT+07, DD00, EJ06, Flo08, Fra06a, Gin05b, Gin06, GG07, GG00, Gra08a, HZPY03, Her07, HCTC07, IBN08, JV05, KN09a, Kel05, KJH09, KZvL09, LV01a, LCL+09b, Luz08, MO06, MNR07, NFT+01, PMHW07, PVW03b, PJS09b, RS09, RS11, SHZGP09, SL05b, SH09, TYY05b, TB09, TPRVC01, VATPR01, VAT03, VTPRA08, VPS+04, YS09, Yar00, YYXC01, ZH06, ZGY+03, vLvL06]. **ordered** [Mar09]. **Ordering** [YYZ05b, RPHG04]. **orders** [CWZ03, DT02b, SSSS09, SMB09]. **Örebro** [ERU07]. **Organic** [BLA00, BN06, BF08a, BK03, CDF06, CRTP05, DDM00, För04, GD00a, JCTD08b, JMEM07, JZZ+08, KZG09, Kel05, KWT06, KS09, OA03, RWW+06, Tor06, YHF+08]. **Organic-inorganic** [BLA00]. **organic-solvent** [Tor06]. **organization** [Brä09a]. **organoaluminum** [CCA+06]. **organolithium** [PJS+09a]. **organometallic** [MW06a, Stu00]. **organophosphinates** [KM05a]. **organoselenium** [BKGF02]. **organoxenon** [LK02]. **orientation** [Kar04, BL04a]. **Orientational** [RPHG04]. **oriented** [YINH00]. **Origin** [HGTW03, SB03, dVHB03, BAZ05, Duf07, Kry02, MZMZ09, She07d, Stu00, ZOK+05, AK02]. **original** [Kry05, SDW07]. **origins** [Nal09b, KS03a]. **ortho** [CNPA04]. **Orthogonal** [DCA03, RBA07, PMZGGR04, SN06b]. **orthogonalization** [May02b, NS04]. **orthogonalized** [PA08]. **orthonormal** [Gus01, Gus02a]. **oscillating** [Lef00]. **oscillation** [MYH03]. **oscillations** [GHG04, GN01, MKZ04b, SCTK+09]. **oscillator** [AC08, BB05b, BKM+02a, BCF03, CCLK04, DLCY+07, KO03, KO04, Mat02a, MAS07, POM+08b, RMM05, RGMP06, SBT+03, SS03a, Sch02, SD06, SK05c, Wyb02, Yam04, Yam05, ZZM09]. **oscillators** [Ban02, Ban05b, BLRT02, CA09, CMS04, MB05b, MB05a, MB02b, WRD03]. **osmium** [TSH03]. **OsO** [UML00]. **other** [ER05, FCC07, IAL06, Lef00, LCK00, NNS+00, PGF+06, TGGV+04, Wen02, Yur07]. **out-of-loop** [YYQ+06]. **out-of-plane** [Buc02b]. **outperform** [CL00a]. **Overhauser** [GGS09a]. **Overlap** [Gus03, HM01a, HM01b, Özt04, Tal04, CDGC05, GM00, GM01, GM02a, GM02b, GM03, GM08, ÖO02, Özd04, ÖÖOY02, Rom08a, Rom08b, RR00, SDB03]. **overlapping** [Kan00b, SSDB06]. **overtones** [LLP05]. **Overview** [ZT04b]. **oxacycloheptane** [FHJ+08]. **oxadiazetidines** [BM04]. **oxadiazole** [AA09b]. **oxalic** [CS00a]. **oxaphosphetane** [PMB08]. **oxazaborolidine** [GP01, LZYT01, LZHT03, LZT03]. **oxazaborolidines** [LXH+00, LXTT00, LXHT00]. **oxazine** [DNC07]. **Oxford** [OC08]. **oxidase** [JG00, ZMS05]. **oxidases** [AG01a]. **oxidation** [ABD06, BPM01, CJB08, DKD+07, EMV05, GARB08, KTN02, LDZ+05, LJL09b, ZLC04]. **Oxidative** [MGMR04, RS08, CCV+07, ĆMTS08]. **oxide** [BR02, Boe07, BKAT00, FTB04, FS05, HSS09, Har02a, HRDM+08, LIBM03, LLZ04, MVL+01, Nav09, NWZ+07b, Oni08, RSFRDNA04, RS08, Rua09, SMM06, SZK07, SZ08, ZHA01, dVHB03]. **oxide-supported** [HRDM+08]. **oxides** [DAA+06, FPJR03, HSN+09, LLX+03, MCF09, Oni07, RRGP05a, RRGP05b, SL09, ZKEE07, Sha07]. **oxime** [LZYT01, LZHT03, LZT03]. **oxirane** [ZYC09]. **oxo**

[GARB08, KSN+04, KFS00, SNM+04, SIS+08a, YYS+09, YYI+09]. **oxo-bridged** [KFS00]. **oxoguanine** [MSS05, SM05b]. **oxy** [CJZZ06]. **oxy-bidentate** [CJZZ06]. **oxygen** [AM07, BPM01, Bau09, EMV05, FVPM05, FAE+05a, FAE+05b, FS05, HR05a, ISK+01, KM05b, KB08, LDZ+05, MVA02, MME09, MSS05, Oni09, PC09, PČH02, PL00, SKN+09a, XYS+03, YYS+09, Yur06]. **oxygen-evolving** [BPM01]. **oxygen-induced** [FS05]. **oxygen-transfer** [XYS+03]. **oxygenation** [BB09, TFS+02]. **oxygenations** [YYS+09]. **oxyorthosilicate** [RSDNSB00]. **oxypictides** [YYI+08]. **OY** [Ano07g, GR07c]. **ozone** [BZH+07, LWW+02, LDXW04].

P [GW06b, IAMY02, KCS02, Met05, SYL05, STW+05, SCHW07, YST+05, YYZ+05c, ZCFD02, ZDQF08, BMMC09a, ÇAK07, GSH02, HBW+08, HP07, IV02, JZZ+08, Nic05a, SI09, BMŁT07, COMA03, DLK00, MJ06, Pud02, SKNN09]. **p-** [HBW+08, Nic05a]. **P-450** [Pud02]. **p-d** [ÇAK07]. **P-NMR** [SKNN09]. **P.** [Sut02]. **P.-O.** [Sut02]. **P173L** [XZGZ06]. **P2** [NPLV05]. **P450** [DKD+07, INS+08, SIS+08b, YYI+09]. **P450nor** [Har02a]. **package** [RSM+04a, THPN03, Wol05]. **packet** [AGBY00, GBA05, GB06a, Gög06, HBKG03, MYH03, PW07, SAM08, SLCW04a, SLCW04b, VWB+03]. **packets** [HBKG03]. **Padé** [BB05c, ISS00, PCF05]. **pages** [ND03, Tem04]. **Pair** [AM05, LMJ00, AGLBM03, AD06, CSA09, DS06, Duf07, DD00, Gda01a, HFGL02, Jal07b, KS03a, KES03, LP00b, MB05b, MSS09, MHGR07, MWXL05, NK06, RHHH00, SKSB08, SM08, SRW+06, TYY04, YL04, ZRRC05, ZWSJ01, SC04]. **Pair-correlated** [LMJ00]. **paired** [PML09b]. **pairing** [BS05b, HM01a, HM01b, Kry02, SM05b]. **pairs** [AH06, Ano07f, EKN04, GR07b, HSRP09, KCGB02, KV01, Kry02, Lu06, SD00a, ZLHL02]. **palladium** [BDMS01, LZW+07, MRMR02, OG00, DKR04]. **pancreatic** [HPC+08, PCML08]. **Panel** [Cas00]. **PANI** [IMTG06]. **para** [BHG+06, CNPA04, CC00b, JSC01, SCB+06]. **para-chlorotoluene** [CC00b]. **para-fluorotoluene** [CC00b]. **para-N** [CNPA04]. **para-nitroaniline** [SCB+06]. **para-phenylene-vinylene** [BHG+06]. **parabolic** [PSML04]. **paracetamol** [ABD06]. **paradigms** [MK01]. **ParaGauss** [FSR02]. **Parallel** [MT03, TŠPJ04, BOW+01, FSR02, KN09a, KM00a, PHK+06, SBT+03, TŠPJ01, Zho07, BZG+02, BZG+04]. **Parallelization** [GBL06]. **paramagnetic** [CC01a]. **paramagnetism** [Col08]. **parameter** [AGSH09, BK09, CD04, Col08, FTM06, GHT09, HCL03, Lat03a, Por02, Yar00]. **parameter-independent** [Col08]. **Parameterization** [CFR07, TGG01, AGN04, CDF00, FV04, GGLS02, SSK+05]. **parameterized** [DTT06]. **parameters** [AK05, BBB02, BDBG09, ÇAK07, DLM+05, GD00b, Irg04, Khe09, KSS00, Lat03a, PNG02, Por03, Por04, PJS09b, RPS+07, SRH02, SM06a, SSZ+07, SSDB06, TYSY07, WSNB00, YYY05, dAMM08]. **parametric** [MBA+04, RSM+04b, RMKS08, RSM+04a]. **parametrization** [DZ01, IG06]. **parametrized** [GH03]. **paraquat** [RFF05]. **paraquat-** [RFF05]. **Parareal** [MT03]. **parathion** [FGML06]. **parent** [FPJR03].

parenthood [Kry07a]. **Pariser** [KF02]. **parity** [BBHQ04, KS08, KH08a]. **parity-violating** [BBHQ04]. **Parr** [KF02]. **Parrinello** [KOH03, YZX+08]. **part** [BK04a, BDBG09, IDM+09, PMBM09, VSI+07, AS01, BR08, BR12, DGD+05, FGdA02, FRK+05, FG01, LXH+00, LXTT00, LXHT00, LZYT01, LZHT03, LZT03, RB08, RB11, ZRRC05]. **Partial** [LS01a, BCWS09, BM07b, Her06, KFD09, Kut08, LWCF08, Pyy01]. **participants** [Ano00f, Ano00g, Ano00h, Ano00i, Ano00j, Ano01e, Ano01f, Ano01g, Ano01h, Ano01i, Ano02b, Ano02h, Ano02j, Ano02i, Ano03b, Ano03c, Ano03d, Ano04a, Ano04b, Ano04c, Ano04d, Ano04f, Ano05b, Ano05c, Ano05e, Ano05d, Ano06b, Ano06c, Ano06d, Ano06e, Ano07b, Ano07c, Ano07d, Ano07i, Ano08b, Ano09e, Ano09f]. **participation** [CJB08, KVT04]. **particle** [AVTPR09, Aze02, Aze05, BN04, Bar08, DFMZO08, Gál07, GB09, GAR08b, HM05b, IAL06, Kat00, KG02, Kut03, Mar87a, MOPdP09, OK04, OdSC05, PO03, VWB+03, VATPR09, WD01]. **particles** [BA01, BA02a, CL05b, HN09, Mar00c, Mar06a, Orl07, SSDM05, SW02, Kar08]. **partite** [CT00]. **partition** [DGD+05, JB07]. **partitional** [Tem02a]. **partitioned** [HW06]. **Partitioning** [MNMV02, MRG02, Vyb08, Cam04, CM05a, CCP00, SS02b, SS03b]. **partners** [POMGM01, PRRMLB05]. **Pasquarello** [RRGP05a]. **path** [AG02b, ART08b, BSR02, Cab05, DCD08, DN06, KFD09, LYP+06, YLZ07, YZY+01, ZSWL07, Gri06]. **path-integral** [Cab05, Gri06]. **paths** [CB00, KV05, SCMS07]. **pathway** [BPM01, FGC04a, MDG07]. **Pathways** [VTS05, BBD08, IAMY02, KVSG02, LCCC08, MPRGLL03, VKIJ06, WSBV05]. **Pattern** [CBRBT03, JZK02]. **patterns** [KS03a, Kry07a, PNN08, ŠK03b]. **Pauli** [Kap02]. **Pauling** [CWZ03]. **Pb** [JLAR07, MTE09]. **PBE** [SBL05b]. **PBE0** [WPB+06]. **PbH** [IMT+02, MST04, MST08]. **PbTi** [UES04]. **PbTiO** [SZSP02, SR07]. **PbZr** [SZSP02, ZSPS03]. **PCM** [CCE+07, DDT06, ICRS08, KBMM08, LTY09, MCF08, SAR08, ZZKS07, dAGD08]. **PCM/COSMO** [DDT06]. **PCM/DFT** [SAR08]. **PCNQM** [PSH00]. **Pd** [HGS03, XD03, YLS+04, BCD+05, BC03, DSW08, HGRL01]. **PDE4** [LSWT05]. **PeCB** [SSK+05]. **peculiar** [DLM+02]. **Peculiarities** [LPV07]. **pendant** [MBM05]. **penetrable** [DGC08, MCLKC02]. **penicillin** [LFZ07]. **penicillins** [SCRRE07]. **Penney** [AC02b]. **penta** [TSH03]. **penta-ammine** [TSH03]. **pentacoordinate** [FAE+05a, FAE+05b]. **pentacoordination** [FS05]. **pentadiene** [SBHF06]. **pentagon** [KLK08, MLW+09]. **pentagon/hexagon** [MLW+09]. **pentagon/hexagon-bearing** [MLW+09]. **pentagonal** [LR01]. **pentagons** [LZXD05, LPZW05]. **Pentalenes** [FRK+05]. **pentane** [DQZ04, TGSK09]. **pentaprismane** [LZXD05]. **pentazenes** [BF09]. **pentazoles** [BF09]. **penten** [RMJ+07]. **pentoxy** [LH03]. **PEO** [BKAT00]. **peptide** [CSL+02, FP02, FCD08, HSW04, HOC00, JTC+03, MET00, SSJ09, SWZ01, VK05]. **peptide/bilayer** [FCD08]. **peptides** [AMOR07, Ano06f, CSL+02, HM01c, HMK05, LAS+07, TS01b]. **Per-Olov** [Ano02k, ÖSB01]. **perceived** [Bec05]. **perchlorate** [CLSD+01].

perchlorocyclopropane [MZN+03]. **perepoxide** [YYS+09]. **perfluoropropanoic** [HDWH09]. **Performance** [DLK00, GSCRO08, ZB05, LP09a, SSK09b]. **performances** [KC09]. **performing** [Obe00]. **perhalocycloalkanes** [MZN+03]. **Pericondensed** [BR08, BR12]. **pericyclic** [Gin08, IYY03]. **period** [Kry07b]. **Periodane** [BvRSS07, Krü06]. **Periodic** [JXC05, QLJ+09, ZKEE07, dD04, AK02, Bau09, DFH02b, DSH01, EB04b, EB04a, FD09, Gar08a, KCGB02, Kry07b, LV01b, LTV05, LTV07, Lef06, MOL03, MNV07, Nég00, ND02, ND03, Pyy01, Sce09, ZWMZ02]. **periodically** [SS04a]. **Periodicity** [IKS08, SH09, IKS10, DFH02a]. **permutation** [LP04b, Tem00]. **perovskite** [CIP+03, EKZ06, Mor04, Oni07, Oni08, Oni09, UES04]. **perovskite-like** [UES04]. **perovskite-type** [Mor04, Oni07, Oni08, Oni09]. **peroxidase** [VCHC07]. **Peroxide** [WQ00, BB05a, BB09, DK04, DZ06b, KN08, YZC09, ZYC09]. **peroxides** [MBRA07]. **peroxy** [HWY+07]. **peroxydisulfate** [ĆMTS08]. **peroxyl** [ETM00, ETEA04, ET05]. **peroxynitrite** [Gog05]. **perpendicular** [BBL09]. **Persilacyclacenes** [KAG08]. **personal** [Tay09]. **Perspective** [Sti06, Dro04, EPSC06, ZFLL00]. **perspectives** [AAB05, PS08, TB06]. **Perturbation** [BTL+02, Ada02, Ada05, ABC+06, BB02a, BB05b, CCL03, CDI02, DCTC03, DGR+00, EJ06, FCS03, Fer02, FHHC00, Fra06a, HH09, HBTW04, IBN08, IVK00, IZ04, KSZČ04, KN09a, KJH09, Khe09, KK02b, Kut09, LP00b, LCL+09b, MGK+09, MVK00, MB00, MTWN09, NM01, Ols04, PMHW07, PCF05, Roh00, RS09, RS11, SJE03, SY06, SH09, SKHY09, SSS02, Yam04, Yam05, ZT02, Zno00]. **Perturbational** [SK03a, SPH00]. **perturbations** [DGD+05, Gin06, Mai05]. **Perturbative** [AAB05, BG00a, BČ02, HMW02, PS03b, SS02b, UP03, ZT04a, RS00]. **perturbed** [DPW00, Gin05b, Gin06, KCGB02, MOL03, MH06]. **perylene** [ABI07, ZNF05]. **PES** [BES08]. **PET** [DKWP04]. **PH** [MOAM07, RD00, YW05, WML08, CSTB08, HW02, FGZ07]. **Ph.D** [Ano02c]. **Ph.D.** [Ano02d]. **pharmacological** [KM03a, KM03b, KM04]. **Phase** [FFFR01, Mar00c, AGM01, Ano07g, Ano07f, Boe09, Bra08, CQN+03, CN03, Cor04, DF07, DLM+04a, DKP+06, FGC04a, FSK05, GR07c, GR07b, GTR+05, GMS01b, GMS01a, HE05, HKE05, HDWH09, IAMY02, JTC+07, JPMM08, JV05, KM06, LDR+08, LS05, LYDK02, MRTT01, MRST01, MTRG04, MMT+07, Mic09, MWW+00, MBK01, MCC08, MGMP01, Mor08, METSH02, NY01, NY04, NSLR04, OA05, PJZ+09, PGF+06, PMLC05, RI05, RJB+06, RF01, RHM05, Rua09, RSTG02, SSC+07, Shi04, SCB+06, SM05c, SM08, SMB09, TGGV+04, USM01, VX04, WAJ04c, XYS+03, XV00, ZR07, ZLL+05, ZDMF08, ZTW+09, ZFD00b, ZMZ+00, FFFR02, Pan05]. **phase-breaking** [JPMM08]. **phase-space** [GMS01b, GMS01a]. **phases** [Bra08, CME07, EYBM03, GM05a, Mar00b, MS05, NNS+00, RI03]. **phenalenyl** [CIT+03]. **phenalenyl-based** [CIT+03]. **phenanthroline** [IABS08, MGMR04]. **phenethylamine** [KM04]. **phenethylamine-type**

[KM04]. **Phenol** [CGCS02, Bar09b, GS01, HEBS00, JWZ+08, LJL09b, SC02b, TW05b, ZRF+09, LJL09b]. **phenol-pyridyl** [ZRF+09]. **phenols** [GSH02, HY04, JB07, KS09, Lav03a, dSNBG08]. **phenomenological** [MC08]. **phenothiazine** [OOD+05, PGNT02]. **phenoxyl** [Bar09b]. **phenyl** [DCO+08, SWSH09, TNJL05, WJLL09]. **phenylalanine** [DSW02]. **phenylalkyl** [ZMB+03]. **phenylazonaphthalenes** [GLX+00]. **phenylboronic** [DDP+07]. **phenylene** [BHG+06, GCG05, RFF05, TOK+00, YYYM01]. **phenylene-linked** [YYYM01]. **phenyleneamine** [GG03]. **phenylenebiscarbene** [Nic05a]. **phenylnitrenes** [JSC01]. **phenylquinoline** [OOD+05]. **philicity** [CSPS05]. **Phonon** [Boh03, Boh01, SKHY09, Tou09, YYK+03]. **phospha** [WW07]. **phospha-naphthalene** [WW07]. **phosphanes** [BBD08]. **phosphasilacyclohexane** [SL09]. **phosphate** [Buc05b, KNO09b, LYDK02, PFSP05]. **phosphides** [GW06b]. **phosphites** [NMNB06]. **phosphodiesterase** [OSW07, SWST04]. **phosphodiesterases** [SOEW08]. **phospholipid** [PFdP08]. **phosphor** [SV08]. **phosphorescence** [Cat05]. **phosphorescent** [ZLL+09b]. **phosphorus** [COMA03, JMP05, LČM01]. **Phosphoryl** [JTC+03, GGLS02, HH03]. **phosphorylation** [CTLZ01, JZW+09]. **Photo** [Ano02l, Ano02g, Ano09g]. **Photoabsorption** [BIP+07, MVL+01, GFMT08, TB03]. **Photoactivated** [ZLS07]. **photoassociation** [NWSC08]. **Photochemical** [CY04, BDMS03, CWY05, Bro00]. **photochemistry** [ZB08]. **photochromic** [PMBM09]. **photoconversion** [SMM02]. **Photodetachment** [MB00, Mon05, Mon08]. **photodimers** [RVR00]. **photodissociation** [Bro07, DGLM09, LBMVDL06, LML02, LA09, LSL+08, MMV04, NWSC08, Sad00, SCSWF04, TSS+09, ZMX+05]. **photodynamic** [KM06]. **photodynamics** [QCC02]. **photoelectron** [HLMH07, LWC01, UMDM06]. **Photoemission** [ZW09a]. **photoexcitation** [MY00]. **photoexcitations** [dFGM08b]. **Photoexcited** [RNS04]. **photoinduced** [DKWP04, LLZ04]. **photointermediates** [SB03]. **Photoionization** [DBLM06, CS07, FM02a, LS01a, MMV05a, VML05]. **photoisomers** [OA02]. **photoluminescence** [CGL+05]. **photolyase** [ZLS07]. **photolysis** [CWY05, ZDAZ03]. **photon** [Gri06, Guo09, MHV00, NNNY01, UKAM04]. **photon-in** [Guo09]. **photon-in/photon-out** [Guo09]. **photon-out** [Guo09]. **photon-stimulated** [MHV00]. **photooxidation** [HZW+08]. **photophysics** [BA06, ICRS08]. **photoproducts** [MUL02]. **photosynthesis** [RHHH00, SN02]. **photosynthetic** [HYC+00, SZZ01]. **photovoltaic** [JMEM07]. **phthalocyanine** [CJB08, GXT02, GXGT02, ZDO09]. **Phthalocyanoiron** [MOAB01]. **phylogenetic** [WLWZ06]. **Physical** [Kry08a, Alc04, CIT+03, GJB02, GS00b, GS01, Kap06, Koz01, NWZ+07b, Pog05, RMB00, ZŠ05]. **Physicochemical** [SCES03, SCRSRE05, SCRSRE06, SCRRE07, SCRE08, ŠK03b]. **physics** [Brä06, DES03, Fri06, GSPT+07, Mat00, NU09, Tem02a, DT02a, GDV05, Nag03c, PČ04a]. **physiological** [KPP01]. **physiologically** [Bec05].

physisorbed [LTV05, RPHG04]. **Physisorption** [ZHS06]. **picosecond** [DBFP05]. **Picture** [Kry08a, CM02b, Kap06, Kry08b]. **piecewise** [MEN+08b]. **pigment** [BL02c]. **pilot** [EBS+09]. **pinene** [Bou03]. **Pinney** [Kry09]. **Piris** [LP07]. **Pitaevskii** [GBL06]. **pK** [GS00b, GS01, HSH02, KS09, Sey08]. **pKa** [SDS04]. **PLA** [DCO+08]. **placed** [SDZ+07]. **Planar** [WW07, GJ03, Kle03, MDBM05, MZMZ09, Nég00, RLB02]. **Planck** [Chu02, Chu04, Chu06, Chu07, Chu09]. **plane** [Buc02b, Čár07, Čár09, ESTU05, MWW+00, NM01, ND02, ND03]. **plane-wave** [Čár07, Čár09, ESTU05, MWW+00]. **plants** [BKM+02b]. **plasma** [Bel04, BSM+07, KPP01, SM05a, SSM05, SM06b, SBM07]. **plasmas** [BVSM04, KH06]. **plasminogen** [DSFS00]. **platelets** [ZHS06]. **platform** [VWSA+04]. **platinum** [AP00, Bou01, DAD+03, Men08a, MRMR02, NWZ+07a, OG00, SD08, XCW07, BZL+09, PBSC04]. **Plesset** [MNMV02, CK09, FHHC00, Fra06a, HH09, IBN08, IVK00, KN09a, RS09, RS11, TB09]. **PLS** [BSKFT07, KFTBS07]. **plus** [DSLC05, DLCY+07, HTN07, Mar03b, Nak07]. **plutonium** [Boe03, BR05]. **PM3** [FRGF04, CDF00, DSFS00, FDL03, KKYT04, MPBM07, PSS05]. **PM3-based** [PSS05]. **PMe** [DR08, WML08]. **PMO** [SPH00]. **PN** [MJ06]. **PNA** [NID+06]. **Pocket** [RGP07, NPLV05]. **pockets** [JCTD08a, Jal08c]. **point** [BL02a, Buc00b, CB04, CFP00, Chu07, Chu08, CTP+08, CT00, DLHP04, Fan01, Fri06, Hog09b, IPPL05, Kry02, LL01, LCK00, Mor04, PC07, SMB09, Tem00, VAS06, YHN+07, ZT04b]. **point-charge** [BL02a, CTP+08, DLHP04]. **point-group** [Fri06, YHN+07]. **points** [BES08, Pup05]. **Poisson** [ND03, AH06, ND02]. **pol** [AYD00]. **polar** [HM05a, LLW+07, LDR+08]. **polarity** [DBB+06]. **Polarizabilities** [CK09, SN06a, ASTO02, BB00, CTS08, DHZ06, JÅM01, JBMP03, JMP06, KCGB02, LCK00, RPB00, SCB+06, YSV05, YCN+07, ZB05, ZWJ02a, ZWJ02b]. **Polarizability** [KMS02, CGG05, JÅM01, JMP04, LFK06, MGC00, OBM06, SO04a, SMS+02, SHE+02, TC07, ZBPD08]. **polarizable** [AYD00, BBDS06, CCM+05, HLP07, SSN01]. **Polarization** [Pai00, PA02, Ada09, BM01a, BTK+05, DC05, ET09, FM02b, GGAMB03, HK09, KM00c, LCT00, LCBC03, MC08, MPIP+01, RRPJ07, SMEA08, WL00]. **polarized** [AZ08, Boe03, LHG00, ZB05]. **Polaron** [LLSY05, PM06b, PM06a, FdONGM08, GDB03]. **Polaron-induced** [LLSY05]. **Polarons** [MD08, AIG02, DM03, SP00, dBM05]. **pole** [AGB06]. **poles** [RE06]. **politics** [Mon00]. **polluting** [PMCOSC00]. **poly** [BHG+06, BKAT00, GCG05, MLD06]. **polyacenes** [ACPG01]. **Polyacetylene** [PM03, För00, GM05b, GM05a, JPA05, KCGB02, MSC05, ZWJ02b, FdONGM08, dFGM08a]. **polyamide** [PVB+03]. **polyamide-6** [PVB+03]. **polyamides** [PVB+02]. **polyaromatic** [HVC08, LSPS01]. **polyaromatics** [VHWM04]. **polyatomic** [ABLL02, CGS01, HN03, May06, MZD+05, MY09, PJ03]. **polyatomics** [Hog09a]. **polyaza** [GBJM01]. **polyaza-compounds** [GBJM01].

polybutatriene [KCGB02]. **polycarbonates** [VWMS03]. **polycarbonyl** [PB03]. **polycyclic** [DFMZO08, GBJM01, RLB02, TCM09, TBCG05, WW08]. **polydiacetylene** [KCGB02]. **polyenals** [PREM04]. **polyendials** [PREM04]. **polyene** [LP09a, MKHP09]. **polyenes** [GB03, GWK+05, PREM05, QC02]. **polyenones** [PREM04]. **polyethylene** [LQC06]. **polyformamide** [TSZW08]. **polyhedral** [CT00, MFA00, Tem00, Tem02c, Tem04]. **polyhedron** [BK04a]. **polyheteroarylethynylenes** [GKE01]. **polyhydrido** [LH07c]. **polyimide** [PRM02]. **polyketides** [dLCRF+08]. **polymer** [FFHD00, HK06, IA06, ITR02, JFC02, JMEM07, SDB03, TDF09]. **polymer-chain** [SDB03]. **polymerization** [CCA+06, ĆMTS08, CP06, CL08, GST+05, HBW+08, KP02, KP05, MGMR04, TBJA03, TVK+02, VHV+05, XFLX+06]. **polymers** [DM03, JC00, MOAB01, PM06a, PM06b, PVZV00, PKB+01, PO05, PGPA09, RCF02, SK05b, Spr00, TVK+02, Ver05, VGM05, dBM05, dFGM08b, JC01]. **polymethine** [IDM+09]. **polymethineimine** [JPA05]. **polymethineimine/polyacetylene** [JPA05]. **polymethines** [TDST07]. **Polymorphism** [KK02a]. **polymorphs** [Seb05]. **Polynitrogen** [CLL04]. **polynitromethanes** [SCLL07]. **polynomial** [Bar08, Fer09, GKYY06, HdMB+05, MBM05, Mar08]. **polynomials** [CXZ09a, DCA03, Fle06b, PMZGGR04, SN06b, WRW02, XZ07, YYZ05a, YY04]. **polynuclear** [BT05, OD03]. **polyoxometalate** [SCW09]. **polyparaphenylene** [VSD+02]. **polypeptide** [HPC+08, PCML08]. **polyphenylene** [GG03]. **polypyridyl** [SMM02]. **polypyrrole** [LLSY05]. **polyradical** [NKS+09, YKT+02]. **polyradicals** [TYY06]. **polysaccharides** [BCFR08]. **polyselenophene** [ML03]. **polysilanes** [PKB+01]. **Polyspherical** [IG06]. **polysulfone** [PRM02]. **polythiophene** [CB03]. **polyvinylformyl** [Por01]. **polyyne** [MBK01, YZW+08, JC00]. **polyynes** [SWSH09]. **Poor** [FWT08]. **Pople** [Ano04e, DKS05, KF02, ÖS05b]. **Population** [CD03b, Gri06, BDMC06, MH05, MCN+05, OYB+00, PTLB00, PC04b, SRA09]. **populations** [AG01b, Kar04]. **pores** [LHTV05]. **porphycene** [WKF+06]. **porphyrin** [CJ03, JLI+01, KSN+04, NIS+05, SE02a, SIS+08a, SPSS07, TN09, YYYM01, ZZKS07]. **porphyrins** [Yam09]. **Pöschl** [DL02]. **posed** [Mar05b]. **Position** [POM+08b, MSJ04, MOPdP09, POM+07, SHZGP09, SMT06]. **Position-dependent** [POM+08b, MSJ04, MOPdP09, POM+07, SHZGP09, SMT06]. **positional** [Pri05]. **positions** [CCR09]. **Positive** [Dou07, CJdC01, PI02]. **positively** [MSC05]. **positron** [GSPT+07, MAS09, VNB+03]. **positronium** [BEL01, CSSB02, DM02a]. **Possibilities** [KKM+01, KTH+05, BvRSS07, Lad00]. **Possibility** [Eva04, KNN+04, MSS09, SGS00b]. **Possible** [CIP+03, GSPT+07, KH01, Sch04, ZSKV04, BJAV08, FGC04b, IK00b, LRB04, MS00, MPBM07, QCC02, SM05b, SMB09, TTM07, VBS+04, YZY+01, ZCZC09]. **post**

[DGRB08, EP02, PRL01, TOK+00, BČZ07, SGHL00, RP09]. **post-Hartree** [DGRB08, PRL01, TOK+00, SGHL00, RP09]. **post-HF** [EP02, BČZ07]. **posteriori** [HMW02, May04]. **postprocessing** [FSLL02]. **postulate** [AT07, Kap02]. **potassium** [BCG09, TRMM04]. **potent** [ASL04, CSL+07]. **Potential** [BS02, BAKK06, BES04, BMMC09b, Gog05, LBSB08, MZD+05, RA03a, ŠŠU+02, TT01, VSS04, YŞ02, ZD08, AS04a, AA04b, ATN09, AD07, AG01a, ARE02, ART08a, BKM+09, BBHQ04, BZ06, BB07, BBC07, BJ00, BBD07a, BFB08, Bou01, CSG06, CBA+06, CNPA04, CDH05, CT05, CCB07, DRPT02, DI05, DBG04, DL02, DLF02, DSLC05, DCLC05, DLCY+07, DN06, DZ06a, DDBF09, DKW09, EB04b, FFFR01, FRGM06, FOM+03, FB07, FTM06, FYSS09, FCD08, GGACT03, GSRL06, GY04, GG07, GMK+09, GGS09b, GSB00, GB06b, HV03, HS02, HM01c, HAL+02, HBTW04, HK09, HLP07, HMMT04, HM05c, IDM+09, JLAR07, JTC+07, Jal07a, JCTA08, KZ08, KM03a, KM03b, KB00, KCS02, KF03b, Koh01, Koh02, KPTŚ03, KDM00, KZ09, LFK06, LFADSF07, Lav03b, LJL09a, LPL04, LSM05, LMSB00, LXY00, LWCF08]. **potential** [MZF05, MGdS+08, MA05, Mar87a, MARK08, MMV04, MSJ04, MK02, MOPdP09, MSC03, NFG05, OdSC05, Pai00, PA02, PRSLA08, PC07, PBS02, Pej03, POM+07, PBI+01, PW09, PHNN09b, PB09, QS00a, QS00b, QTT07, RLBK03, RJB+06, RV05, RJP08, SSDM05, SSMG08, SAM08, SHZGP09, SBM00, SSB00, SSK09a, SSZ+07, Shi05, SD06, Tch07a, TG05, TA06, TR09, TB03, TGG01, VRSF02, VLJ08, VGMN03, VGB05, WAJ04a, WAJ04b, Wyb02, YAŞ00, Yal04, Yam04, Yam05, Yan06, YHD+07, ZLZ05, ZW03, ZW04, ZWM+04, ZLY+09, RA04, FFFR02]. **potential-based** [SAM08]. **potentialities** [DFH02b]. **potentials** [Ada09, AYD00, AK05, ABGS00, BB06, BCdP03, BBM+00, Cou05, Don09, FGR+07, GMPIP01, GSB00, Gus02b, Gus04, HV03, HM03, HWPIM01, Kap06, KAE03, KAE07, KH08a, KM00a, KJW08, KM00c, LME03, LCT00, LSM05, LK02, LZZ+06b, MY08a, MY08b, MGK+09, MOPdP09, MPIP00, MPIP+01, Nes01b, Nes03b, Nes04b, Ort04b, PM06a, PCS09, PS07, POMGM01, PRRMLB05, POM+08a, PGB00, PMPI01, PLC02, PMC02, RBA07, Roy05a, Roy05b, SMY07, SG03, Sch02, SY07, SNH00, SC01, SGS00b, SS09c, STL+09, TTM01b, VTP09, WZ06, Win04, YS06, ZMMK09, Kry08a]. **potentiometric** [EGEDH03]. **power** [CTSÖD03, Mon00, NF02, Por02, Por04, SO09a, WO04]. **powerful** [Mak07, Van06]. **powers** [HM06b, PRM02]. **PPAR** [XCS+03]. **PPh** [YLS+04]. **Pr** [KNO09b, RSFRDNA04, SNN+09]. **Practical** [BBG00]. **pralidoxime** [CFV02]. **prebiotic** [JTC+03]. **precious** [OKY+08]. **precise** [TMPI05, ZWMZ02]. **Precision** [Koz04, JJ00, SH02b]. **precursors** [LRB04]. **predict** [Bar09b, BBSS00, CR08b, CR08a, MC03, Str00]. **predicted** [MLP07, TG01]. **predicting** [GSH02, OD03]. **Prediction** [FGH09, Mal02, NFFA04, PMAA00, ŠK03b, AAB05, DS03, JBMP03, LLR+00, LP00a, MMV04, May02a, Pal00, PGN+05, PLO02, PMLC05, RH03, ŠK01c, YBS05, MST08, WQ00]. **Predictions** [Ano02m, AGM06, LS05, PGF+06, Pol06, VRS01, ZMZ+00, ZWJ02a, CT05, KIK09]. **predissociating**

[ELY09]. **predissociation** [FL04, MB02a, Sha06]. **Preface** [AT03, Ano01j, Ano02m, Ano07h, BCC05, BvL06b, CA06, CB08, ČN07, DL03, DT02a, EL06, GDV05, LSS09, Les04a, Les04b, Les05, Les06, Les07, Les09, MLB04a, MLB04b, Mav05, MMOM09, Nag03c, PČ04a, PMB06, SD03, VM06b, VM07a, WBM09, WV02]. **prefactors** [Pan05]. **preferable** [Sha04]. **preference** [FDLK02, HGTW03, Tri03]. **preferences** [AB08, WT07]. **preferred** [GS05, GI07]. **Preformed** [SM08]. **preliminary** [BSKFT07]. **Preopening** [KV01]. **preorganized** [ELO+07]. **preparation** [KSK+04]. **preparing** [ZFZ+08]. **preresonance** [MP05]. **prescribed** [Ou06]. **presence** [Lef00, Mon05, OR07, SS04a, SS05a]. **present** [SC01, ZA09]. **present-day** [SC01]. **preserved** [DJNH02]. **Pressure** [ZMZ+09, Boe07, CN00, Cor04, Eva04, RHM05, VRA+02]. **pressure-induced** [Eva04, RHM05]. **previous** [Dat04]. **Prigogine** [AGL04a, Ant04, Brä04a, Mar04b]. **prilocaine** [PFdP08]. **primary** [AV02, Irg06, SN02]. **Principal** [CDH05, Gus03, ÖO02, Özd03, Özd04, TPGD02]. **principle** [BSCB04, GD00a, JK00, Kap02, KPSH06, MGG05, Nes04a, VVBT07, ZY06, ZDQF08]. **principles** [Boe07, BKM+02b, DC03, FGFF06, FG03, GWJ05, HCRHM03, IOA+04, IN09, JMEM07, JLM08, JXW+04, KS07, LZW+07, MAS09, MC08, MTO+03, Mor04, MGAS09, Noo03, OCWY09, POV+03, RPPO00, RRGP05a, RRGP05b, RP00, Seb05, SSDB06, SSK+05, SB04, TCM09, TM05, VPS+05, WL00, XR05, YT03, ZXZ+09, ZA09, IG06]. **priori** [May04]. **probabilistic** [Gui06]. **probabilities** [BP04, ÇAK07, GBA05, Gög06, LLR04, PSN08, ŠUKŽŠ07, ZZM09]. **Probability** [ACG04, ZSW+00, dAMM08]. **probe** [KV07, NRS+02, PML09a]. **Probing** [DC06b, HLMH07, MET00, ZW09a]. **problem** [ABB+07, AAB05, BGN+05, CCL03, CDI02, EBR07, FT04, FPJR03, Gin05a, KV02, Kut03, LMJ00, MNR07, Mer04, Muk00, Pan01, Pan02, PMHW07, PCF05, PB04, SB06b, SST+03, TPGD02, VSBD06, VMRA04, Wil04a, Lin06]. **Problems** [Kap07, BBB02, Brä06, BRZ09, CL05a, DMMV00, Fis00, GQ00, HFS04, HFS06, Kar09, Kar10, MNA+99, MSB00, NF03, NU09, Sal09, Zot06]. **procedure** [BvRSS07, GSD+03, LSH08, Man05, MNMV02, NS08]. **procedures** [RS06]. **Proceedings** [Ano02m, BCC05, CA06, CB08, DT02a, Nag03c, PČ04a]. **process** [CDDM05, CL08, FGZ07, GJB02, GARB08, HBW+08, NK06, OMNN04, SMM06, Sko02, SIT+06, TSS+09, YYZ+05c, YWZ+09]. **processes** [AA09a, BK04c, Buc07, CR06, CM05a, CBB01, FPC+03, GMCS04, GKL+09, Mal05b, MVL+01, PD05, PMC02, SINN05, SS03b, TBM04, WKF+06]. **processing** [Bar03, DAA+06, KMM+07, LLB01, SY07]. **produced** [CC01a]. **produces** [Cat05]. **product** [BMMA06, BAG+08, DAD05, Gün06, MBA+08, RA02, TTM01b]. **products** [BB09, CD03a, JRSA08, LH03, PKZN08, Tal07]. **Professor** [JS08]. **profile** [dA08]. **profiles** [ACA02, ADSTS06, NTB02, Tou09, VV05]. **program**

[FSR02, JJWH04, RLA+01, THPN03, TŠPJ01]. **programming** [QW05, SB06b, TŠPJ04]. **programs** [MVG+04]. **progress** [Brä09a, MHV03, SH01, SMB07]. **projected** [KC09, KSN+09]. **projectile** [CTSÖD03, Por03]. **projectile-** [Por03]. **projectiles** [Por01]. **projection** [CD03b, KSI+07]. **projective** [Tem02b]. **projector** [EWCT+05]. **prolapse** [DHCD06]. **prolapse-free** [DHCD06]. **prolate** [LLB01, MCLKC02, Rom08a, Rom08b]. **proline** [CMR05, FWT08, MRTT01]. **promising** [LCCH09b]. **promolecular** [ACD02]. **promoted** [DR08, ZSKV04]. **Promotional** [GBMMSA00]. **Proof** [QS00b, Kry05, Kry06, Pup07, SDW07]. **propagation** [BA02b, HBW+08, Kon04, Wal04b]. **propagator** [AGM06, AM06, DPW00, DZO00, DFMZO08, MY08a, MY08b, MV02, Ort03, SSA07, SMY07, SFZO01, ZDZO07, ZDO00]. **propagators** [DZS+06, SDZ+07]. **propanol** [ZTW+09, ZH05]. **propene** [RD00]. **propenethial** [RJN+08, RJF+09b]. **propensity** [MET00]. **propenyl** [FBC+06, HJT07]. **propenylamine** [RJF+09a]. **proper** [BN04, GSB00]. **Properties** [AFC03, BM01a, KSWR00, SKT05, AV05a, AV06, ABI07, AC07, ALM05, ASL04, ASRL06, AMC07, BZL+09, BF07, BF08a, BČZ07, BBD07a, BBD07b, BBD08, BA01, BA02a, BSCB04, Bor00, Bra08, CJ09, CDV08, CLSD+01, CXZ+09b, CIT+03, CDDM05, CMASC01, DCW03, DT00, DDD02, DW00, DPW00, Den09, DGRB08, DCLC05, DLCY+07, ETEA04, ET05, ES02, ER05, ELG05, EP02, FH02a, FL04, FG01, FPC05, FCLH+06, GBJM01, GBS04, GR05, GLX+00, GXT02, GXGT02, GGPS06, GSPT+07, GS00b, GS01, GP03, GW06a, HCRHM03, HGRL01, HEBS00, Hog04, HLH05, IABS08, IMTG06, Iye09, JJ02, JMEM07, JHLC09a, Koz01, KY00, KZ09, KDF00, KBMM08, LDMR01, LW05, LTV02, LTV03, LDPP05, LDP05, LVM01, LXH+00, LWL+08, Liv02, MMM06, MLW+09, ML05, MLD06, ML08, Mar00a, Mar00b, MCR03]. **properties** [Mar06b, MVdCD00, MOL03, MCLKC02, MNJP05, MD04, MBD05, MWW+00, NFT+01, NID+06, NRK+05, NWZ+07b, dlPOPP03, OBK00a, OBK00b, Oni07, OA05, PRM+06, PK01b, PML09a, PBMA03, PHNN09a, PMO04, PDR+00, Pog05, Pol06, PMAA00, QS00a, QS05, QXJG05, QLJ+09, QZ07, RKM09, RMB00, RBLS04, RdSH08, SR05, SLRS02, SRO02, SYZ+09, SL00, SCW09, SSM05, SM06b, SM07a, SK05b, SSF02, SNdAM08, SWSH09, SCES03, SCRSRE05, SCRSRE06, SCRRE07, SCRE08, SCHH02, Spr00, ŠK03b, SZSP02, SR07, SUH+01, SRHR05, SHM+09b, Sun06, TIV+07, TCS+08, TKS+05, TMAB01, TMPI05, TMS08, TWSK09, TL05, VTA+02, VATPR09, VCF+00, VRFS05, VDF+06, VGB05, VSBD06, VG06, VB04, WRRF03, WZW+09, WGX09, XXJG04, XC07b, YST+05, YHC05, YS09, YZW+08, YNDJ06, YZY+01, YPS05, Yur07, ZSPS03, ZFD05, ZFD+00a, ZXZ+09, ZMZ+09]. **properties** [ZLL+09b, ZNF05, ZDQF08, ZRF+09, dOEG+08, EJ06, LZT03, Bar09b]. **property** [ANJ09, Dya00, KM00b, KSN+04, RW04b, SQZ+02, SNN+09, WGD01, WWW+07]. **property-directed** [KM00b]. **Proposal** [SM05c]. **proposed** [SGLF01]. **propyl** [CdMCS05]. **propylphosphonates**

[CdMCS05]. **propynes** [Iva05]. **propynoic** [NSLR04]. **protease** [FA00, NTB02, NPLV05, TGG01, ZZ05]. **proteases** [ŠFW00]. **Protein** [Han02, HKMM04, JLZY09, SGLF01, WGD01, AV02, BLC09, Bar09b, BBL09, CFM+06, CR08b, CR08a, CBWM09, DCP01, DJNH02, GHK05, JJC+06, JZW+09, KF07, LLR+00, MMR+04, Muñ02, NSZZ04, NSG+06, RO01, SWZ01, ŠK01c, ŠK03b, VED+02, YZX+08, ZZZ+08]. **Protein-folding** [Han02]. **protein-structure** [LLR+00]. **protein-zinc** [DCP01]. **proteinases** [HNR06, HP07, KVSG02]. **proteins** [AT00, DSW00, DSW02, FJK+01, HEBS00, LGJP05, Les03, LW07, RSL+03, SKN+09a, SKMW00, SMOE02, SZZ01, ZMS05, FJK+02]. **proteome** [LLLZ07]. **proteomics** [Ran02]. **Proton** [CNT+09, JM00, QDÖ09, RS06, YWZ+09, ABL03, BVHS05, Bro05, Buc08, DSL06, DLM+04b, GBB06, HKE05, IS03, IKS08, IKS10, KSBK08, Kry02, LTV07, MSS09, Mor06, Mor08, METSH02, NIS+05, SK06, SNT+00, SL05c, SBL05a, WKF+06, XXC08, YZX+08, YYQ+06, ZZDY06, ZZZ+08]. **proton-** [SNT+00]. **proton-substituted** [LTV07]. **proton-transfer** [MSS09]. **protonated** [AG02a, DKC00, SST00, ZTI+07]. **Protonation** [CJZZ06, DDP+07, BRL02, GYS+06, HE05, SCW09, SS09c, TX02, XXC08]. **protonic** [ITN06, ITN08]. **protons** [RLBK03, ST01]. **protoporphyrin** [GdRPLP08, Pud02]. **Prototropic** [TX02]. **prototype** [NTB02]. **prototypical** [PML09c]. **provide** [WLZY08b]. **pseudo** [FTM06]. **pseudo-potential** [FTM06]. **pseudopotential** [DLK00, HDL00, HSB+00, MA05, MWW+00, RBLS04, ZJZ00, RIVB03]. **pseudopotentials** [AA04b]. **Pseudoprecession** [Hag00]. **pseudoresonances** [MSC03]. **Pseudorotational** [Hag01]. **Pseudospin** [DLM+05]. **PsHe** [Str00]. **PSII** [WE01]. **PsLi** [Str00]. **psychedelics** [KM04]. **Pt** [HGS03, MOAM07, MBOA09, SBK+09, MSJ04, SS03b, BLC+00, CBC00, DSW08, GSfLV08, HGRL01, LJL09a, MOAM07, NAE06, BVS+09]. **PT-symmetric** [MSJ04]. **Pt/MFI** [NAE06]. **PTCDA** [ZNF05]. **PtCl** [MLZS06]. **Pu** [HR05a]. **Publications** [Ano09a, Ano02d, Ano02f, Ano06a, Ano09b, Ano09d]. **Publisher** [Ano04e]. **puckering** [FB07]. **pull** [BRR04, GB03, GFMT08, PJ07]. **Pulse** [Mal05a, GLHH09, Mal07, BKM+02b]. **pulsed** [RGMP06, SSA07]. **pulses** [FGM05]. **pulseshaping** [Pöt01]. **Pure** [OA03, Pan02, AV05a, AV06, KSK+04, MSK+05, Sko02, SP00, AML+01]. **pure-jump** [Sko02]. **purine** [MMT+07, MHGR07, SST00, TOC06]. **purine-ring-protonated** [SST00]. **purinic** [ZDZO07]. **push** [BRR04, GB03, GFMT08, PJ07]. **Pushing** [LM02a]. **PW86** [SC01]. **PW86-PW91** [SC01]. **PW91** [SC01]. **pyramidal** [Buc07, GJ03]. **pyran** [YYXC01]. **pyrazolate** [BZL+09, SS08a]. **pyrazolate-bridged** [SS08a]. **pyrazolo** [SSB+07]. **pyrazolone** [DCO+08, WJLL09]. **pyrene** [SBB05, KES03]. **pyridazine** [ZPW+04]. **Pyridine** [IPPL05]. **pyridinyl** [WWW+07]. **pyrido** [DKC00, PCKC08]. **pyrido-di-indoles** [PCKC08]. **pyrido-pyrrolo** [DKC00]. **pyridyl** [BVS+09, PK01a, ZRF+09].

pyridylcarbonyl [BT05]. **pyridylethene** [LTL06]. **pyridylimidazole** [LSK+06]. **pyridylmethyl** [CLSD+01]. **pyridylpyrazolate** [BZL+09]. **pyriformis** [SKSS09b]. **pyrimidine** [MMT+07, RVR00, TOC06]. **pyrimidinetrione** [DB06]. **pyrimidyl** [GMTM02]. **pyrolysis** [CX00, WGX09, ZTW+09]. **Pyrrole** [KVZT04, KVZ+02, Pej03, TTK02]. **pyrrolo** [DKC00]. **PZT** [SM09].

Q [CDB02, dOEG+08, YYYM01]. **q-integral** [dOEG+08]. **Q-like** [YYYM01]. **QB3** [DPS04]. **QCMEE** [JG00]. **QED** [GMCS04, GAL+05, Lin06, LSH08, Mal05b, OY01]. **QED-SCF** [OY01]. **QM** [Han07, AYD00, ALI03, Bol04, CdMCS05, CDS06, CRRL01, FJK+01, FJK+02, KAN+09, LTV07, MMCC02, MPRGLL03, NRK+05, SBB05, Shi04, SBF+04, Swa03, TT04b]. **QM/MM** [AYD00, ALI03, Bol04, CRRL01, FJK+01, FJK+02, KAN+09, MMCC02, MPRGLL03, SBB05, Shi04, SBF+04, Swa03, TT04b, NRK+05]. **QM/MM-pol-vib** [AYD00]. **QM/MM/continuum** [CRRL01]. **QM/QM** [Han07]. **QQSAR** [CD00]. **QR** [BB05d, BB02c, BB04]. **QR-SCMEH-MO** [BB05d, BB04]. **QSAR** [CD00, CDB02, CSL+07, JHR+00, LQC+08, LQM+09, MK01, PSS05, PRS+09, PS04, PBTP06, RACD00, SPS05]. **QSCP** [Ano07i]. **QSCP-XI** [Ano07i]. **QSPR** [CDG05, MK01]. **QSTR** [SKSS09b]. **QTAIM** [NS08]. **Quadratic** [PCF05, BČ02, FZRD07, Pej02]. **quadratically** [YM05]. **quadrature** [BS06, Fuk09]. **Quadricyclane** [LSBDL02]. **Quadrupole** [HL05, LV01b, AC08, GHH03, HW02, KM02, SMS+02]. **quality** [DDD03, RLER04, XVB05]. **Quantal** [SS06, SS01, Mar03a, QS00a, SS04b, SL05b]. **quantification** [BB05c]. **Quantitative** [HSN+09, MEN+08b, SFD09, CDV08, PCKC08, SKSS09a]. **Quantization** [BM01b, Mla02, Don09, MBP01, PSML04, YM05]. **quantized** [NY03, OMC04]. **Quantum** [AV06, AC05, AWZD05b, AKK05b, Ano00d, Ano06g, Ano07a, Ano07g, Ano07e, Ano07f, Ano08c, BPM01, BS00, Boh01, BB05d, Brä04d, BBSS00, Buc05c, BMP+04, CNPA04, CMS04, CSSB02, CS00b, DKD+07, DDW+06, DG04, DT02a, DLTW04, DLM+02, DLM+04b, DCLC05, DDD+00, DK04, DDBF09, ESKB04, FL04, FAE+05b, FPC+08, FYSS09, GJB00, GB09, GMS+05, GBA05, GB06a, Gög06, GSK01, GM05b, Gus03, HGB08, KS03a, LLR04, LBMVDL06, LXH+00, LXTT00, LXHT00, LZYT01, LWW+02, LZHT03, LZT03, LFZ07, LVSG06, MGdS+08, MB05b, MB05a, Mar06a, MHV00, Mic06b, MME09, MBK01, MB01b, MSK+05, NW01, NY01, NY04, NKP+02, ND03, OYYY02, PIGN02, PSK02, PLO02, PW07, PSEP05, Pol06, Pöt01, PSA05, QTT07, RVP06, RACD00, RAdS05, Saa00, SSMG08, SST+02, Sco00, SC02a, SC04, SRO02, SGGBB02]. **Quantum** [SSB00, SSJ09, SZZ01, SK01b, SK00b, SdACAG03, SCRSRE06, SM05c, SM09, SQZ+02, SCMS07, TSN+05, Tem04, TL05, VLJ08, Van06, Var07, VG02, YTS+05, YZ07, ZVVT07, ZTSZ07, AGBY00, AM09b, ABB+07, ASDC08, ASP+05, ASM+03, BGGS08, BFRB07, BF08a, BNS05, BZG+02, BZG+04, BMB02b, BR05, BBPG08, BKRT03, BTK+05, BČ02, Bra08,

BOW+01, CD00, CDB02, CDG05, CDV08, CW08, CSDCCMZT03, CF04, CTP+08, CBRBT03, CHR+06, CMNH07, DK03, DCDW00, DCA03, DL03, DVM06, DFT+07, DM02b, Dun01, DAA+06, EEJ04, EGEDH03, ELY09, FDM09, FZRD07, FJT+05, FGH09, FB01, FT04, FSLL02, Fra03, GTSK07, GC05, GBVD05, GB05, GAIK04, GKL+09, GMK+09, GBL06, GQ00, GSD+03, HBKG03, HZPY03, HM05a, HOIK09, HLP07, HMK06, IS03, ILVMSB+02, ILVMSB+03, Irg04, ITN09]. **quantum** [Iye09, KK02a, Kai09, Kap02, KA05, Kar09, Kar10, KSK+04, KMM+06, KMM+07, KDC09, KJW08, KF03b, Koh02, KS09, Kut09, LPC04, LBSB08, LPL04, MT03, MTRD04, MMV05a, Mat02a, MHI+07, MKZ04a, MMV05b, MVLM05, MLSB06, Mic00, Mon00, MRMR02, MGMP01, MDS04, MVG+04, MW06b, NNNY01, NY03, Nal08, NS08, NS09, NSG+06, OSW07, OY01, OOK03, ÖO02, Özd03, Özd04, Özt04, PNG02, PCKC08, POM+08a, PJZ+09, QG04, QW05, RVR00, RL04, RCD00, RdSH08, RdTdLC+07, Roy05a, Roy05b, RSM+04a, RMKS08, SPN03, Sal05, SFD09, SST+03, SLRS02, SPL03, Sey08, SMM06, SYL05, Sin00, SHG08, SM08, SMB09, Sta00, SZSP02, SV08, SSK+05, SEM05, Tak09, TFS+02, Tap04b, TTFP04, TMM+03, TBJ05, TVK+02, TOB02, TT01, TT02, UC00, VBML04, VWSA+04, Vik07, VRE+04, VG06]. **quantum** [WRD03, WHD+05, Win04, Woo02, XL08, XXY00, Yam04, Yam05, Yan06, YKS+06, YOGR09, YI04, ZSPS03, ZS04a, ZZ05, ZD06, ZD07a, ZSM+01, ZR03, ZKEE07, Živ09, dHG04, dLCPLD+07, Ano06f, Bad03, BL04b, BDA+02, CCM+05, DKP+06, HI06, KP05, LZC04a, MEN+08b, Nag03c, PČ04a, Put09, RLB02, Sok02]. **Quantum-based** [VLJ08]. **Quantum-chemical** [MME09, YZ07, BF08a, BBPG08, DFT+07, GTSK07, GKL+09, SZSP02, SV08]. **quantum-classical** [BMP+04]. **Quantum-controlled** [GM05b]. **Quantum-phase** [NY01, NY04]. **quantum-size** [BR05]. **Quark** [PF06]. **quartet** [Bu02]. **quartic** [POMGM01, TYG05]. **quartz** [LDM09]. **Quasi** [CMNH07, DAA+06, VGB05, BPŠB00, DFMZO08, Gin01, HAL+02, JC00, Lef05, MOL03, MTWN09, ZH06]. **quasi-bound** [BPŠB00]. **Quasi-classical** [DAA+06, VGB05, HAL+02, ZH06]. **quasi-degenerate** [MTWN09]. **quasi-energies** [Lef05]. **quasi-linear** [JC00]. **quasi-one-dimensional** [Gin01]. **quasi-particle** [DFMZO08]. **Quasi-random** [CMNH07]. **Quasiclassical** [VGMN03]. **quasidegenerate** [KK02b]. **quasienergies** [PSML04]. **quasiharmonic** [WAJ04a, WAJ04b]. **Quasilocal** [Kle03]. **quasimodes** [HT05a]. **Quasiparticle** [Ort03, OMY+01, Tem02b]. **quasirectilinear** [Oku01]. **quasirelativistic** [ZT02]. **quaternary** [YYI+08, ZS04b]. **quaternions** [CL05b]. **qubit** [KMM+06, PM03]. **quenching** [RSDNSB00, YYZ+05c]. **quercetin** [VG02]. **question** [JTH02]. **quinolinolato** [GSQ+04]. **quinoxaline** [BHG+06]. **quinoxaline-vinylene** [BHG+06]. **quintet** [CNPA04]. **quintuple** [SYZ+09, SZL+09, XLX+09a].

R [AC05, BBD08, CXZ09a, HH05, TLYW06, WML08, YKT+02, YST+05, TBJ05]. **R-matrix** [TBJ05]. **R12** [FHK06, KMN05]. **Rabi** [GN01, MYH03].

Rabi-oscillations-induced [GN01]. **Racemization** [BF08b]. **Radial** [DGR+00, SBMM03, CF05, MYRNYSB07, VAS05]. **radiation** [KK04, KH05, PVV+04, Pet04]. **radiation-induced** [PVV+04]. **radiations** [Lad00]. **Radiative** [ŠUKŽŠ07, CCM08]. **Radical** [Sok02, SLL06, TVK+02, Bar09b, BK04c, BS02, BHK09, Cab05, CIT+03, CSM02, CCB07, CP06, ETM00, GTSK07, GDB03, GPW06, GST+05, LSBDL02, LZZ+06a, LP08, LZA+09, LH03, MF03, MT04, MSS05, NYU+08, NLD+04, PXZ+09, QBTS05, RHHH00, RNCM05, Sha06, SYZ+09, SE02b, SQZ+02, TS07, TNJL05, TDST07, VHV+05, VVW+03, VHWM04, VPS+05, VG02, VSS04, WE01, YKT+02, YOYY03, YNN+09, ZLML05, ZQF+02, ZLH+08]. **Radical-mediated** [SLL06]. **radical-molecule** [ZLH+08]. **radical-water** [LZA+09]. **radicals** [ADTD05, BG00b, BG00c, CK06, DC05, DDT06, ET01, ETEA04, ET05, GV06, GRC09, HEBS00, HWY+07, KM01, LSM+06, MVL02, NGRR02, PVW03a, PVV+04, RVP09, SBL05a, SD00b, TT05, VB04]. **radii** [Ada05, Ada09, BZ06, MCF08]. **radiolysis** [BKM+02b]. **radius** [Zho07]. **radon** [Mal02]. **Raman** [ASP+05, DBFP05, DI05, JNKMS03, Kel05, LQC06, MP05, MP06, Mal05a, PGNT02, PRM+06, PR05, PSK02, QC02, QCV06, SŚRL07, VV05, ZB05, ZNF05, ZOK+05]. **Ramsperger** [LML02]. **random** [BBO04, CMNH07, GTR+05, Pal01b, SST+02, Zak04b]. **randomness** [CK04]. **Range** [GGS09a, ATN09, GSB00, HJSS09, JC01, KPP01, LLW+05a, LLW+05b, Nes04b, Pet00, QCK04, SWSH09, SBM+05, TSF04, TGGS06, Var08, VPS+04, YJ00]. **range-separated** [ATN09, HJSS09]. **ranitidine** [MPS+02]. **rank** [HLP07, LPL04]. **rapid** [SH00, SH01]. **rare** [BBD07a, BBD07b, BD07, EGEDH03, KBV05, KS03b, LME03, Sme02, STS+00]. **rare-gas** [BBD07a, BBD07b, KS03b]. **RASSI** [DGLM09]. **RASSI-SO** [DGLM09]. **rate** [GA08, GBA05, Gög06, MMV04, NTB02, OM05, VGB05, YLZ07]. **rate-limiting** [NTB02]. **rates** [CCM08, Ghe09, LS01a, SS09c, WBLQ00]. **rational** [RJP08]. **ratios** [MMCC02]. **ray** [AM09a, Guo09, LTV05, OCWY09, RA03b, SMDG09, dVHB03]. **Rayleigh** [Fer09, KSZČ04, Ols04]. **RDX** [BABL09, PM04a]. **Re** [HFS06, NSS09]. **reactant** [RA02]. **reactant-product** [RA02]. **reactants** [Nal00a]. **reacting** [ZFZ+08]. **Reaction** [AG01a, GSPP+06, VK08, Wal04a, XCW07, YLZ07, ZZW+06, AD01, ART08b, AAB05, BGG08, BEM02, BZH+07, BZBT01, BF08b, CQN+03, CB00, Che00, CY04, CWY05, CCH05, CCH06, CCV+07, Cos06, CCB07, CNDÖ00, DCD08, DF07, DRS00, DZ06a, Eva04, FWT08, FYH09, FGC04a, FGC04b, GEB+00, GSRL06, GGLS02, Gog05, GBA05, Gög06, HCZ05, HYC+00, HSN+09, Irg06, IN09, JPA07, JRSA08, JV05, JSvDA06, JG00, KP02, KP05, KS04b, KSN05, KTN02, LP00a, LWW+02, LZHT03, LDXW04, LDZ+05, LZZ+06a, LW08, LYP+06, LCCH09a, Lor08, LYWX07, LXXC08, LYCX08, MSS09, MLZS06, MPRGLL03, MPBM07, NTB02, NWSC08, Oku00, PXZ+09, PMB08, QTT07, REHH07, RRNG05, RA02, RD00, Sak02, Sch04, SK06, SZZ01, SS08a, SLCW04a, SLCW04b, Sok02, Sok04, SSB+07,

STW+05, SHH+06, SZML07, SSK+05, SCMS07, TVK01, TKY00, TLYW06]. **reaction** [TSP+07b, TSP+07a, TWZW09, TGG01, VR01, VGB05, VLK+08, VKIJ06, WGLX02, XFLX+06, YLS+04, Ye01, Yil06, ZLL+05, ZD06, ZLSL06, ZZDY06, ZSWL07, ZLX+07, ZDMF08, ZL00, ZFD00b, ZCZF02, ZCFD02, ZDAZ03, ZLH+08, CK06, ZRRC05, PNBV07]. **reaction-diffusion** [KSN05]. **Reaction-path** [YLZ07]. **Reactions** [JXZ+05, SMS07, TLC06, ARD03, Ano07g, Ano07e, Ano07f, ACDV01, BVG05a, BK04b, BCK04, Buc01, Buc05a, Buc07, Buc08, BF09, CBMRN08, Cas00, CZPJ01, Chr01, DLTW04, DR08, ET01, EGE08, FG06, GR07a, GR07c, GR07b, Gin08, GMS01b, GMS01a, HSW+00, IS03, IAMY02, ISK+01, IYY03, INS+08, Iva05, JFS+09, JM00, KWC09, LRB04, LSBDL02, LBMVDL06, MARK08, MSS09, Met05, Mic09, Now01, ONA05, PSCLGN07, PSN08, PFC02, PGF+06, PMLTL07, RSM+04a, ŠFW00, SRW+06, SLL06, TBJA03, TBM04, TIGD09, TGGV+04, VHV+05, VVW+03, VHWM04, VGMN03, VTS04, VTS05, WWTHF09, Woo02, XYS+03, XVRL04, YYS+09, YOYY03, YW05, YF07, ZZFL00, ZD07a, ZPW+04, ZRRC05, LFZ07, Woo02, ZLF+07]. **Reactivation** [MDG07]. **Reactive** [Bil01, BGJJ01, FRGM06, GB06a, HBKG03, IN09, LWCF08, NFFA04, SSMG08, ZZC09]. **reactivities** [JLC+09, JSC01]. **Reactivity** [CJ03, CMASC01, DBB+06, GWSZ08, MVA02, VHWM04, BGÖ+01, CS03, FCC07, Gin03, LSCC01, LL04, LC05, PMCOSC00, Pri05, SD08, SMOE02, TR00, THP08, VHV+05, VWMS03, VPSH00, YBS05]. **reagent** [Iva05, XYS+03]. **real** [Sko02, SRHÖ06, WS00]. **Real-space** [WS00]. **Realizations** [LKE03, Pan04]. **really** [TKY00, ZW09b]. **reappraisal** [BB02a]. **rearrangement** [IYY03, JRSA08, JFS+09, KZG09, KCU09, Sak00, TNO09, ZFFX05]. **rearrangements** [FBC+06, KPC05, Vrc07, YF07]. **reasonable** [JLC+09]. **reasoning** [Now01]. **received** [Ano00b, Ano01c]. **receptor** [BNHB+02, BSKFT07, BMR+07, DC06b, JHR+00, LAS+07, MESH02, OMMB07, PBTP06, SKSS09a, SLS+05, VED+02]. **receptors** [FH02b, JHR+00, VED+02]. **Reciprocal** [PPP00, AR06, MBM04, MBM05, ZT08]. **recognition** [CBRBT03, FH02b, OSW07, PMCOSC00]. **recombination** [BMŁT07, CR06, YLYD03]. **reconstructed** [HH02]. **Reconstruction** [LDM09]. **Recoordination** [FBGA04]. **Recoupling** [DWF+03, ACC03]. **rectangular** [LM02b]. **Recurrence** [Har05c, HM06b, GM00, GM01, GM02a, GM02b, GM08]. **Recurrent** [Liu02]. **Recursion** [Fle06b, Har04a, HN03, KOT09, Mak07]. **Recursive** [LP05a]. **red** [ABI07, LLYL06, YZG06, DCP06]. **red-** [LLYL06]. **red-shifted** [YZG06]. **Redfield** [SN02]. **Redfield-Davies** [SN02]. **redistribution** [CM09, GBB06]. **Redox** [BKGF02, EGE08, Buc05a, FPC+03, OOD+05, SCW09, SNN+09, ZLHL02]. **redox-couple** [Buc05a]. **Reduced** [Col01, AZ08, BG00a, Har02c, Her07, KV08, LP00b, LP09a, VATPR01, VAT03, ZB05, ZT04b].

reduced-density-matrix [ZT04b]. **reduced-size** [ZB05]. **Reducing** [SS02a]. **reductase** [DDW+06, Har02a, KNRR05, PFSFH06, SHM09a, SIT+07]. **reductio** [Kry05, Kry06, SDW07]. **Reduction** [PRCEM06, CZWZ05, DFMZO08, LXH+00, LXTT00, LXHT00, LZYT01, LZHT03, LZT03, PNBV07, ZHA01]. **reduction/acylation** [PNBV07]. **reductive** [JG00, WB05]. **Reexamination** [Cam04]. **reference** [CSG06, DM08a, Fra06a, JR02, PČH02, RVP09, SFZO01, ŠFW00]. **referential** [Brä09a]. **Refractive** [JV05, FYT09]. **regard** [DLM+05]. **regarded** [OM02, OM03]. **regeneration** [WE01]. **regime** [LS01a, LA09]. **regioisomers** [ZKRS07]. **region** [DBLM06, GFMT08, JLC+09, QS05, SMDG09]. **regioselectivity** [Kor05, LTL05b]. **regression** [MEN+08b]. **regression-discriminant** [MEN+08b]. **regular** [Gin01, Kle03, KZvL09, ZLC04, vLvL06]. **Regularities** [DLZ+03]. **regularity** [ZSM+01]. **regulation** [Wal04b]. **rehybridization** [NLD+04]. **Reinvestigation** [SMM06, BN04]. **related** [AM05, Buc02b, Buc05c, CEÖ02, DD03, DV00, Hua04a, KNN+04, KTH+05, Mar00b, SIT+07, YYT+04]. **relating** [Bou01]. **Relation** [Lav03a, Gin05b, HMMT04, HM05b, Mar00a, Mar09, PMPI01]. **Relations** [KF02, Bel04, GM00, GM01, GM02a, GM02b, GM08, Har05c, HM06b, SK09, TGGS06]. **Relationship** [KM00c, TDS+02, CDG05, DM04, Gra08b, Koh02, MEN+08b, OA03, PRS+09, SKSS09a, eSPM+08]. **relationships** [CDV08, CBRBT03, FCC07, Jal07a, RPS+07, GMPIP01]. **Relative** [ADTD05, AKB06, AT00, FFS04, FAE+05b, FS05, NR09, ABM02, DDT06, FFHT05, GdA01b, HM06a, JBMP03, JMP06, LSC01, LWZ+09, LSCC01, PJZ+09, SLU+06, SUL+07, ZKRS07, FAE+05a]. **Relativistic** [BJS09, BR05, DM02a, Dya00, HdMB+05, IVK00, Khe09, Kut08, MST04, Mar05b, NF03, RW04b, dBKS01, ARH00, BR02, Boe03, BLKJ00, DBd05, DMH+05, DHCD06, DES03, DLK00, GQ00, HSP+09, HDL00, HM05b, ILVMSB+02, ILVMSB+03, LFK06, LVM01, LJL09a, MST08, MKCB05, MTWN09, NF06, PUH+08a, Sap06, Sch05, VMA03, XCW07, YHN+07, BKLB06, NGRR02]. **Relaxation** [BMB02b, BL04b, BFF04, BK03, FBBB06, FYSS09, GMS+05, MB05b, MB07b, SPI04, Whi02a, HK06]. **relaxations** [DNC07]. **released** [PNBV07]. **releasing** [PML09a]. **relevance** [Von00]. **relevant** [LADD00, MVL02, OM04, PPP+08]. **reliably** [SGS00a]. **Remarks** [Bof03]. **Remembering** [Ver09]. **removal** [BJAV08]. **Ren** [Ano07g, Ano07e, Ano07f]. **renormalization** [DCDW00, DJNH02, OK05, WK03]. **renormalizations** [Zak04b]. **renormalized** [Ort05, PHK+06, PGW09, SLE05]. **Rényi** [NR09]. **ReO** [VIGL+05]. **Reorganization** [ELO+07, DST+04, GJ03, RO01, TDS+02, ZLHL02]. **repair** [ZLS07]. **repairing** [BDE+07]. **replaced** [SK09]. **replica** [MVKN06]. **replica-exchange** [MVKN06]. **report** [Brä09a, SMB07]. **representability** [AV05a, AV06, AD06, Pan01, Pan02, VAT03]. **Representation** [KPSH06, RJ08, AG02b, Bil01, CW00, CLL08, Dat04, DLHP04, EJ06, FD09,

Gri06, IPPL05, JLZY09, KK05, LLR04, LLLZ06, LLZH09, LP04b, Luz08, PA04b, RBA07, RVNP09, Ret06, SO09a]. **representations** [Buc00b, Lin09, WRW02]. **representing** [ASO+01, ASO+04, SSR02]. **reproduced** [CRL+02]. **reptation** [YOGR09]. **repulsion** [CC07, CEK01, Fle06b, GSA+09, HM01a, HM01b, Har02b, MNV07, RLER08, YINH00]. **repulsive** [DB04b]. **Requirements** [HT05b]. **Research** [IBB08, Nag03c, BM02, LGJP05, LCCH09b, PL09]. **residue** [CR08a, KF07]. **residues** [PCML08, SLB+08, ST01]. **resin** [Por01]. **Resistance** [BKL+02, Pal01b, ZY07, DFM+02, PMBM09]. **Resistance-distance** [BKL+02]. **resolution** [ASO+01, ASO+04, KN09a, Nal09a, Nal09b, SMDG09]. **resolution-of-identity** [KN09a]. **resolutions** [WZ06]. **resolved** [CN05, DBFP05]. **Resonance** [Ghe09, Kel05, ARBC+05, BB05c, DZ01, DBFP05, DI05, FM02a, HLH05, IYSS07, KAE03, KAE07, LWCF08, MP06, MZD01, Nic02, Orl02, PA08, PKS+00, RE06, SMB09, Tak08, WSK03, MP05]. **Resonances** [MSC03, AR04, AE04, BB02b, Hea00, MV02, SEY07, SEY09]. **Resonant** [BP04, Lef00, BGGS08, Gri08, KK04, NW01, Sal05, VH00]. **Resonating** [NYU+08, TYY06, YNN+09, KM01, TYY07]. **resource** [NU09]. **respect** [AV02, DFM+02, GP08, Özt04, PMC02, VCF+00]. **respective** [BCT+02, DKC00]. **response** [BN06, BK09, CW04, CCE+07, DPW00, JPA05, Kry08b, KZ09, LCT00, MNR07, Nes02a, RMM05, RL04, VH00, VV05, dBKS01]. **Restrained** [HPR09, SKMW00]. **Restricted** [DVM06, FS00, FFHD00, KGA05, LP07, LP09b, WF04, YONY04]. **restriction** [NS04]. **restrictions** [Buc00b]. **result** [SS09a]. **Resultants** [CSWD06]. **results** [BDMS01, BG00b, CSG06, CGG05, CN05, DW05, HVC08, Mar03b, RS08, Saf04, TB09, WF04]. **resveratrol** [DD03]. **Retarded** [Sal00, Sal05]. **retinal** [BL02c, CM09, ESE04]. **retinoic** [SLS+05]. **Retroengineering** [RSL+03]. **revealed** [BvRSS07]. **Revealing** [LTL06]. **reversals** [GB08]. **reverse** [CFR07, GMPIP01, ZT08]. **Review** [ITN09, Kry08a, VAS05, Ano01b, Brä04c, BRZ09, Cal02a, Cal02b, CC09, Deu00, Deu06, DR04, GM09, Kar01, Lar01, Lin01, LM04, Ort04a, Sul00a, Sul00b, Sut00, Tri04, Wil04b, Wil06, BA06, Brä04b, Lun04, PGW09]. **revised** [HSP+09]. **revisited** [AKN09, BTK+05, Brä09b, CS04, KIN09, LH00, MNMV02, MBP01, Nes02b, RV05, TD09, Tem09, WD01, XV01, YYS+09, YYI+09, YKK+05]. **Revisiting** [NS08, NS09]. **reweighted** [KFD09]. **Rg** [LZJ+06, WZJ04, LZJ+06]. **RgX** [WZJ04]. **Rh** [HGS03, LTLS05, XD03, BFAM03, DSW08, LTL06, TLYW06]. **rhenium** [XLX+09a, XLX+09b]. **RhH** [RD00]. **rhodamine** [DNC07]. **rhodium** [BDMS01, LDMR01, LTL05b, RVR00]. **rhodium-catalyzed** [LTL05b]. **Rhodobacter** [DRS00]. **rhodopsin** [BL02c, CM09, SB03]. **rhombohedral** [SM09]. **rhythm** [GHG04]. **RI** [KN09a]. **RI-MP2** [KN09a]. **ribonucleotide** [SIT+07]. **Riccati** [FGF06, CW08, Kry09]. **Rice** [LML02]. **ridge** [PC07]. **Rieske** [SKK+07]. **Rieske-type** [SKK+07]. **right** [MCH02].

rigid [LPV07, Lu06, MVP00, MVKN06]. **rigorous** [NS09, SA09]. **Ring** [BR08, KV07, RB08, Bro00, Buc02a, Buc02b, CJZZ06, DCLC05, För04, FB07, GI07, JPA07, JPA03, JSC01, KM04, LZHT03, MSMS03, NOY+01, NLD+04, PIGN02, RLNA02, SMM06, SWZ01, SST00, TN09, VBT+07, YCS09, ZLL+05, BR12, RB11]. **ring-closing** [ZLL+05]. **ring-expansion** [JSC01]. **ring-opening** [Bro00, SMM06]. **ring-shaped** [DCLC05]. **ring-substituent** [KM04]. **rings** [BR08, BR12, BCdP03, CLL04, DT02b, FS00, GMTM02, PS02, RB08, RB11, WSK03, XVRL04]. **RISM** [CCE+07]. **Ritz** [Fer09]. **RNA** [LLLZ06, MTRG04, MMT+07, RVNP09]. **RNase** [LYDK02, MLSG04]. **RnCO** [Mal02]. **ro** [ŠŠU+02]. **ro-vibrational** [ŠŠU+02]. **robust** [PMHW07]. **rod** [GKE01]. **rod-like** [GKE01]. **Role** [AE04, CDDM05, DGLM09, DS06, Kor05, KP00b, PCML08, SK01a, SEY07, SMM02, UC06, VU02, CJZZ06, CSL+02, Chu02, FYH09, KWC09, MC00, MMR+08, MET00, NU09, PBSC04, QCC02, Sch05, SSJ09, SEY09, SST00, SBM+05, Tem02a, TBB09, YYQ+06, DP06, IAMY02, LYP+06, Mar03a, SBB05]. **roles** [BLC09, New00, PMC02, TN09]. **rolls** [SÖ04b]. **Room** [CGL+05]. **Roothaan** [GE09, WTWT09]. **Rosetta** [CR08a, Luc02]. **rotating** [Oku01, SK05c]. **Rotation** [BJ00, AIG02, Buc02b, CCL03, DI05, GPW02, KCOV07, KZ08, MPBM07, Oku01, SPS06, ZZWM07]. **Rotation-vibration** [BJ00]. **Rotational** [SSN03, SLCW04a, AC06, BFBB06, BDMC06, CC00b, CC01b, GMS+05, ITN08, LIBM03, LN03, MDBM05, MVK00, Moh00, ACDV01]. **Rotationally** [ZYG00, BKRT03]. **rotations** [ABLL02, HQM04]. **rotators** [AGMK02]. **rotor** [MVP00]. **round** [NS04]. **route** [HGB08]. **Rovibrational** [KVF+08, ELY09, MYGD01]. **Rovibrationally** [AC07]. **rovibronic** [TPGD02]. **row** [BMŁT07, BG00b, CJdC01, DNM+08, FTB04, GBS02, PJdC00, PJ03, SDTM02]. **rows** [BG00b]. **RP** [YST+05]. **RPA** [HNKiS01, YSY+00]. **RQDO** [CM05c]. **RSiN** [BBD08]. **RSiP** [BBD08]. **Ru** [AZD06, BPM01, BC03, XD03, BLC+00, DSW08, ZSL+09]. **rubidium** [Obe00]. **Rubisco** [TFS+02]. **rubroflavin** [WRRF03]. **Rüdenberg** [Ano00e, Koc00, Zer00]. **rule** [AK02, CC07, Don09, MHT+08, MBP01, Sce09, YKK+05]. **Rules** [WZJ04, ZWSJ01, BB05b, FZ09, Gos01, PSM07]. **Rumer** [Nég03b]. **ruminations** [NU09]. **rumpled** [QCC05]. **Runge** [HW06, OB02]. **ruthenium** [GL00, SMM02]. **rutile** [EB04a, VG06]. **RVB** [SM04]. **Rychlewski** [CJKK04]. **Rydberg** [DGG09, Hea03, MVL02, MMV05b, SK00a, Van06, VBML01, VBML04, ZSM+01].

S [AC05, Ano07g, Ano07f, Bec02, FWT08, GYF+09, JLAR07, LLW+07, LDR+08, LAQ+09, MB06, SUH+01, TSP+07b, WSC+05, YST+05, YW05, CMR05, GW04, GW07, Har04b, IV02, Nég03a, SI09, YAŞ00, BMŁT07, BK04a, BSH04, CZPJ01, CSTB08, CSM02, DBFP05, DGLM09, DLK00, Els05, GR07c, GR07b, HNKiS01, LLL+07, NFL+02, ONA05, PR09, PYZ09, SH02a, SPS02, Sha07, SRH02, SS09b, SVC+05, SRW+06, TSP+07a,

WSBV05, WSC+05, Ye01, ZRRC05, BD01, KS09, Sey08, CT00, Tem00].
S-CI [BL02a]. **S-monoxide** [PYZ09]. **S-oxides** [Sha07].
S-transferase-catalyzed [SPS02]. **s-type** [GW04, GW07]. **S.S.** [VPS+04].
S2 [LCT00]. **SAANDs** [SWST04]. **saccharin** [BCT+02]. **salicylaldehyde**
[BWS+02]. **salicylamide** [AKK05b]. **salicylic** [AKK05a]. **salsolinol**
[HQL09]. **SAM1** [Pud02]. **same** [CL05b, Man05]. **sample** [GN01]. **samples**
[SSK09b]. **sampling** [BKM+09, SGLF01]. **sandwich**
[CG09, HVC08, HDL00]. **sandwich-type** [HVC08]. **sandwiches** [MABB06].
SAPT [RP09]. **SAR** [CDB02]. **sarcosine** [CSL05b, RST08]. **satellites**
[GMCS04]. **saturated** [FGdA02]. **saturation** [Sch00]. **Sb** [HS05, SYL05].
Scalar [HDL00, DSLC05, VMA03]. **Scalar-relativistic** [HDL00]. **scale**
[BZG+04, MTRD04, MVLM05, Ols04, SMEA08, SK05b, YKGC09]. **scaled**
[CK09, HBTW04, XXY00, YM05]. **scales** [Put06]. **Scaling**
[GWK+05, Pal00, PGN+05, TGGS06, AA09b, Bar09b, BK03, CSA09,
FHHC00, KP09, KN09b, KGI+05, LKE03, LGKN04, PRM03, SS05b, TA06].
scaling-factor [AA09b]. **scars** [LBAB02]. **Scattering**
[Lef07, AR04, AGBY00, ASP+05, Bil01, CGS01, GB06a, GYM+02, HBKG03,
LBSB08, NW01, NK06, Pai00, PA02, PA04a, PSA05, QTT07, RE06, RR02,
RW04c, SAM08, SEY09, VSBD06, YHD00, YYHD01, ZYG00]. **ScBr**
[KH08b]. **SCC** [HEJ+00, KKMS04, KES03, WKF+06]. **SCC-DFTB**
[HEJ+00, KKMS04, WKF+06]. **SCC-DFTB-D** [KES03].
SCC-DFTB/molecular [HEJ+00]. **SCE** [CGS01]. **SCF**
[ACD02, DMMV00, DTT06, Glu04, KGI+05, OY01, Sal09, SCR01, SCRR02].
scheme [BNS05, DZ01, DKM+04, FTW03, FCC07, GTR+05, HZPY03,
HW06, ITN08, KN09b, KDY+02, LZ05, MT03, MGK+09, MB04, SSR02,
Tap04a, YTS+05, YINH00]. **schemes** [GSH02, KIN09, LLZ+00, LSLD01,
May04, Qui05, SRA09, Šat03, SS02b, Tou09]. **Schiff** [AG01a]. **School**
[Nag03c]. **Schrödinger** [FGF06, ACT+05, AVTPR09, Ano06g, GN01, JJ00,
JTB09, KSZČ04, KMS06, LLZ+00, LSLD01, LSD02, LD05, McK04, MSJ04,
MOPdP09, Ols04, POM+07, POM+08b, QLD05, RW00, SBT+03, SHZGP09,
SMT06, SB04, VWB+03, VAT03, VTPRA08, VAS05, WRW02, YAŞ00].
Schur [CT00]. **Schwartz** [RDK02, RDK97]. **ScI** [KKTMA09]. **science**
[Guo09, She07b, Sta00, Ano00d]. **SCMEH** [BB04, BB05d, BB01, BB02c].
ScN [JKU02]. **ScO** [XYS+03, DF07]. **screened**
[BB07, HM01c, KH08a, ZBPD08]. **screening** [KH07, Pyy01, YKK+05].
SCRF [PLA+07]. **ScSb** [RHM05]. **Se**
[GYF+09, HJT07, JLAR07, LLW+07, LDR+08, YST+05, BK04a, SVC+05].
seam [XV01]. **Search** [ONK+05, FM02a, HCZ05, LAS+07, Mor03,
PRBGLL04, SM05b, SS02a, RB06]. **Searching** [FCD08, LYP+06, LAS+07].
sec [CDS06]. **Second**
[ERU07, Gin06, PSML04, ACT+05, Áng09, CK09, DPW00, DD00, EJ06, Flo08,
Fra06a, GG07, GG00, GTR+05, Gra08a, HZPY03, KN09a, Kel05, LCL+09b,
MNR07, NKN+05, PMHW07, PVW03b, PJ03, QC00, SH09, SHE+02,
TYY05b, TB09, VAT03, VTPRA08, Wol05, YS09, YM05, ZGY+03, IBN08].

Second-order [Gin06, ACT+05, CK09, DPW00, DD00, EJ06, Flo08, Fra06a, GG07, GG00, Gra08a, HZPY03, KN09a, Kel05, LCL+09b, MNR07, PMHW07, SH09, TYY05b, TB09, VAT03, VTPRA08, YS09, ZGY+03, IBN08]. **second-row** [PJ03]. **secondary** [HM01c, IS03, JLZY09, LLLZ06, PCML08, PKT05, RVNP09, ŠK03b, VK05]. **section** [LBSB08, PUH+09]. **sections** [AE04, DI05, EMM+02a, GAL+05, GBA05, Gög06, HSP+09, LIBM03, PUH+08a, SEY07, SEY09, SL05d, UBS04, VML05]. **sectors** [CCLK05]. **secular** [SN02]. **segregation** [MB01a]. **selected** [BVHS05, CR08a, KM01, SCRSRE05, SCRSRE06, SCRRE07, BCvzGG04]. **Selection** [WHD+05, LP00b, SEM05]. **Selective** [CNDÖ00, ZHA01, SWST04, YLS+04]. **selectivity** [SOEW08]. **selenide** [FB01]. **selenium** [JWM00, LVM01, LSC02, MLP08]. **selenium-containing** [MLP08]. **selenocysteine** [KSBK08]. **selenoenzymes** [BKGF02]. **Self** [BG00a, BG02a, Pea05, PVW03b, STS+00, VRC04, AKN09, Bli02, Brä09a, CL05e, DKW09, FGC04a, FGC04b, IN07, LE01, MP06, MROA06, Ort05, SMVMC07, TQC05, THP08, TBB09, UT03, UC06, WRD03, WSNB00, YYKY01, YKGC09, YM05, ZZFL00, AIG02]. **self-assembled** [THP08, TBB09]. **Self-assembly** [VRC04, SMVMC07, TQC05]. **self-associate** [MROA06]. **Self-consistent** [Pea05, PVW03b, AKN09, DKW09, MP06, UT03, UC06, YM05]. **self-consistent-field** [CL05e, YKGC09]. **self-diffusion** [WSNB00]. **Self-energy** [BG00a, BG02a, Bli02, Ort05]. **self-exchange** [ZZFL00]. **self-interacting** [WRD03]. **self-interaction** [IN07, LE01, YYKY01]. **Self-interaction-corrected** [STS+00]. **self-organization** [Brä09a]. **self-reaction** [FGC04a, FGC04b]. **self-referential** [Brä09a]. **Self-trapping** [AIG02]. **Semi** [PA04b, CP06, DCP06, Mar87b]. **semi-batch** [CP06]. **Semi-classical** [PA04b]. **semi-empirical** [DCP06]. **semi-infinite** [Mar87b]. **semicarbazide** [AG01a]. **Semiclassic** [Kis04, LLR04]. **Semiclassical** [CR06, DN06, GR04, LDM09, MB02b, MB05c]. **semiconductor** [GSPT+07, KKS+03, PS02]. **semiconductors** [GKL+09]. **semicontinuum** [BF07]. **semiemperical** [Moh00]. **semiempircal** [ZLS07]. **Semiempirical** [Bol04, GG03, JLI+01, LB06, MTE09, NFL+02, NSZZ04, OD03, SPS02, WSK03, BD01, AMC07, ADTD05, BZG+02, BZG+04, CS04, DSFS00, DCW03, FDL03, GH03, Hea03, HH03, KDF00, MK00, MC06a, MPBM07, OOK03, TTM01b, VGM05, ZS04a, ZXX02, vdVM00, KK02a, SMM02, ZFD+00a]. **Semilocalized** [Gin03]. **semiquinonato** [BT05]. **semiquinone** [NGRR02]. **sense** [Now01, Sce09]. **sensitive** [AG01a, Hog04]. **sensitivities** [Nal00a]. **sensitivity** [CX00, EEJ04, ZCZC09]. **sensitized** [LNPL06, SMM02]. **sensor** [DKWP04]. **sensors** [PMCOSC00]. **Separability** [ACF04, ACF05]. **Separable** [AA04b, Lin09, Kar08, Tap04b]. **separated** [ATN09, HJSS09]. **Separation** [IS03, ANM03, DH04a, GGS09a, SN02]. **September** [GDV05]. **Sequence** [MSS09, AV02, CM02a, Chu01, FMBM05, GM09, GKYY06, KF07, LLZH09, MZF05, ZW03, ZW04]. **sequence-specific** [Chu01].

sequence-to-function [KF07]. **sequences** [CLL08, Gar08a, KW03]. **sequential** [NWZ+07b, ZS04a]. **Series** [FS97, AA09a, CC07, COMA03, Fer01, FHHC00, FGF06, FS09, GYF+09, GE09, ITY+09, KM04, KM05a, MDBM05, NJD02, SKSS09b, VBML04, WWTHF09, ZSM+01, ZW03, Zho07]. **series-parallel** [Zho07]. **serinamide** [LZZ+06b]. **serine** [GZD+05, HP07, JAP+05, NTB02, ŠFW00, HT04]. **serotonin** [VED+02]. **sesquifulvalene** [MW06a]. **sesquiterpene** [PRS+09]. **Session** [Har09]. **Set** [DPS04, ABLL02, BML01, BEM02, CJ09, CKM09, Chu07, Chu08, DBd05, DSW08, DW05, FTW03, GSfLV08, HW02, JC00, JCP+08, KCOV07, KP00a, KS09, KS07, KANK00, KWC09, LFK06, LW05, LS01b, MST08, MM07, MM09, PFSFH06, PLU08, QGW02, Ras04, SFD09, SJE03, SST+02, SYZ+09, SZL+09, SGS00a, SEM05, ZŠ05, ZB05, dA08]. **sets** [ACC03, ACCC03, ANJ09, BBM+00, BKM05, CJdC01, DNM+08, DCA03, DMH+05, DHCD06, DDD03, ET09, EYB02, GW02, GW04, GW07, Gus01, Gus02a, HdMB+05, KV02, KW03, LTV07, LJ03, MG05, MDSW07, MW05, NJC02, NJD02, NRJD03, PJdC00, PJ03, PJS+09a, QGW04, RFCG09, RLER04, SS00a, Sha04, Tem00, Tem02a, VD00]. **seven** [BR08, BR12, RB08, RB11, RLNA02]. **seven-membered** [RLNA02]. **Seventh** [PČ04a]. **several** [EEJ04, PIGN02, PGN+05, PML09a]. **sextuple** [KNS+09, VD00]. **Sg** [BB05d, BB04]. **SH** [IAMY02, Pet00, SZL+09, VK08, dSNBG08]. **shakeup** [ZDO00]. **Sham** [AK05, BZ06, BGN+05, CW04, DKM+04, EJ06, FJ00, FCC07, GSB00, KSG03, KDY+02, LSM05, MNR07, MH06, Nal00b, Nes04a, PL00, QS00a, QS00b, RJ08, SG03, SL05b, SFZO01, TKJ09]. **Shannon** [HSW+00]. **Shape** [ASTO02, FTM06, GJ03, Kry08b, MV02, STAO00, SPL03]. **shape-consistent** [FTM06]. **Shape-dependent** [ASTO02]. **shaped** [DCLC05, JPA03]. **shapes** [IROW09, MFA00]. **sharing** [LZXD05, LPZW05]. **Shear** [DCTC03]. **sheet** [SÖ04b]. **sheets** [KTH+05]. **shell** [BKM+02a, CC07, CS07, DM08a, DMH+05, DHCD06, DKM+04, Glu04, GW04, GFMT08, HdMB+05, HSP+09, JNSF04, KGA05, LP07, LP09b, LZ05, MMR+04, MB00, Mon05, OM04, OdSC05, Ort05, PUH+08b, PUH+08a, PUH+09, PVW03b, PGW09, PTLB00, SO09a, SLWS07, TG05, WF04]. **shell-correction** [DKM+04]. **shells** [Koh01, KWG06, SCTK+09]. **Shibuya** [Ave04, RW04a]. **shielding** [Buc05b, MC03, Pea05]. **shieldings** [BSR02, JTH02, KZvL09, Laz02]. **shift** [BCF02, DFM+02, MGK+09, RNVTP09, SB03, Seb05, Tak08, ZKYA04, dVHB03, RFLR00]. **shifted** [LLYL06, LLL+07, RM07, TS07, YZG06, Yan09]. **shifting** [Hob02]. **Shifts** [YSP08, Bou03, Buc04, CVVA08, DDT+03, Gos01, Hes02, Hog04, LCT00, RCF02, Sal05, Sch05, SKNN09, TC05, TCM09, ZOK+05, dBC06]. **Shik** [Ano05f]. **SHO** [Yan09]. **shooting** [JJ00, LD05]. **Short** [TSF04, Ano09g, GSB00, KK02a, Nes04b, TGGS06, VPS+04]. **Short-range** [TSF04, GSB00, Nes04b, TGGS06, VPS+04]. **Shortcomings** [BDL03]. **shortening** [MG08]. **shot** [Mai08a, Mai08b]. **shuttle** [FGZ07]. **shuttles** [RFF05]. **Si**

[HZJ+07, LDR+08, LLYJ09, SYL05, SCHW07, TNET03, ARE02, CB04, GH03, KUS+03, KSG03, LLYJ09, LL04, RKM09, Sha07, SL09, SNZG02, TR00, TNET03, WL00, YHD+07, ZFD05, ZCZ00, ZMZ+09, ZH05, ZLY+09]. **Si-H** [ARE02]. **SiC** [YI04]. **SiCH** [JFS+09]. **SiCl** [MC06b, WCP+00]. **side** [CVPGH+06, KN08, MML+02]. **side-on** [KN08]. **sidechains** [TQC05]. **sidewalls** [KDŁL07]. **sieves** [LV01a, LPV05, LHTV05]. **SiF** [PMLC09]. **sigma** [TC05]. **sigmatropic** [FBC+06, KCU09]. **signal** [CPH04, LLB01]. **signals** [BB05c]. **signatures** [BR08, BR12, RB08, RB11]. **Significance** [ELC08, Buc07, Her07, SM07a, TMS08]. **signs** [Tem02b]. **SiH** [YW05, CSTB08, FF01, MD04]. **Silacycloalkanes** [AKB06, FFS04]. **silacyclohexanes** [WT07]. **silane** [PSCLGN07, TNJL05]. **silathiacyclohexane** [FAE+05a, FAE+05b, FS05, Sha07]. **silatriafulvene** [TSK01]. **silica** [Han07, LPV07]. **silicalites** [ZKYA04]. **silicates** [RRGP05a, RRGP05b]. **SiLiCl** [FFLZ02]. **silico** [MLSG04]. **Silicon** [XBHL04, CK06, Dkh08, FAE+05a, FAE+05b, FS05, GWSZ08, HOIK09, IABS08, KAG08, KUS+03, LJMM09, LLYJ09, LSC02, SMDM03, SPI04, SNZG02, SM03, WFS+01, YF07, YS07]. **silicon-based** [HOIK09]. **silicon-doped** [GWSZ08]. **silicon-sulfur** [WFS+01]. **siliconlike** [IVK00]. **silver** [ESU04, Gur05]. **silyl** [PV09, SWSH09]. **silylalcohols** [YF07]. **silylethyl** [JFS+09]. **silylidyne** [BBD08]. **silylidyne-amines** [BBD08]. **silylidyne-phosphanes** [BBD08]. **silylmethanethiol** [ZFFX05]. **SiMe** [LH07c]. **similarity** [AT07, ART08a, CD00, CDG05, GBVD05, KM03b, RCD00, RACD00, SFD09, WGD01]. **Simos** [Ano06g]. **Simple** [CTP+08, Dei04, DM04, Mak07, MCR03, MMB03, VRSF02, ZWMZ02, AFC03, BK04c, BBL09, BA02b, FA05, FRF02, Gin08, GW07, JCTD08b, Muñ02, Pea08, QW05, Wei08, ZZZ+08]. **Simplest** [Pup07, GV06]. **simplex** [RSM+04b]. **simplified** [CD04]. **simplify** [Oku01]. **simply** [WC04]. **Simulated** [ASH07, CB03, DNM+08, FCD08, dRPFCP08, RSM+04b, SKMW00, VNB+03, dAMM08]. **Simulating** [ART08b, FFF07]. **Simulation** [BDMS01, CC05a, LPL04, ALI03, BKMHP04, BFBB06, BFB08, CR06, CAHl08, CHC05, DKD+07, DMM+02, FFFR01, FFFR02, JLPA09, JZZ+09, JZW+09, KOH03, KUS+03, KSN05, KS07, LFADSF07, LHL+00, LCCH09b, Noo03, NBS04, Now01, PD05, Qui05, QCV06, RNS04, SPS02, VPS+04, YYY+00, ZH06, VG02]. **Simulations** [ASH08, EM05, AMOR07, AP00, BBDS06, BS05b, CRRL01, Dre05, FG03, FDME01, Han02, HLP07, JLM08, KM00a, KBV05, LBMVDL06, MMR+08, Noo06, PRSLA08, PFSFH06, PFdP08, RP00, SRHR05, TS01b, TRMM04, TCM01, TŠPJ04, TWSK09, VPS+05, ZKEE07]. **Simultaneous** [MLP08, Nak02, BFF04, Nak07]. **sinapinic** [PKS+00]. **Sinc** [HBKG03]. **Singer** [CA01]. **Single** [WZL+07, ZLC04, ALM05, BP03, CW00, CAHl08, CC07, CS01, CCR09, CGS01, DM08a, DNN+06, Den09, DGSD07, EB04a, EKZ06, HK06, HT07, IA06, JLC+09, KDŁL07, KG08, KG09, LZC04b, LZA+09, LLSY05, LTW09, MB07b, NY01, NY03, OdSC05, SDZ+07, Tor06, UBS04, VM06a, WKF+06, XR05, YWZ+09, ZWMZ04, GM00, JR02]. **single-**

[DNN+06]. **single-center** [CS01, GM00]. **single-chain** [IA06]. **Single-electron** [WZL+07, CC07, LZA+09]. **single-mode** [NY01, NY03]. **single-molecule** [BP03, XR05]. **single-particle** [OdSC05]. **single-reference** [DM08a]. **Single-reference-state** [JR02]. **single-stranded** [HT07]. **single-wall** [Den09, LZC04b, Tor06, VM06a, ZWMZ04]. **single-walled** [ALM05, CAHl08, DGSD07, JLC+09, KDŁL07, LTW09]. **singles** [IBN08]. **Singlet** [FG06, GL07, BDA+02, BCK04, CMY03, DBPG04a, KS02a, KSN+09, KM05b, MME09, MSS05, PČH02, RSKC08, SLB+08, SD00a, TOH+00, YYI+09]. **Singlet-instability** [TOH+00]. **singlet-state** [CMY03]. **singular** [BB06, DKC00, Roy05a, Roy05b]. **singularity** [Goo03]. **SiO** [CB04, SHC00, FSLL04, MMCC02, MJ06]. **Sir** [Ano04e]. **SiS** [WFS+01, MD04]. **SitCon** [KF07]. **Site** [FDLK02, CDDM05, HKMM04, KF07, KNRR05, KSI+07, LSWT05, LMRT08, MLSG04, NOHN02, OMMB07, PSEP05, SIT+07, SM07a, SSS+05, Whi02a, WRK03]. **sites** [CZWZ05, DD05, DCP01, GYS+06, HE05, Kra00, Loe00, NFFA04, RH03, SWST04, SCW09, SCG07, SCHH01, SCHH02, TC07, XXC08, YWZ+09, Yur07, Yur08, ZSKV04, ZZC09]. **Six** [SGP+07, RPS+07]. **Six-coordinate** [SGP+07]. **sixfold** [CC00b]. **Sixth** [DT02a]. **Size** [CXZ+09b, DFRS07, LP04a, SS05b, ACPG01, BR05, CWZ03, CDG09, Del03, EF03, FCLH+06, SBL05a, VDF+06, ZB05, ZWJ02b, RS09, RS11]. **size-dependent** [ACPG01]. **size-expanded** [FCLH+06]. **Size-extensivity** [RS09, RS11]. **sized** [PHNN09a]. **sketches** [Kry09]. **slab** [EB04a, ESU05, PBMA03]. **slabs** [FA05]. **Slater** [Gus03, GM08, Har03, AM06, AS04c, Bar00, BSH04, Bud04, CD03a, ELF+08, FLE+06a, GSD+03, GM00, GM01, Gus01, GM02a, GM02b, Gus02a, Gus02b, GM03, Gus04, GE09, HS02, HMMT04, HM05c, JJWH04, KZvL09, KANK00, Mar87b, Mar87a, MNA+99, NN09, ÖO02, Özd03, Özd04, ÖKAY03, Özt04, PCT+04, PCT+05, RH09, RLA+01, RLER04, RLRE04, RLER08, RJ08, SH01, Saf04, Tal04]. **Slater-Type** [Gus03, Har03, GM08, AS04c, BSH04, Bud04, ELF+08, FLE+06a, GSD+03, GM00, GM01, Gus01, GM02a, GM02b, KZvL09, KANK00, ÖO02, Özd03, Özd04, ÖKAY03, Özt04, PCT+04, RLA+01, RLRE04, RJ08, SH01, Saf04]. **SLG** [DTT06]. **SLG/SCF** [DTT06]. **sliding** [DFM+02]. **slip** [KIK09]. **small** [AGN04, BLC09, BF08a, BKHPvD01, BA07, CMNH07, Die00, DPS04, FPC05, Guo07, GWSZ08, Gur05, HM01c, HvLJ01, IZ04, KL00, LAS+07, LTL05a, LZW+07, MZN+03, MFA00, MDJ01, PC09, PBI+01, PHNN09a, Put03, QC02, RdSH08, SCR01, SS02a, YYZ05a, YWC07, dlPCLG+00, AYD00]. **small-sized** [PHNN09a]. **smart** [RSL+03]. **Smeyers** [DB04a]. **Sn** [JLAR07, SYL05]. **snake** [DCO+08, HNR06]. **Snijders** [Ano06a, BvL06a]. **SnY** [HS05]. **Sobolev** [CDB02]. **sodium** [ABI07, BNA03, CM02a, IYSS07]. **Soft** [DWD+05, OCAMOHL07, AM09a, GJ03, Guo09, SMDG09]. **soft-X-ray** [Guo09]. **softness** [Put06, SPS05]. **softness-based** [SPS05]. **software**

[CWW09, VWSA+04]. **solar** [SMM02]. **solid** [Cab05, HSB+00, Mat00, MG08, OR09, PMLC05, She07b, SKHY09]. **solid-phase** [PMLC05]. **solids** [Boe04, DP06, DLM+02, Ful00, IOA+04, Mar00a, Mar03a, MCR03, Nes03a, Nes04b, ND02, ND03, Obe00, SBM+05, SM05c, WAJ04b, WAJ04a]. **Solitons** [Vel04, För00]. **soluble** [GGS09b, Sch04]. **solute** [PMAA00]. **solutes** [MC03]. **Solution** [AC02b, ND02, AGM01, AGM02, AG08, ACT+05, AVTPR09, ALI03, CRRL01, DNC07, FGdA02, Fis00, FPJR03, Gin05a, GI07, HEJ+00, HE05, HKE05, Hyd06, IYSS07, JNKMS03, JM00, KK07, KAN+09, LHL+00, LLW+07, LDR+08, LLZ+00, LSLD01, LYDK02, MP00, NOM00, OYYY02, Oku00, Pan01, PVW03b, RW00, SBT+03, SRK01, ŠFW00, SRHR05, TOH+00, VR01, VAS05, YSY+00, YKGC09, ZR07, dAGD08, ND03]. **solution-reaction-surface** [Oku00]. **solutions** [ACM07, BBC07, BG00a, BC06b, CA09, CFP00, DMMV00, DCLC05, Fan01, FZRD07, KP00a, Lef06, MMM06, MKZ04b, MSJ04, NF03, POM+08a, SMT06, YAŞ00, YYY05, YTS+05, YSS08]. **Solvable** [POMGM01, Ada02, FDM09, Mar05a, PRRMLB05, POM+07, POM+08a, SBT+03, SS01]. **solvated** [BCWS09, CSSB02, LCCH09a, PLA+07]. **Solvating** [BDE+07]. **Solvation** [FS08, IYSS07, JCTD08a, SKMW00, AGM02, Cor06, CBWM09, CRL+02, GdRPLP08, IMTG06, Jal08a, KIK09, LS01b, MMR+04, NSG+06, Oku00, PMAA00, PJS+09a, CC00a]. **solvatochromic** [BBVS+06, LCT00]. **solvatochromism** [BD01]. **solve** [ÇKB02]. **solved** [Mer04, QLD05]. **Solvent** [BN06, BRR04, DDT06, MVdCD00, SD08, SSN01, TMS08, BGP+07, CCE+07, DBB+06, FYH09, FG03, FSR02, HM01c, IDM+09, JV05, JSvDA06, KBMM08, LTY09, MRST01, PJ07, SBB05, SPS06, Tor06, WB05, ZWJ02a]. **solvents** [JJFdL08]. **Solving** [BOW+01, Yan06, DM02b, JTB09, LMJ00, NU09]. **Some** [ANJ09, Bra08, Brä06, SH07, Sut02, VTA+02, VCF+00, Wei08, AS04a, AEI00, BMR+07, CMM+07, ÇAK07, CSPS05, EHH09, EGEDH03, FDM09, FRT+00, FS00, FG01, GBS02, GP08, HdMB+05, HNR06, HWPIM01, IDH06, JZZ+08, KZG09, Khe09, LC02, Man05, Mar03b, MCR03, Mat00, MZ09, MESH02, NJC02, dlPOPP03, PRM+06, PCL+03, RSFRDNA04, Roy05a, Roy05b, SCM00, SM07a, VBS+04, WLZY08a, Yal04, YY04, ZCZC09, ZS04b, CL05a, CGG05, DL03, SC01]. **Sommerfeld** [MBP01]. **Sons** [Kry08a]. **SOS** [GG00]. **Space** [CK04, RH02, Yar00, ACCC03, Aze02, Aze05, Bel04, CSG06, CKM09, CP09, Dat04, DFMZO08, EBS+09, EMM+02b, FFHD00, GBS04, GPW06, GMS01b, GMS01a, JFC02, Koh01, KWG06, LP04a, LP05a, Lu06, MP06, MST08, MGMP01, Pan02, Pan06, PHK+06, RVP09, SMY07, ŠPNU08, SRHÖ06, TDF09, WS00, YKGC09]. **Space-group** [Yar00]. **space/bond** [OA02, ONA05]. **spaces** [CDB02, Pan04, Pan05]. **spacetime** [Sco00]. **spaghetti** [PNN08]. **spaghetti-like** [PNN08]. **Spanning** [CKM09]. **Spatial** [BBD04, Cam04, KS04b]. **special** [POM+08a, RHHH00]. **special-pair** [RHHH00]. **speciation** [dAGD08]. **species** [BK04b, DKC00, DBB+06, DM04, LDZ+05, LLL+07, MBRS05, NOM00, SIT+07, SIS+08a, YYS+09, YYI+09].

specific [Chu01, Gin06, KN08, PČH02, TMS08]. **Spectra** [CSP04, För00, AEI00, ASM+03, AA09b, Bec05, BWS+02, BKMHP04, BKRT03, BM07a, BSAL+06, BAG+08, CMR05, CC05a, CHC05, CSTB08, DKC00, DCP06, DS03, DNC07, Don09, Dre05, DKR04, FRT+00, FC05b, För04, FB07, GV06, GMCS04, GBP05, Gos01, Har02a, HLMH07, HRDM+08, IDM+09, IBB08, IOA+04, JLPA09, JNKMS03, KBV05, KVSS05, KNO09b, LSC01, Loe00, MUL02, MKCS05, MVL02, MDS+09, MVK00, MD06, Men08a, MBOA09, MYGD01, NSS09, Noo06, dlPOPP03, OM04, Pal00, PGN+05, PRM+06, PKS+00, PRL01, PLA+07, QBTS05, QC02, QCV06, RSN+07, RBLS04, RJP08, SŚRL07, TWZ03, TW05a, TRF+00, VNB+03, WRRF03, WC04, WSBV05, WSC+05, WPB+06, WT06, XXY00, YW09, YYXC01, ZCZ+07, ZLL+09a, ZNF05, ZTI+07, ZZKS07]. **Spectral** [Ban02, LW05, LVM01, SM06b, ABI07, ASO+01, ASO+04, BVS+09, Ban05b, BSCB04, HLH05, IABS08, MMV04, PGP+07, SRO02, SMDG09, SSM05, SJM08, Zho07, MB05a]. **spectrochemical** [ITY+09]. **spectrometry** [ENGY+07]. **spectrophotometric** [DCP06]. **Spectroscopic** [AC04, BBD07a, Duf07, MD04, OOD+05, SLRS02, BZL+09, BBD07b, BBVS+06, ERC+02, GBJM01, JLAR07, JLI+01, KVF+08, Mar06b, MBD05, MBD09, SSZ+07, SYZ+09, TKS+05, TMAB01, VDF+06, YZW+08, ZLL+09b, AC05]. **spectroscopies** [CÖ05, PGNT02, Qui05]. **spectroscopy** [ARBC+05, AM09a, BB05c, BKHPvD01, BKM+02b, DGQT09, GFMT08, Guo09, HYC+00, JJC+06, Kel05, LMSB00, Mal05a, MAS09, RRC03, SAMBS01, VRA+02, dVHB03]. **Spectrum** [RVNP09, BKAT00, CWF09, CEK01, CEÖ02, CCEÖ06, GXT02, JSvDA06, KFD01, LWC01, LSK+06, Mal05b, MVdCD00, MOA05, MHP04, NFL+02, NF02, Noo03, PRM+06, RLNA02, SBM00, SVDGFC05, SCW09, SKNN08, UMDM06, UC00, WWW+07, XV01, YSS08, ZW03]. **Spectrum-like** [RVNP09]. **Sphaeroides** [DRS00]. **spherands** [Elr09]. **sphere** [DHCD06, Kis04, ZLHL02]. **spherical** [CSP04, CS01, CMNH07, DVM06, DGC08, Eye00, HMB+04, JJWH04, LR01, MG05, SB06a, SK00a]. **spherically** [ANM03, BC06b, MS09, TS01a]. **Spheroidal** [CCR09, CMRMR00, LLB01, MCLKC02, Rom08a, Rom08b]. **sphingomyelin** [SKNN08, SKNN09]. **spices** [BKM+02b]. **spiked** [BB05b, CA09]. **Spin** [AZ08, AV05a, BCK04, Boe03, BSZ07, CL05a, DC05, MW06b, TYY05a, TYSY07, TYY07, Tri03, YTK+03, AV06, AM05, AG02b, ACDV01, ARBD05, BJS09, Boe04, BTK+05, BG00b, BG00c, BG02b, CIP+03, CD03a, CC01a, CK09, CC07, CEÖ02, CCEÖ06, CT00, DMV00, DM08a, DLK00, DB04b, FTM06, FM02b, GS09, GGAMB03, Gri06, Gri08, IAMY02, JHLC09a, JHLC09b, Kap07, KC09, KTK+04, KH01, KYT+04, KSI+07, KSN+09, KB00, KSU04, KSU05, KY05, KF09, LJL09a, LP07, LP00a, LP09b, MY08a, MY08b, MB07b, Mat00, OD03, ONK+05, Orl07, PKS+00, Pen00b, PS03b, RW04b, SMY07, SSR02, SE02a, SGP+07, SNZG02, STS+00, TSN+05, TYY03, Tem00, Tem02c, Tem02b, Tem02a, Tem04, TMAB01, WZW+09, WL00, YSY+01, YYS+00, YYKY01, YSO+01, YYS+01, YOYY03, YYT+04,

YTS$^+$05, YYZ$^+$05c, AV06]. **spin-1** [CCEÖ06, Tem02c, Tem04]. **spin-1/2** [CCEÖ06]. **Spin-adapted** [MW06b, KH01]. **spin-compensated** [AM05]. **spin-component-scaled** [CK09]. **Spin-coupled** [BCK04, KC09]. **spin-degenerate** [YSO$^+$01, YYS$^+$01]. **Spin-density** [CL05a, FM02b, GS09]. **spin-dependent** [CEÖ02]. **spin-forbidden** [IAMY02, YYZ$^+$05c]. **spin-free** [DM08a, SSR02]. **spin-frustrated** [TYY05a, YSY$^+$01, YSO$^+$01, YYS$^+$01]. **Spin-optimized** [TYY07]. **Spin-orbit** [TYSY07, ARBD05, FTM06, KY05, KF09, LJL09a, TMAB01]. **Spin-polarized** [Boe03, AZ08]. **spin-projected** [KC09, KSN$^+$09]. **spin-restricted** [LP09b]. **spin-state** [SE02a]. **spin-tensor** [MY08a, MY08b, SMY07]. **spin-unrestricted** [YTS$^+$05]. **Spindle** [Tac04]. **Spinel** [VPS$^+$04, CGL$^+$05, MTO$^+$03, NWZ$^+$07b, XCC$^+$08]. **spinel-type** [MTO$^+$03]. **spinless** [HN09]. **spinor** [MST08]. **spinors** [MTWN09, YHN$^+$07]. **spins** [Kat00]. **spintoronics** [KTH$^+$05]. **spiral** [KB00]. **split** [XV00]. **splitting** [ITY$^+$09, MK00, MB07b, RVR00, TMAB01, dGS06]. **Spontaneous** [CCM08, Kon04, Kry02, LP08]. **spot** [MFR07]. **spots** [LTL04]. **square** [DLCY$^+$07, GKR00, MZMZ09]. **square-cell** [GKR00]. **squeezed** [NY04]. **squeezing** [UP03]. **Sr** [ZL04, dD04]. **SrFeO** [Yur06]. **SrSe** [Cor04]. **SrTe** [Cor04]. **SrTiO** [EKZ06, ETBA06, Oni08, SVT06, UES04]. **SrZrO** [ETBA06]. **SS** [SBKSS05]. **SSAO** [AG01a]. **SSH** [SÖ04b]. **Stabilities** [TCS$^+$08, CSX$^+$01, DGQT09, GYF$^+$09, RBL04, RBL08, SUA$^+$04, SLU$^+$06, SUL$^+$07, SCHW07]. **Stability** [BBD08, CMW03, DP06, LAQ$^+$09, MBD09, SS08b, ADTD05, Boe09, CZS$^+$05, CMY03, CMNH07, DDT06, Den09, FF01, GWJ05, ILB$^+$08, JK00, JXW$^+$04, JHLC09b, KKMS04, LTV02, LJL$^+$03, LZXL05, LWZ$^+$09, LSK$^+$06, MCF09, MWW$^+$00, MPBM07, PM06b, PI02, PILD07, PJZ$^+$09, PM04b, QMB$^+$06, RJB$^+$06, STN$^+$06, TR00, XXY$^+$05, YS05, ZL04, ZLXL07, FdONGM08]. **Stabilization** [Jal07b, DGSD07, HS05, JdL08, LSC02, SBKSS05, SCMS07, Baň05a]. **stabilized** [FAE$^+$05a, FAE$^+$05b, RFRF05]. **stabilizing** [DS06, PCML08]. **stable** [Krü06, Özd04, PBSC04, ZS04b]. **stabling** [ZLML05]. **stack** [MBOL04, SBBL05]. **stacked** [KM05b, LSPS01, MSS09, SSN01]. **stacking** [KANK00, SKSB08, SS09d]. **stacks** [LY02, SBL05b]. **stage** [NTB02]. **staggered** [EHH09]. **standard** [CL05b, DDD03, PMLC05, PJP08, VD00]. **Stanislaw** [Ano02g, Szu02, Ano02f]. **stannacyclohexane** [FFHT05]. **Stark** [GAIK04, MMV05b]. **starting** [ACD02, Buc00b, NN09]. **Staszek** [Szu02]. **State** [SK00a, SS04b, ABL03, AGSH09, AM09a, AMGN00, AM05, AM09b, ABC$^+$06, AD01, Baň05a, BN04, BDA$^+$02, BM07b, Buc05a, BMMC09b, CA07, CSG06, Chu08, CMY03, CK06, DYD00, DBFP05, Deb08, DW00, DKM$^+$04, DGLM09, DBG04, ER05, FGH09, Fra06a, Fuk09, Ful00, GSQ$^+$04, GSK01, GWK$^+$05, GHT09, HN09, IDM$^+$09, JR02, JXW$^+$04, JSC01, KMM$^+$06, KLI07, KAN$^+$09, KB00, KN08, KV08, KV02, LSL$^+$08, LP04a, LXY00, LWCF08, LCBC03, MZF05, MP05, MA05, Mar04a, Mar07a, Mat00,

MBR07, MG08, MSK+05, NFP05, NSLR04, dlPOPP03, OA03, PK01b, PBS02, PVW03a, PCF05, PČH02, PRBGLL04, PJS+09a, RV05, RJP08, SA09, SE02a, SBB05, SBB06, She07b, SSZ+07, SLB+08, SL00, SL05c, SH02b, ŠŠU+02, SZA07, SM06c, Sun06, SMK08, TMAB01, TGGV+04, VLJ08, VD04, Vrb08, WTWT09, XYS+03, Yal04, YCN+07, ZSM+01]. **state** [ZW04]. **State-changing** [SK00a]. **state-specific** [KN08, PČH02]. **state-universal** [LP04a]. **States** [SE00, AZ08, AAKAF07, AV05a, AV06, AV04, AZD06, AG02b, BL04b, BDA+02, BL02a, BJ00, BKGF02, BDBG09, BBPG08, BABL09, Bu02, BDMS03, BPŠB00, BMP+04, CS03, CB03, CF05, CW08, CTS08, CN05, DL06, DGR+00, DEN02, DD03, DGG09, DBPG04a, DBPG04b, ESE04, Els05, EMV05, FCS03, FDM09, FN04, FS00, FHHC00, GG07, GL00, GSPT+07, Gre09, Gri08, Hag05, HJJ09, HS02, HGB08, Hea03, HGRL01, IN07, IV02, JR02, KS08, KS02a, Kap07, KH06, KH07, KH08a, KPČM05, KSK+04, KMK+05, KH05, KVF+08, KYA03, KF09, Kry06, Kry07a, LW05, Li09, LSM05, LA07, LZ05, MKCS05, Mat02a, MMV05b, MYS+09, MW06b, Muk00, MB02b, Nag04b, NKP+02, NRJD03, Nic02, ND02, ND03, ONK+05, OBM06, OR07, OdSC05, Orl02, OOD+05, PCBA08, PRNM03, PS03b]. **states** [PGW09, PREM04, PRCEM06, PGPA09, PE04, QGW02, QGW04, RCJF00, RdLJ+02, Ret06, RSKC08, RW00, Roh00, SK00a, SKN09b, SYLE07, SFPA03, SASS03, SC04, SSB00, SFZO01, SM05a, SdACAG03, Sjö00, SS01, SUA+04, SLU+06, SBF+04, SE02b, SB04, TN03, TBML06, TKT+05, TPGD02, WRD03, WW08, WO04, WBLQ00, XV00, YAŞ00, YNY01, YTD05, YOM+01, ZZUO05, ZDO00, ZW03, ZLS07, Tap04b]. **Static** [SMS+02, GB08, KCGB02, KZ09, Lef00, LCK00, MOL03, MBOL04, RPB00, SCB+06, ZBPD08]. **stationary** [BES08]. **Statistical** [CDGC05, GYM+02, ZZUO05, BS00, CK04, GSB00, Muñ02, RAdS05, Zak04a, Zak04b]. **statistics** [Mar06a]. **status** [Cas00, ZA09]. **step** [AG01a, TMPI05]. **stepped** [SWL04]. **steps** [Mak07, SKSB08]. **stepwise** [KV05, ZSWL07]. **stereochemistry** [ARD03]. **Stereoelectronic** [AKB06, FFS04, ONA05]. **stereoregular** [JC00, JC01]. **stereoselective** [KVPS05]. **steroid** [BSKFT07]. **steroids** [GP01]. **stilbene** [DI05, KDF00, KFD01]. **stimulated** [Mal05a, MHV00]. **STM** [DND06, LMMB03]. **STO** [Har02b, RFE+00]. **Stochastic** [CD00, CB00, FDME01, GHG04, NCB02, Pet04, GMS+05, HSW04, RT09, Sko02, ZFLL00]. **stockholder** [NB05]. **stoichiometric** [LPC04]. **Stone** [Luc02, SUAL04, TNO09]. **stopping** [CTSÖD03, PRM02, Por02, Por04, SO09a]. **storage** [Gup00, PMBM09]. **storing** [PH07]. **story** [MP05]. **STOs** [MR00]. **strain** [BM04, MZN+03, RO01]. **strained** [ESE04]. **strand** [DNN+06]. **Strandberg** [YST+05]. **stranded** [HT07]. **strands** [NID+06]. **strange** [Wen09]. **strategies** [BKMHP04, SEM05]. **strategy** [CL08, TBJA03]. **strength** [AL09, CCA+06, HEBS00, Kar04, RMJ+07, WLZY08b]. **strengths** [AC08, GAL+05, SI09, ZZM09]. **streptocyanines** [IDM+09]. **stress** [Tac04]. **stretch** [BB05a]. **stretched** [CCM+05]. **stretching**

[KSN+09, LFR+08, Mar00a]. **strictly** [KV02, TTM01b, TT06]. **strip** [ACPG01, CEK01]. **strip-type** [CEK01]. **stripes** [LTL04]. **stripped** [SM05a]. **Strong** [AL09, ZDO09, Ano07a, Deb08, GAIK04, IROW09, KK04, MYH03, MB00, SB06c, VD04]. **stronger** [SK09]. **strongly** [EWCT+05, HVSM02, KDM00, LSE05, SJE03, SLE05, SM06b]. **Structural** [ASO+01, ASO+04, BLZ02, ES02, GP03, GM05a, KM05a, LC02, MP09, NWZ+07a, PI02, PK01a, PHR08, SFK09, SGHL00, SZSP02, Tem02b, VED+02, ZSPS03, ZRF+09, ASRL06, AMC07, AKK05a, AKK05b, AT07, ART08a, BvRSS07, BBD08, Boe09, CVPGH+06, CXZ+09b, CCV+07, Cor04, CHR+06, DKP+06, FB01, FG01, GGPS06, GW06a, JHLC09a, Kan00b, KM00b, LDMR01, LPV02, LGBJ03, Oni07, PGP+07, RHM05, SCES03, SCHH02, Spr00, VDF+06, VBS+04, ZFD05, ZMZ+09, ZDQF08, KM03b, MCF09, SBK+09]. **Structure** [Ano02m, AÖG07, ABM02, BKLB06, Bli02, BBPG08, BGÖ+01, CMY03, DDD02, DGRB08, DBG04, DBPG04b, HWR05, JHLC09b, KP05, LJL+03, LZXL05, Loe00, LMSB00, PILD07, PRS+09, RO01, SE02a, SSSK07, VRFS05, YS05, ZLXL07, ZS04b, ZKRS07, AM07, AZ08, AAKAF07, AKN09, ASH07, AV05a, AV06, AWZD05a, AWZD05b, ASL04, AM09a, AV05b, ARH00, APN02, BVS+09, BE07, BK04a, BBO04, BT05, BBL09, Boe04, Boe07, BCT+02, BAG+08, BLKJ00, BMMC09a, Cab05, CL00a, CZ03, CD04, CDG05, CDV08, CFV02, Cat05, CSL+02, CIT+03, CN00, CBRBT03, Cos06, CR08b, CR08a, CK06, CBWM09, DNMM06, DBFP05, DFH02a, DFH02b, DBL+03, DBPG04a, EFM06, EWCT+05, EP02, EB04a, ESTU05, FH02a, FRT+00, FSGB05, FRNM08, FFHD00, GBJM01, GSQ+04, GS00a, GV06, GB03, GDB03, GD00b, GB05, GT07, Gin01]. **structure** [GG03, GBMMSA00, GXGT02, GWJ05, Guo09, Gup00, HJT07, HM01c, HSH02, IMT+02, IMTG06, JNF+09, JJC+06, JB07, JLZY09, JXW+04, KNRR05, KSH04, Khe09, KLB+05, KSG03, KF03b, KSN+04, KKMS04, KVSS05, KH08b, KKTMA09, KS02b, KSN05, Lav03a, LSPS01, LLR+00, LH07a, LLLZ06, Lin06, LPV07, LWZ+05, LH07b, LADD00, LH00, LSE05, Mal07, MLD06, Mar04a, MBOL04, MS05, MTE09, MOAB01, Mer04, MdlV03, MWW+00, ML01, MS00, MEN+08b, MK01, MW05, MGV00, MBA+08, MESH02, MW06b, Muk00, MGAS09, NSS09, NVA+03, NOHN02, Obe00, PCML08, PT00, Pan05, PKT05, PCKC08, PML09a, PKB+01, Pen00a, Pen06, PSEP05, PBB+02, Pud02, Put03, QLJ+09, QMB+06, QZ07, RVNP09, RA02, RH03, SPN03, SKSS09a, SAM08, SOLI04, SRO02, SSC+07, SNT+00, SNY01, SBM07, SLA+05, SCRRE07, SCRE08]. **structure** [SMM02, ŠK03b, SUH+01, SKT05, SSS+05, STN+06, SDB03, SHM+09b, SÖ04b, SNN+09, Tac04, TNO09, TDF09, TTK02, TT02, Tor02, THPN03, UES04, VRS01, VRA+02, VWMS03, VSD+02, VVBT07, VRC04, VPS+04, WSNB00, Wil04a, XXY+05, XZGZ06, XXY00, YHF+08, YLS+04, Yar00, YPS05, YPD+07, ZFLL00, ZXZ+09, ZTI+07, ZSKV04, ZMZ+00, ZZW+06, ZT04b, dAMM05, dD04, eSPM+08, Har02a, SR07, WW07]. **structure-activity** [eSPM+08]. **structure-antibacterial** [MEN+08b]. **Structure-hepatoprotective** [PRS+09]. **structure-properties** [CDV08].

Structures [BFB08, CK03, EBB06, JAP+05, LSC01, LAK09, LWL+08, SSF02, XXJG04, AdBM06, BGGS08, BFF04, BVHS04, BL04d, Bor00, CSX+01, CC00b, CGMT03, DB06, DLM+02, DJNH02, DK04, ETEA04, ET05, FF01, FFLZ02, FM02a, FAE+05a, FFHT05, FAE+05b, GXT02, GYF+09, HGRL01, IYY03, JTH02, KKS+03, KLI07, KS04b, Kra00, LBP04, LTL04, LLX+03, LLYJ09, MOA02, MS00, MPBM07, NRK+05, OCWY09, Pet00, Pyy01, QD04, QXJG05, QBTS05, RBL04, RSFRDNA04, SIS+08b, SUL+07, SKHY09, SSK09b, SCHW07, SBL05b, TN09, TFS+02, TWZ03, TW05a, TRF+00, TNET03, VK05, Vel04, VNP00, WNW05, WTWT09, WBLQ00, YZW+08, YJ00, ZLL+09a, ZLL+09b, ZWJ02b, ZZKS07, GW06b, LXH+00, LXTT00, LXHT00, LZYT01, LZHT03, RBL08]. **Strutinsky** [BKM+02a, DKM+04, KDY+02]. **studied** [AGLBM03, JXZ+05, Lat03a, SP00, YW09]. **Studies** [DKR04, JK00, KKMS04, Lat03b, dRPFCP08, Por04, Roy05a, Roy05b, SRK01, WT06, ZFD00b, AGN04, AKK05a, AKK05b, BZL+09, BKLB06, BGP+06, BBVS+06, Bou01, Bu02, CTSÖD03, CFV02, CGG05, CBB01, CHC05, CWBM06, DBL+03, DK04, EGEDH03, ELY09, ER05, FRT+00, FF01, FFLZ02, FGML06, FTGH04, GV06, GG03, GLX+00, GXT02, GGPS06, GI07, GFMT08, HEJ+00, HKMM04, Hua04a, HY04, IS03, JRSA08, JHR+00, JWZ+08, KTK+04, KLI07, KJW08, KYT+04, KSS+08, KNS+09, KVSS05, KSWR00, KS03b, LZZ+06a, Li09, LQC+08, LQM+09, LH03, LTL05a, LTW09, LYDK02, LYWX07, LXXC08, MP06, MLZS06, MLSB06, NNS+00, NKK+01, Nag04a, NK05a, NK06, NK05b, ONK+00, OMMWL02, OOD+05, PHR08, PSK02, Pet00, PHNN09a, PHNN09b, PL00, PGP+07, RLB02, SKN+09a, SWL04, SDFM02, SBB06, SSB00, SAMBS01, SSJ09, SPS06, Shi04]. **studies** [SNM+04, SKK+05, SKK+06, SIS+08b, SCW09, SBFV05, SYL05, SZK07, Sta00, SSDB06, ŠFW00, SCHW07, Swa03, TOK+00, TLYW06, TSP+07b, TSP+07a, TWZ03, URBM04, WE01, WB05, WF04, Woo02, XXY00, YKT+02, ZDZO07, ZCZ00, ZXX02, ZD06, ZLSL06, ZD07a, ZCZ+07, ZLL+09a, ZCZF02, ZLF+07, dLCRF+08, MTWN09]. **Study** [CCV+07, CHS09, EMM+02b, FDZ04, GGS09b, IABS08, JFJMR08b, KSS00, KN08, KBUV07, LMX+05, PGNT02, SPI04, SK05a, TN03, TMM+03, VPS+05, WZWC07, ZZWM07, eSPM+08, AEI00, ABBS08, AB08, AGBY00, AG08, AE04, AE07, ARE02, ASL04, ASRL06, AML+01, AMC07, ARD03, ABD06, AV05b, AGFM03, ACB+02, Ano07g, Ano07e, Ano07f, ADTD05, ASO+06, AT00, BM01b, BVS+09, BFRB07, BF08a, BGG08, Baň05a, BK04a, BVG05a, BRL02, BCdP03, BFAM03, BHG+06, BPM01, BP03, BEM02, BK04b, BK04c, BDA+02, BEL01, BVHS04, BVHS05, BČZ07, BBD07a, BBD07b, BGP+07, BCD+05, BBD07c, BL04c, BZH+07, BB09, BCK04, BBPG08, BSKFT07, BZBT01, BCT+02, BMMA06, BAG+08, BLM08, BJAV08, BF08b, BDMS03, Buc05c, Buc08, BSBS06, BSB07, CVPGH+06, CK03, CGL+05, CSX+01, CZ03, CJZZ06, CB04, CdMCS05, CDS06]. **study** [CJ03, CBMRN08, CM05b, CQN+03, CC07, CSPS05, CL05c, CSL05a, CL05d, CL07a, CB03, CC00b, Che00, CC01b, CZPJ01, CY04, CWY05,

CCH05, CSL+07, CCE+07, CTI09, CSDCCMZT03, ĆMTS08, CI06, CN03, Cor04, Cos06, CBC00, CMASC01, CDGC05, CMNH07, DF07, DEN02, DB06, DRD+05, DQZ04, DDT06, DT00, DDD02, DGD+05, DKWP04, DAD+03, DDW+06, DDM00, DBHT01, DH04a, DLTW04, DGRB08, DGLM09, Die00, DSL06, DZS+06, DFT+07, DZTZ05, DFZ04, DFZ05, DZ06b, DZ06a, DSW00, DSW02, DWM+07, ETM00, ET01, ELO+07, ELC08, Els05, EZY00, EKN04, EKZ06, FH02a, FGFF06, FWT08, FYH09, FXHL05, FWZ09, FFF07, FGC04a, FGC04b, FGdA00, FGdA02, FPC+03, FC05a, FOM+03, FF09, FRF02, FRGF04, FGZ07, FGF06, FFDD07, FC04, FAE+05a, FFHT05, FAE+05b, FS05, FBC+06, FG06, FBGA04]. **study** [FYT09, GEB+00, GR07a, GR07c, GR07b, GBJM01, GSQ+04, GSC00, GTSK07, GSPP+06, GJB00, GJB02, GJ03, GDFT01, Gog05, GB06a, GR05, GBMMSA00, GXGT02, GZD+05, GL07, GMTM02, GARB08, GYS+06, GdRPLP08, GW06a, Guo07, GYF+09, GN01, HJT07, Han07, HI06, HGS03, HNR06, HAL+02, HHGSRS02, HCTC07, HDWH09, HDL00, HKY07, HD03, HBW+08, Hua04b, HR05b, HR05a, HP07, IAMY02, IDH06, IN09, IYY03, ITR02, Iva05, JCTA08, JNF+09, JJC+06, JR02, JLI+01, JPA03, JSvDA06, JAP+05, JCP+08, JFS+09, JXW+04, JHLC09a, JFJMR08a, JG09, JG00, KK02a, KDŁL07, KS02a, Kak03, KPC05, KZG09, KNRR05, KRR08, KWWQ04, KFQ+02, KD05, KKK09, KV05, KL03, KDC09, KCOV07, KVSG02, KAN+09, KM04, KF03a, KVZT04, KVT04, KMS02, KWT06, KSK00, KYA03, KS03a, KG08, KES03, KMVR05, KFD09]. **study** [KANK00, KZS07, KB08, KDF00, KBMM08, LDMR01, LCRB01, LRB04, LSBDL02, LDPP05, LDP05, LSWT05, LML02, LMRT08, LHV+09, LXH+00, LXTT00, LXHT00, LXD00, LZYT01, LWW+02, LZHT03, LZT03, LDXW04, LTLS05, LDZ+05, LZJ+06, LFZ07, LZZ+07, LCL+09a, LMDW09, LTY09, LCL+09b, LWC+09, LSCC01, LC02, LSK+06, Lia08, LRS05, LČM01, LQC06, LL04, LC05, LLZ04, LCH05a, LWZ+05, LZXD05, LPZW05, LCH05b, LDG+06, LLYL06, LLL+07, LCCH09a, LJL09b, LDM09, LMSB00, LVSG06, LH00, Lu06, LZWY07, LYCX08, LWCF08, LNPL06, LTL06, LZW+07, LH07c, MUL02, MGdS+08, MZN+03, Mai08a, Mai08b, MP05, MKHP09, MK08, MW06a, MLD06, ML08, MB06, MCR03, MRST01, MTRG04, Mar06b, MARK08, MVL02, MMCC02, MBA+04, MPS+02, MVK00, MHGR07, MOA05, MROA06, MOA07, MOAM07, Men08a, MBOA09, MWXL05, Mey00, MGZL04, MJG+05, MDJ01, MD04, MBD05, MLSG04]. **study** [MdlV03, MGB+06, MWW+00, MME09, MJ00, MSMS03, MMZ02, MLL00, MZMZ09, MBD09, MGMR04, MBRS05, MDG07, MB02b, MSC03, MGAS09, NFFA04, NOY+01, NNNY01, NH00, NMNB06, NID+06, NSLR04, NAE06, NVA+03, Nov07, NOHN02, OSW07, dlPOPP03, OCK07, OKY+08, OM04, OGJdlV03, Oni08, Oni09, OMMB07, POAVdlM08, PIGN02, PNG02, PK01a, PXZ+09, PBSC04, PK01b, PMB08, PBS02, PSS05, PMBM09, PRS+09, PVW03a, PVV+04, Pej02, Pej03, PRNM03, PYZ09, PKZN08, PBI+01, PMCOSC00, PNBV07, PFSP05, PSEP05, PLU08, PDR+00, PREM05, PB03, PRL01, PSB+05, PCM00, QFC04, QCFJ05, QXJG05, QBTS05, QZ07, QC00,

QV01, QCC02, REHH07, RVR00, RRNG05, RVP06, RA03a, RLGB01, RBL04, RBL08, RH09, RWW+01, RFRF05, RSFRB03, RNCM05, RD00, RHM05, RKR+06, RFF05, RAdS05, Rua09, RRD06, SO04a]. **study** [Sad02, SK00a, SL05a, SL07, SKN09b, SPH+03, SSMG08, SLRS02, SB03, SBF03, SK06, SBB05, SVDGFC05, Sha06, Sha07, SKA05, SSK09a, SZZ01, SS08a, SNT+00, SCR01, SCRR02, SY06, SY09, SGHL00, SIT+07, SKK+07, SL05c, SWZ01, SdACAG03, SCG07, SKSS09b, SKHY09, SZ08, SWSH09, SCES03, SCRSRE05, SCRSRE06, SCRE08, SHC00, SCHH02, SCB+06, SPSS07, SPS05, SJM08, SZSP02, SV08, SUH+01, SDZ+07, SVC+05, SMSM02, SQZ+02, SBHF06, SSB+07, SINN05, SIT+06, SKNN08, SKNN09, SHM+09b, SRW+06, SHH+06, SLW+07, SZML07, STL+09, SSK+05, TLC06, TIV+07, TT05, TSK01, TY07, TN09, TNO09, TBJA03, TTK02, TSZW08, TTFP04, TKT+05, TRF+00, TX02, TWZW09, THP08, TUA06, TW05b, TNET03, TL05, TDST07, UMDM06, UML00, USM01, UC00, VHV+05, VWMS03, VVW+03, VR01, VML05, VBT+07, VVBT07]. **study** [VMA03, VK07, VBS+04, VLK+08, VTS04, VTS05, Vrc07, WFS+01, WZL+07, WWW+07, WWTHF09, WHD+05, WJLL09, XD03, XXJG03, XXJG04, XXC08, XFLX+06, XYS+03, XC07a, XCS+03, XVRL04, XXY+05, XCW07, XCC+08, XL08, XC07b, Yam09, YOYY03, YUN+07, YST+05, YMZH04, YSV05, YS05, YYZ+05c, YZG06, YZX+08, Yan09, YS09, YKS+06, YNDJ06, Ye01, YW05, YWC07, YT03, YHD+07, YF07, Yur07, ZSPS03, ZMB+03, ZMMS+00, ZB08, ZR07, ZZFL00, ZZ05, ZLZ05, ZLL+05, ZFFX05, ZH06, ZL06, ZZDY06, ZLX+07, ZZZ+08, ZDMF08, ZFZ+08, ZSL+09, ZXZ+09, ZLL+09b, ZHA01, ZMAL04, ZKYA04, ZNF05, ZOK+05, ZJZ00, ZL04, ZLML05, ZTW+09, ZHS06, ZTI+07, ZSM+01, ZL00, ZQF+02, ZPW+04, ZZC09, ZTSZ07, ZDQF08, ZBPD08, ZNZS00, ZLH+08, ZKRS07, BD01, dlPCLG+00, MMV05a, PČH02, RACD00, VRA+02, VHM+04, RA04]. **studying** [Bol04, MB02a, Mor08, Van06]. **Stueckelberg** [SCTK+09]. **Sturmian** [ACC03, ACCC03, AS00, FGR+07]. **Sturmians** [AS01, Ave04, RFCG09]. **styrene** [DR08]. **sub** [GLHH09]. **sub-100** [GLHH09]. **subcellular** [AG01b]. **subensembles** [Tem02c, Tem04]. **subgroups** [YN04]. **sublimation** [PMLC05]. **submitted** [OB02]. **subnano** [NWZ+07a]. **subphthalocyanines** [FPC+03]. **subspace** [TN03]. **subspaces** [BK09, Pen00b, VNB+03]. **Substituent** [EHN09, GS00b, GS01, HEBS00, HSH02, KKK09, LZWY07, MWXL05, TSK01, dSNBG08, Ess07, HS05, KM04, LTY09, LSC02, MBRA07, MGB+06, MESH02, SST00]. **substituents** [TKS+05, TJAS08, YF07]. **substitute** [HR02]. **substituted** [BCdP03, BHG+06, BDA+02, DCW03, ETM00, ET01, ERC+02, GSH02, JB07, LTV07, dAMdG05, MGG05, MGZL04, SSK09b, TC05, VCHC07, VBS+04, VSI+07, WT07, ZGY+03]. **substitutes** [SYL05]. **substituting** [ZL06]. **Substitution** [ZWJ02b, Buc01, Buc07, GXGT02, JSC01, MMV05a, Nic05a, RJN+08, SAE08, Sok04, VTS04, VTS05, Yur07]. **substitutional** [Cou05, SPI04, SHM+09b, VPS+04]. **substoichiometric** [CB04]. **substrate** [SGLF01]. **substrates** [PKZN08]. **substratum** [BMB02a]. **subsystems**

[Buc02b, MD02, Nal00b]. **subtilis}** [WRK03]. **subunits** [Yur08]. **succeeding** [LZHT03]. **successfully** [HR02]. **Sucher** [AM09b]. **Sudan** [DDD+00]. **sudden** [Baň05a]. **Sufficient** [AP03]. **suggesting** [Mas02]. **suggestions** [YKS+06]. **suitability** [Lu06]. **suitable** [MTWN09]. **sulbactam** [ZLF+07]. **sulfanilamide** [PGP+07]. **sulfenato** [AVBč06]. **sulfenato-** [AVBč06]. **sulfhydryl** [BN01]. **sulfide** [FB01, GG03]. **sulfinato** [AVBč06]. **sulfinato-Co** [AVBč06]. **sulfines** [RM07]. **sulfinyl** [FAE+05a, FAE+05b, FS05]. **sulfobutyl** [DH04a]. **sulfonamide** [ZSWL07]. **sulfonamides** [SCES03]. **sulfotransferase** [LYP+06]. **sulfoxides** [FAE+05a, FAE+05b, FBC+06]. **Sulfur** [FH02a, DV00, DDD03, LXH+00, LXTT00, LXHT00, MLP08, SKK+05, VM06c, WFS+01, WSBV05, WSC+05]. **sulfur-** [MLP08]. **Sulfur-containing** [FH02a, LXH+00, LXTT00, LXHT00]. **sulfuric** [CTI09]. **sulfuryl** [LYP+06]. **Sum** [QC01, AM06, BB05b, FCS03, Gos01, HMMT04, Mar87b, Mar87a, MNA+99, PSM07]. **Sum-frequency** [QC01]. **sum-over-states** [FCS03]. **summation** [Fer01, Goo03]. **summations** [JFC02]. **sums** [BČ02]. **super** [GFDK09, GGDL07]. **super-CI** [GFDK09, GGDL07]. **superalgebra** [Pan06]. **superatom** [SLWS07]. **Superconducting** [BS05b, Baň05a, DB04b, NNS+00, Squ05, Yar00]. **superconductivity** [BS00, KNN+04, LK00b, Lar02, MS03, NNS+00, NKK+01, Nag04a, NK06, PLC04, SC02a, SC04, Shi05, SM04, SM05c, SM07b, SM08, YNN+06, YYT+04]. **superconductor** [DT00, SM06c]. **superconductors** [CDF06, CS00b, FPJR03, KKM+01, LML+04, Liv02, YYK+03, YYI+08]. **supercritical** [FS08]. **superlattices** [JP08]. **supermolecular** [JZL+08, RP09]. **supermolecule** [BF07, GB05, PVZV00]. **superoxide** [MSS05]. **superphane** [MSSM00, MSMS03]. **superposition** [KAE03, KWC09, PA08, SFD09]. **Supershells** [BLRT02]. **supersymmetrical** [DK03]. **Supersymmetry** [CF05]. **support** [CWW09, GI07]. **supported** [HRDM+08, SASS03]. **supports** [HSS09]. **suppresses** [ZTSP00]. **surds** [BČ02]. **Surface** [FA05, MB01a, ACG00, ASP+05, ACHB08, BAKK06, BFB08, BMMC09a, BMMC09b, CR06, CSG06, CCB07, DBG04, DZ06a, EB04b, EB04a, FTB04, FRGM06, FCD08, GGACT03, GSRL06, Gog05, GMPIP01, GSPT+07, GYM+02, HSW04, HR05b, HR05a, JdL08, LPC04, LJMM09, LRS05, LL04, LC05, LPV07, LDM09, LXY00, LWCF08, MGdS+08, MGZL04, MVA02, MPIP00, MPIP+01, NRS+02, Oku00, PA04a, PMPI01, PMC02, QS05, RKM09, RPHG04, RIVB03, SSMG08, SMAL01, She07b, ŠŠU+02, SK05b, SBF+04, SLW+07, Tch07a, TGG01, VG06, WL00, XCC+08, YT03, YHD+07, ZFD05, ZCZ00, ZLZ05, ZYG00, ZD08, ZH05, ZLY+09]. **surface-enhanced** [ASP+05]. **surfaces** [AG01a, AML+01, ART08a, ART08b, BJ00, BS02, BR02, CNPA04, CT05, CS04, DRPT02, DI05, ESU05, FFF07, FOM+03, FYSS09, GY04, HAL+02, HBTW04, HWPIM01, IDM+09, Jal07b, Jal08a, Jal08b, JCTD08a, Jal08c, KZ08, KCS02, KIK09, KDM00, LFADSF07, LB03, MZD+05, MJG+05, Mla02, NH00, PRSLA08, PC07, PLO02, PMAA00,

QTT07, QCC05, RST08, Saa00, SWL04, SSB00, SKA05, SVT06, ŠFW00, TT01, TR09, VLJ08, VGMN03, VGB05, VSS04]. **surfactants** [ZS04b]. **surrounding** [YYQ+06]. **Survey** [PRM03]. **susceptibility** [JV05, She07c]. **SUSY** [PRRMLB05]. **Swart** [Ano07a]. **SWCNT** [SÖ04b, SRHÖ06]. **SWCNTs** [ZMZ+09]. **Sweden** [ERU07]. **Swift** [KZS07]. **switch** [Chu00, Chu01]. **switches** [Chu02]. **switching** [FGZ07, HGB08, Sad00]. **SWKB** [Sin00]. **SY** [Ano07e, Ano07f, GR07a, GR07b]. **Symbolic** [Bar00, BCvzGG04, Fra06b, Gün06, Har06, Her06, SB06b, VAS06, BC06a, Bar06, Gui06, RT06, WK06, Yil06]. **Symmetric** [FB07, BBO04, Brä09b, Buc02a, GB09, May02b, MSJ04]. **symmetrical** [MARK08, SBF03]. **symmetries** [DLCY+07, Fri06, Tem00]. **Symmetrization** [LL01]. **symmetrized** [Ras02]. **Symmetry** [ABCS02, Buc00b, IDM+09, KZB01, LP09b, BE07, BFAM03, CT00, DAD08a, DAD08b, Del03, FGM05, HPR09, Hyd06, KSN+09, LP08, LC02, Liv02, MC00, MDBM05, MYGD01, NYU+08, OBM06, PML09b, Pen00b, RS09, RS11, SSSS09, Sto08, TYY06, WKS03, YHN+07, YN04, ZLY05, DEN02]. **symmetry-forbidden** [Pen00b]. **symmetry-invariant** [WKS03]. **Symplectic** [HW06, JP01, LSD02, Ano06g, HZPY03, KMS06, LLZ+00, LSLD01, QLD05, ZH06]. **Symposium** [CB08, SD03, BCC05, CA06, ERU07, RRUE08]. **Synchronization** [PNN08]. **Synergistic** [PS04]. **synthases** [Cor06]. **Synthesis** [CIT+03, SJM08, LCCH09a, NH00, TVK+02, TUA06]. **synthetic** [BB09, Che00, SUH+01]. **syringic** [PKS+00]. **system** [Apo06, ADK02, BVG05b, BEL01, BGJJ01, CB04, CSL+02, DC06b, FZRD07, GGLS02, Gri06, HT05a, Han07, HZPY03, HLO04, HAL+02, Hog09b, IG06, JMP05, KVF+08, LWCF08, MB05a, May06, NOY+01, NNNY01, NK05a, Nes01a, Orl07, PM03, PGW08, SA09, SNT+00, STN+06, TOH+00, VH00, VHM+04, VGB05, YBS05, YHD00]. **Systematic** [BM07a, CM02a, Mor03, Put06, AE07, KW03]. **Systems** [DT02a, AM05, AG02b, ABLL02, ASO+01, ASO+04, AP03, BR08, BR12, Bar08, BVHS05, BKGF02, BCWS09, BZG+02, BSM+07, BL04c, BA01, BG02a, BKMHP04, Brä04d, Brä09a, Buc00b, Buc02a, Buc02b, Buc05c, Buc08, BCF02, BA02b, BCF03, CCH05, CCH06, Cho08, CF04, Chu00, Chu04, Chu07, CC05c, CMRMR00, CK04, CS01, CDGC05, DMV00, DD05, Deb08, DFH02a, DFH02b, DLK00, DSH01, FRGM06, FRK+05, Fra03, FD09, Gin01, GW04, GKE01, GPW06, Hag00, HdMB+05, HVSM02, HEJ+00, HS02, HH09, HT04, HM03, HRDM+08, IYO+04, Iye09, JLAR07, Kan00a, Kar04, KBV05, KCGB02, KT05, KS04b, KSN05, Kry05, Kry06, KDY+02, LLR04, LME03, LSPS01, LCH05a, LCCH09a, LSE05, Mai08a, Mai08b, MNMV02, MOL03, Mat00, MKZ04a, MHB05, MF03, MVLM05, MLSB06, MT02, Mic06a]. **systems** [MNV07, MDSW07, MB01b, MB05c, NKS+09, NY03, NY04, NJC02, NYU+08, OBM06, OYB+00, OMY+01, Oku01, OR07, Pea08, PVW03b, PKB+01, PGW09, PPP+08, PO03, PRCEM06, PL00, PMPI01, PS03c, PTLB00, Pup07,

RB08, RB11, Roy08, RNS04, SJE03, SLE05, SCP03, SGGBB02, SBB05, SK01b, SH09, Sin00, Stu00, SZJ+04, SDW07, TOK+00, TYY03, TYY05b, TYY05a, Tap04a, Tou09, Tri03, UBS04, UT03, VX04, Var08, VD04, VMRA04, WKF+06, XV00, YŞ02, Yal04, YSO+01, YYS+01, YYT+04, YNN+09, YN04, ZZL04, ZZL05, ZZUO05, ZZFL00, ZR03, Živ09, dD04, Nag03c, PČ04a, BA02a].

T [FHK06, HMW05, JKU02, LVSG06, MLSG04, Mor06, Mor08, RSTG02, ŠPNU08, VGMN03, GBP05, DB04b, EF03, FPJR03, GMS+05, KKM+01, KS03a, Li09, PGF+06, SM04, TCS+08, YYK+03, YNN+06, VG02]. **t-BuOO** [VG02]. **T.** [Ano06g]. **Table** [KH05, Mat07, AK02, Gar08a, Har05b, KH01, Kry07b, Nég00, Sce09, ZWMZ02]. **Table-CI** [KH05, KH01]. **table-driven** [Har05b]. **tables** [SST+02]. **Tabu** [RB06]. **Taft** [Ess07]. **tail** [BNHB+02, JZW+09, MSC03, YZX+08]. **tailoring** [JG09]. **tailoring-based** [JG09]. **tails** [JZZ+09]. **taking** [FBBB06]. **tale** [Bau09]. **Tamm** [WW08, YSY+00]. **tamoxifen** [Hua04a]. **tandem** [PNBV07]. **target** [Por02, Por03, SK00a]. **targets** [CGS01, LLR+00]. **Tautomeric** [AB08, MRST01, KS03a]. **Tautomerism** [LDR+08, ZY06, AEI00, AG08, CME07, DDD+00, LLW+07, SPS06]. **tautomerization** [DFZ04, ZR07]. **tautomers** [Els05, TX02]. **taxol** [Bou03, ZZC09]. **Taylor** [Wen00, Wen02]. **Tayloring** [PJP08]. **TCDD** [SSK+05]. **TCNE** [KBMM08]. **TD** [SL05c, GSQ+04, GL07, PLA+07]. **TD-B3LYP** [GSQ+04]. **TD-DFT** [SL05c, GL07, PLA+07]. **TDA** [HNKiS01]. **TDDFT** [AZD06, Bec05, HCTC07, PJP08, SBM+05, SRHR05, WW08, ZZKS07]. **TDDFT-derived** [Bec05]. **TDDFT-PCM** [ZZKS07]. **TDDFT/MM** [SRHR05]. **TDHF** [Qui05]. **Te** [GYF+09, JLAR07, LLW+07, LDR+08, SZJ+04]. **teaching** [PL09]. **technique** [BGN+05, GTR+05, KGI+05, LPV05, MNMV02, MRG02, SS04c, SS02b, XV00]. **techniques** [Ben05, Glu04, Liv02, Mak07, MC06a, MSC03, QG04, Roh00, RB07, Sal09, Yil06, YOM+01]. **Teller** [Noo06, ADK02, BFAM03, DL02, FMBM05, MP05, MB06, MdlV03, PLC04, Pup05, Pup07, VX04, VIGL+05]. **telluride** [KG08]. **tellurium** [FTM06, LVM01]. **Temperature** [FFDD07, KFD01, FdONGM08, AKN09, AP00, APN02, Boe09, BS05b, CGL+05, CS00b, DKP+06, För00, Gri06, KPP01, Liv02, LB02, NOM00, SKMW00, SC02a, SC04, Shi05, Tou09, dAMM08]. **Temperature-dependent** [FFDD07, AP00]. **tempered** [CKM09, KW03]. **templates** [VAS06]. **Temple** [MB07a]. **tensor** [BKRT03, BG00b, DETA02, Lat03a, MY08a, MY08b, SMY07, Tac04, Tem02b]. **tensorial** [Tem02a]. **tensors** [MC03, MH06, Nee01, NGRR02]. **terephthalato** [BL04c]. **terephthalato-bridged** [BL04c]. **term** [GSCRO08, HM01b, Sce09]. **term-by-term** [GSCRO08]. **terminal** [BP04, ZSL+09]. **terms** [ANM03, BMB02a, BČ02, CDB02, Gin01, GSD+03, Kut03, Lat03a, Lat03b,

MP05, MP06, Mar05b, MC08, NBS04, PA08, PLC02, UB05, VHM+04].
ternary [Mat00, OG00, OHT03]. **tert** [BT05, DAD05, MGZL04, MJG+05].
tert-butyl [MGZL04, MJG+05]. **tertiary** [PCML08]. **Test** [MCF08, BEL01,
BDBG09, CSSB02, DBPG04b, GPW02, LLR+00, LSM05, SPH+03, MMB03].
tested [CBRBT03, DVV05]. **Testing** [SOLI04, DBG04]. **testosterone**
[SPS05]. **Tests** [ZT04a, ZLJ+09]. **tetra**
[DAD05, LAK09, PS03b, RBA07, Pye00]. **tetra-** [LAK09, Pye00].
tetra-atomic [PS03b, RBA07]. **tetra-tert-butyltetrahedrane** [DAD05].
tetraatomic [BDBG09]. **tetrabromomethane** [MdlV03]. **tetracaine**
[BGP+06]. **tetracarboxylic** [ZNF05]. **tetracyanoethylene** [YLYD03].
tetracyanoquinodimethane [MP06]. **tetracycline** [MPIP00].
tetracyclines [HWPIM01]. **tetrafluoroanisole** [KCOV07].
tetrafluoropyridine [TMM+03]. **tetragonal** [PTS03, SM09]. **tetrahedra**
[KZS07]. **tetrahedral** [MGZL04]. **tetrahedrons** [CL05b].
tetrahydroimidazodiazepinone [SKSS09a]. **tetrahydroisoquinoline**
[HQL09]. **tetrahydroquinoxaline** [CSDCCMZT03]. **Tetrahymena**
[SKSS09b]. **tetrakis** [CLSD+01]. **tetramer** [LDMR01, PHR08, ĆMTS08].
tetramethoxybenzene [VBT+07]. **tetramethylammonium** [JWZ+08].
tetramethyleneethane [NLD+04]. **tetramethylsilane**
[DAD08a, DAD08b, Sto08]. **Tetranitrotetraazadecalin** [QXJG05].
tetranuclear [LH07c]. **tetrasulphonated** [CJB08]. **tetrathia** [DCW03].
tetrathiosquaric [ZMZ+00]. **tetratomic** [DWF+03]. **tetrazolate** [Che00].
tetrazole [CX00, Che00]. **texture** [Wal04a]. **Th** [HDL00]. **Th.** [Ano06g].
thallium [RSRMBFR00]. **their** [ABI07, AM09a, BB09, BČ02, BCT+02,
Buc05c, CW00, CD00, CDG05, CJ03, CC00b, DVHJ03, DWF+03, EKN04,
GV06, GT07, Gin05b, Gin06, GW06b, Gus02a, Koc00, LAQ+09, Lu06,
MMCC02, OK05, PRM03, PKT05, PML09a, POMGM01, PRRMLB05,
PGP+07, Put06, Qui05, RFS+00, RS08, Rua09, SBL05a, SSK09b, TKS+05,
TX02, UMDM06, VTPRA08, XC07a, YYY05, Zak04a]. **THEMATICS**
[She07a]. **theorem**
[Brä09b, HM01a, HM01b, KT05, Kry05, Kry06, LSM05, MB05c, PS03a, PS08,
Pan07, Pup02, Pup05, Pup07, RLER04, Sah04, SDW07, TB09, TGGS06].
theorems [ASO+01, ASO+04, QS00c, Wen00, Wen02]. **Theoretical**
[AAKAF07, AEMAO06, ABBS08, AGN04, ALM05, ARE02, AML+01,
ARD03, AZD06, Ano07g, Ano07f, Ano08a, ASO+06, AA09b, BB05a, BGG08,
BVG05a, BVHS05, BBD07b, BGP+06, BBD07c, BL04c, BWS+02, Boe09,
BKHPvD01, BKMHP04, BSAL+06, BZBT01, BMMA06, Bro00, Bro05,
BF08b, BCS01, BHK09, CVPGH+06, CWF09, CB08, CDK01, CJB08,
CM05b, CQN+03, CC07, CL07a, CC00b, Che00, CC01b, CZPJ01, CWY05,
CCH05, CCH06, CL07b, CME07, ĆMTS08, DF07, DYD00, DAD+03, Den09,
DNC07, DFZ05, ETM00, ETEA04, EKN04, ERU07, ELG05, FJT+05,
FRT+00, FF01, FFLZ02, FGC04b, FSLL02, För04, GR07c, GR07b, GD00b,
GDFT01, GLX+00, GRC09, GAR08b, GGPS06, GARB08, GYF+09, HJT07,
HHGSRS02, HKE05, HDWH09, HS05, HY04, Hua04b, HZW+08, IDH06,

ITR02, JFS+09, JHR+00, JWZ+08, KS02a, KPC05, KNRR05, KTK+04].
Theoretical [KL03, KYT+04, KSS+08, KVZ+02, KVT04, KYA03, KH08b, KF09, KKTMA09, KT05, Lad00, LCRB01, LRB04, LXD00, LDXW04, LDZ+05, LZZ+06a, LZZ+07, LCL+09b, LWC+09, LQM+09, LH03, LTL05a, LCH05a, LWZ+05, LZXD05, LPZW05, LCH05b, LLYL06, LYDK02, Lu06, LYWX07, LXXC08, LYCX08, LWCF08, ML05, MLD06, MM02, MARK08, MVL02, MBA+04, MPS+02, MDS+09, MOA05, MOA07, MOAM07, Men08a, MBOA09, MGZL04, MJG+05, MGB+06, MSSM00, MSMS03, MMZ02, NNS+00, NOY+01, NKK+01, NNNY01, Nag04a, NK05a, NK06, NSS09, NSLR04, NVA+03, ONK+00, OM04, Oni09, POAVdlM08, PC09, PNG02, PXZ+09, PMBM09, PML09a, PYZ09, PHNN09b, QCFJ05, QXJG05, QBTS05, QZ07, QCC02, REHH07, RRNG05, RLGB01, RBL04, RFS+00, RWW+01, RSDNSB00, RC05, RHM05, RVD03, SKN+09a, Sak00, Sak02, SHM09a, SDFM02, SMAL01, Šat03, SK06, SAMBS01, SKA05, SSZ+07].
Theoretical
[SZL+09, SNT+00, SY06, SCW09, SWZ01, SD03, SCHH02, SUH+01, SMSM02, SCLL07, SINN05, SIT+06, SHH+06, SLW+07, SZML07, SCHW07, TTK02, TLYW06, TWZ03, TRF+00, TW05b, VATPR09, WFS+01, WB05, WLZY08a, WGX09, WWTHF09, XFLX+06, XYS+03, XXY+05, XR05, XC07b, Yam09, YBS05, YMZH04, YYZ+05c, Yan09, YS09, Ye01, YLYD03, YWC07, YHD+07, YF07, ZZFL00, ZXX02, ZLL+05, ZFFX05, ZLSL06, ZL06, ZZDY06, ZLX+07, ZZM09, ZLL+09a, ZLL+09b, ZLML05, ZTI+07, ZSM+01, ZMZ+00, ZCFD02, ZDAZ03, ZZC09, ZRRC05, ZLF+07, dBC06, dlPCLG+00, AEI00, ASL04, BRL02, Brä06, BAG+08, Buc08, CGL+05, CHMIHS+05, CBC00, DT00, DDD02, DH04a, DR08, DSL06, ERC+02, FF09, FB07, GEB+00, GSCRO08, HBW+08, IROW09, JLAR07, JCTA08, JJC+06, KDŁL07, KKK09, LSBDL02, LDPP05, LDP05, LHV+09, LW08, Liu08, Man05, ML08, MZMZ09, MBD09, MGMR04, MBA+08, OYYY02].
theoretical
[PK01b, QMB+06, Ran02, RFF05, SL07, SKN09b, SŚRL07, SLB+05, SE02a, SY09, SM05b, SCRSRE05, SCRSRE06, SCRE08, SHM+09b, Sun06, TKS+05, TBCG05, VRA+02, VLK+08, Wen09, YLZ07, YN04, ZDMF08, ZFZ+08, ZHA01, dA08, eSPM+08, BK04c, BCC05, CA06, CZ03, DNN+06, DZ06b, FH02a, FRF02, GMS01b, GFMT08, JPA03, LSK+06, LQC06, LLL+07, LH00, LZWY07, MROA06, NJR+09, RJF+09a, RRUE08, SO04a, SIT+07, SCES03, TLC06, TDST07, VBT+07, WSBV05, YZG06, ZMAL04]. **Theories**
[Nag04b, Ada05, AE02, Del03, GQ00, Koc00, Luz08]. **Theory**
[ACDV01, DND06, Fra03, KBV05, LSE05, MK01, OM03, SJE03, SLE05, SNM+04, SKK+05, SKK+06, SIT+07, SKT+07, SKK+07, SIS+08b, SIS+08a, YYI+09, Ada02, AFC03, ABD06, ACG00, ABC+06, Ano07e, AGB06, ASM+03, APN02, BB02a, BB05b, BAZ05, BCG09, BJS09, BKGF02, BK09, BTK+05, BKM+02b, Bu02, BCF02, BA07, CSX+01, CZWZ05, CL05a, CB04, CD03a, CW04, Cas00, CC05a, ÇAK07, CCA+06, CSL05a, CL05d, CDI02, CC05b, CS07, CSTB08, CK06, CRTP05, CSA09, DCTC03, DDA07, DYD03,

DM08a, DGQT09, DBL+03, DLM+04b, DN06, Dre05, DFZ04, DWM+07, EWCT+05, FCS03, FXHL05, Fer02, FJ00, Fra06a, FVPM05, FFHT05, FKR04, FDZ04, GR07a, GBVD05, Glu04, Gog05, GR05, GXT02, GXGT02, GZD+05, GPW02, GE09, Hag00, Hag05, HT05b, HM05a, HH09, HWR05, HBTW04, HTN07, HM05b]. **theory** [HMW05, IYSS07, IABS08, IVK00, ISK+01, INS+08, IZ04, Jal02, JLAR07, JNF+09, JXZ+05, KSZČ04, Kan00a, KN09a, KZB01, KMN05, KK07, KSH04, KJH09, Khe09, KK02b, KSG03, KN09b, KIK09, KSU04, KSU05, KSS00, KMS02, KSK00, KGA05, Kut09, KDF00, Lam07, LDR+05, LML+04, Lat03a, Lat03b, LBSB08, LP00a, LM02a, LCL+09b, LS02, LS05, Liu02, MZF05, MZN+03, Mai05, MP05, MP06, MGK+09, MKHP09, Mar87a, Mar00b, Mar05b, MOL03, MHV00, MLSB06, Mic00, MJ00, Moh00, MC08, MTWN09, MDG07, NK06, NM01, Nag03a, Nag06, Nak02, Nak07, NUY+06, Nal00b, NS08, NS09, Nes00, Nes02a, Nes02b, New00, Nic02, NJR+09, OMC04, OYYY02, OMN+03, OOK03, OM02, Ols04, Ort03, PFC02, PS08, PMHW07, Pea02, Pea08, PW09, PGB00, Pir06, PSB+05, PCL+03, Pom04]. **theory** [Por03, PJS09b, Put06, QS00a, QS00b, QCV06, RA03b, RRC03, RW04b, RW04c, RdSH08, RS09, RS11, SS04b, SS06, SG03, SPH+03, SKSB08, SCP03, SOLI04, Sei03, SBM00, SL05b, SRK01, SPH00, SYZ+09, SZL+09, SY06, SL05c, SS01, SZK07, SWSH09, Son04, SE07, SHE+02, SM04, SBK+09, SCLL07, STL+09, SSS02, TSZW08, Tap04b, TN03, TB06, TGGV+04, TWSK09, UP05, VU02, Van06, VCHC07, VV05, VSBD06, WRRF03, WAJ04a, WAJ04b, WZ06, WWW+07, Wei08, XXY00, YYS+09, YYS+00, YYKY01, YSO+01, YYS+01, YNU+06, Yan06, YOM+01, YCS09, ZT02, ZZL04, Zak04a, ZR07, ZXX02, ZLY05, ZCZ+07, ZZZ+08, ZW09a, ZMAL04, ZKYA04, ZNF05, ZOK+05, ZTW+09, ZSM+01, ZWM+04, ZFD00b, ZCZF02, ZPW+04, Zie02, dBKS01, eSPM+08, EBS+09, GDV05, OD03, PSCLGN07]. **theozymes** [AD01]. **therapeutic** [GP08]. **therapy** [KM06]. **there** [ERC+02]. **thermal** [AMO+01, Buc04, Chu02, Chu04, Chu06, Chu07, Chu08, Chu09, DQZ04, JFS+09, SS03a, SS05a, YF07, PMBM09]. **thermally** [MYS+09, VWMS03]. **thermo** [Cor06]. **thermochemical** [VB04]. **Thermochemistry** [BVG05b, LLX+03, LLYJ09, LK02, SAE08]. **Thermodynamic** [Chu00, Chu01, KIK09, Son04, VSI+07, BA01, BA02a, Bor00, DLCY+07, GR05, GXT02, GdA01b, LS01b, MB01a, MCF09, SE07]. **Thermodynamics** [HLO04, Muñ02, AdWKG00, CCEÖ06, LDZ+05, ZZUO05, DMG09, KBMM08]. **thermoelectric** [SSK09b]. **thermolysis** [CQN+03]. **these** [AV05a, AV06, PKB+01]. **theses** [Ano03a]. **theta** [SPS02]. **theta-class** [SPS02]. **THF** [SL07]. **thiacyclohexane** [FAE+05a, FAE+05b]. **thiadiazole** [ML01]. **thiamin** [FTGH04]. **thiatriazines** [SSB+07]. **thiazide** [Lat03b]. **thiazolidine** [LQC+08]. **Thickness** [MBP03, PBMA03]. **Thickness-dependent** [MBP03]. **thienyl** [ML05, MLD06, ML08]. **thietane** [FB07]. **thietane-1** [FB07]. **thin** [BNA03]. **Thinking** [TA06]. **thioalkanes** [SY05]. **thioamides** [VVBT07]. **thiobiurets** [AB08]. **thiocarbonyl** [PJP08].

thioformaldehyde [BČZ07]. **thioformamide** [BČZ07]. **thiol** [SHM09a, TBB09]. **thiolated** [Den09]. **thiolato** [AVBč06]. **thiolato-** [AVBč06]. **thiols** [ACG00]. **thionylimide** [BAKK06]. **thiophene** [GL07, SCHH02, YYXC01]. **thiophenol** [SBL05a]. **thiophenols** [MGG05, dSNBG08]. **thiosaccharin** [BCT+02]. **thiosaccharinate** [BCT+02]. **thiosemicarbazone** [WJLL09]. **thiosubstituted** [FDL03]. **thiouracil** [MRST01, METSH02]. **thiouracils** [EKN04]. **thiourea** [PJZ+09, PYZ09, PMCOSC00]. **Third** [Cas00, KJH09, NFT+01, BMŁT07, CJdC01, CCH06, JV05, RS09, RS11, Nag03c, VM07a]. **third-** [CJdC01]. **Third-order** [KJH09, NFT+01, JV05]. **Thomas** [Nes02b, Nes04a, PM04b]. **thorium** [Boe09]. **those** [BG00b]. **Thoughts** [Mar05a]. **thousands** [BBG00]. **Three** [ABM01, KS04a, RLER08, SH02a, AS04c, BSH04, Buc08, Bud04, BSK+02, DS07, EB04b, Har05a, HSW04, HGTW03, JJWH04, KLK08, KCS02, LHL+00, LKG09, LAL+08, LPZW05, LDG+06, Mat02b, Mat10, MKDM03, PC04b, RFE+00, Saf04, SA09, SUL+08, SS09b, Wen00, Wen02, WZL+00, YŞ02, Yal04, ZTSP00, SK01b, VLJ08]. **three-** [Buc08, Bud04]. **three-body** [BSK+02, LHL+00, YŞ02, Yal04, SK01b]. **Three-center** [RLER08, SH02a, AS04c, BSH04, Buc08, DS07, JJWH04, PC04b, RFE+00, Saf04, SS09b]. **three-dimensional** [KCS02, LKG09, MKDM03, Wen00, Wen02]. **Three-electron** [KS04a, Har05a]. **three-helix** [HSW04]. **three-periodic** [EB04b]. **three-state** [SA09, VLJ08]. **threefold** [MDBM05]. **threonine** [HT04]. **threshold** [Pup02]. **thrombin** [DGD+05, GdA01b, HNR06, RACD00]. **thrombin-like** [HNR06]. **through-bond** [DD05, OA03]. **through-space** [OA02, ONA05]. **through-space/bond** [OA02, ONA05]. **throughout** [YL04]. **thylakoid** [PD05]. **thymine** [JXZ+05, MHGR07, STL+09]. **Ti** [HDL00, SCW09, SZSP02, ZSPS03, EP02, FTB04, FDLK02, ZZM09, ZKYA04]. **Tight** [FV04, KUS+03, BDMS01, GCG05, SSK+05, ZKB03]. **Tight-binding** [FV04, KUS+03, BDMS01, GCG05, SSK+05, ZKB03]. **Time** [BCG09, FCS03, ICRS08, MYH03, MB02a, Nic02, QS00c, QCV06, RA03b, RW04c, SL05c, SZA07, WRRF03, WWW+07, YYYM01, ZCZ+07, AGB06, BKM+09, BAZ05, BJS09, BB05c, Bel04, Bil01, CW04, CC05a, CDI02, CN05, CK04, DGR+00, DBFP05, Deb08, FZRD07, Fra03, HT05a, HBKG03, HLO04, JTB09, Kar04, KSG03, KDF00, LCT00, LLZ+00, LSLD01, LSD02, MT03, Mai05, MP05, MC00, MMB03, Nag03a, OMN+03, Ols04, PGB00, PA04b, QLD05, QC01, RW00, SG03, SAM08, SS02a, VWB+03, VD04, WRD03, WZ06, dBKS01]. **Time-dependent** [BCG09, FCS03, ICRS08, MYH03, MB02a, QS00c, QCV06, RA03b, RW04c, SL05c, WRRF03, WWW+07, YYYM01, ZCZ+07, AGB06, BKM+09, BAZ05, BJS09, Bil01, CW04, CC05a, DGR+00, Deb08, FZRD07, Fra03, HBKG03, KSG03, KDF00, Mai05, MP05, Nag03a, OMN+03, PGB00, PA04b, QC01, RW00, SG03, VWB+03, VD04, WRD03, WZ06, dBKS01]. **time-independent** [CDI02, HT05a, JTB09, LLZ+00, LSLD01, LSD02, QLD05]. **time-resolved**

[CN05, DBFP05]. **tin** [LDZ+05, JKU02]. **TiO** [CB04, EP02, EB04a, ESU05, LNPL06, SMAL01, VG06]. **tip** [DND06]. **tip-dependent** [DND06]. **tirapazamine** [LZZ+07]. **Titanium** [RRGP05b, CB04, KFS00, KWT06, Oni07, Oni08, SMDG09, RRGP05a]. **Tl** [MOA07, TMAB01]. **TlH** [TMAB01]. **tm** [CDF00, FTB04]. **TM-oxide** [FTB04]. **TNAD** [QXJG05, LCH05b, QLJ+09]. **TNAZ** [LCH05b]. **TNT** [LCCH09a]. **toluene** [BHK09, CC00b, SRS+04]. **tool** [BS06, KF07, PL09, Van06]. **tools** [BM02, PDR+00]. **top** [TYY04]. **topics** [CHN09]. **topographic** [MEN+08b]. **topologic** [SCHH02]. **topological** [Aze02, CBRBT03, Gin08, HLP07, LRS05, LPL04, MEN+08b, NS09, PPP+08, BF08a, BL02b]. **topologies** [ART08a]. **topology** [ACPG01, BLC09, Pri05, RA02, SHC00]. **Toroidal** [LR01]. **torque** [OB02]. **Torsional** [dA08, JCTA08, MBRA07, VTP09, dBM05]. **torus** [SÖ04b]. **Total** [KNO09a, DW05, Fuk09, Gin00, Kap07, LGKN04, Mor02, Mor03, OA03, SLE05, Von00, ZW07, ZT04a]. **toxicity** [DKD+07]. **traceless** [HW02]. **track** [ZFLL00]. **traditional** [UML00]. **trajectories** [AT00, BFBB06, Mic06b, NW01, SGGBB02, Yan06]. **trajectory** [DM02b, VGMN03, ZH06]. **trajectory-based** [DM02b]. **trans** [ML05, MLD06, ML08, TS01b, ZWJ02b, CGMT03, DI05, För00, HvLJ01, HGRL01, KDF00, KFD01, MZMZ09, MCN+05, dFGM08a, BL02c]. **trans-1** [ML05, MLD06, ML08]. **trans}-annulenes** [HvLJ01]. **trans}-influence** [MZMZ09]. **trans}-MeCl** [HGRL01]. **trans-membrane** [TS01b]. **trans}-nicotine** [MCN+05]. **trans}-polyacetylene** [För00, dFGM08a]. **trans}-stilbene** [DI05, KDF00, KFD01]. **Transcorrelated** [UT03, UC06]. **transcriptase** [CFR07, GMPIP01]. **Transfer** [SS09a, ABL03, ATN09, AZD06, BMŁT07, BFBB06, Bro05, Buc05a, Cab05, CBB01, CSDCCMZT03, CDDM05, DKWP04, DNN+06, Dei04, Dei06, EMM+02a, GGLS02, GMS+05, GYM+02, HH03, IS03, JdL08, JM00, KP05, KM00a, Kir08, KL00, Kor05, KTN02, LZT03, LYP+06, LLZ04, LH07b, Lu06, MKHP09, MTRD04, MSS09, MHV00, MHB05, OYB+00, OM02, OM03, QFC04, QCFJ05, QCC02, RVR00, Sal05, SCM00, SASS03, SK06, SBB05, SBB06, SL05c, SMS07, SBL05a, SCTK+09, TFBM02, TBM04, WKF+06, XYS+03, YBS05, YHD00, YWZ+09, YJ00, YLYD03, YYQ+06, ZZFL00, ZZDY06, ZZZ+08, ZW09a, ZFD00b, vdVM00]. **transfer-matrix** [Cab05]. **transferability** [LMGM02, TTM07]. **transferase** [Kra00, SPS02]. **transform** [AS04c, BB05c, CSA09, DFH02b, ELF+08, MK01, NM01, Özt04, RR02]. **transformation** [ARH00, BSH04, CD00, CD04, CCLK04, DS07, MDS04, Nég03b, OMN+03, Rua09, SH02a, UP03, YZY+01]. **transformations** [Kýv09, LKE03, LGKN04, SHZGP09, SS09b, VCF+00]. **Transformed** [Dat04, CD04, Dya00]. **transforms** [PMZGGR04, PCT+04]. **Transient** [VWB+03, NOM00]. **transimination** [SDFM02]. **transistor** [KKM+01]. **Transition** [HSS09, PSN08, ZSW+00, ACF04, ACF05, AD01, Baň05a, BL04b, Bec02, BT05, BKGF02, BB04, BB05d, BB05e, Buc05a, CC00a,

ÇAK07, CMS04, Cor04, CK06, DRPT02, DLM+04a, DFT+07, DSW08, EMV05, FTB04, FV04, FPJR03, GSK01, HJJ09, HT07, IYY03, JKU02, KDC09, KM01, KY05, Kýv09, MKCS05, ML03, NOY+01, Nee01, OD03, OCWY09, OM02, OM03, OM05, PML09a, PRBGLL04, RHM05, ŠUKŽŠ07, SDTM02, SH07, SM08, TTM01a, TGGV+04, Van06, WK03, WWTHF09, WBLQ00, WSNB00, Yam04, Yam05, YZX+08, ZL06, ZZM09, TFS+02].
transition-metal [BT05, BB05e, DSW08, OCWY09, SH07].
transition-state [AD01]. **transitions**
[AT00, ÇAK07, CM02a, DKP+06, Mal05b, Mar00c, PJP08, RF01, SMDM03, SI09, SH07, SM05c, VBML01, VBML04, WAJ04c, ZT02, dFGM08a, HNKiS01].
translation [Del03, Gus01, Gus02a, MR00, FLE+06a]. **translational** [ITN08]. **translations** [Hog09a]. **Transmissivity** [Lef05]. **Transparent** [DC03]. **Transport**
[PD05, BVSM04, BS05c, CIT+03, DG04, Fra03, GSfLV08, GC05, JM07, JPMM08, LJMM09, Mai08a, Mai08b, MLSB06, MRG02, YS07, YL04, Yur06].
trapped [JCTD08a, MCR03, TI05, TTFP04]. **Trapping**
[Jal08c, DRS00, AIG02]. **traps** [Jal08b]. **traversing** [Por01]. **Treating** [MWHZ06]. **Treatment** [MFA00, MV02, AEMAO06, DD00, EMM+02a, GBP05, GSCRO08, Gus02b, Gus04, ITN09, KCGB02, LVM01, MZF05, MC06a, MT02, Özd03, Pau04, SBF+04, SDB03, VNP00, YYHD01, Živ09].
tree [WLWZ06]. **Trees** [LTY00, Ou06, YYZ05b]. **Treilles** [Ano04f]. **Trends** [BG02b, FTB04, FSGB05, ART08b, CM02a, Por02, Por04, Pyy01, RCD00].
tri [LAK09, Men08a]. **tri-** [LAK09]. **tri-heteronuclear** [Men08a]. **Trial** [Gui01, Yam04, HI06, SB04, Yam05]. **trialkylphosphine** [MCF09].
triangular [CEK01, Lef07, WK03, YYT+04]. **triatomic**
[GW05, Hag00, ZD07b]. **triazine** [BABL09, LH07a]. **triazole** [FXHL05].
tribological [Mar00a]. **tribute** [Brä04a]. **tricarbonyl** [LH00]. **trications** [MZD+05]. **trichlorides** [VTS04]. **tricyclo** [DQZ04]. **tridentate** [KWWQ04]. **triepoxides** [TW05a]. **triethylamine** [ZOK+05]. **trifluoride** [GJB02, GJ03]. **trifluoroethanol** [dA08]. **trifluoromethyl** [TCS+08].
trigger [PML09c]. **triggers** [DGSD07]. **Trigonal** [Buc07]. **trihalides** [VTS05]. **trihydrate** [SMSM02]. **trilayer** [PBMA03]. **trilayers** [MBP03].
trimers [GSA+09, KD05, LWC+09, LB02, SYLE07]. **trimethylaluminum** [ZVVT07]. **trimethylbenzene** [DDA07]. **trimethylsilyl** [GXGT02].
trimethylsilylketene [GSPP+06]. **trinitro** [BABL09]. **trinuclear** [NFL+02]. **tripentaprismane** [LDG+06]. **triphosphate** [YZX+08]. **triple** [GB09]. **triples** [FHK06, Mei08]. **Triplet** [ZLZ05, DBPG04a, FG06, KS02a, LSL+08, SD00a, YYI+09, CNPA04, NNS+00]. **trithiacyclohexane** [FC04].
trithiane [FC04]. **trivalent** [FJT+05, SDTM02]. **tropolone** [RLNA02].
tropylium [BHK09]. **Truncated** [LP00b, LP05a]. **Truncation** [MDSW07, PW07]. **trypanocidal** [RAdS05]. **trypsin** [RACD00].
tryptophan [LLZ04]. **Tsallis** [Gra08b]. **TTF** [DETA02, Mar09]. **tube** [KDŁL07]. **tuberculosis** [PFSFH06]. **tubulin** [LQM+09, RT09]. **TUC** [CXZ09a]. **TUNCUR** [ZS04a]. **Tuning** [Mai08b, Mai08a]. **Tunneling**

[SS03a, SS04a, AR04, BP04, DLM+04a, Kry02, Lef00, MMB03, SS05a, Stu00, TGGV+04, VH00, WS00, ZS04a, ZMS05]. **turn** [MET00]. **turned** [JS08]. **twenty** [Tri03]. **twenty-valence** [Tri03]. **Twist** [SKSB08, FAE+05a, FFHT05, FAE+05b, Sha07]. **Twist-dependent** [SKSB08]. **Two** [ABGS00, CCLK05, CMRMR00, DK03, DB04b, GGAMB03, Gus03, Har03, LJL09a, LCT00, MHI+07, McK04, RDK97, SW02, Sme02, TMPI05, Ada05, AM05, Apo06, ACFR05, ART08a, ART08b, BDG01, BSH04, BB09, Buc08, Bud04, CCLK07, CCEÖ06, Dre05, Dya00, ELG05, EB04b, Gin06, GMPIP01, GM09, Gri08, GLHH09, GM02b, Gus04, Har02b, HH02, HH09, HAL+02, HWR05, Hog09a, Hog09b, HN09, JJWH04, KDŁL07, KS04a, KV02, Kut08, Lef00, LC02, LSLD01, LZXD05, LPZW05, MR00, Mak07, MDBM05, MS05, MNV07, MB01b, NK05a, NK06, NY01, NY04, ÖO02, Özd04, ÖKAY03, PRNM03, Pir06, PDR+00, PCL+03, PC04b, Pöt01, PLA+07, PS02, QTT07, RE06, RFE+00, RDK02, SH02a, Saf04, SB06a, SSDM05, Sak02, SEY09, SGS00b, SDZ+07, SSS+05, TNYY03, TOH+00, VGMN03, VGB05]. **two** [Yam09, YNY01, YN04, ZTSP00, GM01, UKAM04]. **two-** [EB04b, PCL+03, RFE+00]. **two-band** [NK05a]. **Two-body** [ABGS00, HN09]. **Two-Center** [Gus03, Har03, Sme02, Bud04, Gin06, GM02b, Har02b, Hog09b, JJWH04, KS04a, MR00, ÖO02, Özd04, ÖKAY03, SB06a, GM01]. **two-channel** [RE06, SEY09]. **two-color** [GLHH09, Pöt01]. **two-component** [Dya00]. **two-crossing** [TOH+00]. **Two-dimensional** [CCLK05, GGAMB03, MHI+07, ACFR05, ART08a, ART08b, CCLK07, Dre05, LSLD01, MB01b, SW02]. **two-dimensionally** [Yam09]. **Two-Electron** [RDK97, CMRMR00, AM05, BDG01, BSH04, Buc08, Gus04, HH02, HH09, Hog09a, Kut08, MR00, Mak07, MNV07, Pir06, PC04b, PS02, RDK02, SH02a, Saf04, YNY01, YN04]. **two-exciton** [NY01, TNYY03]. **Two-fluid** [DB04b]. **two-gap** [NK06]. **two-leg** [CCEÖ06]. **two-level** [Apo06, Gri08]. **two-mode** [Gri08, NY04]. **Two-photon** [UKAM04]. **Two-response-time** [LCT00]. **two-state** [KV02]. **Two-step** [TMPI05]. **Type** [Gus03, Har03, AH06, AS04c, BSH04, Boe03, Boe04, Bud04, CEK01, CBWM09, Don09, ELF+08, ESU04, FLE+06a, GW02, GW04, GW07, GSD+03, GM00, GM01, Gus01, GM02a, GM02b, Gus02a, GM08, GE09, HVC08, Hog09a, HSB+00, ITN06, ITN08, KM04, Koc00, KZvL09, KOT09, KANK00, LLW+05a, LLW+05b, LTL05b, Mak07, Mat02b, Mat10, MTO+03, Mor04, MLP07, Oni07, Oni08, Oni09, ÖO02, Özd03, Özd04, ÖKAY03, Özt04, PI02, PCT+04, PH09, RFLR00, RLA+01, RLRE04, RJ08, RS00, SH01, Saf04, SKN+09a, Sha04, SKT+07, SKK+07, SCW09, SEU02, Str00, TOK+00, Tem02c, Tem04, TS01a, VDF+06, WS00, YAŞ00, YŞ02, Yal04, YHN+07, Gin05a]. **types** [DLZ+03, KS04b, LWC01, LAL+08, ŠK01c]. **tyrosine** [ST01, VR01, WE01]. **tyrosyl** [HEBS00, WE01].

U [HDL00, RSTG02, BSN05, Now01, Sch05, ZD07b]. **UF** [Sch05]. **UHF** [DNMM06, NYU+08]. **UHF-GSA** [DNMM06]. **ulcer** [BMMA06]. **Ultra** [CS08]. **Ultra-high** [CS08]. **ultrafast** [BKHPvD01, HLMH07]. **ultrashort** [HCTC07]. **ultraviolet** [MDS+09]. **umbrella** [BKM+09, GJB00]. **uncertainty** [SK09]. **Unconventional** [Liv02, KS06, QG04, ZW09b]. **undecanethiol** [THP08]. **Understanding** [ASP+05, KSBK08, FCS03, HSN+09, LV01b, PBB+02, BCFR08]. **Unexpectedly** [BML01, Krü06]. **unfolding** [AT00]. **unification** [Zak04a]. **Unified** [Gus02b, Gus04, OOK03, Özd03]. **Uniform** [Tem02a, DM02a, DHCD06, Tem02c, Tem04, TSF04, ZTSP00]. **unimolecular** [KPC05, LCH05b, NSLR04, OCK07]. **unique** [Krü06, WO04]. **uniqueness** [ASO+01, ASO+04]. **unit** [CSDCCMZT03, QFC04, QCFJ05, ZZZ+08]. **Unitarily** [Alc04]. **unitary** [CL05b, Muk00, TB06]. **units** [FB01]. **universal** [BK03, CSL+02, DBd05, LP04a, MW05, MVG+04, Orl07]. **universality** [SM05c]. **Universe** [NU09]. **University** [ERU07]. **Unnatural** [KH08a]. **unpaired** [YKT+02]. **Unrestricted** [Nes05, DVM06, Koc00, WF04, YONY04, YYY05, YTS+05, YNN+09]. **unsaturated** [XLX+09a, XLX+09b]. **unsaturation** [Sch00]. **unscreened** [ZBPD08]. **Unsolved** [Lin06]. **Unusual** [KLK08, LA09, CGG05]. **unusually** [DGSD07]. **UO** [BB02c]. **updated** [Bof03]. **upon** [CWY05, CM09, DJNH02, ELO+07, FL04, LL04, Nov07, PML09c, PM09, QC00, Sad06, YCN+07, Yur07]. **Upper** [Zho07, AC02a]. **uptake** [IN09]. **uracil** [DZO00, DWM+07]. **uranium** [BR00, HR05b, Mat00, Sch05]. **uranyl** [FSR02]. **urea** [BČZ07]. **urease** [KSI+07, LMRT08]. **ureido** [SST00]. **uric** [ASL04, AMC07]. **Use** [ACD02, GE09, JJC+06, Nal08, PS03b, RR02, UB05, WZ06, WK06, WLZY08b, Yil06, BCWS09, BBM+00, BČ02, CD00, ER05, FOM+03, HCZ05, JB07, KH01, Koc00, KZ09, LSD02, MDBM05, PRSLA08, PVZV00, PRCEM06, Swa03, SB04, VD00, CS01, FHHC00, GM02b, XV00]. **used** [CFR07, DTT06, DHCD06, KM06, LS01b, MH09, PMBM09, PMCOSC00, RB06]. **Useful** [HCL03, PT06]. **Using** [AD01, BL02c, CR08b, CR08a, Gui06, Har03, LCN05, RH03, WC04, AH06, AYD00, ATN09, AC02a, AC02b, AC04, AC05, AC06, AC07, AC09, AG01b, AM09a, AM09b, ASDC08, AS04c, ASP+05, AS00, BJS09, Bau09, BSH04, BFB08, Čár09, ÇAK07, CK09, CM05c, CSPS05, CG09, CSL05b, CL07a, Col08, CBRBT03, CDF00, DSFS00, DAD05, DCDW00, DNM+08, DDT06, DGQT09, DFT+07, DC06b, DDD03, EEJ04, ENGY+07, EB04b, FFFR01, FFFR02, FGH09, FTW03, FSLL02, FSLL04, GBS02, GCG05, GBP05, GXT02, Gos01, GTR+05, GdA01b, GM00, GM01, Gus01, GM02a, GM02b, GM03, GM08, HV03, Hea00, HLP07, ISS00, Iye09, JJWH04, JP01, JK00, JXZ+05, JJ00, KS08, KAE03, KA05, KM00a, KYT+04, KT05, KZvL09, KDF00, LCL+09b, LPL04, LS01b, LLZ+00, LSLD01]. **using** [LGBJ03, LCK00, MMM06, MST08, MNMV02, MBA+04, MDJ01, MV02, MSJ04, MP09, MEN+08b, MPRGLL03, MW05, Mor06, MTWN09, MSC03,

MJ06, NF06, ONK+05, ÖKAY03, ÖÖOY02, Pea02, PJZ+09, PCT+05, PSH00, PGB00, dRPFCP08, QGW04, RVP09, RKR+06, RSM+04b, SN02, SH02a, Sal05, SFPA03, SAR08, SAM08, SL05b, SRK01, Sey08, SYZ+09, SZL+09, SMDG09, SMEA08, SNdAM08, SMB09, ŠPNU08, SHM+09b, SÖ04b, SBBL05, TYG05, TMM+03, TG01, TB03, VV05, VSBD06, WGLX02, WW08, YYY05, YOM+01, ZXX02, ZW09a, dOEG+08, eSPM+08].
utilisation [MDBM05]. **Utility** [IYY03]. **utilize** [CD03b]. **UV** [ARBC+05, CC05a, JLPA09, KFD01, Noo03, Nov07, PLA+07, PJP08, UC00, ZNF05].
UV-excitation [Nov07]. **UV-vis** [ZNF05]. **UV-visible** [UC00]. **UV/Vis** [PJP08]. **UV/visible** [CC05a, JLPA09].

V [PBS02, ZZFL00, BL04d, CK03, FTB04, FSK05, GMS+05, ISK+01, KKS+03, MP00, PSB+05, RS00, SMAL01, SY09, SKK+06, ZKYA04]. **V-T** [GMS+05]. **V.** [Ano02c]. **V6.43** [BNHB+02]. **V6.43/I6.46** [BNHB+02].
vacancies [BBO04, MTO+03]. **Vacancy** [FD01, JM07, LTW09, WSNB00].
vacancy-defected [LTW09]. **vacuo** [AG08, RW04b, AT00]. **vacuum** [NY04]. **Valence**
[BB05e, CC07, DVHJ03, QV01, SE00, SE02b, ABC+06, ACF04, ACF05, BB04, BB05d, BG02b, DLZ+03, GGLS02, HvL09, KC09, KCU09, KM01, Koz04, LM02a, OM04, Tri03, TGG01, WSK03, YHC05, ZSM+01, ZKRS07, BB04].
valence-bond [KC09, WSK03]. **valence-core** [BB04, BB05d]. **valency** [DDM00]. **valent** [CPR06, DRD+05, HDL00, ZZUO05]. **Validity** [SCSWF04]. **valley** [PC07]. **value** [CDG09, LLR04, NKS+09]. **valued** [KOT09]. **values** [DSL06, GL01, ITN06, ITN08, Por02, Por04, ZŠ05].
vanadium [BSCB04, KFS00, NFL+02, RIVB03, RS08].
vanadium-containing [BSCB04]. **Van't** [Buc08]. **vapor** [BSAL+06, Chu06, Chu08]. **vaporization** [PMLC05]. **vapors** [KK04].
variable
[ARH00, Bil01, CD04, DCA03, KK05, KM00a, PA04b, WRW02, ZZUO05].
variant [KJH09]. **Variation** [KG02, Fer09, GJ03, RA02]. **Variational** [Ben05, BLKJ00, DVV05, GBS02, GGDL07, MZF05, SB04, TPGD02, AC02b, DES03, GBP05, GFDK09, KPSH06, NS08, Nes03a, PS03b, SH02b, TGGV+04, UT03, MHT+08, VCF+00]. **Variationally** [GW02, GW04].
variations [AV02, GSH02, Jal02, ZW09b]. **variety** [MB07a]. **various** [ART08a, BKM05, CCH05, ESE04, JNKMS03, LY09, OOD+05, VKIJ06, ZLY+09]. **vasoactive** [FP02]. **VAu** [LNSE02]. **VB** [TR09]. **VB2000** [LM02a]. **VCD** [CHC05]. **vector** [BRZ09, GKYY06, OB02, OdSC05].
vectors [GM09]. **Vegetation** [LTL04]. **venom** [DCO+08, HNR06].
verapamil [IDH06]. **Verdet** [BAZ05]. **verification** [YKS+06]. **version** [Gda01a, HdMB+05, HSP+09, KSZČ04, LMJ00, LP00b, NUY+06, Pan07].
versus [Buc02a, CPR06, GGAMB03, LTV07, Lef06, Nes04a, Pye00, SMS07, TS07, TTFP04, SCM00]. **vertex** [Man05]. **vertical** [ASM+03, GDFT01, LCT00, MY08a, MY08b, SC01, SMK08, ZDZO07, BABL09]. **vertices** [MBM05]. **VI** [Sch05, ASO+01]. **via**

[ASO+01, ASO+04, BK04c, DGD+05, DLM+04b, FRGM06, GH03, Har02b, JG09, KM01, KTN02, Kry02, KOT09, Laz02, Lu06, MYGD01, Özt04, QS00a, SSMG08, SRHR05, Tem00, Tem02c, Tem02b, Tem04, Zak04a, ZD08]. **VIB** [BB05d, BB04, AYD00]. **vibration** [BJ00, BZG+04, CCL03, Irg04, KKYT04, MNJP05, Oku01, SKT+07, SIS+08a]. **vibration-rotation** [Oku01]. **Vibrational** [AC06, AE07, CTI09, JNKMS03, KL00, Qui05, SO04a, WSC+05, AA09b, Bar09b, BVHS04, BS05a, BB00, BM07a, BFBB06, Cab05, CMR05, CdMCS05, CDS06, CÖ05, CL05e, DS03, DNC07, DKR04, FG01, För04, FB07, FYSS09, GBP05, GP03, GW06b, HZJ+07, Hea00, HH05, Iye09, Jal02, JNF+09, JJC+06, KVSS05, LSC01, LDPP05, LDP05, LQC06, LCK00, MKCS05, MLW+09, MVK00, MD06, MCLKC02, MY09, MCZWD06, Oku01, Pal00, PNG02, PRM03, PGN+05, PRM+06, PR05, PRL01, Pol06, QBTS05, QZ07, QC00, RPS+07, RNCM05, RLNA02, SAM08, SSB00, SMEA08, SdACAG03, ŠŠU+02, SCHH02, SBK+09, TYG05, VAS06, WC04, YW09, ZB05, ZNF05, ZD07b, ZD08, ZCFD02, ZZW+06, XV01]. **vibrational-rotational** [MVK00]. **vibrations** [CK03, CL05e, DBPG04b, LBAB02, MD08, OK05, Ras02, Sch02, SCRR02, dBM05]. **Vibronic** [AIG02, WHKM04, CPH04, MD02, Noo06, PLC04, PS03b, Tap04b, VBML04, YHC05]. **vicinity** [XV01]. **view** [AE02, Guo09, RHH+02, She07c, XR05, ZT04b]. **viewpoint** [KSS+01, KNS+09, KPTŚ03]. **VII** [ASO+04, SIS+08b]. **VIII** [INS+08, PD05, QGW02, VD00]. **Vikas** [Deb08]. **Villiger** [LJL09b]. **vinyl** [BK04c, LTL05b, RRNG05, Sok02, YYXC01]. **vinylation** [VLK+08]. **vinylene** [BHG+06, GCG05]. **vinylidenecyclopropanes** [ZMAL04]. **vinylidenes** [KPC05]. **vinylogue** [MW06a]. **vinylphosphonic** [OGJdlV03]. **violating** [BBHQ04]. **virial** [KT05, MB05c, QS00c, TB09, TGGS06]. **Virtual** [DFMZO08, MST08, ŠPNU08]. **Virtues** [DFH02b]. **vis** [KV07, ZNF05, KFD01, PJP08]. **vis-à-vis** [KV07]. **viscosity** [DCTC03, KPP01]. **visible** [UC00, CC05a, JLPA09]. **visitation** [dAMM08]. **visual** [BL02c, SB03, CWZ03]. **Visualization** [BB00, BM02, FSLL02, KF07, PL09]. **Visualizing** [AC09]. **vitae** [Ano02k]. **vitamin** [ASRL06, DDW+06, SDFM02]. **vivax** [LVSG06]. **vivo** [MLSG04]. **VKOR** [DDW+06]. **Vleck** [KJH09]. **VN** [JKU02]. **voltage** [EZ05, TRMM04]. **voltage-gated** [TRMM04]. **Volume** [ND03, Tem04]. **vs** [CT00, LLR04, PILD07, RI03, WS00, YYQ+06]. **VUV** [DBLM06]. **vyns** [PRM02].

W [BB05d, GT07, BB04, DS07, HW04, WNW05]. **W1** [PGF+06]. **Waals** [BCG09, BPŠB00, ELY09, FG01, GY04, ILB+08, KCS02, KS03b, LDR+05, MCF08, OSSG07, PLU08, SNH00, WZJ04, ZŠ05, ZNZS00]. **Wales** [SUAL04, TNO09]. **walks** [Pal01b, SST+02]. **wall** [Den09, JLM08, LZC04b, Tor06, VM06a, ZWMZ04]. **walled** [ALM05, CAHl08, DGSD07, JLC+09, KDŁL07, KG08, KG09, LTW09]. **walls** [CS01]. **wanderings** [Mon00]. **Wannier**

[ESU04, ESU05, PTS03, SWC03, SEU02, UES04]. **Wannier-type** [ESU04, SEU02]. **Water** [BGP+07, CFM+06, DM08b, AYD00, AGM02, AG02a, AML+01, BKMS03, BS05a, BGP+06, BSAL+06, CGCS02, CWF09, CC00a, CL05c, CL05d, CSL05b, CHC05, Chu06, Chu08, CBWM09, DKS05, DGD+05, DBHT01, DPS04, FC05b, FC05a, FRGF04, GZD+05, GI07, HEJ+00, HT04, JPA07, JB07, JSvDA06, JAP+05, KAN+09, KS07, KWC09, LTV03, LTV05, LH07a, LZZ+07, LZA+09, LWC+09, LSK+06, LPL04, LCBC03, MK08, MMF00, Nov07, PJZ+09, PYZ09, PHR08, PFSP05, QDÖ09, QCC02, RP09, RFRF05, RC05, Sad02, SKMW00, SLB+08, SBL05a, TI05, TVK01, TYG05, Tou09, TL05, USM01, UC00, YW09, YSV05, YWZ+09, Yur08, ZW09a, ZOK+05, ZMS05, ZQF+02, ZS04b, FGdA02, HT04]. **Water-saturated** [FGdA02]. **waters** [YYQ+06]. **Watson** [GBB06, KS03a, MHGR07]. **Wave** [NY03, Pau04, SLCW04b, AGBY00, ANM03, AM09b, BB06, BM07b, BSZ07, BCS01, Cam04, CDK01, CD03a, Čár07, Čár09, CCLK04, CCLK07, CPH04, DB04b, ER05, ESTU05, Eye00, FGR+07, Ful00, Gál07, GBS02, GBS04, GBA05, GB06a, Gög06, GHT09, Gui01, HBKG03, Har05c, KB00, KMS02, Kut08, LLB01, LKG09, LP09b, LM02b, LFR+08, LP05b, MK00, MNA+99, MYH03, MWW+00, MBR07, MB04, MJ06, Nak02, Nak07, NN09, Nic05b, NF02, ND02, ND03, OMC04, PA08, PSM07, Pea02, PW07, Pup05, RH09, RRC03, RS00, Rui05b, SFPA03, SAM08, SM06a, SMB07, SLCW04a, SSS02, Tap04b, TS01a, VWB+03, WO05, XVB05, YN04, ZSW+00, Zno00, dGS06, KSS00, SS06]. **Wave-function-based** [Pau04]. **wave-functions** [RH09]. **wavefunction** [CDH05]. **wavefunctions** [AGSH09, AC09, DM04, Mic09, Wei03]. **wavelength** [KWWQ04]. **wavelet** [Fis00]. **wavelet-based** [Fis00]. **wavelets** [CF04]. **wavenumbers** [PNG02, RPS+07]. **Wavepacket** [BA02b, Iye09, KDM00, MHI+07, RW04c]. **waves** [NM01]. **Way** [SE00, SE02b]. **WBEPM** [ÇAK07, ZSM+01]. **WDA** [GGACT03]. **weak** [Ano07a, GBB06, SB06c]. **Weakest** [ZWM+04, MZF05, ZSW+00]. **Weakly** [GW05, CCH05, CCH06, EZY00, Kan00b, KJW08, KT05, LME03, LSPS01, SSSK07, Win04]. **wealth** [BvRSS07]. **Web** [MVG+04]. **weight** [Man05, Tem02a, TVK+02]. **weighted** [PA08]. **weights** [Man05]. **Weinstein** [MB07a]. **Weizsäcker** [Mar05c]. **well** [DN06, PGP+07, SS03a, SW02]. **wells** [GB09, SK00b]. **Weyl** [LP04b]. **Where** [LH05, BVG05a]. **Whether** [YZX+08]. **white** [MFR07]. **widely** [CFR07]. **width** [Dou07]. **widths** [Orl02]. **Wiener** [EYY06, GKYY06, LTY00, YY04, ZT08]. **Wigner** [GBO04, HMW02, HMW05, Mar03a, Mar06a, PI02, PMHW07, PČH02, PS02, RI03, RI05, SM05c, SM06c, SK05c, TKT+05]. **Wigner-like** [SM06c]. **Wiley** [Kry08a]. **Will** [Kai09]. **Wilson** [MBP01]. **wire** [BN03]. **wires** [BNA03, DZS+06, KTH+05, MKHP09, SDZ+07, UKAM04]. **within** [ARBD05, BAZ05, BL02a, Bil01, Bou03, CCM+05, CDB02, CMRMR00, CWW09, DZ01, DP06, FCC07, GS09, GGDL07, GFDK09, Kis04, Kry07b, KG08, KG09, LHTV05, LZC04a, LZ05, Put06, SJE03, SI09, SBB05, TTM01b, VBML04, ZSM+01]. **without**

[AML+01, BDMC06, Hog09a, IYO+04, LLLZ06, Nak02, Nak07, RWW+01]. **Wittig** [MPBM07, PMB08]. **Wolfsberg** [CD04]. **Words** [VMRA04]. **work** [Chu02, Chu04, Chu06, Chu07, Chu09]. **Workshop** [Ano04f, DT02a, AGL04a, Nag03c, PČ04a]. **world** [Mon00]. **wreath** [DAD05]. **Wulfman** [Ave04, RW04a].

X [AZD06, Ano07g, Ano07e, Ano07f, ARBD05, BK04a, BL02b, BBD07c, BDBG09, BG00c, BMMC09a, CL07b, CMY06, DLTW04, DETA02, FRNM08, GR07a, GR07c, GR07b, GYF+09, HZJ+07, JLAR07, LSC01, LDXW04, LLW+07, LDR+08, LAQ+09, LC05, Liu08, MGCD01, MMV05a, PT00, Pen00a, RRGP05a, RdTdLC+07, SYZ+09, SZL+09, SYL05, SCHW07, TM05, Var07, VK08, VGMN03, WZJ04, YST+05, YWC07, AM09a, BK04a, BVG05a, BDBG09, CL07b, DLK00, GR07a, GR07c, GDV05, Guo09, HZJ+07, KM02, KPČM05, LTV02, LTV05, LL04, MB06, OCWY09, Pet00, RA03b, RV05, SMDG09, SCHW07, VDF+06, XV00, YWC07, dVHB03, TM05]. **X-ray** [AM09a, LTV05, OCWY09, RA03b, SMDG09, dVHB03]. **Xa** [RACD00]. **XANES** [SNN+09]. **X —** [PT00]. **xC** [FCLH+06]. **XCCY** [Tri03]. **XCN** [BBD07c]. **Xe** [LZJ+06, MGCD01, ZZHL08, ASH08, LJ03]. **xenon** [MH06]. **XF** [VGMN03, MGCD01]. **XH** [LLW+07, LDR+08, CMY06, LL04, Liu08]. **XHX** [BL02b]. **XI** [Ano07i, SIS+08a, SD03]. **XII** [BCC05]. **XIII** [CA06, YYI+09]. **XIV** [CB08]. **XLiX** [BL02b]. **XMg** [Pet00]. **XO** [LTV02]. **XY** [Gri08]. **XYCO** [BDBG09]. **xylene** [HZW+08].

Yb [RSFRDNA04]. **YBa** [Yur06]. **YBr** [AAKAF07]. **years** [Mon09, SÖ09b, Tay09]. **yellow** [CBB01]. **YH** [LH07c]. **Yi** [Ano07g, Ano07e, Ano07f]. **yields** [FJT+05]. **ylide** [LSCC01]. **ylides** [KS04a]. **Young** [PVZV00, PVB+02, PVB+03]. **YSb** [RHM05]. **YTiO** [Oni07]. **ytterbium** [RSDNSB00]. **yttrium** [LH07c, MGAS09, XBHL04]. **Yukawa** [ATN09, PI02, PS07]. **Yukawa-type** [PI02]. **Yuri** [AWZD05b]. **Yves** [DB04a]. **YVO** [PBS02].

Z. [Ano06g]. **Z3PolX** [ZB05]. **Zagreb** [Zho07]. **Zeeman** [Dat04]. **Zeilinger** [KMM+06]. **Zener** [PSCLGN07]. **Zeno** [TTFP04]. **zeolite** [AGFM03, IPPL05, LTV03, MMCC02, ZMMS+00]. **zeolites** [KL03, LTV05, LTV07, MBRS05, SCHH01, SCHH02]. **zeolitic** [SKT05, TC07]. **Zerner** [Ano00a, Ano00k, ÖS00c, RÖ00]. **Zero** [MK00, Tou09, Boe09, DLM+02, EZ05, HDL00, LCK00, NS08, dGS06]. **zero-dimensional** [DLM+02]. **Zero-field** [MK00, dGS06]. **zero-flux** [NS08]. **Zero-phonon** [Tou09]. **zero-point** [LCK00]. **zero-temperature** [Boe09]. **zero-valent** [HDL00]. **zero-voltage** [EZ05]. **zeroth** [KZvL09, vLvL06]. **zeroth-order** [KZvL09, vLvL06]. **zeta** [VD00]. **Ziegler** [CCA+06, MM02]. **zigzag** [CMW03]. **ZILSH** [OD03]. **zinc** [BN01, DCP01, ERC+02, KVSG02, LSK+06, MMT+07, PSN08, YYYM01, Yam09, MWL08]. **ZINDO** [Kir08]. **zintl** [OA05]. **zintl-phase** [OA05]. **zirconium** [CPR06]. **zirconium-imido** [CPR06]. **Zn** [DTT06, KS00, NH00]. **Zn-doped** [KS00]. **Zn/Cu** [NH00].

ZnCu [Mar09]. **ZnO** [PLO02]. **ZnTi** [CGL+05]. **ZnZSM** [ZSKV04]. **ZnZSM-5** [ZSKV04]. **zone** [SH09]. **ZORA** [vLvL06, Sad06]. **Zr** [HDL00]. **ZrO** [AM07]. **ZSM** [SZK07, SZ08]. **ZSM-5** [KZS07, SAE08]. **zwitterion** [JAP+05, PILD07]. **zwitterionic** [GB03, MPIP00].

References

Abarenkov:2004:CBMa

[AA04a] I. V. Abarenkov and I. M. Antonova. Chemical bond modeling with the energy-driven orbital localization. *International Journal of Quantum Chemistry*, 96(3):263–272, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abarenkov:2004:SPE

[AA04b] I. V. Abarenkov and I. M. Antonova. Separable pseudopotentials: Effective core potential and the embedding potential. *International Journal of Quantum Chemistry*, 100(4): 649–660, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Antolin:2009:CAI

[AA09a] J. Antolín and J. C. Angulo. Complexity analysis of ionization processes and isoelectronic series. *International Journal of Quantum Chemistry*, 109(3):586–593, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Avci:2009:TAV

[AA09b] Davut Avci and Yusuf Atalay. Theoretical analysis of vibrational spectra and scaling-factor of 2-aryl-1,3,4-oxadiazole derivatives. *International Journal of Quantum Chemistry*, 109 (2):328–341, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ayers:2005:PPC

[AAB05] Paul W. Ayers, James S. M. Anderson, and Libero J. Bartolotti. Perturbative perspectives on the chemical reaction prediction problem. *International Journal of Quantum Chemistry*, 101(5):520–534, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abdul-Al:2007:TSL

[AAKAF07] S. Abdul-Al, M. Korek, A. R. Allouche, and M. Aubert Frécon. Theoretical structure of the low-laying electronic states of the molecule YBr. *International Journal of Quantum Chemistry*, 107(4):998–1007, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Adane:2008:TPE

[AB08] Legesse Adane and Prasad V. Bharatam. Tautomeric preferences and electron delocalization in biurets, thiobiurets, and dithiobiurets: An ab initio study. *International Journal of Quantum Chemistry*, 108(7):1277–1286, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Angeli:2007:PIC

[ABB+07] C. Angeli, G. L. Bendazzoli, S. Borini, R. Cimiraglia, A. Emerson, S. Evangelisti, D. Maynau, A. Monari, E. Rossi, J. Sanchez-Marin, P. G. Szalay, and A. Tajti. The problem of interoperability: A common data format for quantum chemistry codes. *International Journal of Quantum Chemistry*, 107(11):2082–2091, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Achour:2008:TSH

[ABBS08] M. Nait Achour, M. R. Belmecheri, G. Berthier, and R. Savinelli. Theoretical study of hydrogen-bonded complexes of benzene with hydrides of astrochemical interest. *International Journal of Quantum Chemistry*, 108(3):423–429, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Angeli:2006:DEV

[ABC+06] Celestino Angeli, Stefano Borini, Alex Cavallini, Mirko Cestari, Renzo Cimiraglia, Lara Ferrighi, and Manuel Sparta. Developments in the n-electron valence state perturbation theory. *International Journal of Quantum Chemistry*, 106(3): 686–691, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andre:2002:SAD

[ABCS02] J.-M. André, J. L. Brédas, V. Coropceanu, and R. J. Silbey. Symmetry anomaly in disubstituted benzenes. *Inter-*

national Journal of Quantum Chemistry, 90(4-5):1428–1439, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alves:2006:DFT

[ABD06] C. N. Alves, R. S. Borges, and A. B. F. Da Silva. Density functional theory study of metabolic derivatives of the oxidation of paracetamol. *International Journal of Quantum Chemistry*, 106(13):2617–2623, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

AriasdeSaavedra:2000:TBD

[ABGS00] F. Arias de Saavedra, E. Buendía, F. J. Gálvez, and A. Sarsa. Two-body densities and effective potentials. *International Journal of Quantum Chemistry*, 79(2):75–81, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72508331/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72508331/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72508331&PLACEBO=IE.pdf`.

Aldongarov:2007:CSP

[ABI07] Anuar Aldongarov, Nikolay N. Barashkov, and Irina S. Irgibaeva. Calculated spectral properties of perylene orange, perylene red, and their complex with sodium azide. *International Journal of Quantum Chemistry*, 107(13):2331–2342, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ai:2003:IPT

[ABL03] Hongqi Ai, Yuxiang Bu, and Ping Li. Intramolecular proton transfer induced by divalent alkali earth metal cation in the gas state. *International Journal of Quantum Chemistry*, 94 (4):205–214, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alvarez-Bajo:2006:GAC

[ÁBL06] O. Álvarez-Bajo and R. Lemus. General approach for the construction of hybrid orbitals. *International Journal of Quantum Chemistry*, 106(2):401–414, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aquilanti:2002:HHP

[ABLL02] Vincenzo Aquilanti, Andrea Beddoni, Andrea Lombardi, and Robert Littlejohn. Hyperspherical harmonics for polyatomic systems: Basis set for kinematic rotations. *International Journal of Quantum Chemistry*, 89(4):277–291, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Atticks:2001:TCO

[ABM01] Karissa Atticks, Robert K. Bohn, and H. Harvey Michels. Three conformers observed and characterized in 1-hexyne. *International Journal of Quantum Chemistry*, 85(4–5):514–519, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Atticks:2002:SRE

[ABM02] Karissa A. Atticks, Robert K. Bohn, and H. Harvey Michels. Structure and relative energies of the conformers of n-butyl cyanide and 5-hexynenitrile. *International Journal of Quantum Chemistry*, 90(4-5):1440–1447, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alexander:2002:CUL

[AC02a] S. A. Alexander and R. L. Coldwell. Computing upper and lower bounds using Monte Carlo methods. *International Journal of Quantum Chemistry*, 89(6):489–493, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alexander:2002:SKP

[AC02b] S. A. Alexander and R. L. Coldwell. Solution of the Kronig–Penney model using variational Monte Carlo. *International Journal of Quantum Chemistry*, 86(4):325–329, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86511021/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86511021/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86511021&PLACEBO=IE.pdf`.

Alexander:2004:SCH

[AC04] S. A. Alexander and R. L. Coldwell. Spectroscopic constants of H_2 using Monte Carlo methods. *International Journal of Quantum Chemistry*, 100(6):851–857, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [AC05].

Alexander:2005:ESC

[AC05] S. A. Alexander and R. L. Coldwell. Erratum: Spectroscopic constants of H_2 using Monte Carlo methods, S. A. Alexander and R. L. Coldwell, International Journal of Quantum Chemistry (2004) **100**(6) 851–857. *International Journal of Quantum Chemistry*, 103(1):118, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [AC04].

Alexander:2006:VRE

[AC06] S. A. Alexander and R. L. Coldwell. Vibrational–rotational energies of all H_2 isotopomers using Monte Carlo methods. *International Journal of Quantum Chemistry*, 106(8):1820–1826, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alexander:2007:RAP

[AC07] S. A. Alexander and R. L. Coldwell. Rovibrationally averaged properties of H_2 using Monte Carlo methods. *International Journal of Quantum Chemistry*, 107(2):345–352, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alexander:2008:EQO

[AC08] S. A. Alexander and R. L. Coldwell. Electric quadrupole oscillator strengths of helium. *International Journal of Quantum Chemistry*, 108(15):2813–2818, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alexander:2009:VMW

[AC09] S. A. Alexander and R. L. Coldwell. Visualizing molecular wavefunctions using Monte Carlo methods. *International Journal of Quantum Chemistry*, 109(3):385–400, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Antolin:2002:MCE

[ACA02] J. Antolín, J. C. Cuchí, and J. C. Angulo. Minimum cross-entropy estimation of internally folded densities from Compton profiles. *International Journal of Quantum Chemistry*, 87(4):214–219, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90511630/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90511630/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90511630&PLACEBO=IE.pdf`.

Anguiano:2002:ISC

[ACB+02] A. Anguiano, A. Cruz, V. Bertin, E. Poulain, and S. Castillo. Ab initio study of the $CuPt_3$ cluster with H_2 interaction. *International Journal of Quantum Chemistry*, 89(6):514–524, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aquilanti:2003:HEO

[ACC03] Vincenzo Aquilanti, Andrea Caligiana, and Simonetta Cavalli. Hydrogenic elliptic orbitals, Coulomb Sturmian sets, and recoupling coefficients among alternative bases. *International Journal of Quantum Chemistry*, 92(2):99–117, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aquilanti:2003:HOM

[ACCC03] Vincenzo Aquilanti, Andrea Caligiana, Simonetta Cavalli, and Cecilia Coletti. Hydrogenic orbitals in momentum space and hyperspherical harmonics: Elliptic Sturmian basis sets. *International Journal of Quantum Chemistry*, 92(2):212–228, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Amat:2002:UPA

[ACD02] Lluís Amat and Ramon Carbó-Dorca. Use of promolecular ASA density functions as a general algorithm to obtain starting MO in SCF calculations. *International Journal of Quantum Chemistry*, 87(2):59–67, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.`

wiley.com/cgi-bin/abstract/88510650/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88510650/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88510650&PLACEBO=IE.pdf.

Aquilanti:2001:TEN

[ACDV01] V. Aquilanti, S. Cavalli, D. De Fazio, and A. Volpi. Theory of electronically nonadiabatic reactions: Rotational, Coriolis, spin–orbit couplings and the hyperquantization algorithm. *International Journal of Quantum Chemistry*, 85(4–5):368–381, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Apra:2004:SBV

[ACF04] Edoardo Aprà, Emily A. Carter, and Alessandro Fortunelli. Separability between valence and conduction bands in transition metal clusters. *International Journal of Quantum Chemistry*, 100(3):277–287, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [ACF05].

Apra:2005:ESB

[ACF05] Edoardo Aprà, Emily A. Carter, and Alessandro Fortunelli. Erratum: Separability between valence and conduction bands in transition metal clusters. *International Journal of Quantum Chemistry*, 101(2):230, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [ACF04].

Aquino:2005:AEE

[ACFR05] N. Aquino, G. Campoy, and A. Flores-Riveros. Accurate energy eigenvalues and eigenfunctions for the two-dimensional confined hydrogen atom. *International Journal of Quantum Chemistry*, 103(3):267–277, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andreoni:2000:DFT

[ACG00] Wanda Andreoni, Alessandro Curioni, and Henrik Grönbeck. Density functional theory approach to thiols and disulfides on gold: Au(111) surface and clusters. *International Journal of Quantum Chemistry*, 80(4–5):598–608, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505383/START; http:

//www3.interscience.wiley.com/cgi-bin/fulltext/73505383/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505383&PLACEBO=IE.pdf.

Antoniou:2004:PC

[ACG04] I. Antoniou, Th. Christidis, and K. Gustafson. Probability from chaos. *International Journal of Quantum Chemistry*, 98 (2):150–159, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Atodiresei:2008:IMN

[ACHB08] N. Atodiresei, V. Caciuc, H. Hölscher, and S. Blügel. Ab initio modeling of noncontact atomic force microscopy imaging of benzene on Cu(110) surface. *International Journal of Quantum Chemistry*, 108(15):2803–2812, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aquino:2007:HAS

[ACM07] N. Aquino, G. Campoy, and H. E. Montgomery, Jr. Highly accurate solutions for the confined hydrogen atom. *International Journal of Quantum Chemistry*, 107(7):1548–1558, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andre:2001:LCM

[ACPG01] Jean-Marie André, Benoît Champagne, Eric A. Perpète, and Maxime Guillaume. Linear, cyclic, and Möbius strip polyacenes: The influence of the topology on the size-dependent HOMO-LUMO energy gap. *International Journal of Quantum Chemistry*, 84(6):607–616, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/82502288/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/82502288/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=82502288&PLACEBO=IE.pdf.

Alcoba:2005:CEI

[ACT+05] D. R. Alcoba, F. J. Casquero, L. M. Tel, E. Pérez-Romero, and C. Valdemoro. Convergence enhancement in the iterative solution of the second-order contracted Schrödinger equation. *International Journal of Quantum Chemistry*, 102(5):620–628,

???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arno:2001:UTD

[AD01] Manuel Arnó and Luis R. Domingo. Using theozymes for designing transition-state analogs for the intramolecular aldol reaction ofδ-diketones. *International Journal of Quantum Chemistry*, 83(6):338–347, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/81501979/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/81501979/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=81501979&PLACEBO=IE.pdf`.

Ayers:2006:NCR

[AD06] Paul W. Ayers and Ernest R. Davidson. Necessary conditions for the N-representability of pair distribution functions. *International Journal of Quantum Chemistry*, 106(7):1487–1498, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Al-Dossary:2007:MPE

[AD07] O. M. Al-Dossary. Morse potential eigen-energies through the asymptotic iteration method. *International Journal of Quantum Chemistry*, 107(10):2040–2046, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Adams:2002:IPT

[Ada02] William H. Adams. Intermolecular perturbation theory applied to an exactly solvable model. *International Journal of Quantum Chemistry*, 90(1):54–62, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Adams:2005:CRF

[Ada05] William H. Adams. Convergence radii of five intermolecular perturbation theories applied to the interaction between two hydrogen atoms. *International Journal of Quantum Chemistry*, 105(6):781–793, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Adams:2009:CRP

[Ada09] William H. Adams. Convergence radii of the polarization expansion of intermolecular potentials. *International Journal of Quantum Chemistry*, 109(15):3844–3857, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Azevedo:2006:IEF

[AdBM06] Sérgio Azevedo and Fernando de Brito Mota. Influence of the electric field on BN conical structures. *International Journal of Quantum Chemistry*, 106(8):1907–1911, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Avram:2002:JTA

[ADK02] N. M. Avram, Gh. E. Drăgănescu, and M. R. Kibler. $E \otimes \epsilon$ Jahn–Teller anharmonic coupling for an octahedral system. *International Journal of Quantum Chemistry*, 88(3):303–309, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Asturiol:2006:BFH

[ADSTS06] David Asturiol, Miquel Duran, Pedro Salvador, and Miquel Torrent-Sucarrat. BSSE-free hardness profiles of hydrogen bond exchange in the hydrogen fluoride dimer. *International Journal of Quantum Chemistry*, 106(14):2910–2919, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arantes:2005:RSR

[ADTD05] C. Arantes, M. T. De Araujo, A. G. Taranto, and J. W. De M.Carneiro. Relative stability of radicals derived from artemisinin: A semiempirical and DFT study. *International Journal of Quantum Chemistry*, 103(5):749–762, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alfe:2000:RDI

[AdWKG00] D. Alfè, G. A. de Wijs, G. Kresse, and M. J. Gillan. Recent developments in ab initio thermodynamics. *International Journal of Quantum Chemistry*, 77(5):871–879, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000349/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000349/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000349&PLACEBO=IE.pdf`.

Alferova:2002:MEV

[AE02] T. Alferova and N. Elander. *S*-matrix expansions in view of complex dilation theories. *International Journal of Quantum Chemistry*, 90(4-5):1361–1367, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alferova:2004:RRB

[AE04] Tatjana Alferova and Nils Elander. Role of resonances in building collision cross-sections: Mittag-Leffler-based study. *International Journal of Quantum Chemistry*, 97(5):922–932, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alia:2007:VDH

[AE07] Jose M. Alía and Howell G. M. Edwards. Vibrational dynamics of hydrogen-bonded HCN complexes with OH and NH acids: Computational DFT systematic study. *International Journal of Quantum Chemistry*, 107(5):1170–1180, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abu-Eittah:2000:ETS

[AEI00] Rafie H. Abu-Eittah and Yahya M. Ibrahim. Experimental and theoretical study of the electronic absorption spectra of some 1,2-benzoquinone diazides: Closed-open tautomerism. *International Journal of Quantum Chemistry*, 78(1):52–62, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71001658/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71001658/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71001658&PLACEBO=IE.pdf`.

Abu-Eittah:2006:TID

[AEMAO06] Rafie H. Abu-Eittah, Adel A. Mohamed, and Ahmed M. Al-Omar. Theoretical investigation of the decomposition of acyl azides: Molecular orbital treatment. *International Journal*

of Quantum Chemistry, 106(4):863–875, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Almeida:2003:PSM

[AFC03] L. M. Almeida, Carlos Fiolhais, and M. Causà. Properties of simple metals beyond the local density approximation of density functional theory. *International Journal of Quantum Chemistry*, 91(2):224–229, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alagona:2001:RMB

[AG01a] Giuliano Alagona and Caterina Ghio. Reaction mechanisms between methylamine and a few Schiff bases: Ab initio potential energy surfaces of a catalytic step in semicarbazide sensitive amino oxidases (SSAO). *International Journal of Quantum Chemistry*, 84(6):740–749, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/82003608/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/82003608/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=82003608&PLACEBO=IE.pdf`.

Alexandrov:2001:CPS

[AG01b] Vadim Alexandrov and Mark Gerstein. Calculating populations of subcellular compartments using density matrix formalism. *International Journal of Quantum Chemistry*, 85 (6):693–696, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85008594/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85008594/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85008594&PLACEBO=IE.pdf`.

Alagona:2002:III

[AG02a] Giuliano Alagona and Caterina Ghio. Interplay of intra- and intermolecular H-bonds for the addition of a water molecule to the neutral and N-protonated forms of noradrenaline. *International Journal of Quantum Chemistry*, 90(2):641–656, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anicich:2002:GCS

[AG02b] Pablo G. O. Anicich and Horacio Grinberg. Grassmann coherent states representation of the path integral: Evaluation of the generating function for spin systems. *International Journal of Quantum Chemistry*, 90(6):1562–1576, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alagona:2008:KET

[AG08] Giuliano Alagona and Caterina Ghio. Keto-enol tautomerism in linear and cyclic β-diketones: A DFT study in vacuo and in solution. *International Journal of Quantum Chemistry*, 108 (10):1840–1855, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Appel:2006:DPA

[AGB06] H. Appel, E. K. U. Gross, and K. Burke. Double-pole approximation in time-dependent density functional theory. *International Journal of Quantum Chemistry*, 106(14):2840–2847, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Akpinar:2000:QWP

[AGBY00] Sinan Akpinar, Fahrettin Gogtas, Niyazi Bulut, and Abdulkadir Yildiz. A quantum wave packet study of He-H_2 inelastic scattering. *International Journal of Quantum Chemistry*, 79(5):274–279, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72512625/START;` `http://www3.interscience.wiley.com/cgi-bin/fulltext/72512625/FILE?TPL=ftx_start;` `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72512625&PLACEBO=IE.pdf`.

Andzelm:2003:DSM

[AGFM03] Jan Andzelm, Niranjan Govind, George Fitzgerald, and Amitesh Maiti. DFT study of methanol conversion to hydrocarbons in a zeolite catalyst. *International Journal of Quantum Chemistry*, 91(3):467–473, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Antoniou:2004:CMM

[AGL04a] I. Antoniou, A. Goldbeter, and R. Lefever. Complexity: Microscopic and macroscopic aspects: Workshop in Honor of Ilya Prigogine on the occasion of his 85th birthday. *International Journal of Quantum Chemistry*, 98(2):62–64, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Antoniou:2004:F

[AGL04b] Ioannis Antoniou, Albert Goldbeter, and René Lefever. Foreword. *International Journal of Quantum Chemistry*, 98(2): 68, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aramburu:2003:CDS

[AGLBM03] J. A. Aramburu, J. M. García-Lastra, M. T. Barriuso, and M. Moreno. A complex defect studied through DFT: The Fe^3–O^{2-} pair in $KMgF_3$. *International Journal of Quantum Chemistry*, 91(2):197–201, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alagona:2001:IMC

[AGM01] Giuliano Alagona, Caterina Ghio, and Susanna Monti. Ab initio modeling of competitive drug-drug interactions: 5-fluorouracil dimers in the gas phase and in solution. *International Journal of Quantum Chemistry*, 83(3-4):128–142, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002586/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002586/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002586&PLACEBO=IE.pdf`.

Alagona:2002:FDA

[AGM02] Giuliano Alagona, Caterina Ghio, and Susanna Monti. 5-fluorouracil dimers in aqueous solution: molecular dynamics in water and continuum solvation. *International Journal of Quantum Chemistry*, 88(1):133–146, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/91015567/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91015567/`

FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91015567&PLACEBO=IE.pdf.

Agacino:2006:APE

[AGM06] Esther Agacino, Ricardo Gaitán, and Italo Menconi. Acidity predictions in an electron propagator approach. *International Journal of Quantum Chemistry*, 106(8):1799–1808, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andreev:2002:MMH

[AGMK02] A. G. Andreev, M. Georgiev, M. S. Mladenova, and V. Krastev. Magnetic moments of hindered rotators by off-center impurity ions. *International Journal of Quantum Chemistry*, 89(4):371–376, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alagona:2004:TSE

[AGN04] Giuliano Alagona, Caterina Ghio, and Peter I. Nagy. Theoretical studies on the effects of methods and parameterization on the calculated free energy of hydration for small molecules. *International Journal of Quantum Chemistry*, 99(3):161–178, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Albert:2009:FPE

[AGSH09] Victor V. Albert, Nicolais L. Guevara, John R. Sabin, and Frank E. Harris. Few-parameter exponentially correlated wavefunctions for the ground state of lithium. *International Journal of Quantum Chemistry*, 109(15):3791–3797, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Absi:2006:AEM

[AH06] Noureddine Absi and Philip Hoggan. Analytical evaluation of molecular electronic integrals using Poisson's equation: Exponential-type orbitals and atom pairs. *International Journal of Quantum Chemistry*, 106(14):2881–2888, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andreev:2002:VPS

[AIG02] A. G. Andreev, M. D. Ivanovich, and M. Georgiev. Vibronic polarons: Self-trapping, local rotation, and band features. *International Journal of Quantum Chemistry*, 89(4):405–418, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Allen:2002:LCO

[AK02] Leland C. Allen and Eugene T. Knight. The Löwdin challenge: Origin of the $n + \ell, n$ (Madelung) rule for filling the orbital configurations of the periodic table. *International Journal of Quantum Chemistry*, 90(1):80–88, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arbuznikov:2005:LHE

[AK05] Alexei V. Arbuznikov and Martin Kaupp. Localized hybrid exchange-correlation potentials for Kohn–Sham DFT calculations of NMR and EPR parameters. *International Journal of Quantum Chemistry*, 104(2):261–271, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arnason:2006:CRE

[AKB06] Ingvar Arnason, Ágúst Kvaran, and Andras Bodi. Comment on "Relative Energies, Stereoelectronic Interactions, and Conformational Interconversion in Silacycloalkanes". *International Journal of Quantum Chemistry*, 106(8):1975–1978, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [FFS04].

Anandan:2005:MSC

[AKK05a] K. Anandan, P. Kolandaivel, and R. Kumaresan. Molecular structural conformations and hydration of internally hydrogen-bonded salicylic acid: Ab initio and DFT studies. *International Journal of Quantum Chemistry*, 103(2):127–139, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anandan:2005:QCS

[AKK05b] K. Anandan, P. Kolandaivel, and R. Kumaresan. Quantum chemical studies on molecular structural conformations and hydrated forms of salicylamide and O-hydroxybenzoyl cyanide. *International Journal of Quantum Chemistry*, 104

(3):286–298, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Akama:2009:ETD

[AKN09] Tomoko Akama, Masato Kobayashi, and Hiromi Nakai. Electronic temperature in divide-and-conquer electronic structure calculation revisited: Assessment and improvement of self-consistent field convergence. *International Journal of Quantum Chemistry*, 109(12):2706–2713, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

An:2009:SEM

[AL09] Xiulin An and Qingzhong Li. Strong effect of methyl group on the strength of ionic hydrogen bond between C_2H_2 and H_3O^+. *International Journal of Quantum Chemistry*, 109(4): 870–875, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alcoba:2004:UID

[Alc04] Diego R. Alcoba. Unitarily invariant decomposition of arbitrary Hermitian matrices of physical interest. *International Journal of Quantum Chemistry*, 97(3):776–783, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Amaral:2003:QMH

[ALI03] M. S. Amaral, M. Loos, and A. S. Ito. A QM/MM hybrid simulation of 5-hydroxytryptophan in solution. *International Journal of Quantum Chemistry*, 95(3):289–294, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alford:2005:TEP

[ALM05] J. T. Alford, B. A. Landis, and J. W. Mintmire. Theoretical elastic properties of single-walled carbon nanotubes. *International Journal of Quantum Chemistry*, 105(6):767–771, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Amovilli:2005:PDR

[AM05] C. Amovilli and N. H. March. Pair density related to one-electron information for the ground state of spin-compensated

two-electron systems. *International Journal of Quantum Chemistry*, 102(2):132–138, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Amovilli:2006:FPS

[AM06] Claudio Amovilli and Norman H. March. Feynman propagator and Slater sum for a model Hamiltonian motivated by H in an intense magnetic field. *International Journal of Quantum Chemistry*, 106(2):533–541, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abarenkov:2007:ESN

[AM07] I. V. Abarenkov and I. D. Matyukevich. Electronic structure of negative oxygen ion in ZrO_2 crystal. *International Journal of Quantum Chemistry*, 107(13):2389–2397, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Amano:2009:ESC

[AM09a] Taiji Amano and Yasuji Muramatsu. Electronic structure calculations of carbon nanohorns for their chemical state analysis using soft X-ray spectroscopy. *International Journal of Quantum Chemistry*, 109(12):2728–2733, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Amovilli:2009:IED

[AM09b] Claudio Amovilli and Norman H. March. Inequivalent electron densities derived from an approximate correlated ground-state wave function using the Hiller–Sucher–Feinberg identity: Comparisons with quantum Monte Carlo densities for He and Ne atoms. *International Journal of Quantum Chemistry*, 109 (5):1024–1030, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Altarsha:2007:CSI

[AMC07] Muhannad Altarsha, Gérald Monard, and Bertrand Castro. Comparative semiempirical and ab initio study of the structural and chemical properties of uric acid and its anions. *International Journal of Quantum Chemistry*, 107(1):172–181, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Amovilli:2000:FBD

[AMGN00] C. Amovilli, N. H. March, T. Gál, and Á. Nagy. Force-balance and differential equation for the ground-state electron density in atoms and molecules. *International Journal of Quantum Chemistry*, 77(4):716–720, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70500247/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70500247/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70500247&PLACEBO=IE.pdf`.

Almeida:2001:TSM

[AML+01] A. L. Almeida, J. B. L. Martins, E. Longo, N. C. Furtado, C. A. Taft, J. R. Sambrano, and W. A. Lester, Jr. Theoretical study of MgO(001) surfaces: Pure, doped with Fe, Ca, and Al, and with and without adsorbed water. *International Journal of Quantum Chemistry*, 84(6):705–713, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/82003607/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/82003607/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=82003607&PLACEBO=IE.pdf`.

Arenas:2001:NIT

[AMO+01] J. F. Arenas, J. I. Marcos, J. C. Otero, I. L. Tocón, and J. Soto. Nitrenes as intermediates in the thermal decomposition of aliphatic azides. *International Journal of Quantum Chemistry*, 84(2):241–248, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502329/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502329/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502329&PLACEBO=IE.pdf`.

Alcaro:2007:CBA

[AMOR07] Stefano Alcaro, Tiziana Marino, Francesco Ortuso, and Nino Russo. Conformational behavior of antineoplastic peptides Dolastatin 10 and Dolastatin 15 from Monte Carlo and molecular dynamics simulations. *International Journal of Quantum*

Chemistry, 107(2):318–325, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andre:2005:MCM

[And05] Jean-Marie André. In memory of Carl Moser. *International Journal of Quantum Chemistry*, 105(6):534, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Angyan:2009:ELS

[Áng09] J. G. Ángyán. Electron localization and the second moment of the exchange hole. *International Journal of Quantum Chemistry*, 109(11):2340–2347, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arruda:2009:SCA

[ANJ09] Priscilla M. Arruda, A. Canal Neto, and F. E. Jorge. Some considerations about Gaussian basis sets for electric property calculations. *International Journal of Quantum Chemistry*, 109(6):1189–1199, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Amovilli:2003:AAE

[ANM03] C. Amovilli, Á. Nagy, and N. H. March. Approximate ansatz for the expansion of the spherically averaged wave function in terms of interelectronic separation r_{12} for the Hookean atom, atomic ions, and the H_2 molecule. *International Journal of Quantum Chemistry*, 95(1):21–29, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2000:BMC

[Ano00a] Anonymous. Bibliography of Michael C. Zerner. *International Journal of Quantum Chemistry*, 77(1):3–15, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004272/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004272/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004272&PLACEBO=IE.pdf`.

Anonymous:2000:BR

[Ano00b] Anonymous. Books received. *International Journal of Quantum Chemistry*, 79(6):378, ???? 2000. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72515273/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72515273/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72515273&PLACEBO=IE.pdf.

Anonymous:2000:E

[Ano00c] Anonymous. Erratum. *International Journal of Quantum Chemistry*, 78(1):69, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/71001652/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71001652/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71001652&PLACEBO=IE.pdf.

Anonymous:2000:IAQ

[Ano00d] Anonymous. The International Academy of Quantum Molecular Science elected the following new members. *International Journal of Quantum Chemistry*, 76(4):583, February 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70000688/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000688/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000688&PLACEBO=IE.pdf.

Anonymous:2000:KR

[Ano00e] Anonymous. Klaus Rüdenberg. *International Journal of Quantum Chemistry*, 76(2):113, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/69503180/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503180/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503180&PLACEBO=IE.pdf.

Anonymous:2000:LPa

[Ano00f] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 76(2):131–136, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.

wiley.com/cgi-bin/abstract/69503166/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503166/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503166&PLACEBO=IE.pdf.

Anonymous:2000:LPb

[Ano00g] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 77(1):498–507, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70004292/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004292/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004292&PLACEBO=IE.pdf.

Anonymous:2000:LPc

[Ano00h] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 80(2):85–95, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73001272/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001272/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001272&PLACEBO=IE.pdf.

Anonymous:2000:LPd

[Ano00i] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 80(4–5):508–533, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505375/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505375/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505375&PLACEBO=IE.pdf.

Anonymous:2000:LPe

[Ano00j] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 80(6):1138–1163, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/75502060/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75502060/FILE?TPL=ftx_start;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502060&PLACEBO=IE.pdf.

Anonymous:2000:MCZ

[Ano00k] Anonymous. Michael C. Zerner. *International Journal of Quantum Chemistry*, 77(1):ix, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70004298/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004298/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004298&PLACEBO=IE.pdf.

Anonymous:2001:A

[Ano01a] Anonymous. Announcement. *International Journal of Quantum Chemistry*, 81(4):305, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/76505738/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76505738/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76505738&PLACEBO=IE.pdf.

Anonymous:2001:BRa

[Ano01b] Anonymous. Book review. *International Journal of Quantum Chemistry*, 81(5):370, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/76507292/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76507292/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76507292&PLACEBO=IE.pdf.

Anonymous:2001:BRb

[Ano01c] Anonymous. Books received. *International Journal of Quantum Chemistry*, 81(5):371, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/76507287/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76507287/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76507287&PLACEBO=IE.pdf.

Anonymous:2001:E

[Ano01d] Anonymous. Erratum. *International Journal of Quantum Chemistry*, 85(1):61, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85510914/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85510914/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85510914&PLACEBO=IE.pdf.

Anonymous:2001:LPa

[Ano01e] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 83(3-4):98–103, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/80002585/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002585/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002585&PLACEBO=IE.pdf.

Anonymous:2001:LPb

[Ano01f] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 84(2):311–329, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/84502337/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502337/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502337&PLACEBO=IE.pdf.

Anonymous:2001:LPc

[Ano01g] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 84(5):442–466, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85008760/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85008760/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85008760&PLACEBO=IE.pdf.

Anonymous:2001:LPd

[Ano01h] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 85(4–5):172–195, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2001:LPe

[Ano01i] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 85(6):638–661, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85515912/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85515912/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85515912&PLACEBO=IE.pdf.

Anonymous:2001:P

[Ano01j] Anonymous. Preface. *International Journal of Quantum Chemistry*, 84(1):1, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/84002435/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002435/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002435&PLACEBO=IE.pdf.

Anonymous:2002:EI

[Ano02a] Anonymous. Erratum: Introduction. *International Journal of Quantum Chemistry*, 86(3):323, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/88510558/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88510558/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88510558&PLACEBO=IE.pdf.

Anonymous:2002:ELP

[Ano02b] Anonymous. Erratum: List of participants. *International Journal of Quantum Chemistry*, 86(3):324, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/88510557/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88510557/

FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88510557&PLACEBO=IE.pdf.

Anonymous:2002:GHLb

[Ano02c] Anonymous. Gilda H. Loew, Ph.D., C. V. *International Journal of Quantum Chemistry*, 88(1):17–18, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/91015220/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91015220/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91015220&PLACEBO=IE.pdf.

Anonymous:2002:GHLa

[Ano02d] Anonymous. Gilda H. Loew, Ph.D. list of publications. *International Journal of Quantum Chemistry*, 88(1):5–16, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/91015229/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91015229/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91015229&PLACEBO=IE.pdf.

Anonymous:2002:I

[Ano02e] Anonymous. Introduction. *International Journal of Quantum Chemistry*, 90(4-5):1265, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2002:JSKb

[Ano02f] Anonymous. Józef Stanisław Kwiatkowski: List of publications. *International Journal of Quantum Chemistry*, 90(3): 1253–1264, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2002:JSKa

[Ano02g] Anonymous. Józef Stanislaw Kwiatkowski, photo. *International Journal of Quantum Chemistry*, 90(3):987, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2002:LPa

[Ano02h] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 86(1):2–9, ???? 2002. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/86510680/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86510680/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86510680&PLACEBO=IE.pdf.

Anonymous:2002:LPc

[Ano02i] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 90(4-5):1266–1288, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2002:LPb

[Ano02j] Anonymous. List of the participants. *International Journal of Quantum Chemistry*, 89(4):183–189, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2002:POL

[Ano02k] Anonymous. Per-Olov Löwdin curriculum vitae. *International Journal of Quantum Chemistry*, 90(1):1–11, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2002:PGH

[Ano02l] Anonymous. Photo of Gilda H. Loew. *International Journal of Quantum Chemistry*, 88(1):1, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/91015232/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91015232/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91015232&PLACEBO=IE.pdf.

Anonymous:2002:PPI

[Ano02m] Anonymous. Preface: Proceedings of the international conference on "Electronic Structure: Predictions and Applications". *International Journal of Quantum Chemistry*, 86(1): 1, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/86511424/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86511424/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86511424&PLACEBO=IE.pdf.

Anonymous:2003:LCA

[Ano03a] Anonymous. Leland Cullen Allen: Bibliography and theses. *International Journal of Quantum Chemistry*, 95(6):663–677, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2003:LPa

[Ano03b] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 92(2):96–98, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2003:LPb

[Ano03c] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 95(2):63–78, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2003:LPc

[Ano03d] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 95(4–5):346–364, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2004:LPa

[Ano04a] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 96(6):520–529, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2004:LPb

[Ano04b] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 98(4):344–346, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2004:LPc

[Ano04c] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 99(4):189–197, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2004:LPd

[Ano04d] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 99(6):879–881, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2004:PNS

[Ano04e] Anonymous. Publisher's note: Sir John A. Pople (October 31, 1925–March 15, 2004). *International Journal of Quantum Chemistry*, 98(4):v, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2004:WFT

[Ano04f] Anonymous. Workshop at the Fondation des Treilles, 8–14 July 2002 list of participants. *International Journal of Quantum Chemistry*, 98(2):65–67, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2005:A

[Ano05a] Anonymous. Announcements. *International Journal of Quantum Chemistry*, 102(4):470, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2005:LPa

[Ano05b] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 101(5):472–492, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2005:LPb

[Ano05c] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 103(5):472–492, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2005:LPd

[Ano05d] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 105(6):535–552, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2005:LPc

[Ano05e] Anonymous. List of the participants. *International Journal of Quantum Chemistry*, 104(4):382–386, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2005:OJM

[Ano05f] Anonymous. Obituary: Jhon Mu-Shik. *International Journal of Quantum Chemistry*, 103(2):235, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2006:BJG

[Ano06a] Anonymous. Bibliography of Jaap G. Snijders 1977–2005: List of publications. *International Journal of Quantum Chemistry*, 106(12):2412–2421, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2006:LPa

[Ano06b] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 106(3):556–564, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2006:LPb

[Ano06c] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 106(6):1286–1290, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2006:LPc

[Ano06d] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 106(14):2820–2826, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2006:LPd

[Ano06e] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 106(15):3002–3017, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2006:LHL

[Ano06f] Anonymous. Lulu Huang, Lou Massa, Jerome Karle, "Kernel energy method illustrated with peptides," Internationl Journal of Quantum Chemistry (2005) 103(6) 808–817. *International Journal of Quantum Chemistry*, 106(3):772, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2006:ZKT

[Ano06g] Anonymous. Z. Kalogiratou, Th. Monovasilis, T. E. Simos, Computation of the eigenvalues of the one-dimensional Schrödinger equation by symplectic methods, International Journal of Quantum Chemistry (2006) **106**(4) 795–802. *International Journal of Quantum Chemistry*, 106(5):1283, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2007:EMS

[Ano07a] Anonymous. Erratum: Marcel Swart, Matthias Bickelhaupt, Optimization of strong and weak coordinates, International Journal of Quantum Chemistry (2006) **106**(12), 2536–2544. *International Journal of Quantum Chemistry*, 107(4):1027, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [SB06c].

Anonymous:2007:LPa

[Ano07b] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 107(2):261–264, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2007:LPb

[Ano07c] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 107(8):1653–1656, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2007:LPc

[Ano07d] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 107(11):2048–2056, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2007:NJGb

[Ano07e] Anonymous. Notice: Jing-Gang Gai, Yi Ren, Density functional theory study on the reactions of X^- with CH_3SY (X, Y = F, Cl, Br, I) International Journal of Quantum Chemistry (2006). *International Journal of Quantum Chemistry*, 107(6): 1540, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [GR07a].

Anonymous:2007:NJGc

[Ano07f] Anonymous. Notice: Jing-Gang Gai, Yi Ren, Theoretical study of the gas-phase ion pairs S_N2 reactions of LiX with CH_3SY (X, Y = F, Cl, Br, I) International Journal of Quantum Chemistry (2006). *International Journal of Quantum Chemistry*, 107(6):1541, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [GR07b].

Anonymous:2007:NJGa

[Ano07g] Anonymous. Notice: Jing-Gang Gai, Yi Ren, Theoretical study of the gas-phase S_N2 reactions of X^- with CH_3OY (X,

Y = Cl, Br, I), International Journal of Quantum Chemistry (2006). *International Journal of Quantum Chemistry*, 107(5): 1284, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [GR07c].

Anonymous:2007:P

[Ano07h] Anonymous. Preface. *International Journal of Quantum Chemistry*, 107(14):2565–2566, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2007:QXL

[Ano07i] Anonymous. QSCP-XI: List of participants. *International Journal of Quantum Chemistry*, 107(14):2567–2574, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2008:HCL

[Ano08a] Anonymous. History of the Congress of Latin Expression Theoretical Chemists. *International Journal of Quantum Chemistry*, 108(10):1621, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2008:LP

[Ano08b] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 108(11):1874–1877, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2008:CLE

[Ano08c] Anonymous. "The 33rd Congress of Latin Expression Quantum Chemists". *International Journal of Quantum Chemistry*, 108(10):1622, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2009:FHL

[Ano09a] Anonymous. Frank E. Harris: List of publications. *International Journal of Quantum Chemistry*, 109(13):2803–2816, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2009:IML

[Ano09b] Anonymous. Istvan Mayer: List of publications. *International Journal of Quantum Chemistry*, 109(11):2331–2339,

???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2009:KH

[Ano09c] Anonymous. Kimihiko Hirao. *International Journal of Quantum Chemistry*, 109(9):1767–1769, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2009:KHL

[Ano09d] Anonymous. Kimihiko Hirao: List of publications. *International Journal of Quantum Chemistry*, 109(9):1770–1789, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2009:LPa

[Ano09e] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 109(12):2640–2646, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2009:LPb

[Ano09f] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 109(14):3145–3170, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2009:SPA

[Ano09g] Anonymous. A short photo album of Frank Harris. *International Journal of Quantum Chemistry*, 109(13):2802, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Antoniou:2004:FIP

[Ant04] Ioannis Antoniou. Farewell to Ilya Prigogine. *International Journal of Quantum Chemistry*, 98(2):60–61, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Atis:2007:SEB

[AÖG07] Murat Atiş, Cem Özdoğan, and Ziya B. Güvenç. Structure and energetic of B_n ($n = 2--12$) clusters: Electronic structure calculations. *International Journal of Quantum Chemistry*, 107(3):729–744, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alper:2000:MDS

[AP00] Howard E. Alper and Peter Politzer. Molecular dynamics simulations of the temperature-dependent behavior of aluminum, copper, and platinum. *International Journal of Quantum Chemistry*, 76(5):670–676, February 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000580/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000580/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000580&PLACEBO=IE.pdf`.

Ayers:2003:SCM

[AP03] Paul W. Ayers and Robert G. Parr. Sufficient condition for monotonic electron density decay in many-electron systems. *International Journal of Quantum Chemistry*, 95(6):877–881, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ayers:2002:LKE

[APN02] Paul W. Ayers, Robert G. Parr, and Agnes Nagy. Local kinetic energy and local temperature in the density-functional theory of electronic structure. *International Journal of Quantum Chemistry*, 90(1):309–326, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Apostolova:2006:FCF

[Apo06] E. S. Apostolova. $Fe(CO)_4$ flexible as a two-level system avoided conical intersection. *International Journal of Quantum Chemistry*, 106(5):1225–1236, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Akguc:2004:DTS

[AR04] G. B. Akguc and L. E. Reichl. Dynamic tunneling and scattering resonances. *International Journal of Quantum Chemistry*, 98(2):173–182, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Angulo:2006:BCF

[AR06] J. C. Angulo and E. Romera. Bare Coulomb field and atomic reciprocal form factor. *International Journal of Quantum*

Chemistry, 106(2):485–489, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abo-Riziq:2005:DBD

[ARBC+05] Ali G. Abo-Riziq, John E. Bushnell, Bridgit Crews, Michael P. Callahan, Louis Grace, and Mattanjah S. De Vries. Discrimination between diastereoisomeric dipeptides by IR–UV double resonance spectroscopy and ab initio calculations. *International Journal of Quantum Chemistry*, 105(4):437–445, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Atanasov:2005:CSO

[ARBD05] Mihail Atanasov, Cédrick Rauzy, Pio Baettig, and Claude Daul. Calculation of spin-orbit coupling within the LFDFT: Applications to $[NiX_4]^2-$ (X = F^-, Cl^-, Br^-, I^-). *International Journal of Quantum Chemistry*, 102(2):119–131, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alves:2003:TSS

[ARD03] C. N. Alves, O. A. S. Romero, and A. B. F. Da Silva. Theoretical study on the stereochemistry of intramolecular hetero Diels–Alder cycloaddition reactions of azoalkenes. *International Journal of Quantum Chemistry*, 95(2):133–136, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alkorta:2002:TSS

[ARE02] Ibon Alkorta, Isabel Rozas, and Jose Elguero. Theoretical study of the Si-H group as potential hydrogen bond donor. *International Journal of Quantum Chemistry*, 86(1):122–129, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85011544/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85011544/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85011544&PLACEBO=IE.pdf`.

Andrae:2000:NES

[ARH00] Dirk Andrae, Markus Reiher, and Juergen Hinze. Numerical electronic structure calculations for atoms. II. Generalized variable transformation and relativistic calculations. *In-*

ternational Journal of Quantum Chemistry, 76(4):473–499, February 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70000687/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000687/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000687&PLACEBO=IE.pdf.

Arteca:2008:GED

[ART08a] Gustavo A. Arteca, Jean Pierre Rank, and O. Tapia. Generalized electronic diabatic approach to structural similarity in two-dimensional potential energy surfaces of various topologies. *International Journal of Quantum Chemistry*, 108(4): 651–666, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arteca:2008:STR

[ART08b] Gustavo A. Arteca, Jean Pierre Rank, and Orlando Tapia. Simulating trends in reaction path geometry as a function of external fields. A generalized electronic diabatic model for two-dimensional energy surfaces. *International Journal of Quantum Chemistry*, 108(10):1810–1820, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Avery:2000:CIE

[AS00] John Avery and Rune Shim. Core ionization energies of atoms and ions calculated using the generalized Sturmian method. *International Journal of Quantum Chemistry*, 79(1): 1–7, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72504317/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72504317/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72504317&PLACEBO=IE.pdf.

Avery:2001:MSP

[AS01] John Avery and Rune Shim. Molecular Sturmians. Part 1. *International Journal of Quantum Chemistry*, 83(1):1–10, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/79502656/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/79502656/

FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=79502656&PLACEBO=IE.pdf.

Abarenkov:2004:APA

[AS04a] I. V. Abarenkov and K. V. Smelkov. Adiabatic potential analysis for some carbon-containing molecules. *International Journal of Quantum Chemistry*, 96(3):255–262, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abarenkov:2004:CBMb

[AS04b] I. V. Abarenkov and K. V. Smelkov. Chemical bond modeling with correlation effects included. *International Journal of Quantum Chemistry*, 100(4):661–666, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Antolovic:2004:CTC

[AS04c] Danko Antolovic and Harris J. Silverstone. On the computation of (2-2) three-center Slater-type orbital integrals of $1/r_{12}$ using Fourier-transform-based analytical formulas. *International Journal of Quantum Chemistry*, 100(2):146–154, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Angelotti:2008:KAA

[ASDC08] Wagner Fernando Delfino Angelotti, Lívia Streit, André Luiz Da Fonseca, and Rogério Custodio. Koopmans' approximation applied in atoms and diatomic molecules using the diffusion quantum Monte Carlo method. *International Journal of Quantum Chemistry*, 108(13):2459–2466, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Albert:2007:SSE

[ASH07] Victor V. Albert, John R. Sabin, and Frank E. Harris. Simulated structure and energetics of endohedral complexes of noble gas atoms in buckminsterfullerene. *International Journal of Quantum Chemistry*, 107(15):3061–3066, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Albert:2008:SXC

[ASH08] Victor V. Albert, John R. Sabin, and Frank E. Harris. Simulations of $Xe@C_{60}$ collisions with graphitic films. *Inter-*

national Journal of Quantum Chemistry, 108(15):3010–3015, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Allen:2004:TSS

[ASL04] Reeshemah N. Allen, M. K. Shukla, and Jerzy Leszczynski. A theoretical study of the structure and properties of uric acid: A potent antioxidant. *International Journal of Quantum Chemistry*, 100(5):801–809, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Allen:2006:III

[ASL06] Reeshemah N. Allen, M. K. Shukla, and Jerzy Leszczynski. Ab initio insight on the interaction of ascorbate with Li^+, Na^+, K^+, Be^{2+}, Mg^{2+}, and Ca^{2+} metal cations. *International Journal of Quantum Chemistry*, 106(11):2366–2372, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Austing:2003:DFT

[ASM+03] D. G. Austing, S. Sasaki, K. Muraki, K. Ono, S. Tarucha, M. Barranco, A. Emperador, M. Pi, and F. Garcias. Density functional theory application to double quantum dots: Influence of mismatch on the addition energy spectra of vertical diatomic artificial molecules. *International Journal of Quantum Chemistry*, 91(3):498–503, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arimoto:2001:SAC

[ASO+01] Shigeru Arimoto, Mark Spivakovsky, Hiromu Ohno, Peter Zizler, Keith F. Taylor, Tokio Yamabe, and Paul G. Mezey. Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. VI. *International Journal of Quantum Chemistry*, 84(4):389–400, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502938/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502938/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502938&PLACEBO=IE.pdf`.

Arimoto:2004:SAC

[ASO+04] Shigeru Arimoto, Mark Spivakovsky, Hiromu Ohno, Peter Zizler, Rob A. Zuidwijk, Keith F. Taylor, Tokio Yamabe, and Paul G. Mezey. Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution VII. *International Journal of Quantum Chemistry*, 97(3):765–775, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Araujo:2006:TSC

[ASO+06] Regiane C. M. U. Araújo, Verneck M. Soares, Boaz G. Oliveira, Kelson C. Lopes, Elizete Ventura, Silmar A. Do Monte, Otávio L. Santana, Antônio B. Carvalho, and Mozart N. Ramos. Theoretical study of cooperative effects in the homo- and heteromeric hydrogen bond chains $(HCN)_nHF$ with n = 1, 2, and 3. *International Journal of Quantum Chemistry*, 106(13):2714–2722, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arenas:2005:UCS

[ASP+05] Juan F. Arenas, Juan Soto, Daniel Pelaez, David J. Fernandez, and Juan C. Otero. Understanding complex surface-enhanced Raman scattering, using quantum chemical calculations. *International Journal of Quantum Chemistry*, 104 (5):681–694, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Allen:2006:ISS

[ASRL06] Reeshemah N. Allen, M. K. Shukla, Demarcio Reed, and Jerzy Leszczynski. Ab initio study of the structural properties of ascorbic acid (vitamin C). *International Journal of Quantum Chemistry*, 106(14):2934–2943, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Apell:2002:SDM

[ASTO02] S. Peter Apell, John R. Sabin, S. B. Trickey, and J. Oddershede. Shape-dependent molecular polarizabilities. *International Journal of Quantum Chemistry*, 86(1):35–39, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85011945/START; http:`

//www3.interscience.wiley.com/cgi-bin/fulltext/85011945/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85011945&PLACEBO=IE.pdf.

Arteca:2000:RMG

[AT00] Gustavo A. Arteca and O. Tapia. Relative measure of geometrical entanglement to study folding-unfolding transitions. Application to analysis of molecular dynamics trajectories of proteins *in vacuo*. *International Journal of Quantum Chemistry*, 80(4–5):848–855, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505400/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505400/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505400&PLACEBO=IE.pdf.

Alonso:2003:P

[AT03] J. A.. Alonso and S. B. Trickey. Preface. *International Journal of Quantum Chemistry*, 91(2):65–66, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arteca:2007:GED

[AT07] Gustavo A. Arteca and O. Tapia. Generalized electronic diabatic approach to structural similarity and the Hammond postulate. *International Journal of Quantum Chemistry*, 107 (2):382–395, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arissawa:2003:INA

[ATF03] Márcia Arissawa, Carlton Anthony Taft, and Judith Felcman. Investigation of nucleoside analogs with anti-HIV activity. *International Journal of Quantum Chemistry*, 93(6):422–432, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Akinaga:2009:ICT

[ATN09] Yoshinobu Akinaga and Seiichiro Ten-No. Intramolecular charge-transfer excitation energies from range-separated hybrid functionals using the Yukawa potential. *International Journal of Quantum Chemistry*, 109(9):1905–1914, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arteca:2002:MPN

[AV02] Gustavo A. Arteca and Kalyani Veluri. Metastability of protein native folds with respect to global variations in primary sequence. *International Journal of Quantum Chemistry*, 88(1):220–225, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89013457/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89013457/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89013457&PLACEBO=IE.pdf`.

Amero:2004:NBE

[AV04] José M. Amero and Gabriel J. Vázquez. New bound electronic states of NH^+. *International Journal of Quantum Chemistry*, 99(4):353–372, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alcoba:2005:SSP

[AV05a] D. R. Alcoba and C. Valdemoro. Spin structure and properties of the correlation matrices corresponding to pure spin states: Controlling the S-representability of these matrices. *International Journal of Quantum Chemistry*, 102(5):629–644, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [AV06].

Amero:2005:ESN

[AV05b] José M. Amero and Gabriel J. Vázquez. Electronic structure of NH^+: An ab initio study. *International Journal of Quantum Chemistry*, 101(4):396–410, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alcoba:2006:ESS

[AV06] D. R. Alcoba and C. Valdemoro. Erratum: Spin structure and properties of the correlation matrices corresponding to pure spin states: Controlling the S-representability of these matrices, International Journal of Quantum Chemistry (2005) 102(5) 629–644. *International Journal of Quantum Chemistry*, 106(14):2999, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [AV05a].

Aranyosiova:2006:IHB

[AVBč06] Monika Aranyosiová, Ol'ga Vollárová, Ján Benko, and Ivan černušák. Intramolecular hydrogen bonds in thiolato-, sulfenato-, and sulfinato-Co(III) complexes. *International Journal of Quantum Chemistry*, 106(3):747–763, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Avery:2004:MCC

[Ave04] John Avery. Many-center Coulomb Sturmians and Shibuya–Wulfman integrals. *International Journal of Quantum Chemistry*, 100(2):121–130, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alcoba:2009:CCS

[AVTPR09] D. R. Alcoba, C. Valdemoro, L. M. Tel, and E. Pérez-Romero. The correlation contracted Schrödinger equation: An accurate solution of the G-particle-hole hypervirial. *International Journal of Quantum Chemistry*, 109(14):3178–3190, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alexeev:2005:AHF

[AWZD05a] Yuri Alexeev, Theresa L. Windus, Chang-Guo Zhan, and David A. Dixon. Accurate heats of formation and acidities for H_3PO_4, H_2SO_4, and H_2CO_3 from ab initio electronic structure calculations. *International Journal of Quantum Chemistry*, 102(5):775–784, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [AWZD05b].

Alexeev:2005:YAT

[AWZD05b] Yuri Alexeev, Theresa L. Windus, Chang-Guo Zhan, and David A. Dixon. Yuri Alexeev, Theresa L. Windus, Chang-Guo Zhan, David A. Dixon, Erratum to "Accurate heats of formation and acidities for H_3PO_4, H_2SO_4, and H_2CO_3 from ab initio electronic structure calculations," International Journal of Quantum Chemistry (2005) 102(5) 775–784. *International Journal of Quantum Chemistry*, 104(3):379–380, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [AWZD05a].

Aida:2000:CAH

[AYD00] M. Aida, H. Yamataka, and M. Dupuis. Critical assessment of the hybrid QM/MM-pol-vib approach: Small water clusters using polarizable flexible water potentials. *International Journal of Quantum Chemistry*, 77(1):199–210, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004260/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004260/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004260&PLACEBO=IE.pdf`.

Abarenkov:2008:SSF

[AZ08] I. V. Abarenkov and S. N. Zagoulaev. Spin structure of the first order reduced density matrix and spin-polarized states. *International Journal of Quantum Chemistry*, 108(14):2657–2665, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Amor:2006:TAL

[AZD06] N. Ben Amor, S. Záliš, and C. Daniel. Theoretical analysis of low-lying charge transfer states in [Ru(X) (Me)$(CO)_2$ (Me-DAB)] (X = Cl, I; DAB 1,4-diaza-1,3-butadiene) complexes by TDDFT and CASSCF/CASPT2 methods. *International Journal of Quantum Chemistry*, 106(12):2458–2469, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Azevedo:2002:BPM

[Aze02] Sérgio Azevedo. Bound particle with magnetic moment in a space with topological defect. *International Journal of Quantum Chemistry*, 90(6):1596–1599, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Azevedo:2005:IEF

[Aze05] Sérgio Azevedo. Influence of the electric field on a particle in a space with a disclination. *International Journal of Quantum Chemistry*, 101(2):127–130, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bochicchio:2001:EIT

[BA01] Roberto C. Bochicchio and Diego R. Alcoba. On equilibrium intensive thermodynamic properties of composed p-particles in many-body systems. *International Journal of Quantum Chemistry*, 85(2):63–71, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85510642/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85510642/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85510642&PLACEBO=IE.pdf`. See erratum [BA02a].

Bochicchio:2002:EEI

[BA02a] Roberto C. Bochicchio and Diego R. Alcoba. Erratum: On equilibrium intensive thermodynamic properties of composed p-particles in many-body systems. *International Journal of Quantum Chemistry*, 86(3):313–321, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/88510569/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88510569/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88510569&PLACEBO=IE.pdf`. See [BA01].

Burrows:2002:WPS

[BA02b] B. L. Burrows and A. T. Amos. Wavepacket propagation in simple molecular systems. *International Journal of Quantum Chemistry*, 87(2):68–80, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89010613/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89010613/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89010613&PLACEBO=IE.pdf`.

Boens:2006:CMI

[BA06] Noël Boens and Marcel Ameloot. Compartmental modeling and identifiability analysis in photophysics: Review. *International Journal of Quantum Chemistry*, 106(1):300–315, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burrows:2007:TCT

[BA07] B. L. Burrows and A. T. Amos. The theory of currents through small bridge molecules. *International Journal of Quantum Chemistry*, 107(10):1954–1969, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borges:2009:EES

[BABL09] Itamar Borges, Jr., Adélia J. A. Aquino, Mario Barbatti, and Hans Lischka. The electronically excited states of RDX (hexahydro-1,3,5-trinitro-1,3,5-triazine): Vertical excitations. *International Journal of Quantum Chemistry*, 109(11):2348–2355, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bader:2003:LEQ

[Bad03] R. F. W. Bader. Letter to the editor: Quantum mechanics, or orbitals? *International Journal of Quantum Chemistry*, 94 (3):173–177, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brasil:2008:CST

[BAG+08] Davi S. B. Brasil, Cláudio N. Alves, Giselle M. S. P. Guilhon, Adolfo H. Muller, Ricardo de S. Secco, Gabriel Peris, and Rosa Llusar. Crystal structure and theoretical study of IR and ^{1}H and ^{13}C NMR spectra of cordatin, a natural product with antiulcerogenic activity. *International Journal of Quantum Chemistry*, 108(13):2564–2575, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bharatam:2006:PES

[BAKK06] P. V. Bharatam, Amita, D. Kaur, and P. Senthil Kumar. Potential energy surface of thionylimide. *International Journal of Quantum Chemistry*, 106(5):1237–1249, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bancewicz:2002:SDD

[Ban02] Małgorzata Bancewicz. Spectral density distribution moments of a Hamiltonian of N coupled Morse oscillators: The large-N limit. *International Journal of Quantum Chemistry*, 88 (6):742–749, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Banacky:2005:NSI

[Baň05a] Pavol Baňacký. Nonadiabatic sudden increase of the cooperative kinetic effect at lattice energy stabilization—Microscopic mechanism of superconducting state transition: Model study of MgB_2. *International Journal of Quantum Chemistry*, 101 (2):131–152, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bancewicz:2005:DCF

[Ban05b] Małgorzata Bancewicz. The derivation of the characteristic function and the spectral density distribution of a Hamiltonian of N-coupled Morse oscillators: The large N-limit. *International Journal of Quantum Chemistry*, 102(1):31–37, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barnett:2000:SCA

[Bar00] Michael P. Barnett. Symbolic calculation of auxiliary functions for molecular integrals over Slater orbitals. *International Journal of Quantum Chemistry*, 76(3):464–472, January 20, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000289/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000289/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000289&PLACEBO=IE.pdf`.

Barnett:2003:MII

[Bar03] Michael P. Barnett. Molecular integrals and information processing. *International Journal of Quantum Chemistry*, 95(6): 791–805, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barnett:2006:MMS

[Bar06] Michael P. Barnett. Mathematical methods and symbolic calculation in chemistry and chemical biology—The gathering momentum. *International Journal of Quantum Chemistry*, 106(1):351–354, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bartashevich:2008:CMP

[Bar08] Igor Bartashevich. The connected-moments polynomial approach for Hamiltonian eigenvalues calculation and its application to the one-particle systems. *International Journal of Quantum Chemistry*, 108(2):272–278, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barnett:2009:CCC

[Bar09a] Michael P. Barnett. Chemical calculations and chemicals that might calculate. *International Journal of Quantum Chemistry*, 109(8):1640–1657, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barsberg:2009:ERS

[Bar09b] Søren Barsberg. Evaluation of recent scaling free methods to predict phenol and phenoxyl radical vibrational properties—Guidelines for more complex models of lignin or protein moieties. *International Journal of Quantum Chemistry*, 109(7): 1531–1546, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bauschlicher:2009:CBE

[Bau09] Charles W. Bauschlicher, Jr. Convergence of the binding energy of oxygen on Cu(100): A cautionary tale for computational chemists using periodic bound conditions. *International Journal of Quantum Chemistry*, 109(2):357–361, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Banerjee:2005:GOI

[BAZ05] Arup Banerjee, Jochen Autschbach, and Tom Ziegler. A gauge-origin independent expression for the Verdet constant within the time-dependent density functional theory. *International Journal of Quantum Chemistry*, 101(5):572–578, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bishop:2000:VEV

[BB00] David M. Bishop and Ahmed Bouferguene. Visualization of electronic and vibrational polarizabilities and hyperpolarizabilities. *International Journal of Quantum Chemistry*, 78

(5):348–377, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72001894/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72001894/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72001894&PLACEBO=IE.pdf`.

Boudreaux:2001:SMC

[BB01] Edward A. Boudreaux and Eric Baxter. SCMEH–MO calculations on Cr_2 and Mo_2 molecules. *International Journal of Quantum Chemistry*, 85(4–5):509–513, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bandyopadhyay:2002:LPT

[BB02a] S. K. Bandyopadhyay and K. Bhattacharyya. Logarithmic perturbation theory: A reappraisal. *International Journal of Quantum Chemistry*, 90(1):27–36, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bednarz:2002:FCA

[BB02b] Eugeniusz Bednarz and Mirosław Bylicki. Fast convergent approach for computing atomic resonances. *International Journal of Quantum Chemistry*, 90(3):1021–1030, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boudreaux:2002:QSM

[BB02c] Edward A. Boudreaux and Eric Baxter. QR–SCMEH–MO calculations on NdO and UO. *International Journal of Quantum Chemistry*, 90(2):629–633, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boudreaux:2004:MQS

[BB04] E. A. Boudreaux and E. Baxter. More QR-SCMEH-MO calculations on group VIB transition metal molecules, M_2 (M = Cr, Mo, W, Sg): Valence and valence-core effects. *International Journal of Quantum Chemistry*, 100(6):1170–1178, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [BB05d].

Bacelo:2005:TMP

[BB05a] Daniel E. Bacelo and R. C. Binning, Jr. Theoretical modeling of the peroxide stretch in H_2O_2, F_2O_2, and Fe_2O_4. *International Journal of Quantum Chemistry*, 105(6):740–749, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bandyopadhyay:2005:LPT

[BB05b] S. K. Bandyopadhyay and K. Bhattacharyya. Logarithmic perturbation theory for a spiked oscillator and sum rules. *International Journal of Quantum Chemistry*, 103(1):19–24, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Belkic:2005:FPT

[BB05c] Dževad Belkić and Karen Belkić. Fast Padé transform for optimal quantification of time signals from magnetic resonance spectroscopy. *International Journal of Quantum Chemistry*, 105(5):493–510, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boudreaux:2005:EBB

[BB05d] E. A. Boudreaux and E. Baxter. Erratum: E. A. Boudreaux and E. Baxter, "More QR-SCMEH-MO calculations on group VIB transition metal molecules, M_2 (M = Cr, Mo, W, Sg) valence and valence-core effects," International Journal of Quantum Chemistry (2004) **100**(6) 1170–1178. *International Journal of Quantum Chemistry*, 105(2):199, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [BB04].

Boudreaux:2005:VVC

[BB05e] Edward A. Boudreaux and Eric Baxter. Valence and valence–core interactions in transition-metal diatomic molecules. *International Journal of Quantum Chemistry*, 102(5):866–868, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bandyopadhyay:2006:BDB

[BB06] S. K. Bandyopadhyay and K. Bhattacharyya. Behavior of the Dirichlet boundary for wave functions in a class of singular potentials. *International Journal of Quantum Chemistry*, 106

(2):390–400, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bayrak:2007:AAI

[BB07] O. Bayrak and I. Boztosun. Application of the asymptotic iteration method to the exponential cosine screened Coulomb potential. *International Journal of Quantum Chemistry*, 107 (5):1040–1045, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Binning:2009:DST

[BB09] R. C. Binning, Jr. and Daniel E. Bacelo. A DFT study of two diiron (II) synthetic model compounds and their diiron(III) peroxide oxygenation products. *International Journal of Quantum Chemistry*, 109(15):3533–3540, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bandyopadhyay:2002:EIM

[BBB02] K. Bandyopadhyay, K. Bhattacharyya, and A. K. Bhattacharya. Exploiting the interdependence of maximum entropy parameters in eigenvalue problems. *International Journal of Quantum Chemistry*, 88(6):691–700, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bayrak:2007:EAS

[BBC07] O. Bayrak, I. Boztosun, and H. Ciftci. Exact analytical solutions to the Kratzer potential by the asymptotic iteration method. *International Journal of Quantum Chemistry*, 107 (3):540–544, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borckmans:2004:SBC

[BBD04] P. Borckmans, K. Benyaich, and G. Dewel. Spatial bistability: A chemical idiosyncrasy? *International Journal of Quantum Chemistry*, 98(2):239–247, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bera:2007:SCM

[BBD07a] N. C. Bera, I. Bhattacharyya, and A. K. Das. Spectroscopic constants and molecular properties of rare-gas diatomic

molecule in Lennard-Jones potential: Ab initio and density functional study. *International Journal of Quantum Chemistry*, 107(4):824–831, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bera:2007:TSS

[BBD07b] N. C. Bera, I. Bhattacharyya, and A. K. Das. Theoretical study of spectroscopic constants and molecular properties of rare-gas diatomic cations. *International Journal of Quantum Chemistry*, 107(5):1067–1072, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhattacharyya:2007:TSX

[BBD07c] I. Bhattacharyya, N. C. Bera, and A. K. Das. Theoretical study of XCN^- (X F,Cl) anions. *International Journal of Quantum Chemistry*, 107(3):680–684, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhattacharyya:2008:SSP

[BBD08] I. Bhattacharyya, N. C. Bera, and A. K. Das. Stability, structural properties, and dissociation pathways of silylidyne-amines RSiN and silylidyne-phosphanes RSiP (R = F, Cl). *International Journal of Quantum Chemistry*, 108(3):447–455, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Babin:2006:MDS

[BBDS06] Volodymyr Babin, Jason Baucom, Thomas A. Darden, and Celeste Sagui. Molecular dynamics simulations of polarizable DNA in crystal environment. *International Journal of Quantum Chemistry*, 106(15):3260–3269, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bowler:2000:PMI

[BBG00] D. R. Bowler, I. J. Bush, and M. J. Gillan. Practical methods for ab initio calculations on thousands of atoms. *International Journal of Quantum Chemistry*, 77(5):831–842, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000346/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000346/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000346&PLACEBO=IE.pdf`.

Bakasov:2004:ICP

[BBHQ04] Ayaz Bakasov, Robert Berger, Tae-Kyu Ha, and Martin Quack. Ab initio calculation of parity-violating potential energy hypersurfaces of chiral molecules. *International Journal of Quantum Chemistry*, 99(4):393–407, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bende:2009:SMB

[BBL09] Attila Bende, Ferenc Bogár, and János Ladik. A simple model for the band structure and D.C. conductivity of an infinite CO···HN chain perpendicular to the protein backbone. *International Journal of Quantum Chemistry*, 109(3):612–617, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Blaudeau:2000:AOB

[BBM+00] J.-P. Blaudeau, S. R. Brozell, S. Matsika, Z. Zhang, and R. M. Pitzer. Atomic orbital basis sets for use with effective core potentials. *International Journal of Quantum Chemistry*, 77(2):516–520, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70002210/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70002210/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70002210&PLACEBO=IE.pdf`.

Belavin:2004:MES

[BBO04] V. V. Belavin, L. G. Bulusheva, and A. V. Okotrub. Modifications to the electronic structure of carbon nanotubes with symmetric and random vacancies. *International Journal of Quantum Chemistry*, 96(3):239–246, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bokareva:2008:SDA

[BBPG08] Olga S. Bokareva, Vadim A. Bataev, Vladimir I. Pupyshev, and Igor A. Godunov. Structure and dynamics of acrolein in lowest excited ^{1,3} (n, π *) electronic states: The quantum-chemical study. *International Journal of Quantum Chemistry*, 108(14):2719–2731, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Braunheim:2000:QNN

[BBSS00] Benjamin B. Braunheim, Carey K. Bagdassarian, Vern L. Schramm, and Steven D. Schwartz. Quantum neural networks can predict binding free energies for enzymatic inhibitors. *International Journal of Quantum Chemistry*, 78(3):195–204, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71007688/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71007688/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71007688&PLACEBO=IE.pdf`.

Blice-Baum:2006:CSS

[BBVS+06] Anna Blice-Baum, Aaron Van Dyke, Ian Sigmon, E. Alan Salter, Andrzej Wierzbicki, Y. Pocker, and Greg T. Spyridis. Computational and spectroscopic studies concerning the solvatochromic behavior of 1,3-disubstituted azulenes. *International Journal of Quantum Chemistry*, 106(11):2331–2338, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bracken:2002:EQM

[BČ02] Paul Bracken and Jiri Čížek. Evaluation of quantum mechanical perturbative sums in terms of quadratic surds and their use in the approximation of $\zeta(3)/\pi^3$. *International Journal of Quantum Chemistry*, 90(1):42–53, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bromley:2003:MEB

[BC03] S. T. Bromley and C. R. A. Catlow. Magnetism and energetics of the 4*d* bimetallic cluster Pd_6Ru_6. *International Journal of Quantum Chemistry*, 91(2):270–276, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barnett:2006:MCG

[BC06a] Michael P. Barnett and Joseph F. Capitani. Modular chemical geometry and symbolic calculation. *International Journal of Quantum Chemistry*, 106(1):215–227, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burrows:2006:ESS

[BC06b] B. L. Burrows and M. Cohen. Exact solutions for spherically confined hydrogen-like atoms. *International Journal of Quantum Chemistry*, 106(2):478–484, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:2005:PPX

[BCC05] Erkki Brandas, Rogério Custodio, and Sylvio Canuto. Preface proceedings of the XII Brazilian Symposium of Theoretical Chemistry. *International Journal of Quantum Chemistry*, 103 (5):471, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bertin:2005:HHI

[BCD+05] V. Bertin, A. Cruz, G. Del Angel, M. Castro, and E. Poulain. The H and H_2 interaction with Pd_3Cu, Pd_4, and Cu_4 fcc (111) clusters: A DFT comparative study. *International Journal of Quantum Chemistry*, 102(6):1092–1105, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barrio:2003:DSI

[BCdP03] Laura Barrio, Javier Catalán, and José L. G. de Paz. DFT study of ionization potentials for aza-substituted aromatic rings. *International Journal of Quantum Chemistry*, 91(3): 432–437, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bendito:2008:FKI

[BCEG08] Enrique Bendito, Angeles Carmona, Andres M. Encinas, and Jose M. Gesto. A formula for the Kirchhoff index. *International Journal of Quantum Chemistry*, 108(6):1200–1206, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burrows:2002:TSO

[BCF02] B. L. Burrows, M. Cohen, and T. Feldmann. A theory of shift operators with applications to nonharmonic systems. *International Journal of Quantum Chemistry*, 86(3):245–255, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85513171/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85513171/`

FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85513171&PLACEBO=IE.pdf.

Burrows:2003:CHO

[BCF03] B. L. Burrows, M. Cohen, and Tova Feldmann. Coupled harmonic oscillator systems: Improved algebraic decoupling approach. *International Journal of Quantum Chemistry*, 92 (4):345–354, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bras:2008:CBM

[BCFR08] N. F. Brás, N. M. F. S. A. Cerqueira, P. A. Fernandes, and M. J. Ramos. Carbohydrate-binding modules from family 11: Understanding the binding mode of polysaccharides. *International Journal of Quantum Chemistry*, 108(11):2030–2040, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Banerjee:2009:TDD

[BCG09] Arup Banerjee, Aparna Chakrabarti, and Tapan K. Ghanty. Time-dependent density functional theory calculation of van der Waals coefficient of potassium clusters. *International Journal of Quantum Chemistry*, 109(6):1376–1384, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Blavins:2004:SCS

[BCK04] Joshua J. Blavins, David L. Cooper, and Peter B. Karadakov. Spin-coupled study of addition reactions of singlet dihalocarbenes with ethene. *International Journal of Quantum Chemistry*, 98(5):465–472, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bandrauk:2004:ALE

[BCN04] André D. Bandrauk, Stephane Chelkowski, and Hong Shon Nguyen. Attosecond localization of electrons in molecules. *International Journal of Quantum Chemistry*, 100(6):834–844, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bu:2001:TIC

[BCS01] Yuxiang Bu, Dezhan Chan, and Xinyu Song. Theoretical investigation of the cyclic GaO_2 and GaS_2 molecules

at DFT and correlated wave function levels. *International Journal of Quantum Chemistry*, 81(3):222–231, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76504666/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76504666/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76504666&PLACEBO=IE.pdf`.

Branda:2002:DSE

[BCT+02] M. M. Branda, N. J. Castellani, S. H. Tarulli, O. V. Quinzani, E. J. Baran, and R. H. Contreras. DFT study of electronic structure of saccharin, thiosaccharin, and their respective ions: Effects of metal coordination on thiosaccharinate electronic structure. *International Journal of Quantum Chemistry*, 89 (6):525–534, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barnett:2004:SCC

[BCvzGG04] Michael P. Barnett, Joseph F. Capitani, Joachim von zur Gathen, and Jürgen Gerhard. Symbolic calculation in chemistry: Selected examples. *International Journal of Quantum Chemistry*, 100(2):80–104, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bergonzo:2009:PNE

[BCWS09] Christina Bergonzo, Arthur J. Campbell, Ross C. Walker, and Carlos Simmerling. A partial nudged elastic band implementation for use with large or explicitly solvated systems. *International Journal of Quantum Chemistry*, 109(15):3781–3790, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Benkova:2007:EPF

[BČZ07] Zuzana Benková, Ivan Černušák, and Pavol Zahradník. Electric properties of formaldehyde, thioformaldehyde, urea, formamide, and thioformamide — Post-HF and DFT study. *International Journal of Quantum Chemistry*, 107(11):2133–2152, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burrows:2000:BGF

[BD00] B. L. Burrows and S. G. Davison. Binomial Green functions. *International Journal of Quantum Chemistry*, 78(1): 1–4, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71001661/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71001661/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71001661&PLACEBO=IE.pdf`.

deAlencastro:2001:SIS

[BD01] Ricardo Bicca de Alencastro and Joaquim Delphino Da Motta Neto. Semiempirical INDO/S study on the solvatochromism of merocyanine dyes. *International Journal of Quantum Chemistry*, 85(4–5):529–538, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bertolus:2007:OFR

[BD07] Marjorie Bertolus and Mireille Defranceschi. Optimizing the formula of rare earth-bearing materials: A computational chemistry investigation. *International Journal of Quantum Chemistry*, 107(3):712–721, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bataev:2002:FFS

[BDA+02] Vadim A. Bataev, Eugeniy K. Dolgov, Alexandr V. Abramenkov, Vladimir I. Pupyshev, and Igor A. Godunov. Features of the fluorine-substituted acetaldehydes dynamics in the low-lying electronic states: Quantum mechanical study of the CHF_2CHO molecule lowest excited singlet state. *International Journal of Quantum Chemistry*, 88(4):414–425, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bokarev:2009:MPT

[BDBG09] Sergey I. Bokarev, Evgeny K. Dolgov, Vadim A. Bataev, and Igor A. Godunov. Molecular parameters of tetraatomic carbonyls X_2CO and XYCO (X, Y = H, F, Cl) in the ground and lowest excited electronic states, part 1: A test of ab initio methods. *International Journal of Quantum Chemistry*, 109 (3):569–585, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bunta:2007:SMD

[BDE+07] Juraj Bunta, Martin Dahlberg, Leif Eriksson, Nikolai Korolev, Aatto Laaksonen, Raimo Lohikoski, Alexander Lyubartsev, Miroslav Pinak, and Patric Schyman. Solvating, manipulating, damaging, and repairing DNA in a computer. *International Journal of Quantum Chemistry*, 107(2):279–291, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balint:2001:NAC

[BDG01] Imre Bálint, Gergely Dezs, and Iván Gyémánt. A novel approach for calculating correlation energy based on the two-electron density matrix formalism. *International Journal of Quantum Chemistry*, 84(1):32–38, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84002439/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002439/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002439&PLACEBO=IE.pdf`.

Berthier:2003:SCC

[BDL03] G. Berthier, M. Defranceschi, and C. Le Bris. Shortcomings in computational chemistry. *International Journal of Quantum Chemistry*, 93(3):156–165, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bruhn:2006:LPA

[BDMC06] George Bruhn, Ernest R. Davidson, Istvan Mayer, and Aurora E. Clark. Löwdin population analysis with and without rotational invariance. *International Journal of Quantum Chemistry*, 106(9):2065–2072, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Berthier:2001:SIR

[BDMS01] G. Berthier, M. Defranceschi, R. Montagnani, and O. Salvetti. Simulation of ab initio results for palladium and rhodium clusters by tight-binding calculations. *International Journal of Quantum Chemistry*, 82(1):26–33, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76510761/START; http:`

//www3.interscience.wiley.com/cgi-bin/fulltext/76510761/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76510761&PLACEBO=IE.pdf.

Buchs:2003:DFS

[BDMS03] M. Buchs, C. A. Daul, P. T. Manoharan, and C. W. Schläpfer. Density functional study of nitroprusside: Mechanism of the photochemical formation and deactivation of the metastable states. *International Journal of Quantum Chemistry*, 91(3): 418–431, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balashov:2007:AES

[BE07] Alexander Balashov and Alexandr Yu Ermilov. An alternation of the equilibrium structure symmetry of $\mathrm{Li}[\mathrm{C}_n]_1$ ($n = 7--12$) for different n and the correlation with boundary MO features of isolated hydrocarbons $[\mathrm{C}_n]_1$. *International Journal of Quantum Chemistry*, 107(13):2499–2506, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Beck:2002:ICE

[Bec02] Donald R. Beck. Important correlation effects for the Er^{3+} $4f^{11}{}^4\mathrm{S}_{3/2} \rightarrow {}^4\mathrm{I}_{15/2}$ laser transition energy. *International Journal of Quantum Chemistry*, 90(1):439–444, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Beck:2005:EPP

[Bec05] M. E. Beck. Estimation of physiologically perceived color from TDDFT-derived excitation spectra. *International Journal of Quantum Chemistry*, 101(6):683–689, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Beebe:2009:NML

[Bee09] Nelson H. F. Beebe. A new math library. *International Journal of Quantum Chemistry*, 109(13):3008–3025, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bendazzoli:2001:COE

[BEL01] Gian Luigi Bendazzoli, Stefano Evangelisti, and Thierry Leininger. Convergence of the orbital expansion in a cor-

related system: A test study on positronium. *International Journal of Quantum Chemistry*, 85(3):118–126, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85510866/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85510866/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85510866&PLACEBO=IE.pdf`.

Belyi:2004:FDD

[Bel04] V. V. Belyi. Fluctuation–dissipation–dispersion relations for a time and space nonlocal plasma. *International Journal of Quantum Chemistry*, 98(2):183–190, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Basiuk:2002:BSE

[BEM02] Vladimir A. Basiuk, Alvaro H. Crevenna Escobar, and Héctor M. Montiel Molina. Basis set effects on B3LYP geometries and energies: case study of interstellar reaction $HN{=}{=}CH_2 + {}^{\cdot}C{\equiv}N \rightarrow H_2N{-}C({}^{\cdot})H{-}C{\equiv}N$. *International Journal of Quantum Chemistry*, 87(2):101–109, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/88011404/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88011404/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88011404&PLACEBO=IE.pdf`.

Bendazzoli:2005:VCT

[Ben05] Gian Luigi Bendazzoli. Variational CI techniques for computing dispersion constants. *International Journal of Quantum Chemistry*, 104(1):38–51, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bogomolova:2004:PCM

[BES04] A. Yu. Bogomolova, A. Yu. Ermilov, and A. V. Scherbinin. Potential curves of the Be_2 molecule in cylinder-like cavities. *International Journal of Quantum Chemistry*, 100(4):581–588, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balashov:2008:LMC

[BES08] A. M. Balashov, A. Yu. Ermilov, and A. V. Scherbinin. Lithium mobility in complexes $Li[C_n]_1$ ($n = 5--21$): PES analysis in different stationary points. *International Journal of Quantum Chemistry*, 108(14):2693–2699, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balakina:2007:NCN

[BF07] Marina Yu. Balakina and Olga D. Fominykh. Nonempirical calculations of nonlinear optical properties of *p*-nitroaniline in acetone: Comparison of supermolecule and semicontinuum approaches. *International Journal of Quantum Chemistry*, 107(13):2426–2433, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balakina:2008:QCS

[BF08a] Marina Yu. Balakina and Olga D. Fominykh. The quantum-chemical study of small clusters of organic chromophores: Topological analysis and nonlinear optical properties. *International Journal of Quantum Chemistry*, 108(14):2678–2692, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bruni:2008:TSO

[BF08b] Aline Thais Bruni and Márcia Miguel Castro Ferreira. Theoretical study of omeprazole behavior: Racemization barrier and decomposition reaction. *International Journal of Quantum Chemistry*, 108(6):1097–1106, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burke:2009:CAI

[BF09] Luke A. Burke and Paul J. Fazen. Correlation analysis of the interconversion and nitrogen loss reactions of aryl pentazenes and pentazoles derived from aryl diazonium and azide ions. *International Journal of Quantum Chemistry*, 109(15):3613–3618, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barriuso:2003:DSJ

[BFAM03] M. T. Barriuso, P. García Fernández, J. A. Aramburu, and M. Moreno. DFT study of the Jahn–Teller impurity Rh^{2+}

in octahedral symmetry. *International Journal of Quantum Chemistry*, 91(2):202–207, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borges:2008:SEA

[BFB08] E. Borges, G. G. Ferreira, and J. P. Braga. Structures and energies of Ar_nH_2O ($n = 1--26$) clusters using a nonrigid potential surface: A molecular dynamics simulation. *International Journal of Quantum Chemistry*, 108(13):2523–2529, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borges:2006:CCR

[BFBB06] E. Borges, G. G. Ferreira, J. P. Braga, and J. C. Belchior. Coriolis coupling on the rotational and vibrational energy transfer in H_2O+ Ar collisions: Classical trajectories simulation. *International Journal of Quantum Chemistry*, 106(13): 2643–2649, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bazterra:2004:MGA

[BFF04] Victor E. Bazterra, Marta B. Ferraro, and Julio C. Facelli. Modified genetic algorithm to model crystal structures: III. Determination of crystal structures allowing simultaneous molecular geometry relaxation. *International Journal of Quantum Chemistry*, 96(4):312–320, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balakina:2007:MEO

[BFRB07] Marina Yu. Balakina, Olga D. Fominykh, Federico Rua, and Vicenç Branchadell. Modeling of epoxy oligomers with nonlinear optical chromophores in the main chain: molecular dynamics and quantum chemical study. *International Journal of Quantum Chemistry*, 107(13):2398–2408, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bochicchio:2000:SEF

[BG00a] Roberto C. Bochicchio and Horacio Grinberg. Self-energy fields solutions to the generalized reduced Liouville equation in the perturbative approach. *International Journal of Quantum Chemistry*, 79(5):280–290, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72512623/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72512623/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72512623&PLACEBO=IE.pdf.

Bruna:2000:CES

[BG00b] Pablo J. Bruna and Friedrich Grein. Comparing electron-spin g-tensor results of first-row radicals with those of higher rows. *International Journal of Quantum Chemistry*, 77(1):324–335, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70004274/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004274/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004274&PLACEBO=IE.pdf.

Bruna:2000:ESM

[BG00c] Pablo J. Bruna and Friedrich Grein. The electron-spin magnetic moments (g-factors) of C_2^-, N_2^-, O_2^-, and F_2^- and corresponding M^+ X_2^- radicals (M = alkali metal). *International Journal of Quantum Chemistry*, 76(3):447–457, January 20, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70000287/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000287/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000287&PLACEBO=IE.pdf.

Bochicchio:2002:SEO

[BG02a] Roberto C. Bochicchio and Horacio Grinberg. Self-energy operator and self-energy fields in many-body systems: Liouvillian approach. *International Journal of Quantum Chemistry*, 90(1):148–154, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bruna:2002:THC

[BG02b] Pablo J. Bruna and Friedrich Grein. Trends in hyperfine coupling constants and electron-spin g factors for X diatomics with 1, 3, and 5 valence electrons. *International Journal of Quantum Chemistry*, 90(1):472–481, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ballester:2008:TSH

[BGG08] M. Y. Ballester, Y. O. Guerrero, and J. D. Garrido. Theoretical study of the HS $(v', j' = 1) + O_2$ $(v'' = 0, j'' = 1)$ reaction. *International Journal of Quantum Chemistry*, 108(10):1705–1713, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baccarelli:2008:MAF

[BGGS08] I. Baccarelli, F. A. Gianturco, A. Grandi, and N. Sanna. Metastable anion fragmentations after resonant attachment: Deoxyribosic structures from quantum electron dynamics. *International Journal of Quantum Chemistry*, 108(11):1878–1887, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boyukata:2001:DDN

[BGJJ01] M. Böyükata, Z. B. Güvenç, B. Jackson, and J. Jellinek. Dynamics of the D_2 + Ni(100) collision system: Analysis of the reactive and inelastic channels. *International Journal of Quantum Chemistry*, 84(1):48–57, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84002441/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002441/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002441&PLACEBO=IE.pdf`.

Birkenheuer:2005:MDA

[BGN+05] Uwe Birkenheuer, Aleksei B. Gordienko, Vladimir A. Nasluzov, Monika K. Fuchs-Rohr, and Notker Rösch. Model density approach to the Kohn–Sham problem: Efficient extension of the density fitting technique. *International Journal of Quantum Chemistry*, 102(5):743–761, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boyukata:2001:SRN

[BGÖ+01] M. Böyükata, Z. B. Güvenç, S. Özçelik, P. Durmus, and J. Jellinek. Structure and reactivity of Ni_n $(n = 7--14, 19)$ clusters. *International Journal of Quantum Chemistry*, 84(2):208–215, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502323/START;`

http://www3.interscience.wiley.com/cgi-bin/fulltext/84502323/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502323&PLACEBO=IE.pdf.

Bernardi:2006:TSW

[BGP+06] R. C. Bernardi, D. E. B. Gomes, P. G. Pascutti, A. S. Ito, and A. T. Ota. Theoretical studies on water–tetracaine interaction. *International Journal of Quantum Chemistry*, 106 (5):1277–1282, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bernardi:2007:WSL

[BGP+07] R. C. Bernardi, D. E. B. Gomes, P. G. Pascutti, A. S. Ito, C. A. Taft, and A. T. Ota. Water solvent and local anesthetics: A computational study. *International Journal of Quantum Chemistry*, 107(7):1642–1649, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barnett:2003:LCA

[BH03] Michael P. Barnett and James Harrison. Leland Cullen Allen. *International Journal of Quantum Chemistry*, 95(6):659–662, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bartha:2006:DFC

[BHG+06] F. Bartha, I. A. Howard, P. Geerlings, C. Van Alsenoy, D. Vanderzande, T. J. Cleij, and F. Bogár. Density functional crystal orbital study of cyano-substituted poly(paraphenylene-vinylene) and poly(quinoxaline-vinylene). *International Journal of Quantum Chemistry*, 106(8):1912–1923, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bullins:2009:TIF

[BHK09] Kenneth W. Bullins, Thomas T. S. Huang, and Scott J. Kirkby. Theoretical investigation of the formation of the tropylium ion from the toluene radical cation. *International Journal of Quantum Chemistry*, 109(6):1322–1327, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Billing:2001:RSW

[Bil01] G. D. Billing. Reactive scattering within a time-dependent discrete variable representation. *International Journal of Quantum Chemistry*, 84(5):467–478, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/82003577/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/82003577/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=82003577&PLACEBO=IE.pdf`.

Belyaev:2007:PFI

[BIP+07] A. K. Belyaev, V. K. Ivanov, R. G. Polozkov, A. S. Tiukanov, A. V. Solovyov, and W. Greiner. Photoabsorption of the fullerene ions C and C. *International Journal of Quantum Chemistry*, 107(14):2781–2786, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Belmiloud:2000:RVE

[BJ00] D. Belmiloud and M. Jacon. Rotation-vibration energy levels from recent potential energy surfaces for the ground electronic states of NO_2 and H_2 O. *International Journal of Quantum Chemistry*, 76(4):535–540, February 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000685/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000685/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000685&PLACEBO=IE.pdf`.

Briones-Jurado:2008:PRN

[BJAV08] Claudia Briones-Jurado and Esther Agacino-Valdés. On the possible removal of nitrogen monoxide and carbon monoxide on copper ion-exchanged montmorillonite: A DFT study. *International Journal of Quantum Chemistry*, 108(10):1802–1809, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bast:2009:RAT

[BJS09] Radovan Bast, Hans Jørgen Aa. Jensen, and Trond Saue. Relativistic adiabatic time-dependent density functional theory using hybrid functionals and noncollinear spin magnetization.

International Journal of Quantum Chemistry, 109(10):2091–2112, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bittner:2003:ERD

[BK03] Eric R. Bittner and Stoyan Karabunarliev. Energy relaxation dynamics and universal scaling laws in organic light-emitting diodes. *International Journal of Quantum Chemistry*, 95(4–5):521–531, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baranovski:2004:NME

[BK04a] V. I. Baranovski and D. V. Korolkov. New model of the electronic structure of the $[Mo_6X_8\ (CN)_6]^{6-}$ clusters (X = S, Se) based on the study of electron density distribution in the inner part of the Mo_6 polyhedron. *International Journal of Quantum Chemistry*, 100(4):343–351, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Basiuk:2004:DSH

[BK04b] Vladimir A. Basiuk and Kensei Kobayashi. DFT study of HCN and N C C N reactions with hydrogen species. *International Journal of Quantum Chemistry*, 99(2):91–101, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Basiuk:2004:FIV

[BK04c] Vladimir A. Basiuk and Kensei Kobayashi. Formation of interstellar vinyl alcohol via simple radical processes: Theoretical study. *International Journal of Quantum Chemistry*, 97 (2):713–718, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boman:2009:CCR

[BK09] Linus Boman and Henrik Koch. Coupled cluster response theory in parameter subspaces. *International Journal of Quantum Chemistry*, 109(4):708–716, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandell:2000:COA

[BKAT00] D. Brandell, M. Klintenberg, A. Aabloo, and J. O. Thomas. Calculation of the optical absorption spec-

trum of $ErCl_3$ in poly(ethylene oxide) (PEO). *International Journal of Quantum Chemistry*, 80(4–5):799–806, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505368/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505368/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505368&PLACEBO=IE.pdf.

Benkova:2002:RCO

[BKGF02] Zuzana Benkova, Juraj Kóňa, Gudrun Gann, and Walter M. F. Fabian. Redox chemistry of organoselenium compounds: Ab initio and density functional theory calculations on model systems for transition states and intermediates of the redox cycle of selenoenzymes. *International Journal of Quantum Chemistry*, 90(2):555–565, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bonacic-Koutecky:2001:TEU

[BKHPvD01] V. Bonačić-Koutecký, Michael Hartmann, Jiří Pittner, and Huub van Dam. Theoretical exploration of ultrafast spectroscopy of small clusters. *International Journal of Quantum Chemistry*, 84(6):714–739, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/84502391/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502391/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502391&PLACEBO=IE.pdf.

Babic:2002:RDM

[BKL+02] D. Babić, D. J. Klein, I. Lukovits, S. Nikolić, and N. Trinajstić. Resistance-distance matrix: A computational algorithm and its application. *International Journal of Quantum Chemistry*, 90(1):166–176, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barysz:2006:SHH

[BKLB06] Maria Barysz, Dariusz Kłodziera, Jerzy Leszczyński, and Aleksander Bilewicz. Structure and hydrolysis of the heavy alkaline earth cations: Relativistic studies. *International Journal of Quantum Chemistry*, 106(12):2422–2427, ???? 2006.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bonatsos:2002:DSE

[BKM+02a] D. Bonatsos, A. I. Kuleff, J. Maruani, P. P. Raychev, and P. A. Terziev. Derivation of shell effects and magic numbers in metal clusters by the application of Strutinsky's method to the Clemenger–Nilsson and q-deformed 3-D harmonic oscillator models. *International Journal of Quantum Chemistry*, 89 (4):377–388, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bors:2002:MAP

[BKM+02b] Wolf Bors, Snjezana P. Kazazic, Christa Michel, Vessela D. Kortenska, Kurt Stettmaier, and Leo Klasinc. Methoxyphenols—antioxidant principles in food plants and spices: Pulse radiolysis, EPR spectroscopy, and density functional theory calculations. *International Journal of Quantum Chemistry*, 90(2):969–979, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boese:2005:AVD

[BKM05] A. Daniel Boese, Wim Klopper, and Jan M. L. Martin. Assessment of various density functionals and basis sets for the calculation of molecular anharmonic force fields. *International Journal of Quantum Chemistry*, 104(5):830–845, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Babin:2009:ABM

[BKM+09] Volodymyr Babin, Vadzim Karpusenka, Mahmoud Moradi, Christopher Roland, and Celeste Sagui. Adaptively biased molecular dynamics: An umbrella sampling method with a time-dependent potential. *International Journal of Quantum Chemistry*, 109(15):3666–3678, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bonacic-Koutecky:2004:TAS

[BKMHP04] V. Bonačić-Koutecký, R. Mitrić, M. Hartmann, and J. Pittner. Theoretical approach for simulation of femtosecond spectra: New strategies for optimal control of complex systems. *International Journal of Quantum Chemistry*, 99(4):408–420,

???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bende:2003:BFD

[BKMS03] A. Bende, M. Knapp-Mohammady, and S. Suhai. BSSE-free description of intermolecular force constants in hydrogen fluoride and water dimers. *International Journal of Quantum Chemistry*, 92(2):152–159, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bonatsos:2003:MSR

[BKRT03] Dennis Bonatsos, B. A. Kotsos, P. P. Raychev, and P. A. Terziev. Molecular spectra from rotationally invariant Hamiltonians based on the quantum algebra su_q (2) and irreducible tensor operators under su_q (2). *International Journal of Quantum Chemistry*, 95(1):1–20, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Batista:2002:IPC

[BL02a] Hélcio J. Batista and Ricardo L. Longo. Improved point-charge model within the INDO/S-CI method for describing the ligand excited states of lanthanide coordination compounds. *International Journal of Quantum Chemistry*, 90 (2):924–932, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Berski:2002:CLH

[BL02b] Sławomir Berski and Zdzisław Latajka. Comparison of lithium and hydrogen bonds in $(\mathrm{X}\cdots\mathrm{Li}\cdots\mathrm{X})^-$ and $(\mathrm{X}\cdots\mathrm{H}\cdots\mathrm{X})^-$ (X F, Cl and Br) complexes: Topological analysis of electron localization function. *International Journal of Quantum Chemistry*, 90(3):1108–1120, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Blomgren:2002:UBH

[BL02c] Fredrik Blomgren and Sven Larsson. Using 1,3-butadiene and 1,3,5-hexatriene to model the *cis-trans* isomerization of retinal, the chromophore in the visual pigment rhodopsin. *International Journal of Quantum Chemistry*, 90(4-5):1536–1546, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bandrauk:2004:HGM

[BL04a] André D. Bandrauk and Huizhong Lu. Harmonic generation by molecules in intense laser and magnetic fields: Orientation effects. *International Journal of Quantum Chemistry*, 99 (4):431–438, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baranovski:2004:EST

[BL04b] V. I. Baranovski and O. O. Lubimova. Excited states of transition metal compounds: Quantum chemistry of relaxation effects. *International Journal of Quantum Chemistry*, 96(2):116–122, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bi:2004:TSM

[BL04c] Siwei Bi and Chengbu Liu. Theoretical study of magnetic coupling interaction in terephthalato-bridged Ni(II) binuclear systems. *International Journal of Quantum Chemistry*, 97 (3):802–807, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bogar:2004:CCB

[BL04d] F. Bogar and J. Ladik. Correlation corrected band structures of homopolypeptides v. B3LYP band structures of 19 homopolypeptides. *International Journal of Quantum Chemistry*, 99(1):47–52, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bassani:2000:OIJ

[BLA00] F. Bassani, G. C. La Rocca, and V. M. Agranovich. Organic-inorganic junctions and microcavities: New effects and applications. *International Journal of Quantum Chemistry*, 77 (6):973–981, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000979/START;` `http://www3.interscience.wiley.com/cgi-bin/fulltext/71000979/FILE?TPL=ftx_start;` `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000979&PLACEBO=IE.pdf`.

Binning:2000:DFC

[BLC+00] R. C. Binning, Jr., Meng-Sheng Liao, Carlos R. Cabrera, Yasuyuki Ishikawa, Hakim Iddir, Renxuan Liu, E. S. Smotkin, Antonio J. Aldykiewicz, Jr., and Deborah J. Myers. Density functional calculations on CO attached to Pt_n $Ru_{(10-n)}$ ($n = 6--10$) clusters. *International Journal of Quantum Chemistry*, 77(2):589–598, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70002209/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70002209/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70002209&PLACEBO=IE.pdf`.

Badasyan:2009:IRN

[BLC09] Artem Badasyan, Zhirong Liu, and Hue Sun Chan. Interplaying roles of native topology and chain length in marginally cooperative and noncooperative folding of small protein fragments. *International Journal of Quantum Chemistry*, 109(14): 3482–3499, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Blinder:2002:SSE

[Bli02] S. M. Blinder. Structure and self-energy of the electron. *International Journal of Quantum Chemistry*, 90(1):144–147, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bunge:2000:VIN

[BLKJ00] Carlos F. Bunge, Eugenio Ley-Koo, and Rocio Jáuregui. Variational incorporation of negative-energy orbitals in relativistic electronic structure calculations. *International Journal of Quantum Chemistry*, 80(3):461–470, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501011/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501011/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501011&PLACEBO=IE.pdf`.

Brescansin:2008:CSL

[BLM08] L. M. Brescansin, M.-T. Lee, and L. E. Machado. A comparative study on low-energy elastic electron-NH_x ($x = 1, 2, 3$)

collisions. *International Journal of Quantum Chemistry*, 108 (13):2312–2317, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bonatsos:2002:SDH

[BLRT02] Dennis Bonatsos, D. Lenis, P. P. Raychev, and P. A. Terziev. Supershells in deformed harmonic oscillators and atomic clusters. *International Journal of Quantum Chemistry*, 89(4):299–312, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bi:2002:SMM

[BLZ02] Siwei Bi, Chengbu Liu, and Changqiao Zhang. Structural modeling and magnetostructural correlations for heterobinuclear Cu(II)–Ni(II) complex. *International Journal of Quantum Chemistry*, 88(3):347–354, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bader:2001:PAC

[BM01a] Richard F. W. Bader and Chérif F. Matta. Properties of atoms in crystals: Dielectric polarization. *International Journal of Quantum Chemistry*, 85(4–5):592–607, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baer:2001:QIN

[BM01b] Michael Baer and Alexander M. Mebel. Quantization of the ab initio nonadiabatic coupling matrix: The C_2H molecule as a case study. *International Journal of Quantum Chemistry*, 85 (4–5):315–326, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burewicz:2002:CVT

[BM02] Andrzej Burewicz and Nikodem Miranowicz. Categorization of visualization tools in aspects of chemical research and education. *International Journal of Quantum Chemistry*, 88(5): 549–563, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Benton:2004:CSE

[BM04] Christopher W. Benton and David H. Magers. Conventional strain energy in the oxadiazetidines. *International Journal of Quantum Chemistry*, 100(5):788–800, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bordoni:2007:SCM

[BM07a] Andrea Bordoni and Nicola Manini. Systematic calculation of molecular vibrational spectra through a complete Morse expansion. *International Journal of Quantum Chemistry*, 107 (4):782–797, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bromley:2007:CPW

[BM07b] M. W. J. Bromley and J. Mitroy. Convergence of the partial wave expansion of the He ground state. *International Journal of Quantum Chemistry*, 107(5):1150–1161, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baer:2002:CES

[BMB02a] Michael Baer, Alexander M. Mebel, and Gert D. Billing. Curl equations as substratum for the derivation of the electronic nonadiabatic coupling terms. *International Journal of Quantum Chemistry*, 90(6):1577–1585, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bittner:2002:RQH

[BMB02b] Eric R. Bittner, Jeremy B. Maddox, and Irene Burghardt. Relaxation of quantum hydrodynamic modes. *International Journal of Quantum Chemistry*, 89(4):313–321, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barea:2001:ULB

[BML01] Guada Barea, Feliu Maseras, and Agustí Lledós. Unexpectedly large basis set effects on the binding of O_2 to heme complexes. *International Journal of Quantum Chemistry*, 85(2):100–108, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85008794/START;` `http://www3.interscience.wiley.com/cgi-bin/fulltext/85008794/FILE?TPL=ftx_start;` `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85008794&PLACEBO=IE.pdf`.

Bacchus-Montabonel:2007:CCT

[BMŁT07] M. C. Bacchus-Montabonel, M. Łabuda, and Y. S. Tergiman. Comparison of charge transfer recombination of ($3s^2$ 3p) third row S^{3+} and P^{2+} ions with H. *International Journal of Quantum Chemistry*, 107(14):2672–2678, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brasil:2006:TES

[BMMA06] D. S. B. Brasil, R. Y. O. Moreira, A. H. Müller, and C. N. Alves. Theoretical and experimental study of aparisthman: A natural product with anti-ulcer activity. *International Journal of Quantum Chemistry*, 106(13):2706–2713, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Byrd:2009:ESL

[BMMC09a] Jason N. Byrd, John A. Montgomery, Jr., H. Harvey Michels, and Robin Côté. Electronic structure of the Li_2 [$X\,^1\Sigma$] Li [^{2} p] excited $^2A''$ surface. *International Journal of Quantum Chemistry*, 109(15):3626–3631, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Byrd:2009:PES

[BMMC09b] Jason N. Byrd, John A. Montgomery, Jr., H. Harvey Michels, and Robin Côté. Potential energy surface of the $1^2A\prime$ Li_2 + Li doublet ground state. *International Journal of Quantum Chemistry*, 109(13):3112–3119, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burghardt:2004:QHM

[BMP+04] Irene Burghardt, Klaus B. Møller, Gérard Parlant, Lorenz S. Cederbaum, and Eric R. Bittner. Quantum hydrodynamics: Mixed states, dissipation, and a new hybrid quantum-classical approach. *International Journal of Quantum Chemistry*, 100 (6):1153–1162, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borota:2007:CAS

[BMR+07] Ana Borota, Maria Mracec, Ramona Rad, Liliana Ostopovici, and Mircea Mracec. Conformational analysis for some non-classical antagonists of histamine H3 receptor. *International*

Journal of Quantum Chemistry, 107(8):1803–1813, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bredenberg:2001:MZS

[BN01] Johan Bredenberg and Lennart Nilsson. Modeling zinc sulfhydryl bonds in zinc fingers. *International Journal of Quantum Chemistry*, 83(3-4):230–244, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002596/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002596/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002596&PLACEBO=IE.pdf`.

Baer:2003:IEC

[BN03] Roi Baer and Daniel Neuhauser. Ab initio electrical conductance of a molecular wire. *International Journal of Quantum Chemistry*, 91(3):524–532, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barbosa:2004:GSB

[BN04] André Gustavo Horta Barbosa and Marco Antonio Chaer Nascimento. Ground state of the beryllium atom: Reinvestigation based on a proper independent particle model. *International Journal of Quantum Chemistry*, 99(4):317–324, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balakina:2006:SEG

[BN06] Marina Yu. Balakina and Sergey E. Nefediev. Solvent effect on geometry and nonlinear optical response of conjugated organic molecules. *International Journal of Quantum Chemistry*, 106 (10):2245–2253, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bergara:2003:FIA

[BNA03] A. Bergara, J. B. Neaton, and N. W. Ashcroft. Ferromagnetic instabilities in atomically thin lithium and sodium wires. *International Journal of Quantum Chemistry*, 91(2):239–244, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barnett-Norris:2002:AAT

[BNHB+02] Judy Barnett-Norris, Dow P. Hurst, Kurt Buehner, Juan A. Ballesteros, Frank Guarnieri, and Patricia H. Reggio. Agonist alkyl tail interaction with cannabinoid CB1 receptor V6.43/I6.46 groove induces a helix 6 active conformation. *International Journal of Quantum Chemistry*, 88(1):76–86, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89013458/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89013458/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89013458&PLACEBO=IE.pdf`.

Berente:2005:EDS

[BNS05] Imre Berente and Gábor Náray-Szabó. Energy decomposition scheme for combined ab initio quantum mechanical /molecular mechanical methods. *International Journal of Quantum Chemistry*, 104(3):328–334, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boettger:2003:SPF

[Boe03] Jonathan Carl Boettger. Spin-polarized fully relativistic linear combinations of Gaussian-type orbitals calculations for *fcc* plutonium. *International Journal of Quantum Chemistry*, 95 (4–5):380–386, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boettger:2004:INT

[Boe04] Jonathan C. Boettger. Impact of neglecting p-type spin–orbit coupling during electronic structure calculations on solids. *International Journal of Quantum Chemistry*, 100(6):845–850, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boettger:2007:FPE

[Boe07] Jonathan C. Boettger. First principles electronic structure and band gap pressure coefficient for cadmium-oxide. *International Journal of Quantum Chemistry*, 107(15):2988–2994, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boettger:2009:TZT

[Boe09] Jonathan C. Boettger. Theoretical zero-temperature isotherm and structural phase stability of thorium dioxide. *International Journal of Quantum Chemistry*, 109(15):3564–3569, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bofill:2003:RUH

[Bof03] Josep Maria Bofill. Remarks on the updated Hessian matrix methods. *International Journal of Quantum Chemistry*, 94 (6):324–332, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bohr:2001:QMP

[Boh01] Jakob Bohr. Quantum mode phonon forces between chain molecules. *International Journal of Quantum Chemistry*, 84(2):249–252, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502324/START;` `http://www3.interscience.wiley.com/cgi-bin/fulltext/84502324/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502324&PLACEBO=IE.pdf`.

Bohr:2003:PFC

[Boh03] Jakob Bohr. Phonon forces and cold denaturation. *International Journal of Quantum Chemistry*, 92(2):118–122, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bolton:2004:SQM

[Bol04] Kim Bolton. Semiempirical QM/MM method for studying HCl adsorption on ice. *International Journal of Quantum Chemistry*, 96(6):607–614, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borstnik:2000:IST

[Bor00] B. Borštnik. From interactions to structures and thermodynamic properties. *International Journal of Quantum Chemistry*, 80(3):416–424, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501024/`

START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501024/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501024&PLACEBO=IE.pdf.

Borges:2008:CCD

[Bor08] Itamar Borges, Jr. Conformations and charge distributions of diazocyclopropanes. *International Journal of Quantum Chemistry*, 108(13):2615–2622, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boudreaux:2001:MOS

[Bou01] Edward A. Boudreaux. Molecular orbital studies relating to potential anticancer activity of *cis*-platinum ammines. *International Journal of Quantum Chemistry*, 83(3-4):255–258, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/80002589/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002589/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002589&PLACEBO=IE.pdf.

Bour:2003:CNC

[Bou03] Petr Bouř. Calculation of NMR chemical shifts for taxol and α-pinene within the generalized gradient approximation. *International Journal of Quantum Chemistry*, 91(3):277–283, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brook:2001:SHF

[BOW+01] R. Glenn Brook, Paul E. Oppenheimer, Charles A. Weatherford, Ioana Banicescu, and Jianping Zhu. Solving the hydrodynamic formulation of quantum mechanics: A parallel MLS method. *International Journal of Quantum Chemistry*, 85(4–5):263–271, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baruah:2003:DFS

[BP03] Tunna Baruah and Mark R. Pederson. Density functional study of the conformers of Co_4-based single-molecule magnet. *International Journal of Quantum Chemistry*, 93(5):324–331, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Berman:2004:RTP

[BP04] Lihu Berman and Uri Peskin. Resonant tunneling probabilities for an N-terminal junction by the flux averaging method. *International Journal of Quantum Chemistry*, 99(5):752–757, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bartolotti:2001:QMS

[BPM01] L. J. Bartolotti, L. G. Pedersen, and T. J. Meyer. Quantum mechanical study of the oxidation pathway of the oxygen-evolving catalyst, $[(\mathrm{bpy})_2\ (\mathrm{H_2O})\mathrm{Ru}^{III}\text{-O-}\mathrm{Ru}^{III}\ (\mathrm{H_2O})(\mathrm{bpy})_2]^{+4}$. *International Journal of Quantum Chemistry*, 83(3-4):143–149, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/80002591/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002591/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002591&PLACEBO=IE.pdf.

Burcl:2000:BQB

[BPŠB00] R. Burcl, P. Piecuch, V. Špirko, and O. Bludský. Bound and quasi-bound states of the Li FH van der Waals molecule. *International Journal of Quantum Chemistry*, 80(4–5):916–933, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505371/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505371/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505371&PLACEBO=IE.pdf.

Boettger:2000:AEL

[BR00] J. C. Boettger and A. K. Ray. All-electron LCGTO calculations for uranium dioxide. *International Journal of Quantum Chemistry*, 80(4–5):824–830, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505369/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505369/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505369&PLACEBO=IE.pdf.

Boettger:2002:FRD

[BR02] J. C. Boettger and A. K. Ray. Fully relativistic density functional calculations on hydroxylated actinide oxide surfaces. *International Journal of Quantum Chemistry*, 90(4-5):1470–1477, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boettger:2005:RLF

[BR05] Jonathan C. Boettger and Asok K. Ray. Relativistic LCGTO-FF calculations of quantum-size effects in plutonium films. *International Journal of Quantum Chemistry*, 105(6):564–570, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balaban:2008:RSBb

[BR08] Alexandru T. Balaban and Milan Randić. Ring signatures for benzenoids with up to seven rings, Part 2: Pericondensed systems. *International Journal of Quantum Chemistry*, 108 (5):898–926, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [BR12].

Balaban:2012:ERS

[BR12] Alexandru T. Balaban and Milan Randić. Erratum: Ring signatures for benzenoids with up to seven rings, Part 2: Pericondensed systems. *International Journal of Quantum Chemistry*, 112(10):2342, May 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [BR08].

Brandas:2004:TIP

[Brä04a] Erkki Brändas. A tribute to Ilya Prigogine (1917–2003). *International Journal of Quantum Chemistry*, 98(2):59, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:2004:BRa

[Brä04b] Erkki J. Brändas. Book Review. *International Journal of Quantum Chemistry*, 99(1):59, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:2004:BRb

[Brä04c] Erkki J. Brändas. Book review. *International Journal of Quantum Chemistry*, 99(2):115–116, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:2004:QCC

[Brä04d] Erkki J. Brändas. Quantum concepts and complex systems. *International Journal of Quantum Chemistry*, 98(2):78–86, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:2006:STP

[Brä06] Erkki J. Brändas. Some theoretical problems in chemistry and physics. *International Journal of Quantum Chemistry*, 106(14):2836–2839, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bracken:2008:SGP

[Bra08] Paul Bracken. Some geometric properties of quantum phases and calculation of phase formulas. *International Journal of Quantum Chemistry*, 108(9):1528–1532, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:2009:MSO

[Brä09a] Erkki J. Brändas. Microscopic self-organization and self-referential systems: A progress report. *International Journal of Quantum Chemistry*, 109(14):3500–3504, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:2009:TCS

[Brä09b] Erkki J. Brändas. A theorem for complex symmetric matrices revisited. *International Journal of Quantum Chemistry*, 109 (13):2860–2865, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barrientos:2002:IPM

[BRL02] Carmen Barrientos, Pilar Redondo, and Antonio Largo. Ionization and protonation of MgC_3: A theoretical study. *International Journal of Quantum Chemistry*, 86(1):114–121, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85515907/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85515907/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85515907&PLACEBO=IE.pdf.

Broo:2000:TCM

[Bro00] Anders Broo. Theoretical characterization of a multifunctional electrooptical molecular device: Photochemical ring-opening mechanism of indolinospirobenzopyran. *International Journal of Quantum Chemistry*, 77(1):454–467, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70004289/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004289/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004289&PLACEBO=IE.pdf.

Broo:2005:TIM

[Bro05] Anders Broo. Theoretical investigation of the mechanism of the intermolecular proton transfer in carbanion [1.1]ferrocenophane. *International Journal of Quantum Chemistry*, 102 (5):847–857, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brown:2007:PHI

[Bro07] Alex Brown. The photodissociation of hydrogen iodide: Is it adiabatic? *International Journal of Quantum Chemistry*, 107 (14):2665–2671, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bouchy:2004:SEI

[BRR04] Alain Bouchy, Daniel Rinaldi, and Jean-Louis Rivail. Solvent effect on intramolecular hydrogen bonds in push–pull conjugated molecules. *International Journal of Quantum Chemistry*, 96(3):273–281, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brezinski:2009:RVC

[BRZ09] C. Brezinski and M. Redivo-Zaglia. A review of vector convergence acceleration methods, with applications to linear algebra problems. *International Journal of Quantum Chemistry*,

109(8):1631–1639, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bohm:2000:QSA

[BS00] Michael C. Böhm and Christoph Saal. Quantum statistical analysis of superconductivity, fractional quantum Hall effect, and aromaticity. *International Journal of Quantum Chemistry*, 79(3):125–162, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72508371/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72508371/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72508371&PLACEBO=IE.pdf`.

Beregovaya:2002:PES

[BS02] Irina V. Beregovaya and Lyudmila N. Shchegoleva. Potential energy surfaces of fluorobenzene radical anions. *International Journal of Quantum Chemistry*, 88(4):481–488, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bende:2005:BCG

[BS05a] A. Bende and S. Suhai. BSSE-corrected geometry and harmonic and anharmonic vibrational frequencies of formamide–water and formamide–formamide dimers. *International Journal of Quantum Chemistry*, 103(6):841–853, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bohm:2005:SFO

[BS05b] Michael C. Böhm and Joachim Schulte. Superconducting first-order pairing: Finite-temperature simulations. *International Journal of Quantum Chemistry*, 101(4):411–449, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buttiker:2005:IIM

[BS05c] Markus Büttiker and David Sánchez. Interaction-induced magnetic field asymmetry of nonlinear mesoscopic electrical transport. *International Journal of Quantum Chemistry*, 105 (6):906–913, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bouferguene:2006:GBQ

[BS06] Ahmed Bouferguene and Hassan Safouhi. Gauss–Bessel quadrature: A tool for the evaluation of Barnett–Coulson/ Löwdin functions. *International Journal of Quantum Chemistry*, 106(11):2398–2407, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bautista:2008:HFF

[BS08] Eddy J. Bautista and Jorge M. Seminario. Harmonic force field for glycine oligopeptides. *International Journal of Quantum Chemistry*, 108(1):180–188, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borin:2006:TES

[BSAL+06] Antonio Carlos Borin, Luis Serrano-Andrés, Valdemir Ludwig, Kaline Coutinho, and Sylvio Canuto. Theoretical electronic spectra of 2-aminopurine in vapor and in water. *International Journal of Quantum Chemistry*, 106(13):2564–2577, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buzko:2007:IDS

[BSB07] Vladimir Buzko, Igor Sukhno, and Margarita Buzko. Ab initio and DFT study of La^{3+} hydration. *International Journal of Quantum Chemistry*, 107(13):2353–2360, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buzko:2006:IDS

[BSBS06] Vladimir Y. Buzko, Igor V. Sukhno, Margarita B. Buzko, and Julia O. Subbotina. Ab initio and DFT study of Y^{3+} hydration. *International Journal of Quantum Chemistry*, 106(10): 2236–2244, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borowski:2004:FPC

[BSCB04] Tomasz Borowski, Waldemar Szczepanik, Maksymilian Chruszcz, and Ewa Brocławik. First-principle calculations for the active centers in vanadium-containing chloroperoxidase and its functional models: Geometrical and spectral properties. *International Journal of Quantum Chemistry*, 99 (5):864–875, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Berlu:2004:FAE

[BSH04] Lilian Berlu, Hassan Safouhi, and Philip Hoggan. Fast and accurate evaluation of three-center, two-electron Coulomb, hybrid, and three-center nuclear attraction integrals over Slater-type orbitals using the S D transformation. *International Journal of Quantum Chemistry*, 99(4):221–235, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burcl:2002:ICM

[BSK+02] Rudolf Burcl, M. M. Szcześniak, Jacek Kłos, Grzegorz Chałasiński, and Sławomir M. Cybulski. Ab initio calculations and modeling of three-body forces in Ar_2H_2O. *International Journal of Quantum Chemistry*, 90(3):1215–1231, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bora:2007:PMP

[BSKFT07] Alina Bora, E. Seclaman, L. Kurunczi, and Simona Funar-Timofei. A preliminary MTD-PLS study for androgen receptor binding of steroid compounds. *International Journal of Quantum Chemistry*, 107(8):1707–1713, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bokes:2001:ECE

[BŠM01] P. Bokes, I. Štich, and L. Mitas. Electron correlation effects in ionic hydrogen clusters. *International Journal of Quantum Chemistry*, 83(2):86–95, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002391/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002391/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002391&PLACEBO=IE.pdf`.

Bhattacharyya:2007:EAE

[BSM+07] S. Bhattacharyya, A. N. Sil, T. K. Mukherjee, P. K. Mukherjee, and P. Vasu. Electron affinity of exotic systems under Debye plasma. *International Journal of Quantum Chemistry*, 107(4):946–951, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Blaha:2005:EFG

[BSN05] P. Blaha, K. Schwarz, and P. Novák. Electric field gradients in cuprates: Does LDA+U give the correct charge distribution? *International Journal of Quantum Chemistry*, 101 (5):550–556, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bohm:2002:INF

[BSR02] Michael C. Böhm, Joachim Schulte, and Rafael Ramírez. On the influence of nuclear fluctuations on calculated NMR shieldings of benzene and ethylene: a Feynman path integral-ab initio investigation. *International Journal of Quantum Chemistry*, 86(3):280–296, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89010958/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89010958/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89010958&PLACEBO=IE.pdf`.

Brozell:2007:SOI

[BSZ07] Scott R. Brozell, Ron Shepard, and Zhiyong Zhang. Spin–orbit interaction with nonlinear wave functions. *International Journal of Quantum Chemistry*, 107(15):3191–3202, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bencini:2005:DDM

[BT05] Alessandro Bencini and Federico Totti. DFT description of the magnetic structure of polynuclear transition-metal clusters: The complexes [{Cu(bpca)$_2$ (H_2O)$_2$ }{Cu(NO_3)$_2$ }$_2$], (bpca = Bis(2-pyridylcarbonyl)amine), and [Cu(DBSQ)(C_2H_5O)]$_2$, (DBSQ = 3,5-di-tert-butyl-semiquinonato). *International Journal of Quantum Chemistry*, 101(6):819–825, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borgh:2005:CSP

[BTK+05] M. Borgh, M. Toreblad, M. Koskinen, M. Manninen, S. Åberg, and S. M. Reimann. Correlation and spin polarization in quantum dots: Local spin density functional theory revisited. *International Journal of Quantum Chemistry*, 105(6):817–825,

???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boutreau:2002:PIH

[BTL+02] Laurence Boutreau, Jeanine Tortajada, Alberto Luna, Manuel Alcamí, Otilia Mó, and Manuel Yáñez. Perturbation of the intramolecular hydrogen bonds of glucose by Cu^+ association. *International Journal of Quantum Chemistry*, 86(1):138–144, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85011805/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85011805/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85011805&PLACEBO=IE.pdf`.

Bu:2002:BCI

[Bu02] Yuxiang Bu. The bonding character of AlSO isomers in quartet excited states: Ab initio and density functional theory studies. *International Journal of Quantum Chemistry*, 87 (4):181–191, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90011257/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90011257/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90011257&PLACEBO=IE.pdf`.

Buck:2000:OMC

[Buc00a] Henk Buck. Odd-membered C_2v π-cyclic mono- and dications with internal cross-linking. A Hückel approach for the description of antiaromaticity. *International Journal of Quantum Chemistry*, 78(3):179–185, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71007686/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71007686/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71007686&PLACEBO=IE.pdf`.

Buck:2000:SRS

[Buc00b] Henk Buck. Symmetry restrictions as starting point for the determination of geometric representations and the dynamics of cyclicπ systems. *International Journal of*

Quantum Chemistry, 77(3):641–650, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70004059/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004059/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004059&PLACEBO=IE.pdf.

Buck:2001:EAS

[Buc01] Henk Buck. Elementary addition-substitution reactions. Hückel approach for the description of aromatic and antiaromatic arylmethyl cations. *International Journal of Quantum Chemistry*, 81(1):66–75, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/75502162/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75502162/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502162&PLACEBO=IE.pdf.

Buck:2002:CGC

[Buc02a] Henk Buck. Calculated geometries and charge distributions of $4n$ and $4n+2$ π-ring systems linked with $-$CH: An asymmetric versus symmetric π-delocalization. *International Journal of Quantum Chemistry*, 89(5):464–476, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buck:2002:CGD

[Buc02b] Henk Buck. Calculated geometries of dications of bis odd-membered π-ring systems containing a NCN fragment and related π-systems. An opposite out-of-plane rotation of the $4n\pi$-ring subsystems. *International Journal of Quantum Chemistry*, 87(1):37–48, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85515903/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85515903/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85515903&PLACEBO=IE.pdf.

Buck:2004:CEB

[Buc04] Henk Buck. Critical evaluation of the bond order concept with application to thermal hydrogen shifts. *International Journal*

of Quantum Chemistry, 97(3):808–814, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buck:2005:CMH

[Buc05a] Henk Buck. Charge at the migrating hydrogen in the transition state of hydride transfer reactions from CH groups to hydride acceptors. Dynamics of the redox-couple NADH-NAD^+. *International Journal of Quantum Chemistry*, 101 (4):389–395, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buck:2005:DMP

[Buc05b] Henk Buck. Different models for phosphate anion shielding in DNA duplexes: An elaboration with ab initio and molecular mechanics calculations. *International Journal of Quantum Chemistry*, 103(3):308–313, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buck:2005:QCS

[Buc05c] Henk Buck. Quantum chemical study of alternating N/B and N/C π bonds in (un)charged even-membered 4 n and 4 n +2 cyclic systems and their related open systems. *International Journal of Quantum Chemistry*, 101(1):73–83, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buck:2007:TPC

[Buc07] Henk M. Buck. Trigonal pyramidal carbon geometry as model for electrophilic addition–substitution and elimination reactions and its significance in enzymatic processes. *International Journal of Quantum Chemistry*, 107(1):200–211, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buck:2008:CET

[Buc08] Henk M. Buck. A combined experimental, theoretical, and Van't Hoff model study for identity methyl, proton, hydrogen atom, and hydride exchange reactions. Correlation with three-center four-, three-, and two-electron systems. *International Journal of Quantum Chemistry*, 108(9):1601–1614, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Budzinski:2004:ETC

[Bud04] Jan Budziński. Evaluation of two-center, three- and four-electron integrals over Slater-type orbitals in elliptical coordinates. *International Journal of Quantum Chemistry*, 97(4): 832–843, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barreto:2005:TSR

[BVG05a] Patrícia R. P. Barreto, Alessandra F. A. Vilela, and Ricardo Gargano. Theoretical study of the reactions $BF_3 + BX$, where X = H or N. *International Journal of Quantum Chemistry*, 103(5):685–694, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barreto:2005:TMB

[BVG05b] Patrícia R. P. Barreto, Alessandra F. A. Vilela, and Ricardo Gargano. Thermochemistry of molecules in the B/F/H/N system. *International Journal of Quantum Chemistry*, 103 (5):659–684, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bende:2001:BFD

[BVHS01] A. Bende, Á. Vibók, G. J. Halász, and S. Suhai. BSSE-free description of the formamide dimers. *International Journal of Quantum Chemistry*, 84(6):617–622, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/82003606/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/82003606/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=82003606&PLACEBO=IE.pdf`.

Bende:2004:ISA

[BVHS04] A. Bende, Á. Vibók, G. J. Halász, and S. Suhai. Ab initio study of the ammonia–ammonia dimer: BSSE-free structures and intermolecular harmonic vibrational frequencies. *International Journal of Quantum Chemistry*, 99(5):585–593, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bende:2005:TSH

[BVHS05] A. Bende, Á. Vibók, G. J. Halász, and S. Suhai. Theoretical study of hydrogen bonds between acetylene and selected proton donor systems. *International Journal of Quantum Chemistry*, 101(2):186–200, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Broer:2006:MJG

[BvL06a] Ria Broer and Joop van Lenthe. In memory of Jaap G. Snijders (1951–2003). *International Journal of Quantum Chemistry*, 106(12):2410–2411, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Broer:2006:P

[BvL06b] Ria Broer and Joop van Lenthe. Preface. *International Journal of Quantum Chemistry*, 106(12):2409, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bera:2007:PWS

[BvRSS07] Partha P. Bera, Paul v. R. Schleyer, and Henry F. Schaefer III. Periodane: A wealth of structural possibilities revealed by the Kick procedure. *International Journal of Quantum Chemistry*, 107(12):2220–2223, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bakalova:2009:DSS

[BVS+09] Adriana Bakalova, Hristo Varbanov, Stancho Stanchev, Darvin Ivanov, and Frank Jensen. DFT study of the structure and spectral behavior of new pt(II) complexes with 5-methyl-5(4-pyridyl)hydantoin. *International Journal of Quantum Chemistry*, 109(4):826–836, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balescu:2004:ATP

[BVSM04] R. Balescu, M. Vlad, F. Spineanu, and J. Misguich. Anomalous transport in plasmas. *International Journal of Quantum Chemistry*, 98(2):125–130, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boczar:2002:TMI

[BWS+02] Marek Boczar, Marek J. Wójcik, Krzysztof Szczeponek, Dorota Jamróz, and Susumu Ikeda. Theoretical modeling of infrared spectra of salicylaldehyde and its deuterated derivatives. *International Journal of Quantum Chemistry*, 90(2): 689–698, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barrera:2006:DIR

[BZ06] Mauricio Barrera and Fernando Zuloaga. Determination of the ionic radii by means of the Kohn–Sham potential: Identification of the chemical potential. *International Journal of Quantum Chemistry*, 106(9):2044–2053, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bouhlel:2001:TIS

[BZBT01] O. Bouhlel, M. Zina, S. Boughdiri, and B. Tangour. Theoretical ab initio study of NO and CO depollution reaction catalyzed by copper. *International Journal of Quantum Chemistry*, 84(6):623–629, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85008259/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85008259/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85008259&PLACEBO=IE.pdf`.

Berzigiyarov:2002:NPC

[BZG+02] Parvaz K. Berzigiyarov, Valentin A. Zayets, Ilya Ya. Ginzburg, Vladimir F. Razumov, and Elena F. Sheka. NANOPACK: Parallel codes for semiempirical quantum chemical calculations of large systems in the *sp*- and *spd*-basis. *International Journal of Quantum Chemistry*, 88(4): 449–462, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Berzigiyarov:2004:NPC

[BZG+04] Parvaz K. Berzigiyarov, Valentine A. Zayets, Ilya Y. Ginzburg, Vladimir F. Razumov, and Elena F. Sheka. NANOVIBR: Parallel codes for semiempirical quantum chemical and harmonic vibration large-scale calculations. *International Journal of Quantum Chemistry*, 96(2):73–79, ????

2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bing:2007:ISR

[BZH+07] Dan Bing, Yongfang Zhao, Fengyou Hao, Xinying Li, Fengli Liu, Guohua Zhang, and Pingxia Zhang. Ab initio study on the reaction mechanism of ozone with bromine atom. *International Journal of Quantum Chemistry*, 107(5):1085–1091, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bai:2009:CSS

[BZL+09] Fu-Quan Bai, Xin Zhou, Tao Liu, Guang-Jin Zhao, Jian-Po Zhang, and Hong-Xing Zhang. Computational studies on the spectroscopic properties of the 2-pyridylpyrazolate-based platinum(II) complexes with modified pyrazolate fragment. *International Journal of Quantum Chemistry*, 109(2):308–319, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Budyka:2002:CMC

[BZR02] Mikhayl F. Budyka, Tatyana S. Zyubina, and Alexander G. Ryabenko. Computer modeling of C_2 cluster addition to fullerene C_{60}. *International Journal of Quantum Chemistry*, 88(5):652–662, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cafiero:2001:AGS

[CA01] Mauricio Cafiero and Ludwik Adamowicz. Analytical gradients for Singer's multicenter n-electron explicitly correlated Gaussians. *International Journal of Quantum Chemistry*, 82(4):151–159, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/78503195/START;` `http://www3.interscience.wiley.com/cgi-bin/fulltext/78503195/FILE?TPL=ftx_start;` `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=78503195&PLACEBO=IE.pdf`.

Canuto:2006:PPX

[CA06] Sylvio Canuto and Alfredo Arnóbio Da Gama. Preface: Proceedings of the XIII Brazilian Symposium of Theoretical Chemistry. *International Journal of Quantum Chemistry*,

106(13):2551, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cafiero:2007:NBO

[CA07] Mauricio Cafiero and Ludwik Adamowicz. Non-Born–Oppenheimer calculations of the ground state of H_3. *International Journal of Quantum Chemistry*, 107(14):2679–2686, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Campoy:2009:ASS

[CA09] G. Campoy and N. Aquino. Accurate solutions for the spiked oscillators. *International Journal of Quantum Chemistry*, 109 (6):1267–1273, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cabral:2005:VSO

[Cab05] B. J. Costa Cabral. The vibrational structure of the OH radical in solid argon: A transfer-matrix path-integral approach. *International Journal of Quantum Chemistry*, 103 (5):610–616, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cervellera:2008:MDS

[CAHl08] Víctor Rojas Cervellera, Margarita Albertí, and Fermín Huarte-larrañaga. A molecular dynamics simulation of air adsorption in single-walled carbon nanotube bundles. *International Journal of Quantum Chemistry*, 108(10):1714–1720, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Celik:2007:CTP

[ÇAK07] Gültekin Çelik, Erhan Akin, and Hamdi Şükür Kiliç. Comparison of transition probabilities calculated using different parameters on WBEPM theory for some p-d and d-p transitions in excited atomic nitrogen. *International Journal of Quantum Chemistry*, 107(2):495–500, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Caldwell:2002:BRa

[Cal02a] Dennis Caldwell. Book review. *International Journal of Quantum Chemistry*, 87(3):167, ???? 2002. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/90010532/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90010532/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90010532&PLACEBO=IE.pdf.

Caldwell:2002:BRb

[Cal02b] Dennis Caldwell. Book review. *International Journal of Quantum Chemistry*, 87(3):168–169, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/90010531/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90010531/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90010531&PLACEBO=IE.pdf.

Camparo:2004:SPM

[Cam04] James Camparo. Spatial partitioning of the molecular wave function: Reexamination of the bond-charge model of covalent binding. *International Journal of Quantum Chemistry*, 100 (1):41–52, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carsky:2007:EEC

[Čár07] Petr Čársky. Efficient evaluation of Coulomb integrals in a mixed Gaussian and plane-wave basis. *International Journal of Quantum Chemistry*, 107(1):56–62, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carsky:2009:DFD

[Čár09] Petr Čársky. Density fitting for derivatives of Coulomb integrals in ab initio calculations using mixed Gaussian and plane-wave basis. *International Journal of Quantum Chemistry*, 109 (6):1237–1242, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Castro:2000:PDS

[Cas00] Miguel Castro. Panel discussion: on "The status of the theory of chemical reactions," Third CISTCP, Mexico City, November 8–13, 1999. *International Journal*

of Quantum Chemistry, 80(2):80–84, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73001276/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001276/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001276&PLACEBO=IE.pdf.

Catalan:2005:MSP

[Cat05] J. Catalán. On the molecular structure that produces the phosphorescence of 7-azaindole. *International Journal of Quantum Chemistry*, 102(5):489–497, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cernusak:2009:IMC

[ČAV+09] Ivan Černušák, Monika Aranyosiová, Ol'Ga Vollárová, Dušan Velič, Ol'Ga Kirdajová, and Ján Benko. Interaction of monovalent cations with acetonitrile. *International Journal of Quantum Chemistry*, 109(11):2365–2372, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaudhury:2000:SCR

[CB00] Pinaki Chaudhury and S. P. Bhattacharyya. Stochastic construction of reaction paths: A genetic algorithm-based approach. *International Journal of Quantum Chemistry*, 76(2): 161–168, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/69503169/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503169/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503169&PLACEBO=IE.pdf.

Chaudhury:2003:EDS

[CB03] Pinaki Chaudhury and S. P. Bhattacharyya. Evolution of defect states in doped polythiophene: A study based on the method of simulated annealing. *International Journal of Quantum Chemistry*, 91(6):663–674, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Capron:2004:DFT

[CB04] N. Capron and G. Boureau. Density functional theory study of point defects in the Si SiO_2 system and in substoichiometric titanium dioxide TiO_{2-x}. *International Journal of Quantum*

Chemistry, 99(5):677–684, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Canuto:2008:PPX

[CB08] Sylvio Canuto and Carlos E. Bielchowsky. Preface: Proceedings of the XIV Brazilian Symposium of Theoretical Chemistry. *International Journal of Quantum Chemistry*, 108(13): 2305, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carissan:2006:WCW

[CBA+06] Yannick Carissan, Fabienne Bessac, Fabienne Alary, Jean-Louis Heully, and Romuald Poteau. What can we do with an effective group potential? *International Journal of Quantum Chemistry*, 106(3):727–733, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chateauneuf:2001:CSE

[CBB01] Ginger M. Chateauneuf, Richard E. Brown, and Bette Jo Brown. Computational studies of electron-transfer processes in old yellow enzyme. *International Journal of Quantum Chemistry*, 85(6):685–692, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85513172/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85513172/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85513172&PLACEBO=IE.pdf`.

Cruz:2000:TSP

[CBC00] A. Cruz, V. Bertin, and M. Castro. A theoretical study for the Pt_3-ethylene molecule interaction. *International Journal of Quantum Chemistry*, 80(3):298–306, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501008/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501008/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501008&PLACEBO=IE.pdf`.

Carvalho:2008:DSR

[CBMRN08] Edson F. V. Carvalho, Alessandra N. Barauna, Francisco B. C. Machado, and Orlando Roberto-Neto. DFT study for

the reactions of H atoms with CH_3OH and C_2H_5OH. *International Journal of Quantum Chemistry*, 108(13):2476–2485, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Costa:2003:PRN

[CBRBT03] Maria Cristina Andreazza Costa, Lauro Euclides Soares Barata, Bartira Rossi-Bergmann, and Yuji Takahata. Pattern recognition and neural networks applied to structure–activity relationships of neolignans tested against Leishmania amazonensis using quantum chemical and topological descriptors. *International Journal of Quantum Chemistry*, 95(3):295–302, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cui:2009:ISD

[CBWM09] Jun Cui, Keith Battle, Andrzej Wierzbicki, and Jeffry D. Madura. Investigations of structure and dynamics of water solvation of the type I antifreeze protein. *International Journal of Quantum Chemistry*, 109(1):73–80, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Canuto:2000:HBB

[CC00a] Sylvio Canuto and Kaline Coutinho. From hydrogen bond to bulk: Solvation analysis of the n-π * transition of formaldehyde in water. *International Journal of Quantum Chemistry*, 77(1):192–198, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004259/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004259/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004259&PLACEBO=IE.pdf`.

Chen:2000:TSM

[CC00b] P. C. Chen and F. M. Chang. Theoretical study on the molecular structures of toluene, para-fluorotoluene, para-chlorotoluene, and 4-methylpyridine and their six-fold internal rotational barriers. *International Journal of Quantum Chemistry*, 77(4):772–778, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70500251/START; http://www3.interscience.`

wiley.com/cgi-bin/fulltext/70500251/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70500251&PLACEBO=IE.pdf.

Chong:2000:DFC

[CC00c] Delano P. Chong and Germán Cavigliasso. Density functional calculation of core-electron binding energies of isomers of C_3 H_6 O_2 and C_3 H_5 NO. *International Journal of Quantum Chemistry*, 76(1):44–50, January 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/69503194/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503194/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503194&PLACEBO=IE.pdf.

Cassam-Chenai:2001:AFM

[CC01a] P. Cassam-Chenaï. Analytical formulas for the magnetic field produced by a spin or a paramagnetic current density in the case of Gaussian basis functions. *International Journal of Quantum Chemistry*, 81(1):11–15, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/75502169/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75502169/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502169&PLACEBO=IE.pdf.

Chen:2001:TSI

[CC01b] P. C. Chen and S. C. Chen. Theoretical study of the internal rotational barriers in nitrobenzene, 2-nitrotoluene, 2-nitrophenol, and 2-nitroaniline. *International Journal of Quantum Chemistry*, 83(6):332–337, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/81502112/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/81502112/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=81502112&PLACEBO=IE.pdf.

Clementi:2002:HCM

[CC02] E. Clementi and G. Corongiu. HF–CC model for atoms and molecules. *International Journal of Quantum Chemistry*, 90

(4-5):1295–1308, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cavillot:2005:SUV

[CC05a] Valérie Cavillot and Benoît Champagne. Simulation of UV/visible absorption spectra of (α-diimine)nickel(II) catalysts by time-dependent density functional theory. *International Journal of Quantum Chemistry*, 101(6):840–848, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cheng:2005:DFT

[CC05b] Hsiu-Yao Cheng and Shyang Chang. Density functional theory of the iron–nitrosyl ($S = 3/2$) complex. *International Journal of Quantum Chemistry*, 105(5):511–517, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Clementi:2005:CCC

[CC05c] Enrico Clementi and Giorgina Corongiu. Comments on computational chemistry: From diatomic molecules to large biochemical systems. *International Journal of Quantum Chemistry*, 105(6):709–730, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaquin:2007:TSO

[CC07] Patrick Chaquin and Hilaire Chevreau. Theoretical study of one-electron bonds in a series of high-spin lithium–beryllium–hydrogen clusters: "Valence shell single-electron repulsion" rule and electron localization function analysis. *International Journal of Quantum Chemistry*, 107(1):72–80, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Clementi:2008:AMO

[CC08] Enrico Clementi and Giorgina Corongiu. From atomic and molecular orbitals to chemical orbitals. *International Journal of Quantum Chemistry*, 108(10):1758–1771, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chibotaru:2009:BR

[CC09] Liviu F. Chibotaru and Arnout Ceulemans. Book review. *International Journal of Quantum Chemistry*, 109(3):639–640,

???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Champagne:2006:DFT

[CCA+06] Benoît Champagne, Valérie Cavillot, Jean-Marie André, Philippe François, and Ardéchir Momtaz. Density functional theory investigation of the alkylating strength of organoaluminum co-catalysts for Ziegler–Natta polymerization. *International Journal of Quantum Chemistry*, 106(3):588–598, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cours:2007:FPE

[CCB07] T. Cours, S. Canneaux, and F. Bohr. Features of the potential energy surface for the reaction of HO_2 radical with acetone. *International Journal of Quantum Chemistry*, 107(6):1344–1354, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chiodo:2007:CSE

[CCE+07] S. Chiodo, G. N. Chuev, S. E. Erofeeva, M. V. Fedorov, N. Russo, and E. Sicilia. Comparative study of electrostatic solvent response by RISM and PCM methods. *International Journal of Quantum Chemistry*, 107(2):265–274, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cheranovskii:2006:EST

[CCEÖ06] V. O. Cheranovskii, A. A. Chovpan, E. V. Ezerskaya, and I. Özkan. Energy spectrum and thermodynamics of anisotropic spin-1/2 two-leg ladder. *International Journal of Quantum Chemistry*, 106(10):2254–2261, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cardenas:2007:NFF

[CCGF07] Carlos Cárdenas, Eduardo Chamorro, Marcelo Galván, and Patricio Fuentealba. Nuclear Fukui functions from nonintegral electron number calculations. *International Journal of Quantum Chemistry*, 107(4):807–815, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2005:TSR

[CCH05] Shyh-Jong Chen, Cheng Chen, and Yaw-Shun Hong. Theoretical study of reaction channels for the weakly bound complex systems created with HF, CO_2, and various amines. *International Journal of Quantum Chemistry*, 103(2):198–214, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2006:TIT

[CCH06] Shyh-Jong Chen, Cheng Chen, and Yaw-Shun Hong. Theoretical influence of third molecule on reaction channels of weakly bound complex CO_2 ... HF systems. *International Journal of Quantum Chemistry*, 106(7):1640–1652, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cassam-Chenai:2003:APM

[CCL03] P. Cassam-Chenaï and J. Liévin. Alternative perturbation method for the molecular vibration–rotation problem. *International Journal of Quantum Chemistry*, 93(3):245–264, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaos-Cador:2004:CGF

[CCLK04] L. Chaos-Cador and E. Ley-Koo. Common generating functions of complete harmonic oscillator wave functions and transformation brackets in D dimensions. *International Journal of Quantum Chemistry*, 97(4):844–853, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaos-Cador:2005:TDH

[CCLK05] L. Chaos-Cador and E. Ley-Koo. Two-dimensional hydrogen atom confined in circles, angles, and circular sectors. *International Journal of Quantum Chemistry*, 103(4):369–387, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaos-Cador:2007:CGF

[CCLK07] L. Chaos-Cador and E. Ley-Koo. Common generating function for two-dimensional hydrogen atom complete wave functions. *International Journal of Quantum Chemistry*, 107(1):

12–22, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cappelli:2005:ILD

[CCM+05] Chiara Cappelli, Stefano Corni, Benedetta Mennucci, Jacopo Tomasi, and Roberto Cammi. Infrared linear dichroism in stretched films: Quantum mechanical approach within the polarizable continuum model. *International Journal of Quantum Chemistry*, 104(5):716–726, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Charro:2008:SRD

[CCM08] E. Charro, Z. Curiel, and I. Martín. Spontaneous radiative decay rates in Ga-like ions. *International Journal of Quantum Chemistry*, 108(4):744–753, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cedillo:2000:AMP

[CCP00] Andrés Cedillo, Pratim K. Chattaraj, and Robert G. Parr. Atoms-in-molecules partitioning of a molecular density. *International Journal of Quantum Chemistry*, 77(1):403–407, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004284/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004284/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004284&PLACEBO=IE.pdf`.

Cruz:2009:SCS

[CCR09] Salvador A. Cruz and Ricardo Colín-Rodríguez. Spheroidal confinement of a single electron and of the hydrogen atom, the H and HeH^{++} molecular ions with arbitrary nuclear positions along the major axis. *International Journal of Quantum Chemistry*, 109(13):3041–3054, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cicero:2007:SOH

[CCV+07] Giancarlo Cicero, Chiara Carbonera, Karin Valegård, Janos Hajdu, Inger Andersson, and Graziella Ranghino. Study of the oxidative half-reaction catalyzed by a non-heme ferrous catalytic center by means of structural and computational methodologies. *International Journal of Quantum Chemistry*,

107(6):1514–1522, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carbo-Dorca:2000:STQ

[CD00] Ramon Carbó-Dorca. Stochastic transformation of quantum similarity matrices and their use in quantum QSAR (QQSAR) models. *International Journal of Quantum Chemistry*, 79 (3):163–177, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72508370/START;` `http://www3.interscience.wiley.com/cgi-bin/fulltext/72508370/FILE?TPL=ftx_start;` `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72508370&PLACEBO=IE.pdf`.

Carbo-Dorca:2003:AIM

[CD03a] Ramon Carbó-Dorca. Applications of inward matrix products and matrix wave functions to Hückel MO theory, Slater extended wave functions, spin extended functions, and Hartree method. *International Journal of Quantum Chemistry*, 91 (5):607–617, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Clark:2003:PAU

[CD03b] Aurora E. Clark and Ernest R. Davidson. Population analyses that utilize projection operators. *International Journal of Quantum Chemistry*, 93(6):384–394, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carbo-Dorca:2004:DVW

[CD04] Ramon Carbó-Dorca. Discussion on the variable Wolfsberg–Helmholtz parameter, a new simplified Löwdin transformation and the characteristic structure of the transformed EHT Hamiltonian matrices. *International Journal of Quantum Chemistry*, 98(1):26–32, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carbo-Dorca:2002:FQQ

[CDB02] Ramon Carbó-Dorca and Emili Besalú. Fundamental quantum QSAR (Q^2 SAR) equation: extensions, nonlinear terms, and generalizations within extended Hilbert-Sobolev spaces. *International Journal of Quantum Chemistry*, 88(1):167–182, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/89013453/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89013453/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89013453&PLACEBO=IE.pdf.

Corni:2005:REP

[CDDM05] Stefano Corni, Francesca De Rienzo, Rosa Di Felice, and Elisa Molinari. Role of the electronic properties of azurin active site in the electron-transfer process. *International Journal of Quantum Chemistry*, 102(3):328–342, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cundari:2000:PTP

[CDF00] Thomas R. Cundari, Jun Deng, and Wentao Fu. PM3(tm) parameterization using genetic algorithms. *International Journal of Quantum Chemistry*, 77(1):421–432, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70004286/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004286/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004286&PLACEBO=IE.pdf.

Castet:2006:OSD

[CDF06] Frédéric Castet, Laurent Ducasse, and Alain Fritsch. From organic superconductors to DNA: Fragment orbital-based model. *International Journal of Quantum Chemistry*, 106 (3):734–746, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carbo-Dorca:2005:FQS

[CDG05] Ramon Carbó-Dorca and Xavier Gironés. Foundation of quantum similarity measures and their relationship to QSPR: Density function structure, approximations, and application examples. *International Journal of Quantum Chemistry*, 101(1): 8–20, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carbo-Dorca:2009:EVA

[CDG09] Ramon Carbó-Dorca and Ana Gallegos. Expectation value averages of size consistent Hermitian operators and the definition of Fukui functions. *International Journal of Quantum*

Chemistry, 109(11):2356–2364, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cruz:2005:SAM

[CDGC05] S. A. Cruz, C. Díaz-García, and G. Covarrubias. Statistical atomic models with complete neglect of differential overlap for the study of free and confined systems. *International Journal of Quantum Chemistry*, 102(5):897–910, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carvalho:2005:PCA

[CDH05] Maíra A. Carvalho, João Bosco P. Da Silva, and Marcelo Z. Hernandes. Principal component analysis of the effects of wavefunction modification on the electrostatic potential of indole. *International Journal of Quantum Chemistry*, 102(4): 379–386, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2002:NTI

[CDI02] Feiwu Chen, E. R. Davidson, and Suehiro Iwata. New time-independent perturbation theory for the multireference problem. *International Journal of Quantum Chemistry*, 86(3):256–264, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85514349/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85514349/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85514349&PLACEBO=IE.pdf`.

Carbo-Dorca:2001:TCA

[CDK01] R. Carbó-Dorca and J. Karwowski. Theoretical and computational aspects of extended wave functions. *International Journal of Quantum Chemistry*, 84(3):331–337, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/83002309/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/83002309/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=83002309&PLACEBO=IE.pdf`.

Carauta:2005:CVS

[CdMCS05] Alexandre N. M. Carauta, José Walkimar de M. Carneiro, and Claudio A. Téllez Soto. Conformational and vibrational

study of di-n-propyl and di-i-propylphosphonates by MM/QM method. *International Journal of Quantum Chemistry*, 103 (5):763–774, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carauta:2006:CVS

[CDS06] Alexandre N. M. Carauta, José Walkimar De M.Carneiro, and Claudio A. Téllez Soto. Conformational and vibrational study of di-n-butyl and di-sec-butylphosphonates by MM/QM method. *International Journal of Quantum Chemistry*, 106 (13):2633–2642, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carbo-Dorca:2008:NIQ

[CDV08] Ramon Carbó-Dorca and Sofie Van Damme. A new insight on the quantum quantitative structure-properties relationships. *International Journal of Quantum Chemistry*, 108(10):1721–1734, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cheranovskii:2001:ESH

[CEK01] V. O. Cheranovskii, E. V. Ezerskaya, and M. V. Krikunov. Excitation spectrum of Hubbard model with infinite electron repulsion on strip-type triangular lattices. *International Journal of Quantum Chemistry*, 81(4):253–259, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76505740/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76505740/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76505740&PLACEBO=IE.pdf`.

Cheranovskii:2002:ESE

[CEÖ02] V. O. Cheranovskii, E. V. Ezerskaya, and I. Özkan. Energy spectrum of extended Hubbard model with spin-dependent hopping and related spin ladder model. *International Journal of Quantum Chemistry*, 88(4):398–402, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chuev:2004:DFM

[CF04] G. N. Chuev and M. V. Fedorov. Density functional method based on wavelets for quantum classical systems. *Interna-*

tional Journal of Quantum Chemistry, 100(4):539–547, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chenaghlou:2005:SAR

[CF05] A. Chenaghlou and H. Fakhri. Supersymmetry approaches to the radial bound states of the hydrogen-like atoms. *International Journal of Quantum Chemistry*, 101(3):291–304, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cozzini:2006:WHE

[CFM+06] Pietro Cozzini, Micaela Fornabaio, Andrea Mozzarelli, Francesca Spyrakis, Glen E. Kellogg, and Donald J. Abraham. Water: How to evaluate its contribution in protein–ligand interactions. *International Journal of Quantum Chemistry*, 106 (3):647–651, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2000:ASP

[CFP00] Jin-Quan Chen, Peng-Dong Fan, and Josef Paldus. Algebraic solutions for point groups: Cubic groups G in the group chain $G \supset T \supset D_2 \supset C_2$. *International Journal of Quantum Chemistry*, 76(5):585–599, February 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000589/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000589/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000589&PLACEBO=IE.pdf`.

Carvalho:2007:PAW

[CFR07] Alexandra T. P. Carvalho, Pedro A. Fernandes, and Maria J. Ramos. Parameterization of AZT—A widely used nucleoside inhibitor of HIV-1 reverse transcriptase. *International Journal of Quantum Chemistry*, 107(2):292–298, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Castro:2002:MSC

[CFV02] Alexandre T. Castro and Jose D. Figueroa-Villar. Molecular structure, conformational analysis and charge distribution of pralidoxime: Ab initio and DFT studies. *International Journal of Quantum Chemistry*, 89(3):135–146, ???? 2002.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chattaraj:2009:MDS

[CG09] P. K. Chattaraj and S. Giri. Multi-decker sandwich complexes using Be_3^{2-} and Mg_3^{2-} dianions. *International Journal of Quantum Chemistry*, 109(11):2373–2382, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

CabraldoCouto:2002:PHB

[CGCS02] P. Cabral do Couto, R. C. Guedes, B. J. Costa Cabral, and J. A. Martinho Simões. Phenol O-H bond dissociation energy in water clusters. *International Journal of Quantum Chemistry*, 86(3):297–304, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85514351/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85514351/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85514351&PLACEBO=IE.pdf`.

Chandrakumar:2005:ISP

[CGG05] K. R. S. Chandrakumar, Tapan K. Ghanty, and Swapan K. Ghosh. Ab initio studies on the polarizability of lithium clusters: Some unusual results. *International Journal of Quantum Chemistry*, 105(2):166–173, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Camara:2005:RTP

[CGL+05] M. S. C. Câmara, M. F. C. Gurgel, S. R. Lazaro, T. M. Boschi, P. S. Pizani, E. R. Leite, A. Beltran, and E. Longo. Room temperature photoluminescence of the $Li_2ZnTi_3O_8$ spinel: Experimental and theoretical study. *International Journal of Quantum Chemistry*, 103(5):580–587, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Craig:2003:ESC

[CGMT03] Norman C. Craig, Peter Groner, Donald C. McKean, and Michael J. Tubergen. Equilibrium structures for the *cis* and *trans* isomers of 1,2-difluoroethylene and the *cis,trans* isomer of 1,4-difluorobutadiene. *International Journal of Quantum*

Chemistry, 95(6):837–852, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Curik:2001:CCS

[CGS01] R. Curik, F. A. Gianturco, and N. Sanna. The close-coupling-single center-expansion (CC-SCE) model for electron scattering from polyatomic targets. *International Journal of Quantum Chemistry*, 84(5):565–579, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85004216/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85004216/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85004216&PLACEBO=IE.pdf`.

Choi:2005:AIV

[CHC05] Jun-Ho Choi, Seungsoo Hahn, and Minhaeng Cho. Amide I IR, VCD, and 2d IR spectra of isotope-labeled α-helix in liquid water: Numerical simulation studies. *International Journal of Quantum Chemistry*, 104(5):616–634, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2000:TSS

[Che00] Cheng Chen. Theoretical study of synthetic reaction of tetrazole and tetrazolate anion. *International Journal of Quantum Chemistry*, 80(1):27–37, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72515499/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72515499/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72515499&PLACEBO=IE.pdf`.

Codorniu-Hernandez:2005:EAA

[CHMIHS+05] Edelsys Codorniu-Hernández, Ariel Mesa-Ibirico, Richel Hernández-Santiesteban, Luis A. Montero-Cabrera, Francisco Martínez-Luzardo, Jorge L. Santana-Romero, Tobias Borrmann, and Wolf-D. Stohrer. Essential amino acids interacting with flavonoids: A theoretical approach. *International Journal of Quantum Chemistry*, 103(1):82–104, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cools:2009:RTN

[CHN09] Ronald Cools, Daan Huybrechs, and Dirk Nuyens. Recent topics in numerical integration. *International Journal of Quantum Chemistry*, 109(8):1748–1755, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chojnacki:2008:NCE

[Cho08] Henryk Chojnacki. Nondynamical correlation energy in model molecular systems. *International Journal of Quantum Chemistry*, 108(12):2267–2271, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Christov:2001:NCM

[Chr01] S. G. Christov. Nonlinear coupling model for reactions in dense media. *International Journal of Quantum Chemistry*, 81 (1):1–3, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/75502156/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75502156/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502156&PLACEBO=IE.pdf`.

Costa:2006:KSA

[CHR+06] Luiz Antônio S. Costa, Trevor W. Hambley, Willian R. Rocha, Wagner B. De Almeida, and Hélio F. Dos Santos. Kinetics and structural aspects of the cisplatin interactions with guanine: A quantum mechanical description. *International Journal of Quantum Chemistry*, 106(9):2129–2144, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ciftci:2009:SCH

[CHS09] Hakan Ciftci, Richard L. Hall, and Nasser Saad. Study of a confined hydrogen-like atom by the asymptotic iteration method. *International Journal of Quantum Chemistry*, 109 (5):931–937, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chun:2000:TMS

[Chu00] Paul W. Chun. Thermodynamic molecular switch in biological systems. *International Journal of Quantum Chemistry*, 80 (6):1181–1198, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.`

interscience.wiley.com/cgi-bin/abstract/75501735/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75501735/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75501735&PLACEBO=IE.pdf.

Chun:2001:TMS

[Chu01] Paul W. Chun. Thermodynamic molecular switch in sequence-specific hydrophobic interactions. *International Journal of Quantum Chemistry*, 85(6):697–712, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85513207/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85513207/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85513207&PLACEBO=IE.pdf.

Chun:2002:BPB

[Chu02] Paul W. Chun. Beyond the Planck–Benzinger thermal work function: New insights into the role of molecular switches in biology. *International Journal of Quantum Chemistry*, 87(6):323–353, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/91015589/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91015589/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91015589&PLACEBO=IE.pdf.

Chun:2004:PBT

[Chu04] Paul W. Chun. Planck–Benzinger thermal work function in biological systems. *International Journal of Quantum Chemistry*, 100(6):994–1002, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chun:2006:PBT

[Chu06] Paul W. Chun. The Planck–Benzinger thermal work function in the condensation of water vapor. *International Journal of Quantum Chemistry*, 106(15):3018–3031, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chun:2007:PBT

[Chu07] Paul W. Chun. The Planck–Benzinger thermal work function: Determining the thermal set point in interacting biological systems. *International Journal of Quantum Chemistry*, 107 (15):3272–3279, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chun:2008:TSP

[Chu08] Paul W. Chun. The thermal set point of water vapor and life in the condensed state. *International Journal of Quantum Chemistry*, 108(15):2746–2755, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chun:2009:PBT

[Chu09] Paul W. Chun. Planck–Benzinger thermal work function: Monoclonal antibody–DNA duplex binding interactions. *International Journal of Quantum Chemistry*, 109(15):3827–3839, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chodkiewicz:2004:TCD

[CHW04] Michał L. Chodkiewicz, Siân T. Howard, and Krzysztof Woźniak. Toward a compact description of molecular electron densities. *International Journal of Quantum Chemistry*, 98(1):1–10, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Constantinescu:2006:CSM

[CI06] Mircea Constantinescu and Daniela Ivanov. Computational study of maleamic acid cyclodehydration with acetic anhydride. *International Journal of Quantum Chemistry*, 106(6): 1330–1337, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cacheiro:2003:PSC

[CIP+03] J. López Cacheiro, M. Iglesias, V. Pardo, D. Baldomir, and J. E. Arias. Possible spin configurations and magnetism in $BaCoO_3$ perovskite. *International Journal of Quantum Chemistry*, 91(2):252–256, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chi:2003:SSP

[CIT+03] X. Chi, M. E. Itkis, F. S. Tham, R. T. Oakley, A. W. Cordes, and R. C. Haddon. Synthesis, structure, and physical properties of a new phenalenyl-based neutral radical crystal: Correlation between structure and transport properties in carbon-based molecular conductors. *International Journal of Quantum Chemistry*, 95(6):853–865, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cardenas-Jiron:2003:RDA

[CJ03] Gloria I. Cárdenas-Jirón. Reactivity descriptors applied to the study of cobalt porphyrin and their aza derivatives. *International Journal of Quantum Chemistry*, 91(3):389–397, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Campos:2009:BSC

[CJ09] C. T. Campos and F. E. Jorge. Basis set convergence of electric properties in HF and DFT calculations of nucleic acid bases. *International Journal of Quantum Chemistry*, 109(2): 285–293, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cardenas-Jiron:2008:TEN

[CJB08] Gloria I. Cárdenas-Jirón and Cristhian Berríos. Theoretical evidence of the Ni(III) participation in the chlorophenol oxidation on tetrasulphonated nickel phthalocyanine. *International Journal of Quantum Chemistry*, 108(13):2586–2594, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Centoducatte:2001:GBS

[CJdC01] R. Centoducatte, F. E. Jorge, and E. V. R. de Castro. Gaussian basis sets for first-, third-, and fourth-row positive and negative ions. *International Journal of Quantum Chemistry*, 82(3):126–130, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/77004287/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/77004287/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=77004287&PLACEBO=IE.pdf`.

Chalasinski:2004:OJR

[CJKK04] Grzegorz Chalasinski, Bogumil Jeziorski, Jacek Komasa, and Jerzy Konarski. Obituary: Jacek Rychlewski (1947–2003). *International Journal of Quantum Chemistry*, 99(4):187–188, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2006:PMB

[CJZZ06] Zexing Cao, Xi Jin, Zhaohui Zhou, and Qianer Zhang. Protonation of metal-bound α-hydroxycarboxylate ligand and implication for the role of homocitrate in nitrogenase: Computational study of the oxy-bidentate chelate ring opening. *International Journal of Quantum Chemistry*, 106(9):2161–2168, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Calaminici:2003:SVV

[CK03] Patrizia Calaminici and Andreas M. Köster. Structures and vibrations of V_3O and V_3O^-: A density functional study. *International Journal of Quantum Chemistry*, 91(3):317–320, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Courbage:2004:STI

[CK04] M. Courbage and B. Kamiński. Space–time intrinsic randomness of dynamical systems and statistical mechanics. *International Journal of Quantum Chemistry*, 98(2):145–149, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Crosby:2006:AES

[CK06] Lonnie D. Crosby and Henry A. Kurtz. Application of electronic structure and transition state theory: Reaction of hydrogen with silicon radicals. *International Journal of Quantum Chemistry*, 106(15):3149–3159, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Champagne:2009:PSH

[CK09] Benoît Champagne and Bernard Kirtman. Polarizabilities and second hyperpolarizabilities of hydrogen chains using the spin-component-scaled Møller–Plesset second-order method. *International Journal of Quantum Chemistry*, 109(13):3103–3111,

November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Celik:2002:NMS

[ÇKB02] Ercan Çelik, Erdal Karaduman, and Mustafa Bayram. Numerical method to solve chemical differential-algebraic equations. *International Journal of Quantum Chemistry*, 89(5): 447–451, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cherkes:2009:SHS

[CKM09] Ira Cherkes, Shachar Klaiman, and Nimrod Moiseyev. Spanning the Hilbert space with an even tempered Gaussian basis set. *International Journal of Quantum Chemistry*, 109(13): 2996–3002, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cances:2000:CWO

[CL00a] Eric Cancès and Claude Le Bris. Can we outperform the DIIS approach for electronic structure calculations? *International Journal of Quantum Chemistry*, 79(2):82–90, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72508329/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72508329/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72508329&PLACEBO=IE.pdf`.

Castro:2000:I

[CL00b] Miguel Castro and Janos Ladik. Introduction. *International Journal of Quantum Chemistry*, 80(2):79, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001282/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001282/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001282&PLACEBO=IE.pdf`.

Capelle:2005:SDF

[CL05a] K. Capelle and Valter L. Líbero. Spin-density functional theory: Some open problems and application to inhomogeneous Heisenberg models. *International Journal of Quantum Chem-*

istry, 105(6):679–686, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Capozziello:2005:CTU

[CL05b] S. Capozziello and A. Lattanzi. Chiral tetrahedrons as unitary quaternions: Molecules and particles under the same standard? *International Journal of Quantum Chemistry*, 104 (6):885–893, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaudhari:2005:DFS

[CL05c] Ajay Chaudhari and Shyi-Long Lee. Density functional study of hydrogen-bonded acetonitrile–water complex. *International Journal of Quantum Chemistry*, 102(1):106–111, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaudhari:2005:DFTb

[CL05d] Ajay Chaudhari and Shyi-Long Lee. Density functional theory study of contribution of many-body energies to binding energy for alanine-$(\text{water})_4$ complex. *International Journal of Quantum Chemistry*, 102(2):174–177, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Christiansen:2005:BVS

[CL05e] Ove Christiansen and Josep M. Luis. Beyond vibrational self-consistent-field methods: Benchmark calculations for the fundamental vibrations of ethylene. *International Journal of Quantum Chemistry*, 104(5):667–680, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaudhari:2007:TSM

[CL07a] Ajay Chaudhari and Shyi-Long Lee. Theoretical study of 3d-metal mononitrides using DFT method. *International Journal of Quantum Chemistry*, 107(1):212–218, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chi:2007:TEO

[CL07b] Xian X. Chi and Yong Liu. Theoretical evidence of *d*-orbital aromaticity in anionic metal $\underline{\underline{X}}^3\underline{\ }$ (X = Sc, Y, La) clusters. *International Journal of Quantum Chemistry*, 107(9):1886–1896, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Curteanu:2008:OSB

[CL08] Silvia Curteanu and Florin Leon. Optimization strategy based on genetic algorithms and neural networks applied to a polymerization process. *International Journal of Quantum Chemistry*, 108(4):617–630, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carvajal:2002:LED

[CLA+02] Angels Carvajal, Xiang-Yang Liu, Pere Alemany, Juan J. Novoa, and Santiago Alvarez. Ligand effects and dimer formation in dicoordinated copper(I) complexes. *International Journal of Quantum Chemistry*, 86(1):100–105, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85008815/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85008815/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85008815&PLACEBO=IE.pdf`.

Cheng:2004:PCC

[CLL04] Li Ping Cheng, Se Li, and Qian Shu Li. Polynitrogen clusters containing five-membered rings. *International Journal of Quantum Chemistry*, 97(5):933–943, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2008:GGR

[CLL08] Zhi Cao, Bo Liao, and Renfa Li. A group of 3D graphical representation of DNA sequences based on dual nucleotides. *International Journal of Quantum Chemistry*, 108(9):1485–1490, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2001:EMP

[CLSD+01] Guangju Chen, Ruozhuang Liu, I. Silaghi-Dumitrescu, G. Espinosa-Perez, A. Zentella-Dehesa, and F. Lara-Ochoa. Electronic and magnetic properties of (tetrakis(2-pyridylmethyl)-ethylenediamine)iron(II) perchlorate. A comparison of different computational methods. *International Journal of Quantum Chemistry*, 83(2):60–69, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002390/START; http:`

//www3.interscience.wiley.com/cgi-bin/fulltext/80002390/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002390&PLACEBO=IE.pdf.

Charro:2002:STE

[CM02a] E. Charro and I. Martín. Systematic trends in E2 transitions along the sodium isoelectronic sequence. *International Journal of Quantum Chemistry*, 90(1):403–409, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chernyak:2002:GPC

[CM02b] Vladimir Chernyak and Shaul Mukamel. Geometric picture for coupled electron–nuclear dynamics. *International Journal of Quantum Chemistry*, 90(2):799–811, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carvalho:2005:EPA

[CM05a] Alexandre R. F. Carvalho and André Melo. Energy partitioning in association processes. *International Journal of Quantum Chemistry*, 104(2):240–248, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Castro:2005:TSK

[CM05b] Elton A. S. Castro and João B. L. Martins. Theoretical study of kaolinite. *International Journal of Quantum Chemistry*, 103 (5):550–556, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Charro:2005:CIU

[CM05c] E. Charro and I. Martín. Complementary investigations using the MCDF and RQDO methods. *International Journal of Quantum Chemistry*, 104(4):446–457, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Corn:2009:IAC

[CM09] Brittany Corn and Svetlana A. Malinovskaya. An ab initio analysis of charge redistribution upon isomerization of retinal in rhodopsin and bacteriorhodopsin. *International Journal of Quantum Chemistry*, 109(13):3131–3141, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cruz:2001:RPD

[CMASC01] J. Cruz, L. M. R. Martínez-Aguilera, R. Salcedo, and M. Castro. Reactivity properties of derivatives of 2-imidazoline: an ab initio DFT study. *International Journal of Quantum Chemistry*, 85(4–5):546–556, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cho:2007:TIT

[CME07] Seung Joo Cho, Adel A. Mohamed, and Shaaban A. K. Elroby. Theoretical investigation of the tautomerism of isoorotic acid in gaseous and aqueous phases. *International Journal of Quantum Chemistry*, 107(1):63–71, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Careja:2007:MMS

[CMM+07] Valentin Careja, Simona Muntean, Mircea Mracec, Ludovic Sayti, and Zeno Simon. Molecular modeling of some calcium and magnesium ionic bridges. *International Journal of Quantum Chemistry*, 107(8):1714–1718, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cuenca:2007:QRI

[CMNH07] D. Zorrilla Cuenca, J. Sánchez Márquez, M. Fernández Núñez, and R. Rodríguez Huertas. Quasi-random integration in quantum chemistry: Efficiency, stability, and application to the study of small atoms and molecules constrained in spherical boxes. *International Journal of Quantum Chemistry*, 107 (4):879–893, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cappelli:2005:EEV

[CMR05] Chiara Cappelli, Susanna Monti, and Antonio Rizzo. Effect of the environment on vibrational infrared and circular dichroism spectra of (s)-proline. *International Journal of Quantum Chemistry*, 104(5):744–757, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Corella-Madueno:2000:TEA

[CMRMR00] A. Corella-Madueño, R. A. Rosas, J. L. Marín, and R. Riera. Two-electron atomic systems confined within spheroidal boxes. *International Journal of Quantum Chemistry*, 77

(2):509–515, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70002218/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70002218/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70002218&PLACEBO=IE.pdf`.

Chattaraj:2004:QAK

[CMS04] P. K. Chattaraj, B. Maiti, and S. Sengupta. Quantum analogue of the Kolmogorov–Arnold–Moser transition in different quantum anharmonic oscillators. *International Journal of Quantum Chemistry*, 100(3):254–276, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ciric-Marjanovic:2008:TSO

[ĆMTS08] Gordana Ćirić-Marjanović, Miroslava Trchová, and Jaroslav Stejskal. Theoretical study of the oxidative polymerization of aniline with peroxydisulfate: Tetramer formation. *International Journal of Quantum Chemistry*, 108(2):318–333, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cabria:2003:SNZ

[CMW03] I. Cabria, J. W. Mintmire, and C. T. White. Stability of narrow zigzag carbon nanotubes. *International Journal of Quantum Chemistry*, 91(1):51–56, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Corral:2003:SSC

[CMY03] Inés Corral, Otilia Mó, and Manuel Yáñez. Structure and stability of $[C_2H_4N]^+$ singlet-state cations: Comparison between DFT and high-level ab initio calculations. *International Journal of Quantum Chemistry*, 91(3):438–445, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Corral:2006:ABX

[CMY06] Inés Corral, Otilia Mó, and Manuel Yáñez. Analysis of the bonding in XH_3Cu^+ (X = B, Al, Ga) complexes. *International Journal of Quantum Chemistry*, 106(3):659–663, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Christensen:2000:ESM

[CN00] N. E. Christensen and D. L. Novikov. Electronic structure of materials under pressure. *International Journal of Quantum Chemistry*, 77(5):880–894, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000350/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000350/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000350&PLACEBO=IE.pdf`.

Corongiu:2003:GPG

[CN03] Giorgina Corongiu and Paola Nava. Gas-phase geometries and energies of bis (2,2′-bipyridine) interacting either with Cu(I) or Ag(I): Computational study. *International Journal of Quantum Chemistry*, 93(6):395–404, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Coppens:2005:DCL

[CN05] Philip Coppens and Irina V. Novozhilova. DFT calculations of light-induced excited states and comparison with time-resolved crystallographic results. *International Journal of Quantum Chemistry*, 101(5):611–623, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cernusak:2007:P

[ČN07] Ivan Černušák and Jozef Noga. Preface. *International Journal of Quantum Chemistry*, 107(11):2047, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Campos:2006:DEE

[CNC+06] J. A. Campos, D. L. Nascimento, D. T. Cavalcante, A. L. A. Fonseca, and A. O. C. Nunes. Determination of electronic energy levels for the heteromolecular ions HeH^{2+}, LiH^{3+}, and BeH^{4+} from the Hamilton–Jacobi equation. *International Journal of Quantum Chemistry*, 106(13):2587–2596, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Coutinho-Neto:2000:SBB

[CNDÖ00] Mauricio Coutinho-Neto, Erik Deumens, and Yngve Öhrn. Selective bond breaking in H+HOD reaction. *Inter-*

national Journal of Quantum Chemistry, 77(1):301–304, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004269/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004269/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004269&PLACEBO=IE.pdf`.

Carmona-Novillo:2004:QDC

[CNPA04] Estela Carmona-Novillo, Fernando Pirani, and Vincenzo Aquilanti. Quantum dynamics of clusters on experimental potential energy surfaces: Triplet and quintet O_2-O_2 surfaces and dimers of para-N_2 with ortho — and para-N_2 and with O_2. *International Journal of Quantum Chemistry*, 99(5):616–627, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Czako:2009:PAE

[CNT+09] Gábor Czakó, Balázs Nagy, Gyula Tasi, Árpád Somogyi, Ján Šimunek, Jozef Noga, Bastiaan J. Braams, Joel M. Bowman, and Attila G. Császár. Proton affinity and enthalpy of formation of formaldehyde. *International Journal of Quantum Chemistry*, 109(11):2393–2409, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Champagne:2005:IMV

[CÖ05] Benoît Champagne and Yngve Öhrn. Introduction: Modeling vibrational spectroscopies. *International Journal of Quantum Chemistry*, 104(5):587–588, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Coleman:2001:RDM

[Col01] A. John Coleman. Reduced density matrices — Then and now. *International Journal of Quantum Chemistry*, 85(4–5):196–203, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Collado:2008:CPL

[Col08] J. R. Alvarez Collado. Calculation of the paramagnetism of large carbon nanotubes, using a parameter-independent molecular orbital model. *International Journal of Quantum Chemistry*, 108(2):257–264, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Claeyssens:2003:BPC

[COMA03] Frederik Claeyssens, Josep M. Oliva, Paul W. May, and Neil L. Allan. Binary phosphorus–carbon compounds: The series P_4C_{3+8n}. *International Journal of Quantum Chemistry*, 95 (4–5):546–553, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cortona:2004:ISS

[Cor04] Pietro Cortona. Ab-initio study of the structural phase transition of SrSe and SrTe under pressure. *International Journal of Quantum Chemistry*, 99(5):828–832, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Corongiu:2005:HHM

[Cor05] Giorgina Corongiu. HF–HL method: Combination of Hartree–Fock and Heitler–London approximations. *International Journal of Quantum Chemistry*, 105(6):831–838, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cordeiro:2006:DMT

[Cor06] J. M. M. Cordeiro. Dynamics of meso and thermo citrate synthases with implicit solvation. *International Journal of Quantum Chemistry*, 106(3):652–658, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Costa:2006:ESS

[Cos06] Fabio Costa. Electronic structure study of the reaction $C_2H \rightarrow C_2H + H_2$. *International Journal of Quantum Chemistry*, 106(13):2763–2771, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Coudray:2005:IPM

[Cou05] C. Coudray. Ionization potentials of MgO clusters containing a substitutional atom. *International Journal of Quantum Chemistry*, 104(4):570–577, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Curteanu:2006:NNB

[CP06] Silvia Curteanu and Corneliu Petrila. Neural network-based modeling for semi-batch and nonisothermal free radical polymerization. *International Journal of Quantum Chemistry*, 106

(6):1445–1456, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cooper:2009:ABF

[CP09] David L. Cooper and Robert Ponec. Anatomy of bond formation: Insights from the analysis of domain-averaged Fermi holes in momentum space. *International Journal of Quantum Chemistry*, 109(11):2383–2392, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cusati:2004:EDM

[CPH04] T. Cusati, J. L. Paz, and A. J. Hernández. Effects of the dipole moments behavior on a vibronic coupling model for the four-wave mixing signal. *International Journal of Quantum Chemistry*, 98(5):425–433, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cundari:2006:CHV

[CPR06] Thomas R. Cundari, Aaron W. Pierpont, and Hassan Rabaâ. Carbon hydrogen versus carbon heteroatom activation by a high-valent zirconium-imido complex. *International Journal of Quantum Chemistry*, 106(7):1611–1619, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chamorro:2003:TST

[CQN+03] Eduardo Chamorro, Jairo Quijano, Rafael Notario, Claudia Sánchez, Luis A. León, and Gabriel Chuchani. Theoretical study of the thermolysis reaction of β-hydroxynitriles in the gas phase. *International Journal of Quantum Chemistry*, 91 (5):618–625, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cacciatore:2006:SMD

[CR06] M. Cacciatore and M. Rutigliano. Semiclassical molecular dynamics simulation of surface processes: Application to the hydrogen atom recombination on graphite. *International Journal of Quantum Chemistry*, 106(3):631–635, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Crecca:2008:URA

[CR08a] Christina Crecca and Adrian E. Roitberg. Using the Rosetta algorithm and selected inter-residue distances to predict protein structure. *International Journal of Quantum Chemistry*, 108(15):2793–2802, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Crecca:2008:UDB

[CR08b] Christina R. Crecca and Adrian E. Roitberg. Using distances between α-carbons to predict protein structure. *International Journal of Quantum Chemistry*, 108(15):2782–2792, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Czaplewski:2002:CCH

[CRL+02] Cezary Czaplewski, Daniel R. Ripoll, Adam Liwo, Sylwia Rodziewicz-Motowidło, Ryszard J. Wawak, and Harold A. Scheraga. Can cooperativity in hydrophobic association be reproduced correctly by implicit solvation models? *International Journal of Quantum Chemistry*, 88(1):41–55, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90513477/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90513477/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90513477&PLACEBO=IE.pdf`.

Chalmet:2001:QMC

[CRRL01] S. Chalmet, D. Rinaldi, and M. F. Ruiz-López. A QM/MM/continuum model for computations in solution: Comparison with QM/MM molecular dynamics simulations. *International Journal of Quantum Chemistry*, 84(5):559–564, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502593/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502593/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502593&PLACEBO=IE.pdf`.

Csonka:2005:EOM

[CRTP05] Gábor I. Csonka, Adrienn Ruzsinszky, Jianmin Tao, and John P. Perdew. Energies of organic molecules and atoms

in density functional theory. *International Journal of Quantum Chemistry*, 101(5):506–511, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2000:CIH

[CS00a] Cheng Chen and Shuang-Fuh Shyu. Conformers and intramolecular hydrogen bonding of the oxalic acid monomer and its anions. *International Journal of Quantum Chemistry*, 76(4):541–551, February 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000686/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000686/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000686&PLACEBO=IE.pdf`.

Collins:2000:QDM

[CS00b] T. C. Collins and D. F. Scofield. Quantum dynamical manifolds. 4. High-temperature superconductors. *International Journal of Quantum Chemistry*, 80(3):341–368, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501009/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501009/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501009&PLACEBO=IE.pdf`.

Cruz:2001:CMI

[CS01] S. A. Cruz and J. Soullard. Calculation of molecular integrals for systems confined by hard spherical walls: Use of the single-center expansion of floating spherical Gaussians. *International Journal of Quantum Chemistry*, 83(5):271–278, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/81002392/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/81002392/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=81002392&PLACEBO=IE.pdf`.

Chattaraj:2003:GES

[CS03] P. K. Chattaraj and U. Sarkar. Ground- and excited-states reactivity dynamics of hydrogen and helium atoms. *International Journal of Quantum Chemistry*, 91(5):633–650, ????

2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cortona:2004:CSR

[CS04] Pietro Cortona and Christophe Sapet. The (100), (110), and (111) Cu surfaces revisited by the semiempirical LCAO method. *International Journal of Quantum Chemistry*, 99 (5):713–723, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cherepkov:2007:NDT

[CS07] N. A. Cherepkov and S. K. Semenov. New developments in the theory of molecular K-shell photoionization. *International Journal of Quantum Chemistry*, 107(14):2889–2901, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cencek:2008:UHA

[CS08] Wojciech Cencek and Krzysztof Szalewicz. Ultra-high accuracy calculations for hydrogen molecule and helium dimer. *International Journal of Quantum Chemistry*, 108(12):2191–2198, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cuevas-Saavedra:2009:CSK

[CSA09] Rogelio Cuevas-Saavedra and Paul W. Ayers. Coordinate scaling of the kinetic energy in pair density functional theory: A Legendre transform approach. *International Journal of Quantum Chemistry*, 109(8):1699–1705, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chuan-Song:2003:OCU

[CSDCCMZT03] Qi Chuan-Song, Feng Da-Cheng, Kang Cong-Min, and Cai Zheng-Ting. One-carbon unit transfer quantum study of 1,10-CH^+-tetrahydroquinoxaline analog. *International Journal of Quantum Chemistry*, 92(5):451–456, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cardoen:2006:FHF

[CSG06] Wim Cardoen, Jack Simons, and Robert J. Gdanitz. F + $H_2 \rightarrow$ FH + H potential energy surface: Construction of the reference configuration state function space and MR-ACPF-2

results. *International Journal of Quantum Chemistry*, 106(7): 1516–1527, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chass:2002:TCP

[CSL+02] Gregory A. Chass, Michelle A. Sahai, Jacqueline M. S. Law, Sandor Lovas, Ödön Farkas, Andras Perczel, Jean-Louis Rivail, and Imre G. Csizmadia. Toward a computed peptide structure database: The role of a universal atomic numbering system of amino acids in peptides and internal hierarchy of database. *International Journal of Quantum Chemistry*, 90 (2):933–968, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaudhari:2005:DFTa

[CSL05a] Ajay Chaudhari, Prabhat K. Sahu, and Shyi-Long Lee. Density functional theory study of formaldehyde oligomers. *International Journal of Quantum Chemistry*, 101(1):67–72, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaudhari:2005:HBI

[CSL05b] Ajay Chaudhari, Prabhat K. Sahu, and Shyi-Long Lee. Hydrogen bonding interaction in sarcosine–water complex using ab initio and DFT method. *International Journal of Quantum Chemistry*, 101(1):97–103, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2007:DBQ

[CSL+07] Jincan Chen, Yong Shen, Siyan Liao, Lanmei Chen, and Kangcheng Zheng. DFT-based QSAR study and molecular design of AHMA derivatives as potent anticancer agents. *International Journal of Quantum Chemistry*, 107(6):1468–1478, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cioslowski:2002:CHR

[CSM02] Jerzy Cioslowski, Agnieszka Szarecka, and David Moncrieff. Conformations of the S_5^+ and S_6^+ homocyclic radical cations. *International Journal of Quantum Chemistry*, 90(3):1049–1054, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Changa:2004:SOE

[CSP04] Maris E. Changa, Andrei V. Scherbinin, and Vladimir I. Pupyshev. Spectra of one-electron atom in a spherical cavity. *International Journal of Quantum Chemistry*, 96(2):167–174, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chattaraj:2005:DSS

[CSPS05] P. K. Chattaraj, U. Sarkar, R. Parthasarathi, and V. Subramanian. DFT study of some aliphatic amines using generalized philicity concept. *International Journal of Quantum Chemistry*, 101(6):690–702, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chuev:2002:QMS

[CSSB02] Gennady N. Chuev, D. M. Schrader, Sergey V. Stepanov, and Vsevolod M. Byakov. Quantum mechanics of solvated complexes: A test for positronium. *International Journal of Quantum Chemistry*, 88(5):634–641, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chong:2008:DFT

[CSTB08] Delano P. Chong, Maximiliano Segala, Yuji Takahata, and E. J. Baerends. Density functional theory calculation of 2p spectra of SiH_4, PH_3, H_2S, HCl, and Ar. *International Journal of Quantum Chemistry*, 108(8):1358–1368, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Coutsias:2006:RLC

[CSWD06] Evangelos A. Coutsias, Chaok Seok, Michael J. Wester, and Ken A. Dill. Resultants and loop closure. *International Journal of Quantum Chemistry*, 106(1):176–189, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2001:DFT

[CSX+01] Zexing Cao, Miquel Solà, Hui Xian, Miquel Duran, and Qianer Zhang. Density functional theory study of the structures and stabilities of CuO and CuO_3. *International Journal of Quantum Chemistry*, 81(2):162–168, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/76500937/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76500937/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76500937&PLACEBO=IE.pdf.

Colpa:2000:SFP

[CT00] J. P. Colpa and F. P. Temme. Schur functions over polyhedral lattice-point models: Contrasts in determinacy criteria for $((\lambda_1 \lambda_2) \vdash n)$ vs. $((\lambda_1 \lambda_2, \cdots, \lambda_{m \leq (n/2)}) \vdash n)$ partite SU(m) $\times$ s_n group embeddings: SU(m) $\times$ $s_8 \downarrow d_4$ spin symmetry of [$H^{11}B$]. *International Journal of Quantum Chemistry*, 78(1): 5–14, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/71001653/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71001653/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71001653&PLACEBO=IE.pdf.

Chen:2005:GFE

[CT05] Xin Chen and M. Thachuk. Ground and first-excited global potential energy surfaces of the H_2O^+He complex: Predictions of ion mobilities. *International Journal of Quantum Chemistry*, 101(1):1–7, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Choe:2009:VAA

[CTI09] Yoong-Kee Choe, Eiji Tsuchida, and Tamio Ikeshoji. Vibrational analysis of aqueous sulfuric acid: A computational study. *International Journal of Quantum Chemistry*, 109(9): 1984–1990, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2001:DCC

[CTLZ01] Zhong-Zhou Chen, Bo Tan, Yan-Mei Li, and Yu-Fen Zhao. Differentiation of α-COOH from β-COOH in aspartic acids by N-phosphorylation. *International Journal of Quantum Chemistry*, 83(1):41–51, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/79502660/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/79502660/FILE?TPL=ftx_start;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=79502660&PLACEBO=IE.pdf.

Cisneros:2008:SFI

[CTP+08] G. A. Cisneros, S. Na-Im Tholander, O. Parisel, T. A. Darden, D. Elking, L. Perera, and J.-P. Piquemal. Simple formulas for improved point-charge electrostatics in classical force fields and hybrid quantum mechanical/molecular mechanical embedding. *International Journal of Quantum Chemistry*, 108 (11):1905–1912, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cohen:2008:DDP

[CTS08] S. Cohen, S. I. Themelis, and K. D. Sen. Dynamic dipole polarizabilities of the ground and excited states of confined hydrogen atom computed by means of a mapped Fourier grid method. *International Journal of Quantum Chemistry*, 108 (2):351–361, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cabrera-Trujillo:2003:CPK

[CTSÖD03] R. Cabrera-Trujillo, J. R. Sabin, Y. Öhrn, and E. Deumens. Case for projectile kinetic energy gain in stopping power studies. *International Journal of Quantum Chemistry*, 94(4):215–221, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cabrera-Vivas:2006:TSS

[CVPGH+06] B. M. Cabrera-Vivas, Flor P. Pineda, S. García-Hidalgo, M. G. Múñoz-Arenas, F. J. Meléndez, Y. Reyes-Ortega, and Juan Carlos Ramírez. Theoretical study of structural features of endo, exo double bonds and side chain in 14α-demethylation of lanosterol. *International Journal of Quantum Chemistry*, 106(2):542–549, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Compaan:2008:CDH

[CVVA08] Katherine Compaan, Robert Vergenz, Paul Von Rague Schleyer, and Isis Arreguin. Carbon-donated hydrogen bonding: Electrostatics, frequency shifts, directionality, and bifurcation. *International Journal of Quantum Chemistry*, 108 (15):2914–2923, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2000:AIR

[CW00] Xiaoping Cao and Yan Wang. Analytical irreducible representation bases of the single and double icosahedral groups and their applications. *International Journal of Quantum Chemistry*, 77(3):615–624, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004057/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004057/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004057&PLACEBO=IE.pdf`.

Casida:2004:GKS

[CW04] Mark E. Casida and Tomasz A. Wesołowski. Generalization of the Kohn–Sham equations with constrained electron density formalism and its time-dependent response theory formulation. *International Journal of Quantum Chemistry*, 96 (6):577–588, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chou:2008:RDE

[CW08] Chia-Chun Chou and Robert E. Wyatt. Riccati differential equation for quantum mechanical bound states: Comparison of numerical integrators. *International Journal of Quantum Chemistry*, 108(2):238–248, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Churchill:2006:CSH

[CWBM06] Geoffrey B. Churchill, Kenneth B. Wiberg, Robert K. Bohn, and H. Harvey Michels. Conformational studies of 3-hexyne. *International Journal of Quantum Chemistry*, 106(15):3364–3370, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Campos:2009:TEI

[CWF09] Renan Borsoi Campos, Fernando Wypych, and Harley Paiva Martins Filho. Theoretical estimates of the IR spectrum of water intercalated into kaolinite. *International Journal of Quantum Chemistry*, 109(3):594–604, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Crowley:2009:CCS

[CWW09] Michael F. Crowley, Mark J. Williamson, and Ross C. Walker. CHAMBER: Comprehensive support for CHARMM force fields within the AMBER software. *International Journal of Quantum Chemistry*, 109(15):3767–3772, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2005:TSP

[CWY05] Yishan Chen, Yanxia Wang, and Song Ye. Theoretical study of the photochemical reaction mechanism of bicyclo[4.1.0]hept-2-ene upon direct photolysis. *International Journal of Quantum Chemistry*, 103(1):60–72, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2003:BLF

[CWZ03] Zexing Cao, Wei Wu, and Qianer Zhang. Bond length features of linear carbon chains of finite to infinite size: Visual interpretation from Pauling bond orders. *International Journal of Quantum Chemistry*, 94(3):144–149, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2000:ISA

[CX00] Zhao-Xu Chen and Heming Xiao. Impact sensitivity and activation energy of pyrolysis for tetrazole compounds. *International Journal of Quantum Chemistry*, 79(6):350–357, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72515271/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72515271/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72515271&PLACEBO=IE.pdf`.

Chen:2009:HPT

[CXZ09a] Jianfu Chen, Shoujun Xu, and Heping Zhang. Hosoya polynomials of TUC_4C_8 (R) nanotubes. *International Journal of Quantum Chemistry*, 109(4):641–649, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2009:SDS

[CXZ+09b] Liang Chen, Can Xu, Xiaofang Zhang, Chuan Cheng, and Tao Zhou. Size dependent structural and electronic properties of MgO nanotube clusters. *International Journal of Quantum Chemistry*, 109(2):349–356, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2004:PRM

[CY04] Yishan Chen and Song Ye. Photochemical reaction mechanism of cyclobutanone: CASSCF study. *International Journal of Quantum Chemistry*, 97(2):725–735, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2003:FCL

[CZ03] Zexing Cao and Qianer Zhang. Is the FeC cluster linear? Theoretical study of the equilibrium structure and bonding of FeC. *International Journal of Quantum Chemistry*, 93 (4):275–279, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2001:TSR

[CZPJ01] Xian-Yang Chen, Cheng-Xue Zhao, Yin Ping, and Guan-Zhi Ju. Theoretical study of reactions between MH (M = B, Al) and the H_2S molecule. *International Journal of Quantum Chemistry*, 85(3):127–135, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85511290/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85511290/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85511290&PLACEBO=IE.pdf`.

Chang:2005:GSF

[CZS+05] Y. F. Chang, J. P. Zhang, H. Sun, B. Hong, Z. An, and R. S. Wang. Geometry and stability of fullerene cages: C_{24} to C_{70}. *International Journal of Quantum Chemistry*, 105 (2):142–147, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2005:ECR

[CZWZ05] Zexing Cao, Zhaohui Zhou, Huilin Wan, and Qianer Zhang. Enzymatic and catalytic reduction of dinitrogen to ammo-

nia: Density functional theory characterization of alternative molybdenum active sites. *International Journal of Quantum Chemistry*, 103(3):344–353, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deAmorim:2008:TPT

[dA08] Mauro B. de Amorim. Torsional profile of 2,2,2-trifluoroethanol: A theoretical analysis with basis set extrapolation. *International Journal of Quantum Chemistry*, 108(13):2550–2556, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dunne:2006:QCF

[DAA+06] Lawrence J. Dunne, Anna-Karin Axelsson, Neil McN. Alford, Jonathan Breeze, Xavi Aupi, and Erkki J. Brändas. Quasi-classical fluctuation–dissipation description of dielectric loss in oxides with implications for quantum information processing. *International Journal of Quantum Chemistry*, 106(4): 986–993, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeSouza:2003:TSA

[DAD+03] P. R. N. De Souza, D. A. G. Aranda, J. W. De M.Carneiro, C. Da S. B. De Oliveira, O. A. C. Antunes, and F. B. Passos. Theoretical study on the adsorption of aromatic compounds on platinum clusters. *International Journal of Quantum Chemistry*, 92(4):400–411, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Darafsheh:2005:CFN

[DAD05] Mohammad Reza Darafsheh, Ali Reza Ashrafi, and Arash Darafsheh. Computing the full nonrigid group of tetra-tert-butyltetrahedrane using wreath product. *International Journal of Quantum Chemistry*, 105(5):485–492, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Darafsheh:2008:ESG

[DAD08a] Mohammad Reza Darafsheh, Ali Reza Ashrafi, and Arash Darafsheh. Erratum: The symmetry group of nonrigid tetramethylsilane. *International Journal of Quantum Chemistry*, 108(8):1411–1413, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [DAD08b].

Darafsheh:2008:SGN

[DAD08b] Mohammad Reza Darafsheh, Ali Reza Ashrafi, and Arash Darafsheh. The symmetry group of nonrigid tetramethylsilane. *International Journal of Quantum Chemistry*, 108(3): 440–446, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [DAD08a].

deAbreu:2008:DPI

[dAGD08] Heitor Avelino de Abreu, Luciana Guimarães, and Hélio Anderson Duarte. DFT/PCM investigation of the Mn(II) chemical speciation in aqueous solution. *International Journal of Quantum Chemistry*, 108(13):2467–2475, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Machado:2005:LFH

[dAMdG05] A. E. de A. Machado and A. A. S. da Gama. Large first hyperpolarizabilities of substituted aniline oligomers. *International Journal of Quantum Chemistry*, 103(5):625–631, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deAndrade:2005:GAA

[dAMM05] M. D. de Andrade, K. C. Mundim, and L. A. C. Malbouisson. GSA algorithm applied to electronic structure: Hartree–Fock–GSA method. *International Journal of Quantum Chemistry*, 103(5):493–499, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deAndrade:2008:CGS

[dAMM08] M. D. de Andrade, K. C. Mundim, and L. A. C. Malbouisson. Convergence of the generalized simulated annealing method with independent parameters for the acceptance probability, visitation distribution, and temperature functions. *International Journal of Quantum Chemistry*, 108(13):2392–2397, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Datta:2004:TDE

[Dat04] Sambhu N. Datta. Transformed Dirac equation for the hydrogen atom, comparison with previous approaches in momentum space, and the anomalous Zeeman effect in momentum representation. *International Journal of Quantum Chemistry*,

96(1):42–55, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Davidson:2003:LID

[Dav03] Ernest R. Davidson. Linear inequalities for density matrices: III. *International Journal of Quantum Chemistry*, 91(1):1–4, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Davidson:2004:BFH

[Dav04] Ernest R. Davidson. Bonding in FHF^-, $(HF)_2$, and FHF. *International Journal of Quantum Chemistry*, 98(3):317–324, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Delgado–Barrio:2004:OYG

[DB04a] Gerardo Delgado-Barrio. Obituary: Yves G. Smeyers (1931–2003). *International Journal of Quantum Chemistry*, 99(4): 185–186, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dunne:2004:TFM

[DB04b] Lawrence J. Dunne and Erkki J. Brändas. Two-fluid model of superconducting condensates and spin gaps in d-wave high T_c cuprates from repulsive electronic correlations. *International Journal of Quantum Chemistry*, 99(5):798–804, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Daskalova:2006:CSE

[DB06] Lalka I. Daskalova and Ivan Binev. Computational study of energies and structures of 2,4,6-pyrimidinetrione and its anions. *International Journal of Quantum Chemistry*, 106(6): 1338–1345, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Derat:2006:RDS

[DBB+06] Etienne Derat, James Bouquant, Philippe Bertus, Jan Szymoniak, and Stéphane Humbel. Reactivity of dialkylzirconium species and solvent polarity. *International Journal of Quantum Chemistry*, 106(3):704–711, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

dAntuono:2006:TIC

[dBC06] Philippe d'Antuono, Edith Botek, and Benoît Champagne. Theoretical investigation of the chain length effects on the NMR chemical shifts of oligomers. *International Journal of Quantum Chemistry*, 106(15):3113–3121, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeMacedo:2005:HAR

[DBd05] L. G. M. De Macedo, R. C. Barbosa, and A. B. F. da Silva. Highly accurate relativistic universal Gaussian basis set for Dirac–Fock–Breit calculations. *International Journal of Quantum Chemistry*, 102(1):1–7, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeWaele:2005:ASE

[DBFP05] V. De Waele, G. Buntinx, J-P. Flament, and O. Poizat. Asymmetric structure for the excited S_1 state of 2,2′-bipyridine evidenced by picosecond time-resolved resonance Raman experiments and ab initio calculation. *International Journal of Quantum Chemistry*, 104(5):794–807, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolgov:2004:SNM

[DBG04] Eugeniy K. Dolgov, Vadim A. Bataev, and Igor A. Godunov. Structure of the nitrosomethane molecule (CH_3NO) in the ground electronic state: Testing of ab initio methods for the description of potential energy surface. *International Journal of Quantum Chemistry*, 96(3):193–201, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Demuth:2001:AWM

[DBHT01] Th. Demuth, L. Benco, J. Hafner, and H. Toulhoat. Adsorption of water in mordenite — An ab initio study. *International Journal of Quantum Chemistry*, 84(1):110–116, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84002446/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002446/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002446&PLACEBO=IE.pdf`.

deBoeij:2001:REO

[dBKS01] P. L. de Boeij, F. Kootstra, and J. G. Snijders. Relativistic effects in the optical response of HgSe by time-dependent density functionals theory. *International Journal of Quantum Chemistry*, 85(4–5):449–454, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dkhissi:2003:DFT

[DBL+03] A. Dkhissi, D. Beljonne, R. Lazzaroni, F. Louwet, L. Groenendaal, and J. L. Brédas. Density functional theory and Hartree–Fock studies of the geometric and electronic structure of neutral and doped ethylenedioxythiophene (EDOT) oligomers. *International Journal of Quantum Chemistry*, 91 (3):517–523, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DosSantos:2006:PCV

[DBLM06] A. S. Dos Santos, L. M. Brescansin, M.-T. Lee, and L. E. Machado. Photoionization of C_2F_4 in the VUV region. *International Journal of Quantum Chemistry*, 106(13):2552–2557, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deBrito:2005:DIB

[dBM05] Alexandre Naves de Brito and Geraldo Magela e Silva. Dynamic interaction between polarons and torsional vibrations in conjugated polymers. *International Journal of Quantum Chemistry*, 103(5):604–609, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolgov:2004:IDS

[DBPG04a] Eugeniy K. Dolgov, Vadim A. Bataev, Vladimir I. Pupyshev, and Igor A. Godunov. Ab initio description of the structure and dynamics of the nitrosomethane molecule in the first excited singlet and triplet electronic states. *International Journal of Quantum Chemistry*, 96(6):589–597, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolgov:2004:SVC

[DBPG04b] Eugeniy K. Dolgov, Vadim A. Bataev, Vladimir I. Pupyshev, and Igor A. Godunov. Structure and vibrations of the CF_3NO

molecule in the ground and lowest excited electronic states: A test of ab initio methods. *International Journal of Quantum Chemistry*, 100(4):509–518, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Du:2003:TIB

[DC03] Mao-Hua Du and Hai-Ping Cheng. Transparent interface between classical molecular dynamics and first-principles molecular dynamics. *International Journal of Quantum Chemistry*, 93(1):1–8, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Davidson:2005:SPA

[DC05] Ernest R. Davidson and Aurora E. Clark. Spin polarization and annihilation for radicals and diradicals. *International Journal of Quantum Chemistry*, 103(1):1–9, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DelRe:2006:MLA

[DC06a] Giuseppe Del Re and Amedeo Capobianco. MO-LCAO approach and ab initio computations. *International Journal of Quantum Chemistry*, 106(9):2014–2025, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dottorini:2006:PBL

[DC06b] T. Dottorini and P. Cozzini. Probing the binding of ligands to estrogen receptor using an empirical system. *International Journal of Quantum Chemistry*, 106(3):641–646, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeFazio:2003:OPD

[DCA03] Dario De Fazio, Simonetta Cavalli, and Vincenzo Aquilanti. Orthogonal polynomials of a discrete variable as expansion basis sets in quantum mechanics: Hyperquantization algorithm. *International Journal of Quantum Chemistry*, 93(2):91–111, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DaSilva:2008:IRP

[DCD08] Valdilei José Da Silva, Luiz Antônio S. Costa, and Hélio F. Dos Santos. Ab initio reaction path for cisplatin interaction

with L-cysteine and L-methionine. *International Journal of Quantum Chemistry*, 108(2):401–414, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Daul:2000:FCQ

[DCDW00] S. Daul, I. Ciofini, C. Daul, and Steven R. White. Full-CI quantum chemistry using the density matrix renormalization group. *International Journal of Quantum Chemistry*, 79(6):331–342, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72515274/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72515274/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72515274&PLACEBO=IE.pdf`.

Dong:2005:QPC

[DCLC05] Shi-Hai Dong, Chang-Yuan Chen, and M. Lozada-Cassou. Quantum properties of complete solutions for a new noncentral ring-shaped potential. *International Journal of Quantum Chemistry*, 105(5):453–462, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DaSilva:2008:MMI

[DCO+08] S. L. Da Silva, M. Comar, Jr., K. M. T. Oliveira, J. S. Chaar, E. R. M. Bezerra, A. K. Calgarotto, P. A. Baldasso, C. L. Veber, J. A. F. P. Villar, A. R. M. Oliveira, and S. Marangoni. Molecular modeling of the inhibition of enzyme PLA_2 from snake venom by dipyrone and 1-phenyl-3-methyl-5-pyrazolone. *International Journal of Quantum Chemistry*, 108(13):2576–2585, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deerfield:2001:MPZ

[DCP01] David W. Deerfield II, Charles W. Carter, Jr., and Lee G. Pedersen. Models for protein-zinc ion binding sites. II. The catalytic sites. *International Journal of Quantum Chemistry*, 83(3-4):150–165, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002601/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002601/FILE?TPL=ftx_start;`

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002601&PLACEBO=IE.pdf.

Dias:2006:INR

[DCP06] Lauro C. Dias, Jr., Rogério Custodio, and Francisco B. T. Pessine. Investigation of the Nile Red spectra by semi-empirical calculations and spectrophotometric measurements. *International Journal of Quantum Chemistry*, 106(13):2624–2632, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DaCostaSilva:2003:SVC

[DCTC03] Fabrício Da Costa Silva, Luiz A. F. Coelho, Frederico W. Tavares, and Márcio J. E. M. Cardoso. Shear viscosity calculated by perturbation theory and molecular dynamics for dense fluids. *International Journal of Quantum Chemistry*, 95(2):79–87, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Daul:2003:INP

[DCW03] Claude A. Daul, Ilaria Ciofini, and Valery Weber. Investigation of NLO properties of substituted (M)-tetrathia-[7]-helicenes by semiempirical and DFT methods. *International Journal of Quantum Chemistry*, 91(3):297–302, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dykstra:2000:ESO

[DD00] Clifford E. Dykstra and Ernest R. Davidson. Enhanced second-order treatment of electron pair correlation. *International Journal of Quantum Chemistry*, 78(4):226–236, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72000076/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72000076/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72000076&PLACEBO=IE.pdf.

DelNero:2003:IES

[DD03] Jordan Del Nero and Celso P. De Melo. Investigation of the excited states of resveratrol and related molecules. *International Journal of Quantum Chemistry*, 95(3):213–218, ????

2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

dePinhoRibeiroMoreira:2004:PAE

[dD04] Ibério de Pinho Ribeiro Moreira and Roberto Dovesi. Periodic approach to the electronic structure and magnetic coupling in $KCuF_3$, K_2CuF_4, and $Sr_2CuO_2Cl_2$ low-dimensional magnetic systems. *International Journal of Quantum Chemistry*, 99 (5):805–823, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeSantana:2005:GFC

[DD05] O. L. De Santana and A. A. S. Da Gama. Green's function calculation of through-bond electronic coupling in donor–bridge–acceptor model systems II: Importance factors applied to atomic sites. *International Journal of Quantum Chemistry*, 102(3):265–274, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Darafsheh:2007:NGT

[DDA07] Mohammad Reza Darafsheh, Arash Darafsheh, and Ali Reza Ashrafi. Nonrigid group theory for 1,3,5-trimethylbenzene. *International Journal of Quantum Chemistry*, 107(2):340–344, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dufty:2009:QPD

[DDBF09] James Dufty, Sandipan Dutta, Michael Bonitz, and Alexei Filinov. Quantum potential for diffraction and exchange effects. *International Journal of Quantum Chemistry*, 109(13):3082–3092, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DosSantos:2000:QMI

[DDD+00] Hélio F. Dos Santos, Luiz F. C. De Oliveira, Sócrates O. Dantas, Paulo S. Santos, and Wagner B. De Almeida. Quantum mechanical investigation of the tautomerism in the azo dye Sudan III. *International Journal of Quantum Chemistry*, 80(4–5):1076–1086, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505380/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505380/FILE?TPL=ftx_start;`

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505380&PLACEBO=IE.pdf.

DeOliveira:2002:SEP

[DDD02] Marcos A. De Oliveira, Hélio F. Dos Santos, and Wagner B. De Almeida. Structure and electronic properties of cyanothiophene derivatives: A theoretical ab initio and DFT study. *International Journal of Quantum Chemistry*, 90(2):603–610, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Duani:2003:IQS

[DDD03] Helena Duani, Hélio A. Duarte, and Wagner B. De Almeida. Investigation of the quality of standard sulfur basis sets for molecules using a new generator coordinate method approach: Application to 2,2′-bithiophene. *International Journal of Quantum Chemistry*, 95(2):194–204, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dehareng:2000:ISO

[DDM00] Dominique Dehareng, Georges Dive, and Alec Moradpour. Ab initio study of organic mixed valency. *International Journal of Quantum Chemistry*, 76(4):552–573, February 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70000683/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000683/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000683&PLACEBO=IE.pdf.

De:2007:PPA

[DDP+07] Senjuti De, Michael G. B. Drew, David W. Price, Samik Nag, and Dipankar Datta. Protonation of phenylboronic acid: Comparison of G3B3 and G2MP2 methods. *International Journal of Quantum Chemistry*, 107(1):182–188, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeMCarneiro:2003:HEH

[DDT+03] José Walkimar De M.Carneiro, Jacques F. Dias, José Glauco R. Tostes, Peter R. Seidl, and Carlton A. Taft. Hyperconjugation effects of hydroxyl and amine groups on chemical shifts of neighboring carbon nuclei. *International Journal*

of Quantum Chemistry, 95(3):322–328, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeAraujo:2006:SER

[DDT06] M. T. De Araujo, J. W. De M.Carneiro, and A. G. Taranto. Solvent effects on the relative stability of radicals derived from artemisinin: DFT study using the PCM/COSMO approach. *International Journal of Quantum Chemistry*, 106(13):2804–2810, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deerfield:2006:QCS

[DDW+06] David Deerfield II, Charles H. Davis, Troy Wymore, Darrel W. Stafford, and Lee G. Pedersen. Quantum chemical study of the mechanism of action of vitamin K epoxide reductase (VKOR). *International Journal of Quantum Chemistry*, 106(14):2944–2952, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deb:2008:EVB

[Deb08] B. M. Deb. Erratum: Vikas, B. M. Deb: Ground-state electronic energies and densities of atomic systems in strong magnetic fields through a time-dependent hydrodynamical equation. *International Journal of Quantum Chemistry*, 108(4): 820, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [VD04].

Defranceschi:2000:I

[Def00] M. Defranceschi. Introduction. *International Journal of Quantum Chemistry*, 77(5):v, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000340/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000340/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000340&PLACEBO=IE.pdf`.

Deineka:2004:SMH

[Dei04] G. B. Deineka. Simple model of H^+ and H(1s) collision: Application to charge transfer. *International Journal of Quantum Chemistry*, 100(4):677–680, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deineka:2006:MHH

[Dei06] G. B. Deineka. 2D model of H^+ and H(1s) collision: Application to charge transfer. *International Journal of Quantum Chemistry*, 106(10):2262–2267, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deleuze:2003:ISC

[Del03] Michael S. Deleuze. The issues of size and charge consistency and the implications of translation symmetry in advanced Green's function theories. *International Journal of Quantum Chemistry*, 93(3):191–211, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Das:2002:ESA

[DEN02] A. K. Das, M. Ehara, and H. Nakatsuji. Excited states of Na and Al iso-electronic ions: Symmetry adapted cluster-configuration interaction study. *International Journal of Quantum Chemistry*, 87(2):81–88, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85515904/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85515904/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85515904&PLACEBO=IE.pdf`.

Denis:2009:TIS

[Den09] Pablo A. Denis. Theoretical investigation of the stability, electronic and magnetic properties of thiolated single-wall carbon nanotubes. *International Journal of Quantum Chemistry*, 109 (4):772–781, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolbeault:2003:VMR

[DES03] Jean Dolbeault, Maria J. Esteban, and Eric Séré. A variational method for relativistic computations in atomic and molecular physics. *International Journal of Quantum Chemistry*, 93(3):149–155, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dhouib:2002:GTI

[DETA02] A. Dhouib, K. Essalah, B. Tangour, and M. Abderraba. Gyroscopic tensor ab initio calculation of the molecular crystals:

$(Mo_6\ X_{14})^{2-}\ Y^{-}\ (TTF^{+})_3$ (X = Br, Cl and Y = Br, Cl, I). *International Journal of Quantum Chemistry*, 87(4):220–224, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89016146/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89016146/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89016146&PLACEBO=IE.pdf`.

Deumens:2000:BR

[Deu00] Erik Deumens. Book review. *International Journal of Quantum Chemistry*, 77(4):797, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70500244/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70500244/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70500244&PLACEBO=IE.pdf`.

Deumens:2006:BR

[Deu06] Erik Deumens. Book review. *International Journal of Quantum Chemistry*, 106(9):2169, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dai:2007:TSR

[DF07] Guo-Liang Dai and Kang-Nian Fan. Theoretical study of the reaction of Cr^{+} with SCO in gas phase. *International Journal of Quantum Chemistry*, 107(7):1598–1607, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deOliveiraNeto:2008:CLE

[dFGM08a] Pedro Henrique de Oliveira Neto, Wiliam Ferreira da Cunha, Ricardo Gargano, and Geraldo Magela e Silva. Chain length effects on nonlinear excitation transitions in *trans*-polyacetylene. *International Journal of Quantum Chemistry*, 108(13):2507–2511, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deOliveiraNeto:2008:DPI

[dFGM08b] Pedro Henrique de Oliveira Neto, Wiliam Ferreira da Cunha, Ricardo Gargano, and Geraldo Magela e Silva. Dynamics of

photoexcitations with interchain coupling in conjugated polymers. *International Journal of Quantum Chemistry*, 108(13): 2442–2447, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Delhalle:2002:ECE

[DFH02a] Joseph Delhalle, Joseph G. Fripiat, and Frank E. Harris. Exchange contributions in the electronic structure of systems with 1D-periodicity: Importance and computation. *International Journal of Quantum Chemistry*, 90(2):587–593, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Delhalle:2002:VPF

[DFH02b] Joseph Delhalle, Joseph G. Fripiat, and Frank E. Harris. Virtues and potentialities of the Fourier transform method for electronic structure calculations of 1-D periodic systems at the Hartree–Fock level and beyond. *International Journal of Quantum Chemistry*, 90(4-5):1326–1333, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dorfman:2002:IMB

[DFM+02] Simon Dorfman, David Fuks, Luiz A. C. Malbouisson, Kleber C. Mundim, and Donald E. Ellis. Influence of many-body interactions on resistance of a grain boundary with respect to a sliding shift. *International Journal of Quantum Chemistry*, 90(4-5):1448–1456, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolgounitcheva:2008:VSR

[DFMZO08] O. Dolgounitcheva, R. Flores-Moreno, V. G. Zakrzewski, and J. V. Ortiz. Virtual space reduction in quasi-particle electron propagator calculations: Applications to polycyclic aromatic hydrocarbons. *International Journal of Quantum Chemistry*, 108(15):2862–2869, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dinh:2007:SCE

[DFRS07] P. M. Dinh, F. Fehrer, P.-G. Reinhard, and E. Suraud. Size and charge effects on the deposition of Na on Ar clusters. *International Journal of Quantum Chemistry*, 107(14):2828–2837, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolin:2007:SHD

[DFT+07] S. P. Dolin, I. S. Flyagina, M. V. Tremasova, T. Yu. Mikhailova, A. B. Gavrilyuk, and A. A. Levin. The study of H/D isotope-dependent order–disorder transition in crystalline α-chromous acid using quantum-chemical modeling. *International Journal of Quantum Chemistry*, 107(13):2409–2416, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Du:2004:DFT

[DFZ04] Dongmei Du, Aiping Fu, and Zhengyu Zhou. Density functional theory study of formamide–formamidic acid tautomerization. *International Journal of Quantum Chemistry*, 99(1): 1–10, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Du:2005:TSC

[DFZ05] Dongmei Du, Aiping Fu, and Zhengyu Zhou. Theoretical study of chiral discrimination in the hydrogen bonding complexes of the hydrazine dimer. *International Journal of Quantum Chemistry*, 101(3):340–347, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Delaney:2004:QET

[DG04] P. Delaney and J. C. Greer. Quantum electronic transport in a configuration interaction basis. *International Journal of Quantum Chemistry*, 100(6):1163–1169, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Diaz-Garcia:2008:MEA

[DGC08] C. Díaz-García and S. A. Cruz. Many-electron atom confinement by a penetrable spherical box. *International Journal of Quantum Chemistry*, 108(9):1572–1588, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeOliveira:2005:MDS

[DGD+05] César Augusto Fernandes De Oliveira, Cristiano Ruch Werneck Guimarães, Heloisa De Mello, Aurea Echevarria, and Ricardo Bicca De Alencastro. A molecular dynamics study on liquid 1-octanol. Part 3. Evaluating octanol/water partition coefficients of novel thrombin inhibitors via free-energy perturbations. *International Journal of Quantum Chemistry*, 102

(5):542–553, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deng:2009:RSH

[DGG09] Jia Deng, Andrew T. B. Gilbert, and Peter M. W. Gill. Rydberg states of the helium atom. *International Journal of Quantum Chemistry*, 109(9):1915–1919, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Devarajan:2009:REC

[DGLM09] Ajitha Devarajan, Alexander Gaenko, Roland Lindh, and Per-Åke Malmqvist. Role of electronic curve crossing of benzene S_1 state in the photodissociation of aryl halides, effect of fluorination: RASSI-SO MS-CASPT2 study. *International Journal of Quantum Chemistry*, 109(9):1962–1974, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeLaLande:2008:HOC

[DGP08] A. De La Lande, H. Gérard, and O. Parisel. How to optimize a C — H cleavage with a mononuclear copper–dioxygen adduct? *International Journal of Quantum Chemistry*, 108 (11):1898–1904, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ding:2009:ISS

[DGQT09] Yuqi Ding, Peng Gao, Lichao Qin, and Qiwen Teng. Investigation on stabilities and spectroscopy of $C_{80}O_2$ based on C_{80} (D_{5d}) using density functional theory. *International Journal of Quantum Chemistry*, 109(4):693–700, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Das:2000:RAC

[DGR+00] A. K. Das, T. K. Ghosh, D. Ray, T. K. Mukherjee, and P. K. Mukherjee. Radial and angular correlations in doubly excited states: A time-dependent perturbation approach. *International Journal of Quantum Chemistry*, 76(1):99–104, January 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503199/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503199/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503199&PLACEBO=IE.pdf`.

Derzi:2008:SPD

[DGRB08] Afaf R. Al Derzi, Adriana Gregušová, Keith Runge, and Rodney J. Bartlett. Structure and properties of disiloxane: An ab initio and post-Hartree–Fock study. *International Journal of Quantum Chemistry*, 108(12):2088–2096, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deGraaf:2006:AZF

[dGS06] Coen de Graaf and Carmen Sousa. Assessing the zero-field splitting in magnetic molecules by wave function-based methods. *International Journal of Quantum Chemistry*, 106(12): 2470–2478, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dinadayalane:2007:CIT

[DGSD07] T. C. Dinadayalane, Leonid Gorb, Tomekia Simeon, and Helena Dodziuk. Cumulative π-π interaction triggers unusually high stabilization of linear hydrocarbons inside the single-walled carbon nanotube. *International Journal of Quantum Chemistry*, 107(12):2204–2210, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deng:2004:CES

[DH04a] Yuanjian Deng and Ming-Ju Huang. Capillary electrophoretic separation and theoretical study of inclusion complexes of sulfobutyl ether β-cyclodextrin with estrogens. *International Journal of Quantum Chemistry*, 100(5):746–752, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Driebe:2004:EDC

[DH04b] Dean J. Driebe and Hiroshi H. Hasegawa. Ensemble dynamics of chaos. *International Journal of Quantum Chemistry*, 98 (2):131–137, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeMacedo:2006:ARP

[DHCD06] Luiz Guilherme M. De Macedo, Roberto L. A. Haiduke, Moacyr Comar, Jr., and Albérico B. F. Da Silva. Adapted relativistic prolapse-free Gaussian basis sets for closed shell atoms up to nobelium and to be used with the uniform sphere nucleus model. *International Journal of Quantum Chemistry*,

106(13):2790–2803, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deHaan:2004:DEQ

[dHG04] M. de Haan and C. D. George. Dissipative extension of quantum mechanics. *International Journal of Quantum Chemistry*, 98(2):112–117, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ding:2006:ELN

[DHZ06] Fu-Jiang Ding, Yun-Qing He, and Ke-Qing Zhao. Extrapolation of the linear and nonlinear polarizabilities from ab initio finite oligomer calculations. *International Journal of Quantum Chemistry*, 106(8):1934–1942, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dehestani:2005:EDR

[DI05] M. Dehestani and R. Islampour. Effects of distortion–rotation of potential energy surfaces on absorption and resonance Raman cross sections of *trans*-stilbene molecule. *International Journal of Quantum Chemistry*, 103(2):119–126, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Diez:2000:DFS

[Die00] Reinaldo Pis Diez. Density functional study of small molybdenum clusters. *International Journal of Quantum Chemistry*, 76(1):105–112, January 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503200/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503200/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503200&PLACEBO=IE.pdf`.

Doruker:2002:IFD

[DJNH02] Pemra Doruker, Robert L. Jernigan, Isabelle Navizet, and Rigoberto Hernandez. Important fluctuation dynamics of large protein structures are preserved upon coarse-grained renormalization. *International Journal of Quantum Chemistry*, 90(2):822–837, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Daoud:2003:TAF

[DK03] M. Daoud and M. Kibler. Two approaches to fractional supersymmetrical quantum mechanics. *International Journal of Quantum Chemistry*, 91(4):551–565, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Drougas:2004:QMS

[DK04] Evangelos Drougas and Agnie M. Kosmas. Quantum mechanical studies of isomeric and conformeric structures of methylchloro-peroxide. *International Journal of Quantum Chemistry*, 98(3):335–341, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DelValle:2000:SCF

[DKC00] Juan Carlos Del Valle, Michael Kasha, and Javier Catalán. The singular coincidence of fluorescence spectra of the anionic and cationic species formed by the respective deprotonated and protonated pyrido-pyrrolo bases. *International Journal of Quantum Chemistry*, 77(1):118–127, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004252/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004252/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004252&PLACEBO=IE.pdf`.

DYachkov:2007:QCS

[DKD+07] P. N. D'Yachkov, N. V. Kharchevnikova, A. V. Dmitriev, A. V. Kuznetsov, and V. V. Poroikov. Quantum chemical simulation of cytochrome P450 catalyzed aromatic oxidation: Metabolism, toxicity, and biodegradation of benzene derivatives. *International Journal of Quantum Chemistry*, 107(13): 2454–2478, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dkhissi:2008:EEC

[Dkh08] Ahmed Dkhissi. Evaluation of exchange-correlation functionals in comparison to B3LYP for the description of silicon and Cu-doped silicon clusters. *International Journal of Quantum Chemistry*, 108(5):996–1003, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Delchev:2004:SSC

[DKM+04] Ya. I. Delchev, A. I. Kuleff, Tz. Mineva, F. Zahariev, and J. Maruani. Strutinsky's shell-correction method in the extended Kohn–Sham scheme for the investigation of binding energies of atoms and cations in the ground state. *International Journal of Quantum Chemistry*, 99(4):265–276, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolin:2006:LTS

[DKP+06] S. P. Dolin, A. A. Khrulev, E. V. Polyakov, T. Yu. Mikhailova, and A. A. Levin. Low-temperature structural phase transitions in crystalline bromo and iodo 9-hydroxyphenalenone derivatives: Quantum chemistry employment. *International Journal of Quantum Chemistry*, 106(10):2297–2304, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Drozdzewski:2004:SMI

[DKR04] Piotr M. Drożdżewski, Ewa Kordon, and Szczepan Roszak. Studies of metal isotope and deuteration effects in vibrational spectra of palladium(II) complex with histamine. *International Journal of Quantum Chemistry*, 96(4):355–364, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Day:2005:PGM

[DKS05] Mary Beth Day, Karl N. Kirschner, and George C. Shields. Pople's Gaussian-3 model chemistry applied to an investigation of $(H_2O)_8$ water clusters. *International Journal of Quantum Chemistry*, 102(5):565–572, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dulak:2009:LOF

[DKW09] Marcin Dułak, Jakub W. Kamiński, and Tomasz A. Wesołowski. Linearized orbital-free embedding potential in self-consistent calculations. *International Journal of Quantum Chemistry*, 109(9):1886–1897, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeSilva:2004:CSF

[DKWP04] S. A. De Silva, M. L. Kasner, M. A. Whitener, and S. L. Pathirana. A computational study of a fluorescent photoinduced electron transfer (PET) sensor for cations. *International Journal of Quantum Chemistry*, 100(5):753–757, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dong:2002:LOMa

[DL02] Shi-Hai Dong and R. Lemus. Ladder operators for the modified Pöschl–Teller potential. *International Journal of Quantum Chemistry*, 86(3):265–272, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86011318/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86011318/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86011318&PLACEBO=IE.pdf`.

Defranceschi:2003:PSN

[DL03] M. Defranceschi and Cl. Le Bris. Preface: Some numerical methods and modeling issues in quantum chemistry. *International Journal of Quantum Chemistry*, 93(2):49, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DaCosta:2006:EBE

[DL06] R. F. Da Costa and M. A. P. Lima. Excitation of the $a^1\ \Pi_g$ and $B^3\ \Pi_g$ electronic states of the nitrogen molecule by electron impact. *International Journal of Quantum Chemistry*, 106 (13):2664–2676, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deLara-Castells:2007:DHC

[dLCPLD+07] M. P. de Lara-Castells, R. Prosmiti, D. López-Durán, G. Delgado-Barrio, P. Villarreal, F. A. Gianturco, and J. Jellinek. Doped helium clusters analyzed through quantum chemistry methods. *International Journal of Quantum Chemistry*, 107(14):2902–2921, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deLazaro:2008:CND

[dLCRF+08] Sergio de Lazaro, Francinete Ramos Campos, Edson Rodrigues-Fo, Andersson Barison, Cristina Daolio, Antonio G. Ferreira, Victor Polo, Elson Longo, and Juan Andrés. Combined ^{13}C NMR and DFT/GIAO studies of the polyketides Aurasperone A and Fonsecinone A. *International Journal of Quantum Chemistry*, 108(13):2408–2416, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dong:2007:HST

[DLCY+07] Shi-Hai Dong, M. Lozada-Cassou, Jiang Yu, Felipe Jiménez-Ángeles, and A. L. Rivera. Hidden symmetries and thermodynamic properties for a harmonic oscillator plus an inverse square potential. *International Journal of Quantum Chemistry*, 107(2):366–371, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dong:2002:LOMb

[DLF02] Shi-Hai Dong, R. Lemus, and A. Frank. Ladder operators for the Morse potential. *International Journal of Quantum Chemistry*, 86(5):433–439, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86011230/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86011230/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86011230&PLACEBO=IE.pdf`.

Dungsrikaew:2004:CMP

[DLHP04] Virasak Dungsrikaew, Jumras Limtrakul, Kersti Hermansson, and Michael Probst. Comparison of methods for point-charge representation of electrostatic fields. *International Journal of Quantum Chemistry*, 96(1):17–22, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolg:2000:PRD

[DLK00] M. Dolg, W. Liu, and S. Kalvoda. Performance of relativistic density functional and ab initio pseudopotential approaches for systems with high-spin multiplicities: Gadolinium diatomics GdX (X = H, N, O, F, P, S, Cl, Gd). *International Journal of Quantum Chemistry*, 76(3):359–370, January 20, 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000279/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000279/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000279&PLACEBO=IE.pdf`.

Dolin:2002:QCF

[DLM+02] S. P. Dolin, A. A. Levin, T. Yu. Mikhailova, M. V. Solin, and L. I. Trakhtenberg. Quantum chemistry of ferroelectric solids: Electronic structures and peculiar behavior of zero-dimensional $K_3H(SO_4)_2$-like materials. *International Journal of Quantum Chemistry*, 88(4):463–471, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolin:2004:DTP

[DLM+04a] S. P. Dolin, A. A. Levin, T. Y. Mikhailova, M. V. Solin, E. V. Polyakov, and N. S. Strokach. Deuteron tunneling and phase transition in $M_3D(AO_4)_2$ antiferroelectrics. *International Journal of Quantum Chemistry*, 100(4):589–594, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolin:2004:QCA

[DLM+04b] S. P. Dolin, A. A. Levin, T. Yu. Mikhailova, M. V. Solin, N. S. Strokach, and N. I. Kirillova. Quantum chemistry application to H-bonded ferroelectrics via mean field theory involving proton correlation. *International Journal of Quantum Chemistry*, 96(3):247–254, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolin:2005:PHP

[DLM+05] S. P. Dolin, A. A. Levin, T. Yu. Mikhailova, M. V. Solin, A. B. Gavriluyk, and E. V. Polyakov. Pseudospin Hamiltonian parameters evaluated with regard to alkali metal ions in $K_3(H/D)(SO_4)_2$ materials. *International Journal of Quantum Chemistry*, 104(2):197–202, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

delaPortilla:2000:TSI

[dlPCLG+00] C. de la Portilla, A. Cruz, H. Luna-García, E. Poulain, V. Bertin, and S. Castillo. Theoretical study of interaction of small clusters of IrPt with H_2. *Interna-*

tional Journal of Quantum Chemistry, 80(4–5):657–663, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505385/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505385/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505385&PLACEBO=IE.pdf.

OShea:2003:DSE

[dlPOPP03] V. A. de la Peña O'Shea, A. Pardo, and J. M. L. Poyato. DFT study of electronic spectra and excited-state properties of some 1,8-naphthalimide derivatives. *International Journal of Quantum Chemistry*, 91(3):446–450, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deng:2004:QSE

[DLTW04] Ping Deng, Lai-Cai Li, An-Min Tian, and Ning-Bew Wong. Quantum study on the electrocyclic reactions of $CH_2CHCHCHX$ (X = H, F, Cl). *International Journal of Quantum Chemistry*, 100(3):288–292, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deakyne:2003:RBD

[DLZ+03] Carol A. Deakyne, Le Li, Wencui Zheng, Danyu Xu, and Joel F. Liebman. Regularities in the bond dissociation enthalpies of molecules of types AB and BAB: Energetics of 10- and 16-valence electron ions of groups 13, 15, and 16. *International Journal of Quantum Chemistry*, 95(6):713–718, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dobrowolski:2000:CCH

[DM00] Jan Cz. Dobrowolski and Aleksander P. Mazurek. C_{60} Cyclized hook-and-ladder carbynes. *International Journal of Quantum Chemistry*, 80(4–5):1087–1098, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505392/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505392/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505392&PLACEBO=IE.pdf.

Datta:2002:RDP

[DM02a] Sambhu N. Datta and Anirban Misra. Relativistic dynamics of positronium atom in uniform magnetic field. *International Journal of Quantum Chemistry*, 90(2):812–821, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Donoso:2002:CTB

[DM02b] Arnaldo Donoso and Craig C. Martens. Classical trajectory-based approaches to solving the quantum Liouville equation. *International Journal of Quantum Chemistry*, 90(4-5):1348–1360, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DaSilvaPinheiro:2003:DPB

[DM03] Cleber Da Silva Pinheiro and Geraldo Magela e Silva. Dynamics of polarons and bipolarons with interchain coupling in conjugated polymers. *International Journal of Quantum Chemistry*, 95(2):153–158, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dunne:2004:SWD

[DM04] Lawrence J. Dunne and John N. Murrell. Simple wavefunctions for dipositronium and the relationship between this species and the hydrogen molecule. *International Journal of Quantum Chemistry*, 96(5):512–517, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Datta:2008:CSF

[DM08a] Dipayan Datta and Debashis Mukherjee. A compact spin-free combinatoric open-shell coupled cluster theory applied to single-reference doublets. *International Journal of Quantum Chemistry*, 108(12):2211–2222, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DiLeo:2008:WFT

[DM08b] Julio Marañón Di Leo and Julio Marañón. Water flow through nanopore. *International Journal of Quantum Chemistry*, 108 (10):1623–1628, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dogaru:2009:IFF

[DMG09] Daniela Dogaru, Stefan Motiu, and Valentin Gogonea. Inactivation of [Fe Fe]-hydrogenase by O_2. Thermodynamics and frontier molecular orbitals analyses. *International Journal of Quantum Chemistry*, 109(4):876–889, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeMacedo:2005:NAG

[DMH+05] L. G. M. De Macedo, N. H. Morgon, R. L. A. Haiduke, R. C. Barbosa, and A. B. F. Da Silva. New adapted Gaussian basis sets for the relativistic closed shell atoms from helium to barium generated with the generator coordinate Dirac–Fock method. *International Journal of Quantum Chemistry*, 103 (5):523–528, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Duque:2002:CSC

[DMM+02] F. Duque, A. Mañanes, L. M. Molina, M. J. López, and J. A. Alonso. Computer simulation of cluster assembling. *International Journal of Quantum Chemistry*, 86(2):226–238, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86510683/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86510683/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86510683&PLACEBO=IE.pdf`.

Dardenne:2000:MIS

[DMMV00] L. E. Dardenne, N. Makiuchi, L. A. C. Malbouisson, and J. D. M. Vianna. Multiplicity, instability, and SCF convergence problems in Hartree–Fock solutions. *International Journal of Quantum Chemistry*, 76(5):600–610, February 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000581/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000581/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000581&PLACEBO=IE.pdf`.

Datta:2000:HSB

[DMV00] Sambhu N. Datta, Anirban Misra, and R. Vinodhkumar. High-spin behavior of molecular crystals and extendedπ sys-

tems. *International Journal of Quantum Chemistry*, 79 (5):308–324, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72512627/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72512627/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72512627&PLACEBO=IE.pdf`.

Douvropoulos:2006:SPI

[DN06] Theodosios G. Douvropoulos and Cleanthes A. Nicolaides. Semiclassical path integral theory of a double-well potential in an electric field. *International Journal of Quantum Chemistry*, 106(5):1032–1042, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dong:2007:TAF

[DNC07] Li-Qing Dong, Kai Niu, and Shu-Lin Cong. Theoretical analysis of femtosecond fluorescence depletion spectra and vibrational relaxations of dye oxazine 750 and rhodamine 700 molecules in acetone solution. *International Journal of Quantum Chemistry*, 107(5):1205–1214, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Drakova:2006:TTD

[DND06] D. Drakova, M. Nedjalkova, and G. Doyen. Theory of tip-dependent imaging of adsorbates in the STM: CO on Cu(111). *International Journal of Quantum Chemistry*, 106(6):1419–1431, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeAndrade:2008:ABS

[DNM+08] M. D. De Andrade, M. A. C. Nascimento, K. C. Mundim, A. M. C. Sobrinho, and L. A. C. Malbouisson. Atomic basis sets optimization using the generalized simulated annealing approach: New basis sets for the first row elements. *International Journal of Quantum Chemistry*, 108(13):2486–2498, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeAndrade:2006:GAA

[DNMM06] Micael Dias De Andrade, Marco Nascimento, Kleber Mundim, and Luiz Malbouisson. GSA algorithm applied to electronic

structure II: UHF-GSA method. *International Journal of Quantum Chemistry*, 106(13):2700–2705, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dedachi:2006:CTS

[DNN+06] Kenichi Dedachi, Takayuki Natsume, Taisuke Nakatsu, Yasuyuki Ishikawa, and Noriyuki Kurita. Charge transfer in single- and double-strand DNAs: Theoretical analysis based on molecular orbital method. *International Journal of Quantum Chemistry*, 106(15):3270–3277, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deOliveira:2008:MPC

[dOEG+08] Heibbe C. B. de Oliveira, Cristiano S. Esteves, Ricardo Gargano, Marco A. Chaer Do Nascimento, Luiz A. C. Malbouisson, and Kleber C. Mundim. Molecular properties calculations using the q-integral method. *International Journal of Quantum Chemistry*, 108(13):2540–2549, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dong:2009:NQR

[Don09] Shi-Hai Dong. A new quantization rule to the energy spectra for modified hyperbolic-type potentials. *International Journal of Quantum Chemistry*, 109(4):701–707, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Douvropoulos:2007:PWF

[Dou07] Theodosios G. Douvropoulos. Positive width function and energy indeterminacies in ammonia molecule. *International Journal of Quantum Chemistry*, 107(8):1673–1687, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Datta:2006:SCH

[DP06] Ayan Datta and Swapan K. Pati. Stability of cyclic $(H_2O)_n$ clusters within molecular solids: Role of aromaticity. *International Journal of Quantum Chemistry*, 106(7):1697–1702, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dunn:2004:AGG

[DPS04] Meghan E. Dunn, Emma K. Pokon, and George C. Shields. The ability of the Gaussian-2, Gaussian-3, Complete Basis Set–QB3, and Complete Basis Set–APNO model chemistries to model the geometries of small water clusters. *International Journal of Quantum Chemistry*, 100(6):1065–1070, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deleuze:2000:CMR

[DPW00] Michael S. Deleuze, Barry T. Pickup, and David J. Wilton. Calculation of molecular response properties with the second-order coupled perturbed electron propagator. *International Journal of Quantum Chemistry*, 77(3):625–640, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004058/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004058/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004058&PLACEBO=IE.pdf`.

Davis:2004:MST

[DQZ04] Steven R. Davis, Changyong Qin, and Zhendong Zhao. MCSCF study of the thermal isomerization of tricyclo[2.1.0.$0^{2,5}$] pentane to 1,3-cyclopentadiene. *International Journal of Quantum Chemistry*, 96(4):411–415, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Diaz-Rivera:2004:BR

[DR04] L. M. Diaz-Rivera. Book review. *International Journal of Quantum Chemistry*, 97(6):1012–1013, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dias:2008:ICR

[DR08] Roberta P. Dias and Willian R. Rocha. Insertion and carbonylation reactions of styrene promoted by [$HRh(CO)_x$ — $(PMe_3)_{3-x}$] ($x = 1, 2$) compounds: A theoretical investigation. *International Journal of Quantum Chemistry*, 108(13): 2358–2373, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Daul:2005:DSM

[DRD+05] Claude Daul, Cédrick Rauzy, Silvio Decurtins, Patrick Franz, and Andreas Hauser. DFT study of mixed-valent Mn(II/III) hexacyanide clusters. *International Journal of Quantum Chemistry*, 101(6):753–760, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dreyer:2005:DFT

[Dre05] Jens Dreyer. Density functional theory simulations of two-dimensional infrared spectra for hydrogen-bonded acetic acid dimers. *International Journal of Quantum Chemistry*, 104 (5):782–793, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dronskowski:2004:IFA

[Dro04] Richard Dronskowski. Itinerant ferromagnetism and antiferromagnetism from the perspective of chemical bonding. *International Journal of Quantum Chemistry*, 96(2):89–94, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pita:2008:SMD

[dRPFCP08] Samuel Silva da Rocha Pita, Tácio Vinício Amorim Fernandes, Ernesto Raul Caffarena, and Pedro Geraldo Pascutti. Studies of molecular docking between fibroblast growth factor and heparin using generalized simulated annealing. *International Journal of Quantum Chemistry*, 108(13):2608–2614, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Darhovskii:2002:HMM

[DRPT02] M. B. Darhovskii, M. G. Razumov, I. V. Pletnev, and A. L. Tchougréeff. Hybrid molecular mechanics: For effective crystal field method for modeling potential energy surfaces of transition metal complexes. *International Journal of Quantum Chemistry*, 88(5):588–605, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Damjanovic:2000:EET

[DRS00] Ana Damjanović, Thorsten Ritz, and Klaus Schulten. Excitation energy trapping by the reaction center of *Rhodobacter Sphaeroides*. *International Journal of Quantum Chemistry*,

77(1):139–151, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70004254/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004254/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004254&PLACEBO=IE.pdf.

Dimitrova:2003:IPV

[DS03] Yordanka Dimitrova and Bistra A. Stamboliyska. Ab initio prediction of the vibrational spectra of the hydrogen-bonded complexes between CO and $HONO_2$. *International Journal of Quantum Chemistry*, 92(6):506–515, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Difley:2006:RAE

[DS06] Seth Difley and Jack Simons. Role of angular electron pair correlation in stabilizing C. *International Journal of Quantum Chemistry*, 106(2):507–513, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Duret:2007:WAD

[DS07] Stefan Duret and Hassan Safouhi. The W algorithm and the D transformation for the numerical evaluation of three-center nuclear attraction integrals. *International Journal of Quantum Chemistry*, 107(5):1060–1066, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Daniels:2000:GOK

[DSFS00] Andrew D. Daniels, Gustavo E. Scuseria, Ödön Farkas, and H. Bernhard Schlegel. Geometry optimization of Kringle 1 of plasminogen using the PM3 semiempirical method. *International Journal of Quantum Chemistry*, 77(1):82–89, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70004297/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004297/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004297&PLACEBO=IE.pdf.

Doll:2001:AHF

[DSH01] K. Doll, V. R. Saunders, and N. M. Harrison. Analytical Hartree–Fock gradients for periodic systems. *In-*

ternational Journal of Quantum Chemistry, 82(1):1–13, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76510762/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76510762/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76510762&PLACEBO=IE.pdf`.

Dinadayalane:2006:CTS

[DSL06] T. C. Dinadayalane, G. Narahari Sastry, and Jerzy Leszczynski. Comprehensive theoretical study towards the accurate proton affinity values of naturally occurring amino acids. *International Journal of Quantum Chemistry*, 106(14):2920–2933, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dong:2005:DEC

[DSLC05] Shi-Hai Dong, Guo-Hua Sun, and M. Lozada-Cassou. Dirac equation with a Coulomb plus scalar potential in $D + 1$ dimensions. *International Journal of Quantum Chemistry*, 102 (2):147–157, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

dosSantos:2008:SEO

[dSNBG08] Daniel J. V. A. dos Santos, Ana S. Newton, Raul Bernardino, and Rita C. Guedes. Substituent effects on O — H and S — H bond dissociation enthalpies of disubstituted phenols and thiophenols. *International Journal of Quantum Chemistry*, 108(4):754–761, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Davydova:2004:CEI

[DST+04] E. I. Davydova, T. N. Sevastianova, A. Y. Timoshkin, A. V. Suvorov, and G. Frenking. Chelate effect: The importance of reorganization energy. *International Journal of Quantum Chemistry*, 100(4):419–425, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Duan:2000:DMI

[DSW00] Guilin Duan, Vedene H. Smith, Jr., and Donald F. Weaver. A data mining and ab initio study of the interaction between the aromatic and backbone amide groups in proteins. *International Journal of Quantum Chemistry*, 80(1):44–60,

???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72515502/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72515502/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72515502&PLACEBO=IE.pdf.

Duan:2002:DMI

[DSW02] Guilin Duan, Vedene H. Smith, Jr., and Donald F. Weaver. Data mining, ab initio, and molecular mechanics study on conformation of phenylalanine and its interaction with neighboring backbone amide groups in proteins. *International Journal of Quantum Chemistry*, 90(2):669–683, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Du:2008:CAC

[DSW08] Jiguang Du, Xiyuan Sun, and Hongyan Wang. The confirmation of accurate combination of functional and basis set for transition-metal dimers: Fe_2, Co_2, Ni_2, Ru_2, Rh_2, Pd_2, Os_2, Ir_2, and Pt_2. *International Journal of Quantum Chemistry*, 108(9):1505–1517, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeLaMora:2000:TSM

[DT00] Pablo De La Mora and Gustavo Tavizón. A theoretical study of the magnetic properties of the infinite-layer superconductor. *International Journal of Quantum Chemistry*, 80(3):499–506, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73501027/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501027/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501027&PLACEBO=IE.pdf.

Delchev:2002:PPS

[DT02a] Yavor Delchev and Alia Tadjer. Preface: Proceedings of the Sixth European Workshop on Quantum Systems in Chemistry and Physics. *International Journal of Quantum Chemistry*, 89 (4):181–182, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Doerksen:2002:BOH

[DT02b] Robert J. Doerksen and Ajit J. Thakkar. Bond orders in heteroaromatic rings. *International Journal of Quantum Chemistry*, 90(2):534–540, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Darkhovskii:2006:MPH

[DTT06] M. B. Darkhovskii, A. M. Tokmachev, and A. L. Tchougréeff. MNDO parameterized hybrid SLG/SCF method as used for molecular modeling of Zn(II) complexes. *International Journal of Quantum Chemistry*, 106(10):2268–2280, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dufey:2007:CEP

[Duf07] Florian Dufey. Comment on "The electron-pair origin of antiaromaticity: Spectroscopic manifestations". *International Journal of Quantum Chemistry*, 107(3):764–768, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dunlap:2001:DQC

[Dun01] Brett I. Dunlap. Direct quantum chemical integral evaluation. *International Journal of Quantum Chemistry*, 81(6):373–383, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76509320/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76509320/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76509320&PLACEBO=IE.pdf`.

Denis:2000:DFI

[DV00] Pablo A. Denis and Oscar N. Ventura. Density functional investigation of atmospheric sulfur chemistry. I. Enthalpy of formation of HSO and related molecules. *International Journal of Quantum Chemistry*, 80(3):439–453, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501020/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501020/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501020&PLACEBO=IE.pdf`.

deVries:2003:OCS

[dVHB03] A. H. de Vries, L. Hozoi, and R. Broer. Origin of the chemical shift in X-ray absorption near-edge spectroscopy at the Mn K-edge in manganese oxide compounds. *International Journal of Quantum Chemistry*, 91(1):57–61, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dijkstra:2003:VBD

[DVHJ03] Fokke Dijkstra, Joop H. Van Lenthe, Remco W. A. Havenith, and Leonardus W. Jenneskens. Valence bond descriptions of benzene and cyclobutadiene and their counterparts with localized bonds. *International Journal of Quantum Chemistry*, 91(4):566–574, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Destefani:2006:RUH

[DVM06] C. F. Destefani, J. D. M. Vianna, and G. E. Marques. Restricted and unrestricted Hartree–Fock approaches applied to spherical quantum dots in a magnetic field. *International Journal of Quantum Chemistry*, 106(9):2090–2099, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dahlen:2005:VEF

[DVV05] Nils Erik Dahlen, Robert Van Leeuwen, and Ulf Von Barth. Variational energy functionals of the Green function tested on molecules. *International Journal of Quantum Chemistry*, 101 (5):512–519, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DelBene:2000:BPH

[DW00] Janet E. Del Bene and John D. Watts. Base properties of H_2CO in the excited $^3n \rightarrow \pi*$ state. *International Journal of Quantum Chemistry*, 77(1):187–191, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004258/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004258/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004258&PLACEBO=IE.pdf`.

Dulak:2005:BSE

[DW05] Marcin Dulak and Tomasz A. Wesolowski. The basis set effect on the results of the minimization of the total energy bifunctional $E = [\rho_A, \rho_B]$. *International Journal of Quantum Chemistry*, 101(5):543–549, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dobson:2005:SCF

[DWD+05] John F. Dobson, Jun Wang, Bradley P. Dinte, Keith McLennan, and Hung M. Le. Soft cohesive forces. *International Journal of Quantum Chemistry*, 101(5):579–598, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ding:2003:RCG

[DWF+03] Shiliang Ding, Meishan Wang, Dongtai Feng, Bofu Li, and Jiazhong Sun. Recoupling coefficients of group SO (4) and their application to linear tetratomic molecules. *International Journal of Quantum Chemistry*, 94(6):293–301, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Duan:2007:DFT

[DWM+07] Chunsheng Duan, Qunyan Wu, Hongkun Ma, Xinming Zhou, and Zhengyu Zhou. Density functional theory study of the interaction between formamide and uracil. *International Journal of Quantum Chemistry*, 107(5):1253–1260, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dyall:2000:REM

[Dya00] Kenneth G. Dyall. Relativistic electric and magnetic property operators for two-component transformed Hamiltonians. *International Journal of Quantum Chemistry*, 78(6):412–421, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72502336/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72502336/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72502336&PLACEBO=IE.pdf`.

Das:2000:TME

[DYD00] G. P. Das, A. T. Yeates, and D. S. Dudis. Theoretical model for excited-state absorption. *International Journal of Quantum Chemistry*, 80(4–5):1039–1042, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505373/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505373/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505373&PLACEBO=IE.pdf`.

Das:2003:IFO

[DYD03] G. P. Das, A. T. Yeates, and D. S. Dudis. Ab initio fragment orbital-based theory. *International Journal of Quantum Chemistry*, 92(1):22–28, March 5, 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DaMottaNeto:2001:NPS

[DZ01] Joaquim Delphino Da Motta Neto and Michael C. Zerner. New parametrization scheme for the resonance integrals (H_μ) within the INDO/1 approximation. Main group elements. *International Journal of Quantum Chemistry*, 81(3):187–201, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76504665/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76504665/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76504665&PLACEBO=IE.pdf`.

Du:2006:IMS

[DZ06a] Benni Du and Weichao Zhang. Ab initio MO study of potential energy surface of NH_2 with CN reaction. *International Journal of Quantum Chemistry*, 106(8):1827–1843, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Du:2006:CDH

[DZ06b] Dongmei Du and Zhengyu Zhou. Chiral discrimination in hydrogen-bonded complexes of hydrogen peroxide with methyl hydroperoxide: Theoretical study. *International Journal of Quantum Chemistry*, 106(4):935–942, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolgounitcheva:2000:EPC

[DZO00] O. Dolgounitcheva, V. G. Zakrzewski, and J. V. Ortiz. Electron propagator calculations on uracil and adenine ionization energies. *International Journal of Quantum Chemistry*, 80(4–5):831–835, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505424/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505424/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505424&PLACEBO=IE.pdf`.

Dolgounitcheva:2002:EBE

[DZO02] O. Dolgounitcheva, V. G. Zakrzewski, and J. V. Ortiz. Electron binding energies of nucleobases and nucleotides. *International Journal of Quantum Chemistry*, 90(4-5):1547–1554, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolgounitcheva:2006:CIE

[DZS+06] O. Dolgounitcheva, V. G. Zakrzewski, Mark R. Sterling, A. Kletsov, Yu. Dahnovsky, and J. V. Ortiz. Correlated Ab initio electron propagators in the study of molecular wires. *International Journal of Quantum Chemistry*, 106(15):3387–3392, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dong:2005:DFS

[DZTZ05] Xiu-Li Dong, Zheng-Yu Zhou, Lai-Jin Tian, and Gang Zhao. Density functional study of $HO(H_2O)_n$ ($n = 1 - -3$) clusters. *International Journal of Quantum Chemistry*, 102(4):461–469, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Evarestov:2004:HFC

[EB04a] R. A. Evarestov and A. V. Bandura. Hartree–Fock calculations of electronic structure of (110)-surface of rutile TiO_2: Comparison of single (2D) and periodic (3D) slab models. *International Journal of Quantum Chemistry*, 96(3):282–291, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Evarestov:2004:HDC

[EB04b] R. A. Evarestov and A. V. Bandura. HF and DFT calculations of MgO surface energy and electrostatic potential using two- and three-periodic models. *International Journal of Quantum Chemistry*, 100(4):452–459, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Elkner:2006:SGE

[EBB06] Kenneth Elkner, R. C. Binning, Jr., and Daniel E. Bacelo. Structures and G3X energies of $C_3H_3N^+$ intermediates. *International Journal of Quantum Chemistry*, 106(15):3043–3047, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Exley:2007:CAB

[EBR07] Christopher Exley, James Beardmore, and Gordon Rugg. Computational approach to the blood–aluminum problem? *International Journal of Quantum Chemistry*, 107(2):275–278, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Eliav:2009:IHH

[EBS+09] Ephraim Eliav, Anastasia Borschevsky, K. R. Shamasundar, Sourav Pal, and Uzi Kaldor. Intermediate Hamiltonian Hilbert space coupled cluster method: Theory and pilot application. *International Journal of Quantum Chemistry*, 109 (13):2909–2915, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Eckard:2009:IGH

[EE09] Simon Eckard and Thomas E. Exner. Improvements in the generalized hybrid orbital method. *International Journal of Quantum Chemistry*, 109(7):1451–1463, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Edwards:2004:CBS

[EEJ04] Jesse Edwards, Claudia Eybl, and Brian Johnson. Correlation between sensitivity and approximated heats of detonation of several nitroamines using quantum mechanical methods. *International Journal of Quantum Chemistry*, 100(5):713–719, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Eskandari:2003:MBE

[EF03] M. R. Eskandari and F. Faghihi. Minimum binding energy and size of the doubly muonic T_3 molecule. *International Journal of Quantum Chemistry*, 93(6):377–383, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Emiris:2006:AAS

[EFM06] Ioannis Z. Emiris, Epaminondas D. Fritzilas, and Dinesh Manocha. Algebraic algorithms for structure determination in biological chemistry. *International Journal of Quantum Chemistry*, 106(1):190–210, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Eriksson:2008:RDR

[EGE08] Emma S. E. Eriksson, Rita C. Guedes, and Leif A. Eriksson. Redox and debromination reactions of brominated hypericin. *International Journal of Quantum Chemistry*, 108(11):1921–1929, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

El-Gogary:2003:MMQ

[EGEDH03] T. M. El-Gogary, A. El-Dissouky, and A. S. Hilali. Molecular mechanics, quantum mechanics, potentiometric, and conductometric studies on the complexes of some rare earth metals with 5-azorhodanine derivatives. *International Journal of Quantum Chemistry*, 91(6):685–694, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ebrahimi:2009:DES

[EHH09] Ali Ebrahimi, Mostafa Habibi, and Nahid Hesabi. Development of eclipsed and staggered forms in some hydrogen bonded complexes. *International Journal of Quantum Chemistry*, 109(3):629–638, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ebrahimi:2009:SEI

[EHN09] A. Ebrahimi, S. M. Habibi, and R. S. Neyband. Substituent effect on intramolecular hydrogen bonding in 2-hydroxybenzaldehyde. *International Journal of Quantum Chemistry*, 109(6):1274–1282, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Engel:2006:ODR

[EJ06] E. Engel and H. Jiang. Orbital-dependent representation of the correlation energy functional: Properties of second-order Kohn–Sham perturbation expansion. *International Journal of Quantum Chemistry*, 106(15):3242–3259, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Eriksson:2004:TSH

[EKN04] Leif A. Eriksson, Eugene S. Kryachko, and Minh T. Nguyen. Theoretical study of hydrogenation of thiouracils and their base pairs with adenine. *International Journal of Quantum Chemistry*, 99(5):841–853, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Evarestov:2006:DSS

[EKZ06] R. A. Evarestov, E. A. Kotomin, and Yu. F. Zhukovskii. DFT study of a single F center in cubic $SrTiO_3$ perovskite. *International Journal of Quantum Chemistry*, 106(10):2173–2183, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Evangelisti:2006:P

[EL06] Stefano Evangelisti and Thierry Leininger. Preface. *International Journal of Quantum Chemistry*, 106(3):555, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Elroby:2008:SCD

[ELC08] Shabaan A. K. Elroby, Kyu Hwan Lee, and Seung Joo Cho. Significance of charge-dipolar moiety interaction: Computational study of cyanospherands. *International Journal of Quantum Chemistry*, 108(4):779–787, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ema:2008:AFM

[ELF+08] I. Ema, R. López, J. J. Fernández, G. Ramírez, and J. F. Rico. Auxiliary functions for molecular integrals with Slater-type orbitals. II. Gauss transform methods. *International Journal of Quantum Chemistry*, 108(1):25–39, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Evangelista-Lara:2005:TEN

[ELG05] Aurelio Evangelista-Lara and Patricia Guadarrama. Theoretical evaluation of the nanocarrier properties of two families of functionalized dendrimers. *International Journal of Quantum Chemistry*, 103(4):460–470, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Elroby:2007:RHP

[ELO+07] Shabaan A. K. Elroby, Kyu Hwan Lee, Jung Soo Oh, Hwan Won Chung, Seung Joo Cho, and Kyungsoo Paek. Reorganization of highly preorganized hosts upon cation complexation: Ab initio study of fluorospherands. *International Journal of Quantum Chemistry*, 107(4):930–936, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Elroby:2009:EDA

[Elr09] Shabaan A. K. Elroby. The effect of donor atoms on the complexation of alkali cations with spherands: A density functional investigation. *International Journal of Quantum Chemistry*, 109(7):1515–1521, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Elshakre:2005:ISG

[Els05] Mohamed Elshakre. Ab initio study of guanine tautomers in the S_0 and D_0 states. *International Journal of Quantum Chemistry*, 104(1):1–15, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Elander:2009:CQN

[ELY09] Nils Elander, Sergey B. Levin, and Evgeny Yarevsky. Convergence and quantum number assignment studies of rovibrational eigenstates in a model of predissociating NeICl van der Waals complex. *International Journal of Quantum Chemistry*, 109(3):459–468, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Elizondo:2005:SMN

[EM05] S. L. Elizondo and J. W. Mintmire. Simulations of metal nanowires. *International Journal of Quantum Chemistry*, 105 (6):772–780, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Errea:2002:MTC

[EMM+02a] L. F. Errea, A. Macías, L. Méndez, I. Rabadán, A. Riera, and P. Sanz. Molecular treatment of charge transfer cross sections in N^{5+} collisions with H_2. *International Journal of Quantum Chemistry*, 86(2):182–189, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85510857/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85510857/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85510857&PLACEBO=IE.pdf`.

Errea:2002:SMO

[EMM+02b] L. F. Errea, A. Macías, L. Méndez, A. Riera, B. Pons, and I. Sevila. Study of molecular orbitals in momentum space. *International Journal of Quantum Chemistry*, 86(1):46–58, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85514352/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85514352/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85514352&PLACEBO=IE.pdf`.

Ermakov:2005:FAT

[EMV05] A. I. Ermakov, V. Y. Mashutin, and A. V. Vishnjakov. Forms of adsorption and transition states of oxidation of carbon monoxide by molecular oxygen and dissociation of nitrogen monooxide, catalyzed by monovalent copper. *International Journal of Quantum Chemistry*, 104(2):181–188, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

El-Nakat:2007:DBD

[ENGY+07] John Hanna El-Nakat, Noha Ghanem, Paolo Yammine, Gary Willett, and Keith Fisher. Determination of bond dissociation energies using mass spectrometry. *International Journal of Quantum Chemistry*, 107(6):1367–1372, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Evarestov:2002:EEC

[EP02] R. A. Evarestov and A. I. Panin. Effects of electronic correlation on local properties of electronic structure of TiO_2 and

Ti_2O_3 crystals: DFT and post-HF approaches. *International Journal of Quantum Chemistry*, 88(4):472–480, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Elango:2006:AEE

[EPSC06] M. Elango, R. Parthasarathi, V. Subramanian, and P. K. Chattaraj. Alkylation of enolates: An electrophilicity perspective. *International Journal of Quantum Chemistry*, 106 (4):852–862, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Eskandari:2005:CGS

[ER05] M. R. Eskandari and B. Rezaie. Calculation of the ground-state energy and studies of other properties of exotic helium atoms with the use of boundary conditions of wave function. *International Journal of Quantum Chemistry*, 101(3): 320–324, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Estiu:2002:TBL

[ERC+02] Guillermina L. Estiú, Rodolfo M. Rasia, Julia A. Cricco, Alejandro J. Vila, and Michael C. Zerner. Is there a bridging ligand in metal-substituted zinc β-lactamases? A spectroscopic and theoretical answer. *International Journal of Quantum Chemistry*, 88(1):118–132, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90010554/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90010554/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90010554&PLACEBO=IE.pdf`.

Eriksson:2007:SIT

[ERU07] Leif A. Eriksson, Nino Russo, and Jesus M. Ugalde. Second International Theoretical Biophysics Symposium, Örebro University, Sweden, June 28–July 1, 2005. *International Journal of Quantum Chemistry*, 107(2):259–260, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Estrada:2006:ABM

[ERVR06] Ernesto Estrada, Juan A. Rodríguez-Velázquez, and Milan Randić. Atomic branching in molecules. *International Journal*

of Quantum Chemistry, 106(4):823–832, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Erazo:2002:SEP

[ES02] Franklin Erazo and Arvids Stashans. Structural and electronic properties of La-doped $CaTiO_3$ crystal. *International Journal of Quantum Chemistry*, 87(4):225–231, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/91012823/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91012823/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91012823&PLACEBO=IE.pdf`.

Eick:2006:ACG

[ES06] Bettina Eick and Bernd Souvignier. Algorithms for crystallographic groups. *International Journal of Quantum Chemistry*, 106(1):316–343, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Escobedo:2008:CLC

[Esc08] Ramón Escobedo. A CFL-like constraint for the fast marching method in inhomogeneous chemical kinetics. *International Journal of Quantum Chemistry*, 108(5):848–857, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Egorova:2004:MDS

[ESE04] K. B. Egorova, K. V. Shaitan, and A. Y. Ermilov. Molecular dynamics of strained retinal in various electronic states. *International Journal of Quantum Chemistry*, 96(3):219–225, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Evarestov:2004:QCC

[ESKB04] R. A. Evarestov, V. E. Stefanov, V. A. Karasev, and A. V. Bandura. Quantum chemical calculation of crystalline model of biomembrane. *International Journal of Quantum Chemistry*, 96(2):106–115, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

eSilva:2008:SSA

[eSPM+08] Tânia B. e Silva, Mariano A. Pereira, Valéria S. Malta, Edson S. Bento, Miguel A. San-Miguel, Roberta L. Ziolli, João B. L. Martins, Andre Sih, and Carlton A. Taft. Study of the structure-activity relationship for theoretical molecular descriptors using density functional theory and chemometric methods in cannabinoid metabolites. *International Journal of Quantum Chemistry*, 108(13):2530–2539, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Essa:2007:HMT

[Ess07] Ali Hashem Essa. Hammett MSP and Taft DSP analysis of substituent effects on Mulliken charges of 1-(arylmethylene)-1 H-cyclopropanaphthalene. *International Journal of Quantum Chemistry*, 107(7):1574–1577, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Evarestov:2005:LCE

[ESTU05] R. A. Evarestov, V. P. Smirnov, I. I. Tupitsyn, and D. E. Usvyat. Local characteristics of the electronic structure of MgO: LCAO and plane-wave calculations. *International Journal of Quantum Chemistry*, 104(2):110–113, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Evarestov:2004:CBC

[ESU04] R. A. Evarestov, V. P. Smirnov, and D. E. Usvyat. Chemical bonding in crystalline silver halides: Wannier-type atomic functions approach. *International Journal of Quantum Chemistry*, 96(2):95–105, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Evarestov:2005:WFC

[ESU05] R. A. Evarestov, V. P. Smirnov, and D. E. Usvyat. Wannier functions and chemical bonding in a slab model: MgO (001) and TiO_2 (110) surfaces. *International Journal of Quantum Chemistry*, 104(2):102–109, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

El-Taher:2001:ISR

[ET01] S. El-Taher. Ab initio study of reactions of hydroxyl radicals with chloro- and fluoro-substituted methanes. *In-*

ternational Journal of Quantum Chemistry, 84(4):426–440, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85005090/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85005090/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85005090&PLACEBO=IE.pdf`.

El-Taher:2005:IDI

[ET05] S. El-Taher. Ab initio and DFT investigation of the structures and properties of chloromethyl and chlorofluoromethyl peroxyl radicals. *International Journal of Quantum Chemistry*, 102(2):178–188, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

ElSohly:2009:CPC

[ET09] Adel M. ElSohly and Gregory S. Tschumper. Comparison of polarization consistent and correlation consistent basis sets for noncovalent interactions. *International Journal of Quantum Chemistry*, 109(1):91–96, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Evarestov:2006:ICA

[ETBA06] R. A. Evarestov, I. I. Tupitsyn, A. V. Bandura, and V. E. Alexandrov. Ab initio calculations and analysis of chemical bonding in $SrTiO_3$ and $SrZrO_3$ cubic crystals. *International Journal of Quantum Chemistry*, 106(10):2191–2200, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

El-Taher:2004:TIS

[ETEA04] S. El-Taher and Adel A. El-Azhary. Theoretical investigation of the structures and properties of fluoromethyl peroxyl radicals. *International Journal of Quantum Chemistry*, 98 (6):502–514, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

El-Taher:2000:TSP

[ETM00] S. El-Taher and Adel A. Mohamed. Theoretical study on peroxyl radical additions to methyl-substituted ethenes. *International Journal of Quantum Chemistry*, 77(4):761–771, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70500250/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70500250/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70500250&PLACEBO=IE.pdf.

Evangelisti:2004:PPI

[Eva04] Stefano Evangelisti. Possibility of a pressure-induced $2N_2 \rightarrow N_4$ reaction. *International Journal of Quantum Chemistry*, 96 (6):598–606, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Eriksson:2005:MBP

[EWCT+05] O. Eriksson, J. M. Wills, M. Colarieti-Tosti, S. Lebègue, and A. Grechnev. Many-body projector orbitals for electronic structure theory of strongly correlated electrons. *International Journal of Quantum Chemistry*, 105(2):160–165, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Englman:2002:HCF

[EYB02] R. Englman, A. Yahalom, and M. Baer. Hierarchical construction of finite diabatic sets by Mathieu functions. *International Journal of Quantum Chemistry*, 90(1):266–272, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Englman:2003:ECC

[EYBM03] R. Englman, A. Yahalom, M. Baer, and A. M. Mebel. Experimental and calculational consequences of phases in molecules with multiple conical intersections. *International Journal of Quantum Chemistry*, 92(2):135–151, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Eyert:2000:BNA

[Eye00] Volker Eyert. Basic notions and applications of the augmented spherical wave method. *International Journal of Quantum Chemistry*, 77(6):1007–1031, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/71000982/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000982/FILE?TPL=ftx_start;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000982&PLACEBO=IE.pdf.

Eu:2006:GWI

[EYY06] Sen-Peng Eu, Bo-Yin Yang, and Yeong-Nan Yeh. Generalized Wiener indices in hexagonal chains. *International Journal of Quantum Chemistry*, 106(2):426–435, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ernzerhof:2005:DFM

[EZ05] Matthias Ernzerhof and Min Zhuang. A density functional method for the calculation of the zero-voltage conductance of molecular electronic devices. *International Journal of Quantum Chemistry*, 101(5):557–563, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Enkvist:2000:DFS

[EZY00] Christer Enkvist, Yingkai Zhang, and Weitao Yang. Density functional study of a weakly hydrogen-bonded benzene-ammonia complex: The importance of the exchange functional. *International Journal of Quantum Chemistry*, 79 (5):325–329, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72512624/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72512624/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72512624&PLACEBO=IE.pdf.

Figueiredo:2000:CCH

[FA00] Luciana J. O. Figueiredo and O. A. C. Antunes. Chemometric classification of HIV-1 protease inhibitors. *International Journal of Quantum Chemistry*, 76(6):744–755, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70001600/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70001600/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70001600&PLACEBO=IE.pdf.

Fiolhais:2005:SES

[FA05] Carlos Fiolhais and L. M. Almeida. Surface energies of simple metals from slabs: Comparison of exchange-correlation den-

sity functionals. *International Journal of Quantum Chemistry*, 101(6):645–650, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Freeman:2005:CSS

[FAE+05a] Fillmore Freeman, Nina Asgari, Behrooz Entezam, Faranak Gomarooni, Jolene Mac, Monet H. Nguyen, Nhu N. T. Nguyen, Thao P. Nguyen, Ngoc B. Pham, Perveen Sultana, Timothy S. Welch, and Bagrat A. Shainyan. Computational study of sulfoxides of thiacyclohexane, 4-silathiacyclohexane, 4-fluoro-4-silathiacyclohexane, and 4,4-difluoro-4-silathiacyclohexane: Relative energies of conformations and sulfinyl oxygen stabilized pentacoordinate silicon in boat and twist structures. *International Journal of Quantum Chemistry*, 101(1):40–54, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [FAE+05b].

Freeman:2005:ECS

[FAE+05b] Fillmore Freeman, Nina Asgari, Behrooz Entezam, Faranak Gomarooni, Jolene Mac, Monet H. Nguyen, Nhu N. T. Nguyen, Thao P. Nguyen, Ngoc B. Pham, Perveen Sultana, Timothy S. Welch, and Bagrat A. Shainyan. Erratum: Computational study of sulfoxides of thiacyclohexane, 4-silathiacyclohexane, 4-fluoro-4-silathiacyclohexane, and 4,4-difluoro-4-silathiacyclohexane: Relative energies of conformations and sulfinyl oxygen stabilized pentacoordinate silicon in boat and twist structures, International Journal of Quantum Chemistry (2005). *International Journal of Quantum Chemistry*, 101(1):118, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [FAE+05a].

Fan:2001:ASP

[Fan01] Peng-Dong Fan. Algebraic solutions for point groups: The octahedral group for the group chain $O \supset T \supset C_3$. *International Journal of Quantum Chemistry*, 83(5):259–270, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/81002391/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/81002391/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=81002391&PLACEBO=IE.pdf`.

Fan:2003:AEC

[Fan03] Peng-Dong Fan. Algebraic expressions of Clebsch–Gordon coefficients for the group chain $O\dagger \supset C$. *International Journal of Quantum Chemistry*, 91(4):541–550, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fejes:2001:ISU

[FB01] István Fejes and Ferenc Billes. Investigation of the structural units of germanium sulfide and selenide by quantum chemical methods. *International Journal of Quantum Chemistry*, 85(2):85–91, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85004526/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85004526/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85004526&PLACEBO=IE.pdf`.

Forner:2007:SRP

[FB07] Wolfgang Förner and Hassan M. Badawi. Symmetric ring puckering potential in thietane-1,1-dioxide compared with experiment and analysis of theoretical vibrational spectra. *International Journal of Quantum Chemistry*, 107(2):469–479, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ferreira:2006:CAA

[FBBB06] G. G. Ferreira, E. Borges, J. P. Braga, and J. C. Belchior. Comparative analysis of Ar_nCl_2 ($2 \leq n \leq 30$) clusters taking into account molecular relaxation effects. *International Journal of Quantum Chemistry*, 106(13):2752–2762, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Freeman:2006:SRH

[FBC+06] Fillmore Freeman, Radha M. Bathala, Jessica E. Cavillo, Angela C. Huang, Tara K. Jackson, Angelica Zavala Lopez-Mercado, Sandy Phung, Jenny Suh, and Diego O. Valencia, Jr. [2,3]-sigmatropic rearrangements of hydrogen and alkyl 3-propenyl sulfoxides: A computational study. *International Journal of Quantum Chemistry*, 106(11):2390–2397, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Freidzon:2004:RMI

[FBGA04] A. Ya. Freidzon, A. A. Bagatur'Yants, S. P. Gromov, and M. V. Alfimov. Recoordination of a metal ion in the cavity of an arylazacrown ether: Model study of the conformations and microsolvation of calcium complexes of arylazacrown ethers. *International Journal of Quantum Chemistry*, 100 (4):617–625, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Freeman:2004:CSC

[FC04] Fillmore Freeman and Chansa Cha. Computational study of the conformational interconversion of 5,5-dimethyl-1,2,3-trithiacyclohexane (5,5-dimethyl-1,2,3-trithiane). *International Journal of Quantum Chemistry*, 96(4):443–455, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fileti:2005:INS

[FC05a] Eudes E. Fileti and Sylvio Canuto. Ab initio NMR study of the isomeric hydrogen-bonded methanol–water complexes. *International Journal of Quantum Chemistry*, 102(5):554–564, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fileti:2005:CIS

[FC05b] Eudes E. Fileti and Sylvio Canuto. Calculated infrared spectra of hydrogen-bonded methanol–water, water–methanol, and methanol–methanol complexes. *International Journal of Quantum Chemistry*, 104(5):808–815, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuentealba:2007:FEF

[FCC07] P. Fuentealba, E. Chamorro, and C. Cárdenas. Further exploration of the Fukui function, hardness, and other reactivity indices and its relationships within the Kohn–Sham scheme. *International Journal of Quantum Chemistry*, 107(1):37–45, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuzo:2008:SGM

[FCD08] C. A. Fuzo, J. R. M. Castro, and L. Degrève. Searching the global minimum of a peptide/bilayer potential energy sur-

face by fast heating and cooling cycles of simulated annealing. *International Journal of Quantum Chemistry*, 108(13):2403–2407, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuentes-Cabrera:2006:AIC

[FCLH+06] Miguel Fuentes-Cabrera, Pawel Lipkowski, Oscar Huertas, Bobby G. Sumpter, Modesto Orozco, F. Javier Luque, Jack C. Wells, and Jerzy Leszczynski. Aromaticity-induced changes in electronic properties of size-expanded DNA bases: Case of xC. *International Journal of Quantum Chemistry*, 106(11):2339–2346, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fadda:2003:TDD

[FCS03] Elisa Fadda, Mark E. Casida, and Dennis R. Salahub. Time-dependent density functional theory as a foundation for a firmer understanding of sum-over-states density functional perturbation theory: "Loc.3" approximation. *International Journal of Quantum Chemistry*, 91(2):67–83, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuks:2001:VIC

[FD01] David Fuks and Simon Dorfman. Vacancy interactions in cluster expansion formalism. *International Journal of Quantum Chemistry*, 85(4–5):301–306, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fripiat:2009:ECE

[FD09] Joseph G. Fripiat and Joseph Delhalle. Efficient calculation of the exchange in the Fourier representation of HF-LCAO-CO equations for 1D periodic systems. *International Journal of Quantum Chemistry*, 109(13):2960–2967, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Faria:2003:CAE

[FDL03] Luciano Emerich Faria, Claudio Luis Donnici, and Júlio César Dias Lopes. Conformational analysis and electronic interactions of 2-thiosubstituted cyclohexanones by semiempirical method PM3. *International Journal of Quantum Chem-*

istry, 95(3):313–321, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuks:2002:SPO

[FDLK02] David Fuks, Simon Dorfman, Vlad Liubich, and Larisa Kutsenko. Site preference occupation of Ti, Ni, and Cr in Fe_3Al compound. *International Journal of Quantum Chemistry*, 90 (4-5):1478–1490, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fakhri:2009:AAL

[FDM09] H. Fakhri, A. Dehghani, and B. Mojaveri. Approach of the associated Laguerre functions to the $su(1,1)$ coherent states for some quantum solvable models. *International Journal of Quantum Chemistry*, 109(6):1228–1236, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuks:2001:SMD

[FDME01] David Fuks, Simon Dorfman, Kleber C. Mundim, and Donald E. Ellis. Stochastic molecular dynamics in simulations of metalloid impurities in metals. *International Journal of Quantum Chemistry*, 85(4–5):354–367, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

daCunha:2008:TEP

[FdONGM08] Wiliam Ferreira da Cunha, Pedro Henrique de Oliveira Neto, Ricardo Gargano, and Geraldo Magela e Silva. Temperature effects on polaron stability in polyacetylene. *International Journal of Quantum Chemistry*, 108(13):2448–2453, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fu:2004:SFM

[FDZ04] Aiping Fu, Dongmei Du, and Zhengyu Zhou. Study of the formamide–methanol dimer with ab initio and density functional theory methods. *International Journal of Quantum Chemistry*, 97(4):865–875, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fernandez:2001:FAM

[Fer01] Francisco M. Fernández. Fast and accurate method for summation of divergent series. *International Journal of*

Quantum Chemistry, 81(4):268–279, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/76505743/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76505743/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76505743&PLACEBO=IE.pdf.

Fernandez:2002:CPT

[Fer02] Francisco M. Fernández. On canonical perturbation theory in classical mechanics. *International Journal of Quantum Chemistry*, 90(1):37–41, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fernandez:2009:RRV

[Fer09] Francisco M. Fernández. Rayleigh–Ritz variation method and connected-moments polynomial approach. *International Journal of Quantum Chemistry*, 109(4):717–719, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Feng:2001:TSC

[FF01] Shengyu Feng and Dacheng Feng. Theoretical studies of cyclopropylsilylenes: The structures and stability of cyclopropylsilylene C_3 H_5 SiH. *International Journal of Quantum Chemistry*, 85(2):92–99, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85011808/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85011808/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85011808&PLACEBO=IE.pdf.

Florez:2009:TSA

[FF09] Elizabeth Florez and Patricio Fuentealba. A theoretical study of alkali metal atomic clusters: From Li_n to Cs_n ($n = 2--8$). *International Journal of Quantum Chemistry*, 109(5):1080–1093, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Franco:2007:TDC

[FFDD07] Mauro L. Franco, Dalva E. C. Ferreira, Hélio F. Dos Santos, and Wagner B. De Almeida. Temperature-dependent confor-

mational analysis of cyclononane: An ab initio study. *International Journal of Quantum Chemistry*, 107(3):545–555, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fartaria:2007:FFS

[FFF07] Rui P. S. Fartaria, Filomena F. M. Freitas, and Fernando M. S. Silva Fernandes. A force field for simulating ethanol adsorption on Au(111) surfaces. A DFT study. *International Journal of Quantum Chemistry*, 107(11):2169–2177, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fartaria:2001:PBC

[FFFR01] Rui P. S. Fartaria, Fernando M. S. Silva Fernandes, Filomena F. M. Freitas, and Pedro C. R. Rodrigues. Phase behavior of C_{60} by computer simulation using ab-initio interaction potential. *International Journal of Quantum Chemistry*, 84(3):375–387, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/83502023/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/83502023/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=83502023&PLACEBO=IE.pdf`. See erratum [FFFR02].

Fartaria:2002:EPB

[FFFR02] Rui P. S. Fartaria, Fernando M. S. Silva Fernandes, Filomena F. M. Freitas, and Pedro C. R. Rodrigues. Erratum: Phase behavior of C_{60} by computer simulation using ab-initio interaction potential. *International Journal of Quantum Chemistry*, 88(3):355, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [FFFR01].

Fripiat:2000:CAP

[FFHD00] Joseph G. Fripiat, Isabelle Flamant, Frank E. Harris, and Joseph Delhalle. Computational aspects of polymer band structure calculations by the Fourier space restricted Hartree–Fock method. *International Journal of Quantum Chemistry*, 80(4–5):856–862, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505378/START; http://www3.interscience.`

wiley.com/cgi-bin/fulltext/73505378/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505378&PLACEBO=IE.pdf.

Freeman:2005:DFT

[FFHT05] Fillmore Freeman, Christine Fang, David V. Hoang, and Khue M. Trinh. Density functional theory study of the relative energies and structures of the chair, twist, and boat conformations of stannacyclohexane, 1-methylstannacyclohexane, and 1,1-dimethylstannacyclohexane. *International Journal of Quantum Chemistry*, 105(4):416–428, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Feng:2002:TSS

[FFLZ02] Shengyu Feng, Dacheng Feng, Meijiang Li, and Yufang Zhou. Theoretical studies on the structures and isomerization of methylene lithium-chlorosilylenoid H_2 C SiLiCl. *International Journal of Quantum Chemistry*, 87(6):360–365, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/91015491/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91015491/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91015491&PLACEBO=IE.pdf.

Freeman:2004:RES

[FFS04] Fillmore Freeman, Christine Fang, and Bagrat A. Shainyan. Relative energies, stereoelectronic interactions, and conformational interconversion in silacycloalkanes. *International Journal of Quantum Chemistry*, 100(5):720–732, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [AKB06].

Ford:2001:ICS

[FG01] Thomas A. Ford and Leslie Glasser. Ab initio calculations of the structural, energetic, and vibrational properties of some hydrogen bonded and van der Waals dimers. Part 4. The acetonitrile dimer. *International Journal of Quantum Chemistry*, 84(2):226–240, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/84502334/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502334/FILE?TPL=ftx_start;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502334&PLACEBO=IE.pdf.

Fattebert:2003:FPM

[FG03] Jean-Luc Fattebert and François Gygi. First-principles molecular dynamics simulations in a continuum solvent. *International Journal of Quantum Chemistry*, 93(2):139–147, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Freeman:2006:STG

[FG06] Fillmore Freeman and Mahshid Gomarooni. Singlet–triplet gaps and insertion reactions of aminocyanocarbenes: A computational study of hydrogen cyanide covalent dimers. *International Journal of Quantum Chemistry*, 106(11):2379–2389, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Feria:2004:ISC

[FGC04a] L. Feria, C. Gonzalez, and M. Castro. Ab initio study of the CH_3O_2 self-reaction in gas phase: Elucidation of the $CH_3O_2CH_3O_2 \rightarrow 2CH_3OO_2$ pathway. *International Journal of Quantum Chemistry*, 99(5):605–615, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Feria:2004:TSE

[FGC04b] Leticia Feria, Carlos Gonzalez, and Miguel Castro. Theoretical study of the energetic and possible intermediates of the $CH_3CH_2O_2$ self-reaction. *International Journal of Quantum Chemistry*, 96(4):380–393, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

FernandesdeOliveira:2000:MDS

[FGdA00] César Augusto Fernandes de Oliveira, Cristiano Ruch Werneck Guimarães, and Ricardo Bicca de Alencastro. Molecular dynamics study on liquid 1-octanol. *International Journal of Quantum Chemistry*, 80(4–5):999–1006, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505426/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505426/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505426&PLACEBO=IE.pdf.

FernandesdeOliveira:2002:MDS

[FGdA02] César Augusto Fernandes de Oliveira, Cristiano Ruch Werneck Guimarães, and Ricardo Bicca de Alencastro. Molecular dynamics study on liquid 1-octanol. Part 2. Water-saturated 1-octanol solution. *International Journal of Quantum Chemistry*, 90(2):786–791, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fraga:2006:SRE

[FGF06] Serafin Fraga, José M. García De La Vega, and Eric S. Fraga. Schrödinger–riccati equation: Feasibility study for the Heisoelectronic series. *International Journal of Quantum Chemistry*, 106(2):458–464, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fagan:2006:FPS

[FGFF06] Solange B. Fagan, E. C. Girão, J. Mendes Filho, and A. G. Souza Filho. First principles study of 1,2-dichlorobenzene adsorption on metallic carbon nanotubes. *International Journal of Quantum Chemistry*, 106(13):2558–2563, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fayton:2009:PES

[FGH09] Floyd A. Fayton, Jr., Ainsley A. Gibson, and John A. W. Harkless. Prediction of excited state energies for molecular nitrogen using quantum Monte Carlo methods. *International Journal of Quantum Chemistry*, 109(1):43–49, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fleischer:2005:DSA

[FGM05] Avner Fleischer, Ashish Kumar Gupta, and Nimrod Moiseyev. Dynamical symmetry analysis of ionization and harmonic generation of atoms in bichromatic laser pulses. *International Journal of Quantum Chemistry*, 103(6):824–840, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ford-Green:2006:CSP

[FGML06] Jason Ford-Green, D. Majumdar, and Jerzy Leszczynski. Conformational studies on parathion. *International Journal of*

Quantum Chemistry, 106(11):2356–2365, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Frapiccini:2007:DSW

[FGR+07] A. L. Frapiccini, V. Y. Gonzalez, J. M. Randazzo, F. D. Colavecchia, and G. Gasaneo. L^2 discretization of Sturmian wave functions for Coulomb-like potentials. *International Journal of Quantum Chemistry*, 107(4):832–844, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fomine:2007:DLM

[FGZ07] Serguei Fomine, Patricia Guadarrama, and Mikhail Zolotukhin. DFT and local MP2 study of switching process in a pH controllable molecular "shuttle". *International Journal of Quantum Chemistry*, 107(3):685–693, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fabian:2002:SCM

[FH02a] Jürgen Fabian and B. Andes Hess, Jr. Sulfur-containing mesoionic compounds: Theoretical study on structure and properties. *International Journal of Quantum Chemistry*, 90 (3):1055–1063, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Filizola:2002:MDR

[FH02b] Marta Filizola and Danni L. Harris. Molecular determinants of recognition and activation at $GABA_A$/benzodiazepine receptors. *International Journal of Quantum Chemistry*, 88(1): 56–64, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90010558/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90010558/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90010558&PLACEBO=IE.pdf`.

Forsberg:2000:CBM

[FHHC00] Björn Forsberg, Zhi He, Yuan He, and Dieter Cremer. Convergence behavior of the Møller–Plesset perturbation series: Use of Feenberg scaling for the exclusion of backdoor intruder states. *International Journal of Quantum Chemistry*, 76(3):306–330, January 20,

2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70000276/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000276/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000276&PLACEBO=IE.pdf.

Freeman:2008:CAC

[FHJ+08] Fillmore Freeman, Jung H. Hwang, Eun Hae Junge, Prem Dinesh Parmar, Zhongwei Renz, and James Trinh. Conformational analysis of cycloheptane, oxacycloheptane, 1,2-dioxacycloheptane, 1,3-dioxacycloheptane, and 1,4-dioxacycloheptane. *International Journal of Quantum Chemistry*, 108(2):339–350, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fliegl:2006:ITC

[FHK06] Heike Fliegl, Christof Hättig, and Wim Klopper. Inclusion of the (T) triples correction into the linear-r_{12} corrected coupled-cluster model CCSD(R12). *International Journal of Quantum Chemistry*, 106(11):2306–2317, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fischer:2000:NSE

[Fis00] Patrick Fischer. Numerical solution of eigenvalue problems by means of a wavelet-based Lanczos decomposition. *International Journal of Quantum Chemistry*, 77(2):552–562, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70002215/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70002215/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70002215&PLACEBO=IE.pdf.

Fournier:2000:MHD

[FJ00] René Fournier and Nan Jiang. Model Hamiltonians derived from Kohn–Sham theory. *International Journal of Quantum Chemistry*, 80(4–5):582–590, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505366/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505366/FILE?TPL=ftx_start;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505366&PLACEBO=IE.pdf.

French:2001:QMD

[FJK+01] Alfred D. French, Glenn P. Johnson, Anne-Marie Kelterer, Michael K. Dowd, and Christopher J. Cramer. QM/MM distortion energies in di- and oligosaccharides complexed with proteins. *International Journal of Quantum Chemistry*, 84 (4):416–425, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85004547/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85004547/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85004547&PLACEBO=IE.pdf. See erratum [FJK+02].

French:2002:EQM

[FJK+02] Alfred D. French, Glenn P. Johnson, Anne-Marie Kelterer, Michael K. Dowd, and Christopher J. Cramer. Erratum: QM/MM distortion energies in di- and oligosaccharides complexed with proteins. *International Journal of Quantum Chemistry*, 86(3):322, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/88510560/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88510560/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88510560&PLACEBO=IE.pdf. See [FJK+01].

Faustino:2005:TEL

[FJT+05] Wagner M. Faustino, Severino A. Junior, Larry C. Thompson, Gilberto F. De Sá, Oscar L. Malta, and Alfredo M. Simas. Theoretical and experimental luminescence quantum yields of coordination compounds of trivalent europium. *International Journal of Quantum Chemistry*, 103(5):572–579, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fritsche:2004:BCD

[FKR04] L. Fritsche, J. Koller, and Th. Reinert. Borderline cases in density functional theory. *International Journal of Quantum Chemistry*, 100(4):681–694, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Farias:2004:QIE

[FL04] Patricia M. A. Farias and Ricardo L. Longo. Quantum interference effects in the Br_2 electronic predissociation: Dependence upon the molecular properties. *International Journal of Quantum Chemistry*, 97(5):944–948, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fernandez:2006:AFM

[FLE+06a] J. J. Fernández, R. López, I. Ema, G. Ramírez, and J. Fernández Rico. Auxiliary functions for molecular integrals with Slater-type orbitals. I. Translation methods. *International Journal of Quantum Chemistry*, 106(9):1986–1997, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fletcher:2006:RFE

[Fle06b] G. D. Fletcher. Recursion formula for electron repulsion integrals over Hermite polynomials. *International Journal of Quantum Chemistry*, 106(2):355–360, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Flores:2008:NBS

[Flo08] Jesús R. Flores. New benchmarks for the second-order correlation energies of Ne and Ar through the finite element MP2 method. *International Journal of Quantum Chemistry*, 108 (12):2172–2177, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fernandez:2002:SNR

[FM02a] J. Fernández and F. Martín. In search of new resonance structures in dissociative photoionization of H_2. *International Journal of Quantum Chemistry*, 86(2):145–150, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86510681/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86510681/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86510681&PLACEBO=IE.pdf`.

Fuentealba:2002:ASD

[FM02b] P. Fuentealba and Junia Melin. Atomic spin-density polarization index and atomic spin-density information entropy

distance. *International Journal of Quantum Chemistry*, 90 (1):334–341, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fessatidis:2005:CSA

[FMBM05] Vassilios Fessatidis, Jay D. Mancini, Samuel P. Bowen, and William J. Massano. A canonical sequence approach to the $E \otimes \epsilon$ Jahn–Teller effect. *International Journal of Quantum Chemistry*, 103(6):792–797, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Filippov:2004:CSI

[FN04] D. A. Filippov and I. S. Nikiforov. Calculation of states of an ion Fe^3 in crystal $FeBO_3$. *International Journal of Quantum Chemistry*, 100(1):13–15, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Filho:2003:UNN

[FOM+03] T. M. Rocha Filho, Z. T. Oliveira, Jr., L. A. C. Malbouisson, R. Gargano, and J. J. Soares Neto. The use of neural networks for fitting potential energy surfaces: A comparative case study for the H molecule. *International Journal of Quantum Chemistry*, 95(3):281–288, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Forner:2000:SCS

[För00] Wolfgang Förner. Spectra of charged solitons and temperature dependence of the mobility of neutral solitons in *trans*-polyacetylene. *International Journal of Quantum Chemistry*, 80(2):153–183, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001289/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001289/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001289&PLACEBO=IE.pdf`.

Forner:2004:TVS

[För04] Wolfgang Förner. Theoretical vibrational spectra of organic ring compounds compared to experiment. *International Journal of Quantum Chemistry*, 99(4):533–555, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Filizola:2002:ABC

[FP02] Marta Filizola and Juan J. Perez. Assessment of the bioactive conformation of the vasoactive intestinal peptide by computational methods. *International Journal of Quantum Chemistry*, 88(1):201–210, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90510850/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90510850/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90510850&PLACEBO=IE.pdf`.

Ferro:2003:DFS

[FPC+03] V. R. Ferro, L. A. Poveda, C. G. Claessens, R. H. González-Jonte, and J. M. García de la Vega. Density functional study of the redox processes in subphthalocyanines. *International Journal of Quantum Chemistry*, 91(3):369–375, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuentealba:2005:EPS

[FPC05] Patricio Fuentealba and Luis Padilla-Campos. Electronic properties of small bimetallic Li_nCu_m $(n, m \leq 4)$ clusters. A comparison with Li_n and Cu_n clusters. *International Journal of Quantum Chemistry*, 102(5):498–505, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuentes:2008:QMM

[FPC+08] María E. Fuentes, Brisa Peña, César Contreras, Ana L. Montero, Russell Chianelli, Manuel Alvarado, Ramón Olivas, Luz M. Rodríguez, Héctor Camacho, and Luis A. Montero-Cabrera. Quantum mechanical model for Maya Blue. *International Journal of Quantum Chemistry*, 108(10):1664–1673, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fritsche:2003:DBS

[FPJR03] L. Fritsche, A. J. Pérez-Jiménez, and T. Reinert. DFT-based solution to the gap problem of antiferromagnetic transition metal oxides and parent compounds of high-T_c superconductors. *International Journal of Quantum Chemistry*, 91(2):216–

223, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fransson:2003:TTD

[Fra03] J. Fransson. Theory of time-dependent transport in quantum dot systems. *International Journal of Quantum Chemistry*, 92(6):471–477, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Franz:2006:MSM

[Fra06a] Jan Franz. Multi-state multi-reference Møller–Plesset second-order perturbation theory for molecular calculations. *International Journal of Quantum Chemistry*, 106(4):773–786, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fraser:2006:SMI

[Fra06b] Simon J. Fraser. Symbolic methods for invariant manifolds in chemical kinetics. *International Journal of Quantum Chemistry*, 106(1):228–243, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fomina:2002:CCF

[FRF02] Lioudmila Fomina, Abraham Reyes, and Serguei Fomine. Complexes of C60 fullerene with simple donor molecules: Theoretical study. *International Journal of Quantum Chemistry*, 89(5):477–483, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fomina:2004:OMP

[FRGF04] Lioudmila Fomina, Abraham Reyes, Patricia Guadarrama, and Serguei Fomine. Oniom (MP2:PM3) study of C_{60}–water complex. *International Journal of Quantum Chemistry*, 97 (1):679–687, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

FerreiraDaCunha:2006:FPE

[FRGM06] Wiliam Ferreira Da Cunha, Luiz Fernando Roncaratti, Ricardo Gargano, and Geraldo Magela E.Silva. Fitting potential energy surface of reactive systems via genetic algorithm. *International Journal of Quantum Chemistry*, 106(13):2650–2657, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fritzsche:2006:APG

[Fri06] S. Fritzsche. Application of point-group symmetries in chemistry and physics: A computer-algebraic approach. *International Journal of Quantum Chemistry*, 106(1):98–129, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fleischhauer:2005:MNA

[FRK+05] Jörg Fleischhauer, Gerhard Raabe, Kenneth A. Klingensmith, Udo Höweler, Prabir K. Chatterjee, Klaus Hafner, Emanuel Vogel, and Josef Michl. MCD of non-aromatic cyclic π-electron systems. Part 6: Pentalenes and heptalenes. *International Journal of Quantum Chemistry*, 102(5):925–939, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ferrao:2008:ESC

[FRNM08] Luiz Fernando A. Ferrão, Orlando Roberto-Neto, and Francisco B. C. Machado. Electronic structure of CuX^y (X = B, C, N, O, F; y = 0, +1, −1). *International Journal of Quantum Chemistry*, 108(13):2512–2522, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Feng:2000:TSS

[FRT+00] Jikang Feng, Aimin Ren, Weiquan Tian, Maofa Ge, Zhiru Li, Chiachung Sun, Xuehe Zheng, and Michael C. Zerner. Theoretical studies on the structure and electronic spectra of some isomeric fullerene derivatives C_{60} O_n ($n = 2, 3$). *International Journal of Quantum Chemistry*, 76(1):23–43, January 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503193/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503193/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503193&PLACEBO=IE.pdf`.

Frolov:1997:EFS

[FS97] Alexei M. Frolov and Vedene H. Smith, Jr. Exact finite series for the few-body auxiliary functions. *International Journal of Quantum Chemistry*, 63(1):269–278, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-`

bin/abstract?ID=42572; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42572&PLACEBO=IE.pdf. See erratum [FS09].

Flocke:2000:IAH

[FS00] N. Flocke and T. G. Schmalz. IPM approach to Hubbard model. Applications and limitations of restricted CI calculations to ground states of someπ networks containing fused 5- and 6-membered rings. *International Journal of Quantum Chemistry*, 76(1):83–98, January 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/69503198/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503198/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503198&PLACEBO=IE.pdf.

Freeman:2005:REC

[FS05] Fillmore Freeman and Bagrat A. Shainyan. Relative energies of conformations and sulfinyl oxygen-induced pentacoordination at silicon in 4-bromo- and 4,4-dibromo-4-silathiacyclohexane 1-oxide: A computational study. *International Journal of Quantum Chemistry*, 105(4):313–324, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Furlan:2008:SFS

[FS08] Ana C. Furlan and Munir S. Skaf. Solvation of 5-fluorouracil in supercritical CO_2. *International Journal of Quantum Chemistry*, 108(13):2557–2563, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Frolov:2009:EEF

[FS09] Alexei M. Frolov and Vedene H. Smith, Jr. Erratum: Exact finite series for the few-body auxiliary functions. *International Journal of Quantum Chemistry*, 109(2):384, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [FS97].

Fernandez:2005:TSB

[FSGB05] E. M. Fernández, J. M. Soler, I. L. Garzón, and L. C. Balbás. Trends in the structure and bonding of neutral and

charged noble metal clusters. *International Journal of Quantum Chemistry*, 101(6):740–745, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuks:2005:BCV

[FSK05] D. Fuks, A. Strutz, and A. Kiv. Bonding of Cr and V in FeAl B2 phase. *International Journal of Quantum Chemistry*, 102 (5):606–611, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fleisher:2002:TIB

[FSLL02] M. Fleisher, V. Stonkus, L. Leite, and E. Lukevics. Theoretical investigations of 1,4-butanediol and 2-butene-1,4-diol cyclodehydration using postprocessing visualization of quantum chemical calculation data. *International Journal of Quantum Chemistry*, 88(5):670–675, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fleisher:2004:IBD

[FSLL04] M. Fleisher, V. Stonkus, L. Leite, and E. Lukevics. Investigation of the 1,4-butanediol dehydrogenation over SiO_2 using AM1 method. *International Journal of Quantum Chemistry*, 100(4):407–411, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuchs:2002:HUD

[FSR02] Monika S. K. Fuchs, Alexey M. Shor, and Notker Rösch. The hydration of the uranyl dication: Incorporation of solvent effects in parallel density functional calculations with the program ParaGauss. *International Journal of Quantum Chemistry*, 86(5):487–501, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/88010694/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88010694/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88010694&PLACEBO=IE.pdf`.

Fidder:2004:QMP

[FT04] Henk Fidder and O. Tapia. The quantum measurement problem. *International Journal of Quantum Chemistry*, 97(1):670–678, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fernandez:2004:TBF

[FTB04] E. M. Fernández, M. B. Torres, and L. C. Balbás. Trends in the bonding of the first-row transition metal compounds: V(001) surface, TM-oxide and nitride molecules, and Au_nTi ($2 \leq n \leq 7$) clusters. *International Journal of Quantum Chemistry*, 99(1):39–46, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Friedemann:2004:DSK

[FTGH04] Rudolf Friedemann, Kai Tittmann, Ralph Golbik, and Gerhard Hübner. DFT studies on key intermediates in thiamin catalysis. *International Journal of Quantum Chemistry*, 99 (2):109–114, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fromager:2006:ESC

[FTM06] Emmanuel Fromager, Christian Teichteil, and Laurent Maron. Extraction of shape-consistent spin-orbit pseudo-potential from an effective spin-orbit parameter and application to the tellurium atom. *International Journal of Quantum Chemistry*, 106(3):764–771, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fernandez:2003:DEE

[FTW03] J. J. Fernández, C. Tablero, and P. Wahnón. Development of the exact exchange scheme using a basis set framework. *International Journal of Quantum Chemistry*, 91(2):157–164, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fukushima:2009:GQM

[Fuk09] Kimichika Fukushima. A Gaussian quadrature method for total energy analysis in electronic state calculations. *International Journal of Quantum Chemistry*, 109(12):2664–2671, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fulde:2000:GSW

[Ful00] Peter Fulde. Ground-state wave functions and energies of solids. *International Journal of Quantum Chemistry*, 76(3): 385–395, January 20, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.`

interscience.wiley.com/cgi-bin/abstract/70000281/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000281/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000281&PLACEBO=IE.pdf.

Fortunelli:2004:TBP

[FV04] Alessandro Fortunelli and Ana Marìa Velasco. Tight-binding parameterization of transition and noble metal clusters. *International Journal of Quantum Chemistry*, 99(5):654–666, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Frayret:2005:DFT

[FVPM05] Christine Frayret, Antoine Villesuzanne, Michel Pouchard, and Samir Matar. Density functional theory calculations on microscopic aspects of oxygen diffusion in ceria-based materials. *International Journal of Quantum Chemistry*, 101(6):826–839, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fan:2008:PED

[FWT08] Jian-Fen Fan, Li-Fen Wu, and Fu-Ming Tao. Poor enantioselectivity of the direct aldol reaction catalyzed by (S, S)-proline dipeptide: A density functional study. *International Journal of Quantum Chemistry*, 108(1):66–74, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fang:2009:DFS

[FWZ09] Hua Fang, Shu-Guang Wang, and Xiao-Gang Zhang. Density functional study of aurophilic interaction in $Cl(AuPH_3)$ and in its dimerization. *International Journal of Quantum Chemistry*, 109(3):526–533, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fang:2005:DFT

[FXHL05] Guo-Yong Fang, Li-Na Xu, Xin-Gen Hu, and Xin-Hua Li. Density functional theory study of the interaction between 3-nitro-1,2,4-triazole-5-one and ammonia. *International Journal of Quantum Chemistry*, 105(2):148–153, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fan:2009:DSR

[FYH09] Jian-Fen Fan, Chun-Hong Yang, and Liang-Jun He. DFT study on the role of methanol solvent in Morita–Baylis–Hillman reaction. *International Journal of Quantum Chemistry*, 109(6):1311–1321, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fujisaki:2009:QCV

[FYSS09] Hiroshi Fujisaki, Kiyoshi Yagi, John E. Straub, and Gerhard Stock. Quantum and classical vibrational relaxation dynamics of N-methylacetamide on ab initio potential energy surfaces. *International Journal of Quantum Chemistry*, 109(10):2047–2057, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fujiwara:2009:MOS

[FYT09] Yasuhiro Fujiwara, Tomohiko Yoshioka, and Junzo Tanaka. Molecular orbital study on a mechanism of adhesion between carbides and optical glass with high refractive index. *International Journal of Quantum Chemistry*, 109(12):2780–2787, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Firouzi:2009:CEI

[FZ09] Rohoullah Firouzi and Mansour Zahedi. Conclusive evidence on the insensitivity of additive rules to the combinational details of exchange and correlation functional in hybrid DFT methods. *International Journal of Quantum Chemistry*, 109 (2):160–170, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fan:2007:EQS

[FZRD07] Kaimin Fan, Yujun Zheng, Weiyi Ren, and Shiliang Ding. Exact quantum solutions of general driven time-dependent quantum quadratic system. *International Journal of Quantum Chemistry*, 107(6):1355–1366, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gheisari:2008:NFR

[GA08] R. Gheisari and A. Avazpour. Nuclear fusion rate for ddμ muonic molecule. *International Journal of Quantum Chem-*

istry, 108(2):378–382, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Glushkov:2004:DSF

[GAIK04] Alexander V. Glushkov, Sergey V. Ambrosov, Anna V. Ignatenko, and Dmitry A. Korchevsky. DC strong field Stark effect for nonhydrogenic atoms: consistent quantum mechanical approach. *International Journal of Quantum Chemistry*, 99(6):936–939, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Glushkov:2005:CQA

[GAL+05] Alexander V. Glushkov, Sergey V. Ambrosov, Andrey V. Loboda, Elena P. Gurnitskaya, and Georgy P. Prepelitsa. Consistent QED approach to calculation of electron-collision excitation cross sections and strengths: Ne-like ions. *International Journal of Quantum Chemistry*, 104(4):562–569, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gal:2007:PWF

[Gál07] Tamás Gál. The N-particle wave function as a homogeneous functional of the density. *International Journal of Quantum Chemistry*, 107(14):2586–2594, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garai:2008:MFD

[Gar08a] Jozsef Garai. Mathematical formulas describing the sequences of the periodic table. *International Journal of Quantum Chemistry*, 108(4):667–670, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gonzalez:2008:TII

[GAR08b] Sergio A. González, Néstor F. Aguirre, and Andrés Reyes. Theoretical investigation of isotope effects: The any-particle molecular orbital code. *International Journal of Quantum Chemistry*, 108(10):1742–1749, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Griffe:2008:TSO

[GARB08] Beulah Griffe, Giuseppe Agrifoglio, Fernando Ruette, and Joaquín L. Brito. Theoretical study of olefin oxidation process on a dioxo-μ-oxo Mo catalyst. *International Journal of*

Quantum Chemistry, 108(10):1674–1683, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Geskin:2003:GES

[GB03] V. M. Geskin and J. L. Bredas. Geometric and electronic structure of zwitterionic push–pull polyenes for nonlinear optics. *International Journal of Quantum Chemistry*, 91(3):303–310, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2005:CQM

[GB05] Dulal C. Ghosh and Soma Bhattacharyya. Computation of quantum mechanical hybridization and dipole correlation of the electronic structure of the F_3B–NH_3 supermolecule. *International Journal of Quantum Chemistry*, 105(3):270–279, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gogtas:2006:QWPa

[GB06a] Fahrettin Gogtas and Niyazi Bulut. Quantum wave packet study of $N(^2D) + H_2$ reactive scattering. *International Journal of Quantum Chemistry*, 106(4):833–838, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gritsenko:2006:CDL

[GB06b] Oleg Gritsenko and Evert Jan Baerends. Correct dissociation limit for the exchange-correlation energy and potential. *International Journal of Quantum Chemistry*, 106(15):3167–3177, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2008:DDM

[GB08] S. Ghosh and S. P. Bhattacharyya. Dissociation of a diatomic molecule induced by discontinuous reversals of a static electric field. *International Journal of Quantum Chemistry*, 108(7):1209–1219, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2009:QDD

[GB09] S. Ghosh and S. P. Bhattacharyya. Quantum dynamics of a discontinuously kicked charged particle in harmonic, symmetric double, or triple wells. *International Journal of Quantum*

Chemistry, 109(6):1177–1188, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gogtas:2005:QWP

[GBA05] Fahrettin Gogtas, Niyazi Bulut, and Sinan Akpinar. Quantum wave packet calculation of reaction probabilities, cross sections, and rate constants for the C(^{1}D) + HD reaction. *International Journal of Quantum Chemistry*, 105(5):478–484, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guerra:2006:OIC

[GBB06] Célia Fonseca Guerra, Evert Jan Baerends, and F. Matthias Bickelhaupt. Orbital interactions and charge redistribution in weak hydrogen bonds: Watson–Crick GC mimic involving C H proton donor and F proton acceptor groups. *International Journal of Quantum Chemistry*, 106(12):2428–2443, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guillaume:2002:EEF

[GBC+02] Maxime Guillaume, Edith Botek, Benoît Champagne, Frédéric Castet, and Laurent Ducasse. Electronic excitations and first hyperpolarizability of 2-methyl-4-nitroaniline clusters. *International Journal of Quantum Chemistry*, 90(4-5): 1378–1387, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Galasso:2001:SMS

[GBJM01] V. Galasso, F. Benedetti, D. Jones, and A. Modelli. A study of the molecular structure and spectroscopic properties of polycyclic polyaza-compounds with diamond-lattice conformations. *International Journal of Quantum Chemistry*, 84 (6):630–641, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/82502286/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/82502286/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=82502286&PLACEBO=IE.pdf`.

Gorecki:2006:PQD

[GBL06] Adam Gorecki, Piotr Bala, and Bogdan Lesyng. Parallelization of the quantum dynamics code for cluster architecture and its applications to the Gross–Pitaevskii equation. *International Journal of Quantum Chemistry*, 106(3):664–669, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gomez-Balderas:2000:PEC

[GBMMSA00] R. Gómez-Balderas, J. M. Martínez-Magadán, R. Santamaria, and C. Amador. Promotional effect of Co or Ni impurity in the catalytic activity of MoS_2: An electronic structure study. *International Journal of Quantum Chemistry*, 80(3):406–415, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501019/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501019/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501019&PLACEBO=IE.pdf`.

Gill:2004:WIK

[GBO04] Peter M. W. Gill, Nicholas A. Besley, and Darragh P. O'Neill. Wigner intracule for the Kellner helium-like ions. *International Journal of Quantum Chemistry*, 100(2):166–171, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gohaud:2005:AVS

[GBP05] Neil Gohaud, Didier Begue, and Claude Pouchan. Accurate vibrational spectra of methylpotassium using a hybrid CCSD(t)/b3LYP approach and a variational treatment. *International Journal of Quantum Chemistry*, 104(5):773–781, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Galvez:2002:VMC

[GBS02] F. J. Gálvez, E. Buendía, and A. Sarsa. Variational Monte Carlo calculations for some cations and anions of the first-row atoms using explicitly correlated wave functions. *International Journal of Quantum Chemistry*, 87(5):270–274, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90512105/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90512105/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90512105&PLACEBO=IE.pdf`.

Galvez:2004:MSP

[GBS04] F. J. Gálvez, E. Buendía, and A. Sarsa. Momentum space properties for the atoms helium to neon from energy-optimized explicitly correlated wave functions. *International Journal of Quantum Chemistry*, 99(4):247–255, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Geerlings:2005:DFT

[GBVD05] P. Geerlings, G. Boon, C. Van Alsenoy, and F. De Proft. Density functional theory and quantum similarity. *International Journal of Quantum Chemistry*, 101(6):722–732, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gebauer:2005:ETD

[GC05] Ralph Gebauer and Roberto Car. Electron transport with dissipation: A quantum kinetic approach. *International Journal of Quantum Chemistry*, 101(5):564–571, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gaffney:2003:CDM

[GCCM03] Shannon M. Gaffney, Joseph F. Capitani, Lyana Castaldo, and Abhijit Mitra. Critical distance model for the energy of activation of the Bergman cyclization of enediynes. *International Journal of Quantum Chemistry*, 95(6):706–712, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Giro:2005:BGE

[GCG05] R. Giro, M. J. Caldas, and D. S. Galvão. Band gap engineering for poly(*p*-phenylene) and poly(*p*-phenylene vinylene) copolymers using the tight-binding approach. *International Journal of Quantum Chemistry*, 103(5):588–596, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Geerlings:2000:HPA

[GD00a] P. Geerlings and F. De Proft. HSAB principle: Applications of its global and local forms in organic chemistry. *International Journal of Quantum Chemistry*, 80(2):227–235, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001279/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001279/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001279&PLACEBO=IE.pdf`.

Ghanty:2000:TIE

[GD00b] Tapan K. Ghanty and Ernest R. Davidson. Theoretical investigation of electronic structure and ESR hyperfine parameters for the CuH^+ molecule. *International Journal of Quantum Chemistry*, 77(1):291–300, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004268/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004268/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004268&PLACEBO=IE.pdf`.

Gdanitz:2001:NVM

[Gda01a] Robert J. Gdanitz. A new version of the multireference averaged coupled-pair functional (MR-ACPF-2). *International Journal of Quantum Chemistry*, 85(4–5):281–300, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guimaraes:2001:ERF

[GdA01b] Cristiano Ruch Werneck Guimarães and Ricardo Bicca de Alencastro. Evaluating the relative free energy of hydration of new thrombin inhibitor candidates using the finite difference thermodynamic integration (FDTI) method. *International Journal of Quantum Chemistry*, 85(6):713–726, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85008800/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85008800/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85008800&PLACEBO=IE.pdf`.

Geskin:2003:ORC

[GDB03] V. M. Geskin, A. Dkhissi, and J. L. Brédas. Oligothiophene radical cations: Polaron structure in hybrid DFT and MP2 calculations. *International Journal of Quantum Chemistry*, 91(3):350–354, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Giuffreda:2001:TSV

[GDFT01] M. G. Giuffreda, M. S. Deleuze, J.-P. François, and A. B. Trofimov. Theoretical study of the vertical electron excitation of linear carbon clusters C_3, C_5, and C_7. *International Journal of Quantum Chemistry*, 85(4–5):475–491, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guizado:2008:CSS

[GdRPLP08] Teobaldo Cuya Guizado, Samuel da Rocha Pita, Sonia R. Wanderley Louro, and Pedro Geraldo Pascutti. Computational study of the solvation of protoporphyrin IX and its Fe^{2+} complex. *International Journal of Quantum Chemistry*, 108(13):2603–2607, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Geerlings:2005:PXI

[GDV05] P. Geerlings, F. De Proft, and C. Van Alsenoy. Preface: X International Conference on the Applications of Density Functional Theory in Chemistry and Physics 7–12 September 2003, Brussels, Belgium. *International Journal of Quantum Chemistry*, 101(5):469–471, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guseinov:2009:UNS

[GE09] I. I. Guseinov and M. Ertürk. Use of noninteger n-Slater type orbitals in combined Hartree–Fock–Roothaan theory for calculation of isoelectronic series of atoms Be to Ne. *International Journal of Quantum Chemistry*, 109(2):176–184, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gagliardi:2000:DRA

[GEB+00] Laura Gagliardi, Stefano Evangelisti, Anders Bernhardsson, Roland Lindh, and Björn O. Roos. Dissociation reaction of N_8 azapentalene to $4N_2$: A theoretical study. *In-*

ternational Journal of Quantum Chemistry, 77(1):311–315, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004271/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004271/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004271&PLACEBO=IE.pdf`.

Gusarov:2009:VEE

[GFDK09] Sergey Gusarov, Tatiana A. Fedorova, Yuri Yu. Dmitriev, and Andriy Kovalenko. On variational estimates for exchange-correlation interaction obtained within super-CI approach to MCSCF approximation. *International Journal of Quantum Chemistry*, 109(8):1672–1675, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guerra:2008:ISP

[GFMT08] Antonio C. O. Guerra, Glaucio B. Ferreira, Sérgio P. Machado, and Cássia C. Turci. Inner-shell photoabsorption spectroscopy of push–pull nitroanilines—Theoretical and experimental studies at N 1*s* region. *International Journal of Quantum Chemistry*, 108(13):2340–2357, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goller:2000:INC

[GG00] Andreas Göller and Ulrich-Walter Grummt. Implementation of an NDDO/CI/SOS approach for second-order hyperpolarizabilities. *International Journal of Quantum Chemistry*, 77(4):727–760, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70500249/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70500249/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70500249&PLACEBO=IE.pdf`.

Giro:2003:SSE

[GG03] R. Giro and D. S. Galvão. Semiempirical studies of the electronic structure of polyphenylene sulfide phenyleneamine. *International Journal of Quantum Chemistry*, 95(3):252–259, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Glushkov:2007:COP

[GG07] Vitaly N. Glushkov and Nikitas Gidopoulos. Constrained optimized potential method and second-order correlation energy for excited states. *International Journal of Quantum Chemistry*, 107(14):2604–2615, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garcia-Gonzalez:2003:NWF

[GGACT03] P. García-González, J. E. Alvarellos, E. Chacón, and P. Tarazona. Nonlocal WDA functional capable of describing the image potential of a metallic surface. *International Journal of Quantum Chemistry*, 91(2):139–144, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gori-Giorgi:2003:TDE

[GGAMB03] Paola Gori-Giorgi, Claudio Attaccalite, Saverio Moroni, and Giovanni B. Bachelet. Two-dimensional electron gas: Correlation energy versus density and spin polarization. *International Journal of Quantum Chemistry*, 91(2):126–130, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gusarov:2007:VEE

[GGDL07] S. I. Gusarov, I. A. Goidenko, Yu. Yu. Dmitriev, and L. N. Labzowsky. Variational estimates for exchange-correlation interaction obtained within Super-CI approach to MCSCF approximation. *International Journal of Quantum Chemistry*, 107(14):2616–2621, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ginalski:2002:DCP

[GGLS02] Krzysztof Ginalski, Pawel Grochowski, Bogdan Lesyng, and David Shugar. DFT calculations and parameterization of the approximate valence bond method to describe the phosphoryl transfer reaction in a model system. *International Journal of Quantum Chemistry*, 90(3):1129–1139, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goswami:2006:TSS

[GGPS06] Biplab Goswami, Chanchal Ghosh, Sougata Pal, and Pranab Sarkar. Theoretical studies of structural and electronic properties of Al_nAs_n clusters. *International Journal of Quantum*

Chemistry, 106(4):887–893, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gori-Giorgi:2009:RSC

[GGS09a] Paola Gori-Giorgi and Andreas Savin. Range separation combined with the Overhauser model: Application to the H_2 molecule along the dissociation curve. *International Journal of Quantum Chemistry*, 109(9):1950–1961, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gori-Giorgi:2009:SDE

[GGS09b] Paola Gori-Giorgi and Andreas Savin. Study of the discontinuity of the exchange-correlation potential in an exactly soluble case. *International Journal of Quantum Chemistry*, 109(11): 2410–2415, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ge:2003:GOS

[GH03] Yingbin Ge and John D. Head. Global optimization of Si_xH_y at the ab initio level via an iteratively parametrized semiempirical method. *International Journal of Quantum Chemistry*, 95(4–5):617–626, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gheisari:2009:REF

[Ghe09] Rouhollah Gheisari. Resonance energies and fusion rates of mass-nonsymmetric dtμ* molecule. *International Journal of Quantum Chemistry*, 109(5):1070–1073, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gonze:2004:SMC

[GHG04] Didier Gonze, José Halloy, and Albert Goldbeter. Stochastic models for circadian oscillations: Emergence of a biological rhythm. *International Journal of Quantum Chemistry*, 98 (2):228–238, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gearhart:2003:MQM

[GHH03] Dorothy J. Gearhart, James F. Harrison, and Katharine L. C. Hunt. Molecular quadrupole moments of HCCH, FCCF, and ClCCCl. *International Journal of Quantum Chemistry*, 95

(6):697–705, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gront:2005:EPE

[GHK05] Dominik Gront, Ulrich H. E. Hansmann, and Andrzej Kolinski. Exploring protein energy landscapes with hierarchical clustering. *International Journal of Quantum Chemistry*, 105 (6):826–830, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guevara:2009:AFP

[GHT09] Nicolais L. Guevara, Frank E. Harris, and Alexander V. Turbiner. An accurate few-parameter ground state wave function for the lithium atom. *International Journal of Quantum Chemistry*, 109(13):3036–3040, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gotsev:2007:LRC

[GI07] Martin G. Gotsev and Petko M. Ivanov. Large-ring cyclodextrins. Further support for the preferred conformations of CD26 in water solution: Molecular dynamics studies on CD26-derived conformations of CDn ($n = 24, 25, 27, 28, 29, 30$). *International Journal of Quantum Chemistry*, 107(8):1657–1672, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gineityte:2000:GDF

[Gin00] V. Gineityte. Generalization of the Dewar formula for total energies of molecules. *International Journal of Quantum Chemistry*, 77(2):534–543, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70002213/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70002213/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70002213&PLACEBO=IE.pdf`.

Gineityte:2001:IEB

[Gin01] V. Gineitytė. Interpretation of energy bands of regular quasi-one-dimensional systems in terms of local structure. *International Journal of Quantum Chemistry*, 81(5):321–331, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76507291/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76507291/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76507291&PLACEBO=IE.pdf`.

Gineityte:2003:SAI

[Gin03] V. Gineityte. Semilocalized approach to investigation of chemical reactivity. *International Journal of Quantum Chemistry*, 94(6):302–316, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gineityte:2005:BDP

[Gin05a] V. Gineityte. Block-diagonalization problem for the common Hückel-type Hamiltonian matrix of alternant hydrocarbons and its nonperturbative solution. *International Journal of Quantum Chemistry*, 101(3):274–282, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gineityte:2005:LMO

[Gin05b] V. Gineityte. Localized molecular orbitals in the Hückel model of perturbed alternant hydrocarbons and their relation to the charge–bond order matrix. *International Journal of Quantum Chemistry*, 105(3):232–245, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gineityte:2006:SOE

[Gin06] V. Gineityte. Second-order effects in the Hückel model of perturbed alternant hydrocarbons and their coincidence for specific one- and two-center perturbations. *International Journal of Quantum Chemistry*, 106(9):2145–2160, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gineityte:2008:STF

[Gin08] V. Gineityte. A simple topological factor determining the allowance of pericyclic reactions. *International Journal of Quantum Chemistry*, 108(6):1141–1154, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2003:FOD

[GJ03] Dulal C. Ghosh and Jibanananda Jana. Frontier orbital and density functional study of the variation of the hard–soft be-

havior of monoborane (BH_3) and boron trifluoride (BF_3) as a function of angles of reorganization from planar (D_{3h}) to pyramidal (C_{3v}) shape. *International Journal of Quantum Chemistry*, 92(6):484–505, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2000:QCS

[GJB00] Dulal C. Ghosh, Jibanananda Jana, and Raka Biswas. Quantum chemical study of the umbrella inversion of the ammonia molecule. *International Journal of Quantum Chemistry*, 80(1):1–26, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72515501/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72515501/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72515501&PLACEBO=IE.pdf`.

Ghosh:2002:DFM

[GJB02] Dulal C. Ghosh, Jibanananda Jana, and Soma Bhattacharyya. Density functional and molecular orbital study of physical process of inversion of nitrogen trifluoride (NF_3) molecule. *International Journal of Quantum Chemistry*, 87(3):111–134, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89013462/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89013462/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89013462&PLACEBO=IE.pdf`.

Godfrey-Kittle:2006:EDM

[GKC06] Andrew Godfrey-Kittle and Mauricio Cafiero. Evaluation of DFT methods for computing the interaction energies of homomolecular and heteromolecular dimers of monosubstituted benzene. *International Journal of Quantum Chemistry*, 106 (9):2035–2043, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goller:2001:MSR

[GKE01] Andreas Göller, E. Klemm, and D. A. M. Egbe. Model systems for rod-like polyheteroarylethynylenes. *International Journal of Quantum Chemistry*, 84(1):86–98, ????

2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/84002444/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002444/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002444&PLACEBO=IE.pdf.

Glushkov:2009:EQC

[GKL+09] A. V. Glushkov, P. A. Kondratenko, Ya. I. Lepikh, A. P. Fedchuk, L. Lovett, and A. A. Svinarenko. Electrodynamical and quantum-chemical approaches to modeling the electrochemical and catalytic processes on metals, metal alloys, and semiconductors. *International Journal of Quantum Chemistry*, 109(14):3473–3481, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gutman:2000:ADS

[GKR00] Ivan Gutman, Sandi Klavžar, and Amal Rajapakse. Average distances in square-cell configurations. *International Journal of Quantum Chemistry*, 76(5):611–617, February 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70000582/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000582/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000582&PLACEBO=IE.pdf.

Grembecka:2001:EMI

[GKSL01] J. Grembecka, P. Kedzierski, W. A. Sokalski, and J. Leszczyński. Electrostatic models of inhibitory activity. *International Journal of Quantum Chemistry*, 83(3-4):180–192, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/80002587/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002587/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002587&PLACEBO=IE.pdf.

Guo:2006:HWV

[GKYY06] Xiaofeng Guo, D. J. Klein, Weigen Yan, and Yeong-Nan Yeh. Hyper-Wiener vector, Wiener matrix sequence, and Wiener polynomial sequence of a graph. *International Journal of*

Quantum Chemistry, 106(8):1756–1761, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gorelsky:2000:MSR

[GL00] Sergey I. Gorelsky and A. B. P. Lever. Metastable states of ruthenium (II) nitrosyl complexes and comparison with $[Fe(CN)_5\ NO]^{2-}$. *International Journal of Quantum Chemistry*, 80(4–5):636–645, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505419/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505419/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505419&PLACEBO=IE.pdf`.

Gadella:2001:GDE

[GL01] M. Gadella and R. Laura. Gamow dyads and expectation values. *International Journal of Quantum Chemistry*, 81(5):307–320, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76511022/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76511022/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76511022&PLACEBO=IE.pdf`.

Gong:2007:SEE

[GL07] Zhijun Gong and Jolanta B. Lagowski. Singlet excitation energies of thiophene derivatives of fluorene: TD-DFT study. *International Journal of Quantum Chemistry*, 107(1):159–171, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghiotto:2004:AAF

[GLF04] R. C. T. Ghiotto, F. C. Lavarda, and F. J. B. Ferreira. Antioxidant activity of flavonols. *International Journal of Quantum Chemistry*, 97(5):949–952, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:2009:GIS

[GLHH09] Ya-Hui Guo, Rui-Feng Lu, Ke-Li Han, and Guo-Zhong He. Generation of an isolated sub-100 attosecond pulse in a two-color laser field. *International Journal of Quantum Chemistry*,

109(14):3410–3415, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Glushkov:2004:ATO

[Glu04] V. N. Glushkov. Alternative techniques in open-shell SCF theory. *International Journal of Quantum Chemistry*, 99(4):236–246, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gong:2000:TSC

[GLX+00] Xue Dong Gong, Ya Lin Lu, He Ming Xiao, Kong Chang Chen, and He Tian. Theoretical studies on the conformations and properties of phenylazonaphthalenes. *International Journal of Quantum Chemistry*, 79(1):25–33, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72504319/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72504319/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72504319&PLACEBO=IE.pdf`.

Guseinov:2000:CAM

[GM00] I. I. Guseinov and B. A. Mamedov. On the calculation of arbitrary multielectron molecular integrals over Slater-type orbitals using recurrence relations for overlap integrals I. Single-center expansion method. *International Journal of Quantum Chemistry*, 78(3):146–152, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71007683/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71007683/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71007683&PLACEBO=IE.pdf`.

Guseinov:2001:CAM

[GM01] I. I. Guseinov and B. A. Mamedov. On the calculation of arbitrary multielectron molecular integrals over Slater-type orbitals using recurrence relations for overlap integrals. II. Two-center expansion method. *International Journal of Quantum Chemistry*, 81(2):117–125, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76500933/START; http:`

//www3.interscience.wiley.com/cgi-bin/fulltext/76500933/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76500933&PLACEBO=IE.pdf.

Guseinov:2002:CAMa

[GM02a] I. I. Guseinov and B. A. Mamedov. On the calculation of arbitrary multielectron molecular integrals over Slater-type orbitals using recurrence relations for overlap integrals. III. Auxiliary functions $Q^q_{nn'}$ and $G^q_{-nn'}$. *International Journal of Quantum Chemistry*, 86(5):440–449, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/86510685/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86510685/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86510685&PLACEBO=IE.pdf. See erratum [GM08].

Guseinov:2002:CAMb

[GM02b] I. I. Guseinov and B. A. Mamedov. On the calculation of arbitrary multielectron molecular integrals over Slater-type orbitals using recurrence relations for overlap integrals. IV. Use of recurrence relations for basic two-center overlap and hybrid integrals. *International Journal of Quantum Chemistry*, 86(5):450–455, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/88011407/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88011407/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88011407&PLACEBO=IE.pdf.

Guseinov:2003:CME

[GM03] I. I. Guseinov and B. A. Mamedov. Calculation of molecular electric and magnetic multipole moment integrals of integer and noninteger n Slater orbitals using overlap integrals. *International Journal of Quantum Chemistry*, 93(1):9–19, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guimaraes:2005:SPC

[GM05a] Paulo Henrique Alves Guimarães and Geraldo Magela e Silva. Structural phases of coupled polyacetylene chains with im-

purities. *International Journal of Quantum Chemistry*, 103 (5):597–603, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guimaraes:2005:QCG

[GM05b] Paulo Henrique Vales Guimarães and Geraldo Magela e Silva. Quantum-controlled NOT gate made of coupled polyacetylene chains. *International Journal of Quantum Chemistry*, 103(5):543–549, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guseinov:2008:ECA

[GM08] I. I. Guseinov and B. A. Mamedov. Erratum: On the calculation of arbitrary multielectron molecular integrals over Slater-type orbitals using recurrence relations for overlap integrals. III. Auxiliary functions $Q^q_{nn'}$ and $G^q_{-nn'}$. *International Journal of Quantum Chemistry*, 108(1):202, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [GM02a].

Graves-Morris:2009:RTA

[GM09] P. R. Graves-Morris. A review of two algorithms for acceleration of convergence of a sequence of vectors. *International Journal of Quantum Chemistry*, 109(8):1658–1665, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Glushkov:2004:CLE

[GMCS04] Alexander V. Glushkov, Svetlana V. Malinovskaya, Yulia G. Chernyakova, and Andrey A. Svinarenko. Cooperative laser-electron-nuclear processes: QED calculation of electron satellites spectra for multi-charged ion in laser field. *International Journal of Quantum Chemistry*, 99(6):889–893, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Glushkov:2009:GFM

[GMK+09] A. V. Glushkov, S. V. Malinovskaya, O. Yu. Khetselius, A. V. Loboda, D. E. Sukharev, and L. Lovett. Green's function method in quantum chemistry: New numerical algorithm for the Dirac equation with complex energy and Fermi-model nuclear potential. *International Journal of Quantum Chemistry*,

109(8):1717–1727, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gonzalez:2001:CMS

[GMPIP01] Oscar Galvez Gonzalez, Jane S. Murray, Zenaida Peralta-Inga, and Peter Politzer. Computed molecular surface electrostatic potentials of two groups of reverse transcriptase inhibitors: Relationships to anti-HIV-1 activities. *International Journal of Quantum Chemistry*, 83(3-4):115–121, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002594/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002594/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002594&PLACEBO=IE.pdf`.

Gross:2001:PSMb

[GMS01a] A. Gross, K. V. Mikkelsen, and W. R. Stockwell. A phase-space method for arbitrary bimolecular gas-phase reactions: Application to the CH_3 CHO+HO and CH_3 OOH+HO reactions. *International Journal of Quantum Chemistry*, 84 (5):493–512, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/83502022/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/83502022/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=83502022&PLACEBO=IE.pdf`.

Gross:2001:PSMa

[GMS01b] A. Gross, K. V. Mikkelsen, and W. R. Stockwell. A phase-space method for arbitrary bimolecular gas-phase reactions: Theoretical description. *International Journal of Quantum Chemistry*, 84(5):479–492, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/83502021/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/83502021/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=83502021&PLACEBO=IE.pdf`.

Glushkov:2005:QSM

[GMS+05] Alexander V. Glushkov, Svetlana V. Malinovskaya, Iryna M. Shpinareva, Valya P. Kozlovskaya, and Vlad I. Gura. Quantum stochastic modeling energy transfer and effect of rotational and V-T relaxation on multiphoton excitation and dissociation for CF_3Br molecules. *International Journal of Quantum Chemistry*, 104(4):512–516, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gonzalez-Moa:2002:ASP

[GMTM02] María J. González-Moa, Carmen Terán, and Ricardo A. Mosquera. AIM study of pyrimidyl carbocyclic analogues of nucleosides based on cyclopentene rings. *International Journal of Quantum Chemistry*, 86(1):67–78, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85011559/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85011559/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85011559&PLACEBO=IE.pdf`.

Gupta:2001:ROI

[GN01] Ashish K. Gupta and Daniel Neuhauser. Rabi-oscillations-induced multiharmonic emission in a Maxwell–Schrödinger study of a dense sample of molecules. *International Journal of Quantum Chemistry*, 81(4):260–267, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76505737/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76505737/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76505737&PLACEBO=IE.pdf`.

Gogonea:2005:PES

[Gog05] Valentin Gogonea. Potential energy surface of the reaction of imidazole with peroxynitrite: Density functional theory study. *International Journal of Quantum Chemistry*, 104(3):342–353, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gogtas:2006:QWPb

[Gög06] Fahrettin Gögtas. Quantum wave packet calculation of reaction probabilities, cross sections, and rate constants for H^+ +

LiH $\rightarrow$ Li + H reaction. *International Journal of Quantum Chemistry*, 106(9):1979–1985, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goodson:2003:IAI

[Goo03] David Z. Goodson. Improving the accuracy of ab initio methods with summation approximants and singularity analysis. *International Journal of Quantum Chemistry*, 92(1):35–46, March 5, 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goscinski:2001:CDE

[Gos01] Osvaldo Goscinski. Calculation of dispersion energy shifts in molecular electronic spectra using sum rules. *International Journal of Quantum Chemistry*, 81(3):202–205, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76504670/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76504670/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76504670&PLACEBO=IE.pdf`.

Gondos:2001:CCE

[GP01] Gy. Göndös and I. Pálinkó. Combined computational and experimental investigations on the diastereoselective hydrogenation of steroids by chiral oxazaborolidine. *International Journal of Quantum Chemistry*, 84(2):253–258, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502341/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502341/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502341&PLACEBO=IE.pdf`.

Guerini:2003:SEV

[GP03] Silvete Guerini and Paulo Piquini. Structural, electronic, and vibrational properties of B_xN_y ($x + y = 6$) clusters. *International Journal of Quantum Chemistry*, 95(3):329–335, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gourlaouen:2008:CCB

[GP08] C. Gourlaouen and O. Parisel. Competitive coordination between lead and oligoelements with respect to some therapeutic heavy-metal chelators. *International Journal of Quantum Chemistry*, 108(11):1888–1897, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goodman:2002:DDE

[GPW02] Lionel Goodman, Vojislava Pophristic, and Windy Wang. Does digermane exhibit free rotation? A test of barrier theory. *International Journal of Quantum Chemistry*, 90(2):657–662, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gour:2006:EAS

[GPW06] Jeffrey R. Gour, Piotr Piecuch, and Marta Włoch. Extension of the active-space equation-of-motion coupled-cluster methods to radical systems: The EA-EOMCCSDt and IP-EOMCCSDt approaches. *International Journal of Quantum Chemistry*, 106(14):2854–2874, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grant:2000:ART

[GQ00] Ian P. Grant and Harry M. Quiney. Application of relativistic theories and quantum electrodynamics to chemical problems. *International Journal of Quantum Chemistry*, 80(3):283–297, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501012/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501012/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501012&PLACEBO=IE.pdf`.

Garashchuk:2004:ACS

[GR04] Sophya Garashchuk and Vitaly A. Rassolov. Applicability criterion for semiclassical Bohmian dynamics. *International Journal of Quantum Chemistry*, 100(6):1057–1064, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gomes:2005:DFT

[GR05] José R. B. Gomes and Manuel A. V. Ribeiro Da Silva. Density functional theory study on the thermodynamic properties of aminophenols. *International Journal of Quantum Chemistry*, 101(6):860–868, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gai:2007:DFT

[GR07a] Jing-Gang Gai and Yi Ren. Density functional theory study on the reactions of X^- with CH_3SY (X, Y = F, Cl, Br, I). *International Journal of Quantum Chemistry*, 107(6):1373–1381, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See notice [Ano07e].

Gai:2007:TSGb

[GR07b] Jing-Gang Gai and Yi Ren. Theoretical study of the gas-phase ion pairs S_N2 reactions of LiX with CH_3SY (X, Y = F, Cl, Br, I). *International Journal of Quantum Chemistry*, 107(6): 1487–1494, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See notice [Ano07g, Ano07f].

Gai:2007:TSGa

[GR07c] Jing-Gang Gai and Yi Ren. Theoretical study of the gas-phase S_N2 reactions of X^- with CH_3OY (X, Y = Cl, Br, I). *International Journal of Quantum Chemistry*, 107(5):1142–1149, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See notice [Ano07g].

Grabowski:2008:CSO

[Gra08a] Ireneusz Grabowski. Comparison of second-order orbital-dependent DFT correlation functionals. *International Journal of Quantum Chemistry*, 108(12):2076–2087, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grassi:2008:RBA

[Gra08b] A. Grassi. A relationship between atomic correlation energy and Tsallis entropy. *International Journal of Quantum Chemistry*, 108(4):774–778, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gonzalez-Rivas:2009:TEE

[GRC09] Nelly González-Rivas and Andrés Cedillo. Theoretical estimation of the electron affinity of enolate radicals. *International Journal of Quantum Chemistry*, 109(5):1031–1035, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grein:2009:GLL

[Gre09] Friedrich Grein. Ground and low-lying excited C_{2v} states of FeO_2 — A challenge to computational methods. *International Journal of Quantum Chemistry*, 109(3):549–558, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grinberg:2006:PIT

[Gri06] Horacio Grinberg. Population inversion, temperature, and photon distributions of the generalized fermionic Ising ferromagnetic model: Path-integral representation of the spin system. *International Journal of Quantum Chemistry*, 106(8): 1769–1781, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grinberg:2008:ITL

[Gri08] Horacio Grinberg. Interaction of a two-level cyclic XY n-spin model with a two-mode cavity field in off-resonant states. *International Journal of Quantum Chemistry*, 108(2):210–218, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gauss:2000:ESL

[GS00a] Jürgen Gauss and John F. Stanton. Equilibrium structure of LiCCH. *International Journal of Quantum Chemistry*, 77(1):305–310, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004270/START;` `http://www3.interscience.wiley.com/cgi-bin/fulltext/70004270/FILE?TPL=ftx_start;` `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004270&PLACEBO=IE.pdf`.

Gross:2000:SEP

[GS00b] Kevin C. Gross and Paul G. Seybold. Substituent effects on the physical properties and pK_a of aniline. *International Journal of Quantum Chemistry*, 80(4–5):1107–1115, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505418/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505418/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505418&PLACEBO=IE.pdf`.

Gross:2001:SEP

[GS01] Kevin C. Gross and Paul G. Seybold. Substituent effects on the physical properties and pK_a of phenol. *International Journal of Quantum Chemistry*, 85(4–5):569–579, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goodman:2005:EAP

[GS05] Lionel Goodman and Ronald R. Sauers. Ethyl anion preferred conformation. *International Journal of Quantum Chemistry*, 102(5):829–837, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gidofalvi:2009:ESD

[GS09] Gergely Gidofalvi and Ron Shepard. The evaluation of spin-density matrices within the graphically contracted function method. *International Journal of Quantum Chemistry*, 109 (15):3552–3563, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guerout:2009:CRE

[GSA+09] R. Guérout, P. Soldán, M. Aymar, J. Deiglmayr, and O. Dulieu. Core repulsion effects in alkali trimers. *International Journal of Quantum Chemistry*, 109(14):3387–3398, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gritsenko:2000:EPS

[GSB00] O. V. Gritsenko, P. R. T. Schipper, and E. J. Baerends. Ensuring proper short-range and asymptotic behavior of the exchange-correlation Kohn–Sham potential by modeling with

a statistical average of different orbital model potentials. *International Journal of Quantum Chemistry*, 76(3):407–419, January 20, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000283/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000283/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000283&PLACEBO=IE.pdf`.

Garcia-Sosa:2000:DFS

[GSC00] Alfonso T. García-Sosa and Miguel Castro. Density functional study of FeO_2, FeO, and FeO. *International Journal of Quantum Chemistry*, 80(3):307–319, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501022/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501022/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501022&PLACEBO=IE.pdf`.

Guadarrama:2008:PDH

[GSCRO08] Patricia Guadarrama, Delia Soto-Castro, and Jesús Rodríguez-Otero. Performance of DFT hybrid functionals in the theoretical treatment of H-bonds: Analysis term-by-term. *International Journal of Quantum Chemistry*, 108(2):229–237, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guidotti:2003:CQC

[GSD+03] C. Guidotti, O. Salvetti, N. Durante, U. T. Lamanna, and G. P. Arrighini. Computational quantum chemistry in terms of multicenter Slater-type orbitals: Entirely numerical procedure for the accurate evaluation of the basic integrals. *International Journal of Quantum Chemistry*, 93(2):59–71, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garcia:2008:EMB

[GSfLV08] Y. García, E. San-fabián, E. Louis, and J. A. Vergés. Effects of methods and basis set on ab initio calculations of electronic transport through hydrogenated Pt nanocontacts. *International Journal of Quantum Chemistry*, 108(10):1637–

1644, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gross:2002:CDA

[GSH02] Kevin C. Gross, Paul G. Seybold, and Christopher M. Hadad. Comparison of different atomic charge schemes for predicting p K_a variations in substituted anilines and phenols. *International Journal of Quantum Chemistry*, 90(1):445–458, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grembecka:2001:QCA

[GSK01] J. Grembecka, W. A. Sokalski, and P. Kafarski. Quantum chemical analysis of the interactions of transition state analogs with leucine aminopeptidase. *International Journal of Quantum Chemistry*, 84(2):302–310, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502331/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502331/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502331&PLACEBO=IE.pdf`.

Gaudel-Siri:2006:RTH

[GSPP+06] Anouk Gaudel-Siri, Jean-Marc Pons, Nathalie Piétri, Isabelle Tamburelli-Couturier, and Jean-Pierre Aycard. Reaction of trimethylsilylketene with HCl: Mechanistic study. *International Journal of Quantum Chemistry*, 106(3):719–726, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grafutin:2007:PPP

[GSPT+07] V. I. Grafutin, E. P. Svetlov-Prokop'ev, S. P. Timoshenkov, V. V. Kalugin, and E. I. Artemov. Possible properties of positron states in physics and chemistry of a surface and in semiconductor nanotechnologies. *International Journal of Quantum Chemistry*, 107(14):2844–2848, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2004:ESM

[GSQ+04] Hong-Ze Gao, Zhong-Min Su, Chun-Sheng Qin, Ri-Gen Mo, and Yu-He Kan. Electronic structure and molecular orbital study of the first excited state of the high-efficiency blue

OLED material bis(2-methyl-8-quinolinolato)aluminum(III) hydroxide complex from ab initio and TD-B3LYP. *International Journal of Quantum Chemistry*, 97(6):992–1001, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garcia:2006:MMP

[GSRL06] Ernesto Garcia, Carlos Sánchez, Aurelio Rodríguez, and Antonio Laganà. MEP–MPE potential energy surface for the $Cl + CH_4 \rightarrow HCl + CH_3$ reaction. *International Journal of Quantum Chemistry*, 106(3):623–630, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gunaydin:2005:MFR

[GST+05] Hakan Günaydin, Seyhan Salman, Nurcan Şenyurt Tüzün, Duygu Avci, and Víktorya Avíyente. Modeling the free radical polymerization of acrylates. *International Journal of Quantum Chemistry*, 103(2):176–189, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gili:2007:ESC

[GT07] Pedro Gili and Athanassios C. Tsipis. Electronic structure calculations on multiply charged anions containing M — S bonds (M = Cr, Mo, W) and their heterobimetallic cluster complexes. *International Journal of Quantum Chemistry*, 107 (2):418–439, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gotoh:2005:FSD

[GTR+05] Masashi Gotoh, Masanori Tachikawa, Kotaro Ryuo, Kotoku Sasagane, Kazunari Suzuki, Kazuhide Mori, and Shinichiro Nakamura. The first and second derivative matrices in the random phase approximation scheme by using the Lagrangian technique. *International Journal of Quantum Chemistry*, 105 (3):225–231, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garifzianova:2007:QCS

[GTSK07] Guzel G. Garifzianova, Roman V. Tsyshevskii, Alexander G. Shamov, and Grigorii M. Khrapkovskii. A quantum-chemical study of *n*-butane and of butane cation radical. *International Journal of Quantum Chemistry*, 107(13):2489–2493,

???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guiasu:2001:TWF

[Gui01] Silviu Guiasu. Trial wave functions for multielectron atoms. *International Journal of Quantum Chemistry*, 81(6):389–408, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76509322/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76509322/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76509322&PLACEBO=IE.pdf`.

Guiasu:2006:USC

[Gui06] Silviu Guiasu. Using symbolic computing in building probabilistic models for atoms. *International Journal of Quantum Chemistry*, 106(1):4–26, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guntert:2006:SNP

[Gün06] Peter Güntert. Symbolic NMR product operator calculations. *International Journal of Quantum Chemistry*, 106(1): 344–350, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:2007:DFS

[Guo07] Ling Guo. Density functional study of carbon monoxide adsorption on small cationic, neutral, and anionic aluminum nitride clusters. *International Journal of Quantum Chemistry*, 107(7):1624–1631, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:2009:ISN

[Guo09] Jinghua Guo. Interface science in nanoparticles: An electronic structure view of photon-in/photon-out soft-X-ray spectroscopy. *International Journal of Quantum Chemistry*, 109(12):2714–2721, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gupta:2000:ESH

[Gup00] M. Gupta. Electronic structure of hydrogen storage materials. *International Journal of Quantum Chemistry*, 77(6):982–990, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/71000980/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000980/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000980&PLACEBO=IE.pdf.

Gurin:2005:ESS

[Gur05] V. S. Gurin. Endofullerenes with small silver and copper clusters. *International Journal of Quantum Chemistry*, 104 (2):249–255, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guseinov:2001:EEC

[Gus01] I. I. Guseinov. Evaluation of expansion coefficients for translation of Slater-type orbitals using complete orthonormal sets of exponential-type functions. *International Journal of Quantum Chemistry*, 81(2):126–129, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/76500931/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76500931/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76500931&PLACEBO=IE.pdf.

Guseinov:2002:NCO

[Gus02a] I. I. Guseinov. New complete orthonormal sets of exponential-type orbitals and their application to translation of Slater orbitals. *International Journal of Quantum Chemistry*, 90 (1):114–118, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guseinov:2002:UAT

[Gus02b] I. I. Guseinov. Unified analytical treatment of one-electron multicenter integrals of central and noncentral potentials over Slater orbitals. *International Journal of Quantum Chemistry*, 90(2):980–985, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guseinov:2003:CET

[Gus03] I. I. Guseinov. Comment on "Evaluation of Two-Center Overlap and Nuclear-Attraction Integrals over Slater-Type Orbitals with Integer and Noninteger Principal Quantum Numbers". *International Journal of Quantum Chemistry*, 91(1):

62–64, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [ÖO02].

Guseinov:2004:UAT

[Gus04] I. I. Guseinov. Unified analytical treatment of two-electron multicenter integrals of central and noncentral interaction potentials over Slater orbitals. *International Journal of Quantum Chemistry*, 100(2):206–207, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Georgieva:2006:CES

[GV06] Miglena K. Georgieva and Evelina A. Velcheva. Computational and experimental studies on the IR spectra and structure of the simplest nitriles (C_1 and C_2), their anions, and radicals. *International Journal of Quantum Chemistry*, 106 (6):1316–1322, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Glushkov:2002:DGB

[GW02] V. N. Glushkov and S. Wilson. Distributed Gaussian basis sets: Variationally optimized s-type sets for H_2, LiH, and BH. *International Journal of Quantum Chemistry*, 89(4):237–247, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Glushkov:2004:DGB

[GW04] V. N. Glushkov and S. Wilson. Distributed Gaussian basis sets: Variationally optimized s-type sets for the open-shell systems HeH and BeH. *International Journal of Quantum Chemistry*, 99(6):903–913, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gou:2005:WBT

[GW05] Bingcong Gou and Fei Wang. Weakly bound triatomic $^4He_2^3He$ and $^3He_2^4He$ molecules. *International Journal of Quantum Chemistry*, 101(2):169–173, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:2006:DFS

[GW06a] Ling Guo and Hai-Shun Wu. Density functional study of structural and electronic properties of Al_nN ($1 \leq n \leq 12$) clusters.

International Journal of Quantum Chemistry, 106(5):1250–1257, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:2006:GPG

[GW06b] Ling Guo and Haishun Wu. Gallium phosphides GA_mP_n $(m+n=2--5)$ and their anions: Structures, electron affinities, and vibrational frequencies. *International Journal of Quantum Chemistry*, 106(4):968–980, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Glushkov:2007:DBS

[GW07] V. N. Glushkov and S. Wilson. Distributed basis sets of s-type Gaussian functions for simple diatomics: Anharmonic-model distribution. *International Journal of Quantum Chemistry*, 107(14):2632–2642, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:2005:FPI

[GWJ05] Ling Guo, Hai-Shun Wu, and Zhi-Hao Jin. First-principles investigation of structure and stability of Al_nN_m clusters. *International Journal of Quantum Chemistry*, 103(3):291–298, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Griffin:2005:SBG

[GWK+05] L. L. Griffin, Jian Wu, D. J. Klein, T. G. Schmalz, and L. Bytautas. Scaling behavior of ground-state energy cluster expansion for linear polyenes. *International Journal of Quantum Chemistry*, 102(4):387–397, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:2008:RSD

[GWSZ08] Guanlun Guo, Fang Wang, Hui Sun, and Dongju Zhang. Reactivity of silicon-doped carbon nanotubes toward small gaseous molecules in the atmosphere. *International Journal of Quantum Chemistry*, 108(2):203–209, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gong:2002:ETS

[GXGT02] Xue Dong Gong, He Ming Xiao, Pin Gao, and He Tian. Effect of trimethylsilyl substitution on the structure and properties

of phthalocyanine: A density functional theory study. *International Journal of Quantum Chemistry*, 88(3):331–341, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gong:2002:CSS

[GXT02] Xue Dong Gong, He Ming Xiao, and He Tian. Comparative studies on the structures, infrared spectrum, and thermodynamic properties of phthalocyanine using ab initio Hartree–Fock and density functional theory methods. *International Journal of Quantum Chemistry*, 86(6):531–540, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89010621/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89010621/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89010621&PLACEBO=IE.pdf`.

Giese:2004:HLI

[GY04] Timothy J. Giese and Darrin M. York. High-level ab initio methods for calculation of potential energy surfaces of van der Waals complexes. *International Journal of Quantum Chemistry*, 98(4):388–408, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guohua:2009:TSS

[GYF+09] Zhang Guohua, Zhao Yongfang, Hao Fengyou, Zhang Pingxia, and Song Xiudan. Theoretical study on structures and stabilities of N_4X (X = O, S, Se, Te) series. *International Journal of Quantum Chemistry*, 109(2):226–235, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guan:2002:SME

[GYM+02] Daren Guan, Xizhang Yi, Qingtian Meng, Yujun Zheng, Jianzhong Wu, and Jiazhong Sun. Statistical mechanics of energy transfer in gas-surface scattering: A dynamical Lie algebraic approach. *International Journal of Quantum Chemistry*, 86(6):518–530, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86011223/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86011223/FILE?TPL=ftx_start;`

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86011223&PLACEBO=IE.pdf.

Guan:2006:DFS

[GYS+06] Wei Guan, Li-Kai Yan, Zhong-Min Su, En-Bo Wang, and Xiao-Hong Wang. Density functional study of protonation sites of α-Keggin isopolyanions. *International Journal of Quantum Chemistry*, 106(8):1860–1864, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gong:2005:DFT

[GZD+05] Xiaoli Gong, Zhengyu Zhou, Dongmei Du, Xiuli Dong, and Shuzhen Liu. Density functional theory study of the hydrogen bonding interaction of 1:1 complexes of serine with water. *International Journal of Quantum Chemistry*, 103(1):105–117, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hagelberg:2000:PTS

[Hag00] F. Hagelberg. Pseudoprecession of triatomic systems by electron nuclear dynamics theory. *International Journal of Quantum Chemistry*, 80(4–5):966–988, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505396/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505396/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505396&PLACEBO=IE.pdf.

Hagelberg:2001:PDH

[Hag01] F. Hagelberg. Pseudorotational dynamics of H_3^+ and Li_3^+. *International Journal of Quantum Chemistry*, 85(2):72–84, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85011547/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85011547/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85011547&PLACEBO=IE.pdf.

Hagelberg:2005:NEE

[Hag05] Frank Hagelberg. Nonadiabatic evolution of electronic states by electron nuclear dynamics theory. *International Journal*

of Quantum Chemistry, 102(5):869–879, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hernandez:2002:ICQ

[HAL+02] María Luz Hernández, José María Alvariño, Antonio Laganà, Marzio Rosi, and Antonio Sgamellotti. Ab initio calculation and quasi-classical dynamics study of the two lowest potential energy surfaces of the $O(^1D)$ + HBr system. *International Journal of Quantum Chemistry*, 86(1):79–89, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86510682/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86510682/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86510682&PLACEBO=IE.pdf`.

Hansmann:2002:PFS

[Han02] Ulrich H. E. Hansmann. Protein-folding simulations in generalized ensembles. *International Journal of Quantum Chemistry*, 90(4-5):1515–1521, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Handzlik:2007:AOQ

[Han07] Jarosław Handzlik. Application of the ONIOM (QM/QM) method in the study of molybdena–silica system active in olefin metathesis. *International Journal of Quantum Chemistry*, 107(11):2111–2119, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2001:KFL

[Har01] Frank E. Harris. On Kryachko's formula for the leaky aquifer function. *International Journal of Quantum Chemistry*, 81 (5):332–334, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76507286/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76507286/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76507286&PLACEBO=IE.pdf`.

Harris:2002:CPN

[Har02a] Danni L. Harris. Cytochrome P450nor: A nitric oxide reductase — Structure, spectra, and mechanism. *Inter-*

national Journal of Quantum Chemistry, 88(1):183–200, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90010557/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90010557/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90010557&PLACEBO=IE.pdf`.

Harris:2002:AET

[Har02b] Frank E. Harris. Analytic evaluation of two-center STO electron repulsion integrals via ellipsoidal expansion. *International Journal of Quantum Chemistry*, 88(6):701–734, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2002:CBA

[Har02c] Frank E. Harris. Cumulant-based approximations to reduced density matrices. *International Journal of Quantum Chemistry*, 90(1):105–113, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2003:CCT

[Har03] Frank E. Harris. Comment on "Computation of Two-Center Coulomb Integrals over Slater-Type Orbitals Using Elliptical Coordinates". *International Journal of Quantum Chemistry*, 93(5):332–334, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [ÖKAY03].

Harris:2004:EEM

[Har04a] Frank E. Harris. Efficient evaluation of the molecular auxiliary function B_n by downward recursion. *International Journal of Quantum Chemistry*, 100(2):142–145, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2004:ER

[Har04b] Frank E. Harris. Expansion(s) of r_{12}^{-2}. *International Journal of Quantum Chemistry*, 97(5):908–913, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2005:GET

[Har05a] Frank E. Harris. Gegenbauer expansions for three-electron integrals. *International Journal of Quantum Chemistry*, 102

(5):940–947, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2005:IET

[Har05b] Frank E. Harris. Improving the efficiency of table-driven CI. *International Journal of Quantum Chemistry*, 105(1):34–36, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2005:RRM

[Har05c] Frank E. Harris. Recurrence relations for matrix elements of few-body correlated wave functions. *International Journal of Quantum Chemistry*, 105(6):857–865, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2006:MMS

[Har06] Frank E. Harris. Mathematical methods and symbolic calculation in chemistry and chemical biology — introduction. *International Journal of Quantum Chemistry*, 106(1):1–2, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2009:BAM

[Har09] Frank E. Harris. Bill Adams Memorial Session. *International Journal of Quantum Chemistry*, 109(15):3840, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hankel:2003:SWP

[HBKG03] Marlies Hankel, Gabriel G. Balint-Kurti, and Stephen K. Gray. Sinc wave packets: New form of wave packet for time-dependent quantum mechanical reactive scattering calculations. *International Journal of Quantum Chemistry*, 92(2): 205–211, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hodges:2004:EMS

[HBTW04] Matthew P. Hodges, Elena Bichoutskaia, Akyl S. Tulegenov, and Richard J. Wheatley. Extrapolation methods and scaled perturbation theory for determining intermolecular potential energy surfaces. *International Journal of Quantum Chemistry*, 96(6):537–546, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hua:2008:TSA

[HBW+08] Xiao Hua, Feng-Li Bei, Xin Wang, Xu-Jie Yang, and Lu-De Lu. The theoretical study on anionic polymerization mechanism of maleimide: Chain propagation by p-π conjugation process. *International Journal of Quantum Chemistry*, 108 (7):1257–1265, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2002:EOB

[HC02] Haiquan Hu and Zhida Chen. Effect of the orbitals of the bridging group on magnetic coupling. *International Journal of Quantum Chemistry*, 88(2):275–279, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2003:UPD

[HCL03] Haiquan Hu, Zhida Chen, and Chengbu Liu. Useful parameter describing magnetic interactions in extended bis-bidentate bridged dimers. *International Journal of Quantum Chemistry*, 92(5):428–432, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Herrera-Cabrera:2003:FPE

[HCRHM03] M. J. Herrera-Cabrera, P. Rodríguez-Hernández, and A. Muñoz. First-principles elastic properties of BAs. *International Journal of Quantum Chemistry*, 91(2):191–196, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Heslar:2007:HOH

[HCTC07] John Heslar, Juan Carrera, Dmitry Telnov, and Shih-I Chu. High-order harmonic generation of heteronuclear diatomic molecules in intense ultrashort laser fields: An all-electron TDDFT study. *International Journal of Quantum Chemistry*, 107(15):3159–3168, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Haas:2005:UER

[HCZ05] Yehuda Haas, Semyon Cogan, and Shmuel Zilberg. The use of elementary reaction coordinates in the search for conical intersections. *International Journal of Quantum Chemistry*, 102(5):961–970, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Honorio:2003:ASE

[HD03] K. M. Honório and A. B. F. Da Silva. An AM1 study on the electron-donating and electron-accepting character of biomolecules. *International Journal of Quantum Chemistry*, 95(2):126–132, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hong:2000:SRD

[HDL00] Gongyi Hong, Michael Dolg, and Lemin Li. Scalar-relativistic density functional and ab initio pseudopotential study of zero-valent d and f metal bis-η^6-benzene sandwich complexes $M(C_6\ H_6)_2$ (M = Sc, Ti, Y, Zr, La, Lu, Hf, Th, U). *International Journal of Quantum Chemistry*, 80(2):201–209, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001285/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001285/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001285&PLACEBO=IE.pdf`.

Haiduke:2005:RGB

[HdMB+05] R. L. A. Haiduke, L. G. M. de Macedo, R. C. Barbosa, N. H. Morgon, and A. B. F. da Silva. Relativistic Gaussian basis sets obtained with a polynomial version of the generator coordinate Dirac–Fock method: Ionization energies of some closed-shell atomic systems. *International Journal of Quantum Chemistry*, 103(5):529–536, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Holmes:2009:TSI

[HDWH09] Tiffani M. Holmes, Jacek Doskocz, Terrance Wright, and Glake A. Hill. Theoretical study of interactions between cysteine and perfluoropropanoic acid in gas and aqueous phase. *International Journal of Quantum Chemistry*, 109(1):119–123, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hilal:2005:DIS

[HE05] Rifaat Hilal and Shabaan A. K. Elroby. DFT investigation of sites of protonation of antitumor of 2-(4-aminophenyl)benzazoles in the gas phase and in solution. *International Journal of Quantum Chemistry*, 103(4):449–459,

???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Head:2000:VAF

[Hea00] John D. Head. A vibrational analysis with Fermi resonances for methoxy adsorption on Cu(111) using ab initio cluster calculations. *International Journal of Quantum Chemistry*, 77(1):350–357, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004277/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004277/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004277&PLACEBO=IE.pdf`.

Head:2003:IRO

[Hea03] John D. Head. Inclusion of Rydberg orbitals in semiempirical calculations on excited states? *International Journal of Quantum Chemistry*, 95(4–5):580–592, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Himo:2000:SEO

[HEBS00] Fahmi Himo, Leif A. Eriksson, Margareta R. A. Blomberg, and Per E. M. Siegbahn. Substituent effects on OH bond strength and hyperfine properties of phenol, as model for modified tyrosyl radicals in proteins. *International Journal of Quantum Chemistry*, 76(6):714–723, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70001602/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70001602/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70001602&PLACEBO=IE.pdf`.

Han:2000:HSD

[HEJ+00] Wen-Ge Han, Marcus Elstner, K. J. Jalkanen, Thomas Frauenheim, and Sándor Suhai. Hybrid SCC-DFTB/molecular mechanical studies of H-bonded systems and of N-acetyl-(L-Ala)$_n$ N'-methylamide helices in water solution. *International Journal of Quantum Chemistry*, 78(6):459–479, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72502341/START; http:`

//www3.interscience.wiley.com/cgi-bin/fulltext/72502341/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72502341&PLACEBO=IE.pdf.

Hereman:2006:SCC

[Her06] Willy Hereman. Symbolic computation of conservation laws of nonlinear partial differential equations in multi-dimensions. *International Journal of Quantum Chemistry*, 106(1):278–299, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Herbert:2007:MSH

[Her07] John M. Herbert. Magnitude and significance of the higher-order reduced density matrix cumulants. *International Journal of Quantum Chemistry*, 107(3):703–711, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hess:2002:HSM

[Hes02] B. Andes Hess, Jr. 1,5-hydrogen shifts in methyl-1,3-cycloheptadienes. *International Journal of Quantum Chemistry*, 90(3):1064–1070, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2009:MIB

[HF09] Frank E. Harris and J. G. Fripiat. Methods for incomplete Bessel function evaluation. *International Journal of Quantum Chemistry*, 109(8):1728–1740, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hill:2002:CDI

[HFGL02] Glake A. Hill, Gareth Forde, Leonid Gorb, and Jerzy Leszczynski. cis-Diamminedichloropalladium and its interaction with guanine and guanine–cytosine base pair. *International Journal of Quantum Chemistry*, 90(3):1121–1128, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2004:NMO

[HFS04] Frank E. Harris, Alexei M. Frolov, and Vedene H. Smith, Jr. New methods for old Coulomb few-body problems. *International Journal of Quantum Chemistry*, 100(6):1086–1091, ????

2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2006:RCN

[HFS06] Frank E. Harris, Alexei M. Frolov, and Vedene H. Smith, Jr. Re: Comment on "New methods for old Coulomb few-body problems". *International Journal of Quantum Chemistry*, 106 (2):552–553, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hazra:2008:QAS

[HGB08] Ram Kuntal Hazra, Manas Ghosh, and S. P. Bhattacharyya. Quantum adiabatic switching route to the impurity modulated states of 2-D quantum dots with different switching functions. *International Journal of Quantum Chemistry*, 108 (4):719–730, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hill:2001:SPC

[HGRL01] Glake Hill, Robert W. Gora, Szczepan Roszak, and Jerzy Leszczyński. The structures and properties of *cis*- and *trans*-$MeCl_2$ $(NH_3)_2$, Me = Pd and Pt complexes, in ground and excited states. *International Journal of Quantum Chemistry*, 83(3-4):213–219, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002588/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002588/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002588&PLACEBO=IE.pdf`.

Heiberg:2003:HAC

[HGS03] Hanne Heiberg, Odd Gropen, and Ole Swang. Heterolytic activation of C H bond in methane with (HN CHCH NH)M(CH_3) (M = Pd^+, Pt^+, Rh^+, Ir^+, Rh, Ir): Comparative density functional study of activation mechanisms. *International Journal of Quantum Chemistry*, 92(4):391–399, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2003:OCP

[HGTW03] Hai-Rong Hu, Mao-Chu Gong, Anmin Tian, and Ning-Bew Wong. Origin of *cis* preference among the three isomers of 1,4-

difluorobutadiene. *International Journal of Quantum Chemistry*, 91(6):675–684, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Herbert:2002:CTE

[HH02] John M. Herbert and John E. Harriman. Comparison of two-electron densities reconstructed from one-electron density matrices. *International Journal of Quantum Chemistry*, 90(1): 355–369, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hutter:2003:MPT

[HH03] Michael C. Hutter and Volkhard Helms. Mechanism of phosphoryl transfer in kinases investigated by semiempirical calculations. *International Journal of Quantum Chemistry*, 95 (4–5):479–486, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hug:2005:VOA

[HH05] Werner Hug and Jacques Haesler. Is the vibrational optical activity of (R)-[^{2}H$_1$,^{2}H$_2$,^{2}H$_3$]-neopentane measurable? *International Journal of Quantum Chemistry*, 104(5):695–715, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Herman:2009:DMP

[HH09] Mark S. Herman and George A. Hagedorn. Does Møller–Plesset perturbation theory converge? A look at two-electron systems. *International Journal of Quantum Chemistry*, 109 (2):210–225, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hernandez:2002:TSM

[HHGSRS02] J. M. Hernández, Ana M. Herrera, J. García-Serrano, and J. F. Rivas-Silva. Theoretical study of *p*-methacryloylaminophenylarsonic acid. *International Journal of Quantum Chemistry*, 88(3):342–346, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harkless:2006:MDT

[HI06] J. A. W. Harkless and K. K. Irikura. Multi-determinant trial functions in the determination of the dissociation energy of

the beryllium dimer: Quantum Monte Carlo study. *International Journal of Quantum Chemistry*, 106(11):2373–2378, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hansen:2009:MET

[HJJ09] M. B. Hansen, H. J. A. Jensen, and F. Jensen. Modeling enzymatic transition states by force field methods. *International Journal of Quantum Chemistry*, 109(2):373–383, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Henderson:2009:LRS

[HJSS09] Thomas M. Henderson, Benjamin G. Janesko, Gustavo E. Scuseria, and Andreas Savin. Locally range-separated hybrids as linear combinations of range-separated local hybrids. *International Journal of Quantum Chemistry*, 109(9):2023–2032, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hameed:2007:TSM

[HJT07] Ali Jameel Hameed, Abraham F. Jalbout, and Bartosz Trzaskowski. Theoretical study of molecular and electronic structure of 2-Se-(2-methyl-2-propenyl)-1-benzoic acid. *International Journal of Quantum Chemistry*, 107(1):152–158, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hanke:2006:NDS

[HK06] Felix Hanke and Hans Jürgen Kreuzer. Nonequilibrium dynamics of single polymer molecules: Relaxation close to and far from equilibrium. *International Journal of Quantum Chemistry*, 106(14):2953–2959, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Holt:2009:INP

[HK09] Asbjørn Holt and Gunnar Karlström. Improvement of the NEMO potential by inclusion of intramolecular polarization. *International Journal of Quantum Chemistry*, 109(6):1255–1266, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hilal:2005:TIP

[HKE05] Rifaat Hilal, Ahmed A. Abdel Khalek, and Shabaan A. K. Elroby. Theoretical investigation of the proton affinities of benzazoles in the gas phase and in solution. *International Journal of Quantum Chemistry*, 103(3):332–343, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hoffmann:2004:PEB

[HKMM04] Marcin Hoffmann, Ilja V. Khavrutskii, Djamaladdin G. Musaev, and Keiji Morokuma. Protein effects on the O_2 binding to the active site of the methane monooxygenase: ONIOM studies. *International Journal of Quantum Chemistry*, 99(6):972–980, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Holt:2009:CCC

[HKR09] Asbjørn Holt, Gunnar Karlström, and Björn O. Roos. The charge capacitance of the chemical bond: Application to bonds containing metals. *International Journal of Quantum Chemistry*, 109(3):618–628, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hongo:2007:DMC

[HKY07] Kenta Hongo, Yoshiyuki Kawazoe, and Hiroshi Yasuhara. Diffusion Monte Carlo study of correlation in the hydrogen molecule. *International Journal of Quantum Chemistry*, 107 (6):1459–1467, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harrison:2005:QMA

[HL05] James F. Harrison and Daniel B. Lawson. Quadrupole moments of the alkali dimers, Li_2, Na_2, and K_2. *International Journal of Quantum Chemistry*, 102(6):1087–1091, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2005:NMR

[HLH05] Ming-Ju Huang, Ken S. Lee, and Sharon J. Hurley. Nuclear magnetic resonance spectral analysis and molecular properties of berberine. *International Journal of Quantum Chemistry*, 105(4):396–409, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2007:PUP

[HLMH07] Jie Hu, Feng Liu, Qing-Tian Meng, and Ke-Li Han. Probing the ultrafast photoelectron spectra of Br_2 molecule. *International Journal of Quantum Chemistry*, 107(10):1994–1998, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hasegawa:2004:TSL

[HLO04] Hiroshi H. Hasegawa, Chun-Biu Li, and Yoshikazu Ohtaki. Thermodynamics of a system with long-time correlations. *International Journal of Quantum Chemistry*, 98(2):138–144, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Houlding:2007:PHR

[HLP07] S. Houlding, S. Y. Liem, and P. L. A. Popelier. A polarizable high-rank quantum topological electrostatic potential developed using neural networks: Molecular dynamics simulations on the hydrogen fluoride dimer. *International Journal of Quantum Chemistry*, 107(14):2817–2827, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hamza:2001:ORLa

[HM01a] A. Hamza and I. Mayer. Overlap repulsion with Löwdin's pairing theorem. *International Journal of Quantum Chemistry*, 82(2):53–59, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/77502751/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/77502751/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=77502751&PLACEBO=IE.pdf`.

Hamza:2001:ORLb

[HM01b] A. Hamza and I. Mayer. Overlap repulsion with Löwdin's pairing theorem II. The leading term. *International Journal of Quantum Chemistry*, 82(3):105–112, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/77004286/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/77004286/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=77004286&PLACEBO=IE.pdf`.

Hassan:2001:GSC

[HM01c] Sergio A. Hassan and Ernest L. Mehler. A general screened Coulomb potential based implicit solvent model: Calculation of secondary structure of small peptides. *International Journal of Quantum Chemistry*, 83(3-4):193–202, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002595/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002595/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002595&PLACEBO=IE.pdf`.

Howard:2003:MFS

[HM03] I. A. Howard and N. H. March. Many-fermion systems: Differential equations and kinetic energy functionals for different confining potentials. *International Journal of Quantum Chemistry*, 91(2):119–125, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See also [Mar87a, Mar87b, MNA+99, HMMT04].

Hassan:2005:QCC

[HM05a] Sergio A. Hassan and Ernest L. Mehler. From quantum chemistry and the classical theory of polar liquids to continuum approximations in molecular mechanics calculations. *International Journal of Quantum Chemistry*, 102(5):986–1001, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Howard:2005:FPD

[HM05b] I. A. Howard and N. H. March. Fermion particle density equations in relation to relativistic density functional theory. *International Journal of Quantum Chemistry*, 101(6):651–657, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Howard:2005:SNE

[HM05c] I. A. Howard and N. H. March. Slater's nonlocal exchange potential and beyond. *International Journal of Quantum Chemistry*, 102(1):64–71, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2006:IFC

[HM06a] Frank E. Harris and Hendrik J. Monkhorst. Integrals for fully correlated Gaussians in relative coordinates. *International Journal of Quantum Chemistry*, 106(1):54–64, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2006:RRF

[HM06b] Frank E. Harris and Hendrik J. Monkhorst. Recurrence relations for fully correlated Gaussians with odd powers of interparticle coordinates. *International Journal of Quantum Chemistry*, 106(15):3186–3189, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Howard:2004:DMF

[HMB+04] I. A. Howard, N. H. March, F. Bartha, A. K. Ray, and M.-L. Zhang. Density matrix force-balance equation applied to He, Be, and Ne atoms and to almost-spherical methane-like molecules. *International Journal of Quantum Chemistry*, 100 (2):155–165, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2005:KEM

[HMK05] Lulu Huang, Lou Massa, and Jerome Karle. Kernel energy method illustrated with peptides. *International Journal of Quantum Chemistry*, 103(6):808–817, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2006:KEM

[HMK06] Lulu Huang, Lou Massa, and Jerome Karle. Kernel energy method: Basis functions and quantum methods. *International Journal of Quantum Chemistry*, 106(2):447–457, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Howard:2004:SSO

[HMMT04] I. A. Howard, A. Minguzzi, N. H. March, and M. P. Tosi. Slater sum for the one-dimensional sech^2 potential in relation to the kinetic energy density. *Journal of Mathematical Physics*, 45(6):2411–2419, June 2004. CODEN JMAPAQ. ISSN 0022-2488 (print), 1089-7658 (electronic), 1527-

2427. URL `http://jmp.aip.org/resource/1/jmapaq/v45/i6/p2411_s1`.

Hubac:2002:PCM

[HMW02] I. Hubać, P. Mach, and S. Wilson. A posteriori corrections to multireference limited configuration interaction based on a Brillouin–Wigner perturbative analysis. *International Journal of Quantum Chemistry*, 89(4):198–207, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hubac:2005:MBW

[HMW05] I. Hubač, P. Mach, and S. Wilson. Multireference Brillouin–Wigner coupled cluster (MR-BWCC) theory applied to the H8 model: Comparison with CCSD(T) theory. *International Journal of Quantum Chemistry*, 104(4):387–396, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hazra:2003:DEI

[HN03] Anirban Hazra and Marcel Nooijen. Derivation and efficient implementation of a recursion formula to calculate harmonic Franck–Condon factors for polyatomic molecules. *International Journal of Quantum Chemistry*, 95(4–5):643–657, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huntington:2009:IHT

[HN09] Lee M. J. Huntington and Marcel Nooijen. An SO(4) invariant Hamiltonian and the two-body bound state. I: Coulomb interaction between two spinless particles. *International Journal of Quantum Chemistry*, 109(13):2885–2896, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hara:2001:CTR

[HNKiS01] Toshiki Hara, Susumu Narita, Sukeyuki Kumei, and Tai ichi Shibuya. Complete TDA and RPA Calculations on the Electronic Transitions of Fullerene-C_{60} in the CNDO/S and INDO/S Approximations. *International Journal of Quantum Chemistry*, 85(3):136–161, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/88011599/START; http://www3.interscience.`

wiley.com/cgi-bin/fulltext/88011599/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88011599&PLACEBO=IE.pdf.

Henriques:2006:CSS

[HNR06] Elsa S. Henriques, Marco A. C. Nascimento, and Maria João Ramos. Computational study of some benzamidine-based inhibitors of thrombin-like snake venom proteinases. *International Journal of Quantum Chemistry*, 106(9):2107–2121, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hobza:2002:HIB

[Hob02] Pavel Hobza. N-H$\cdots$F improper blue-shifting H-bond. *International Journal of Quantum Chemistry*, 90(3):1071–1074, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Herz:2000:BGP

[HOC00] Thomas Herz, Peter Otto, and Timothy Clark. On the band gap in peptide α-helices. *International Journal of Quantum Chemistry*, 79(2):120–124, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72508330/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72508330/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72508330&PLACEBO=IE.pdf.

Hoggan:2004:CAO

[Hog04] Philip E. Hoggan. Choice of atomic orbitals to evaluate sensitive properties of molecules: An example of NMR chemical shifts. *International Journal of Quantum Chemistry*, 100 (2):214–220, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hoggan:2009:GTE

[Hog09a] Philip E. Hoggan. General two-electron exponential type orbital integrals in polyatomics without orbital translations. *International Journal of Quantum Chemistry*, 109(13):2926–2932, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hogreve:2009:PIT

[Hog09b] H. Hogreve. The δ point interaction two-center system. *International Journal of Quantum Chemistry*, 109(7):1430–1441, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hayafuji:2009:LED

[HOIK09] Yoshinori Hayafuji, Kengo Ohmori, Kazushi Igei, and Nobuo Kambara. Light emission due to the quantum confinement of carriers in silicon-based nanostructures. *International Journal of Quantum Chemistry*, 109(12):2764–2772, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hudaky:2007:PKO

[HP07] Péter Hudáky and András Perczel. p K_a optimized catalysis in serine proteinases, an ab initio study on the catalytic His. *International Journal of Quantum Chemistry*, 107(11):2178–2183, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hatfield:2008:EMC

[HPC+08] Marcus P. D. Hatfield, Nicholas Y. Palermo, József Csontos, Richard F. Murphy, and Sándor Lovas. Evaluation of methods to cap molecular fragments in calculating energies of interaction in avian pancreatic polypeptide. *International Journal of Quantum Chemistry*, 108(5):1017–1021, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Herrmann:2009:ROB

[HPR09] Carmen Herrmann, Maren Podewitz, and Markus Reiher. Restrained optimization of broken-symmetry determinants. *International Journal of Quantum Chemistry*, 109(11):2430–2446, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2009:CMI

[HQL09] Ming-Ju Huang, Zhe Quan, and Yi-Ming Liu. Computational modeling of inclusion complexes of β-cyclodextrin with enantiomers of salsolinol, N-methyl-salsolinol, and 1-benzyltetrahydroisoquinoline. *International Journal of Quantum*

Chemistry, 109(1):81–90, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Herve:2004:ERG

[HQM04] Stephen Hervé, Frédéric Le Quéré, and Roberto Marquardt. Effect of rotations on the generation of coherent internal molecular motion. *International Journal of Quantum Chemistry*, 99(4):439–451, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hoffmann:2002:WCD

[HR02] Marcin Hoffmann and Jacek Rychlewski. When, in the context of drug design, can a fluorine atom successfully substitute a hydroxyl group? *International Journal of Quantum Chemistry*, 89(4):419–427, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huda:2005:ISM

[HR05a] M. N. Huda and A. K. Ray. Ab initio study of molecular oxygen adsorption on Pu (111) surface. *International Journal of Quantum Chemistry*, 105(3):280–291, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huda:2005:DFS

[HR05b] M. N. Huda and A. K. Ray. Density functional study of O_2 adsorption on (100) surface of γ-uranium. *International Journal of Quantum Chemistry*, 102(1):98–105, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hall:2007:AMC

[HR07] G. G. Hall and D. Rees. Atomic and molecular cubature grids. *International Journal of Quantum Chemistry*, 107(4): 845–857, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huix-Rotllant:2008:COS

[HRDM+08] Miquel Huix-Rotllant, Ajanta Deka, Alexei V. Matveev, Sergey I. Bosko, Lyudmila V. Moskaleva, and Notker Rösch. Characterization of optical spectra of interacting systems: Application to oxide-supported metal clusters. *International Journal of Quantum Chemistry*, 108(15):2978–2990, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harbola:2002:MSP

[HS02] Manoj K. Harbola and K. D. Sen. Modified Slater potential and its application to the ground-states and excited-states of atomic systems. *International Journal of Quantum Chemistry*, 90(1):327–333, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2005:TES

[HS05] Ya-Hui Hu and Ming-Der Su. Theoretical examination of substituent effects on the stabilization of a SnY (Y = Sb and Bi) multiple bond. *International Journal of Quantum Chemistry*, 102(1):72–79, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2000:AEP

[HSB+00] Anguang Hu, Markus Staufer, Uwe Birkenheuer, Valentin Igoshine, and Notker Rösch. Analytical evaluation of pseudopotential matrix elements with Gaussian-type solid harmonics of arbitrary angular momentum. *International Journal of Quantum Chemistry*, 79(4):209–221, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72512059/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72512059/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72512059&PLACEBO=IE.pdf`.

Hollingsworth:2002:SEE

[HSH02] Chad A. Hollingsworth, Paul G. Seybold, and Christopher M. Hadad. Substituent effects on the electronic structure and pK_a of benzoic acid. *International Journal of Quantum Chemistry*, 90(4-5):1396–1403, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hirate:2009:QAU

[HSN+09] H. Hirate, Y. Saito, I. Nakaya, H. Sawai, Y. Shinzato, H. Yukawa, M. Morinaga, T. Baba, and H. Nakai. Quantitative approach to the understanding of catalytic effect of metal oxides on the desorption reaction of MgH_2. *International Journal of Quantum Chemistry*, 109(12):2793–2800, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Haque:2009:MVR

[HSP+09] A. K. F. Haque, M. S. I. Sarker, M. A. R. Patoary, M. Shahjahan, M. Ismail Hossain, M. Alfaz Uddin, A. K. Basak, and B. C. Saha. Modified version of revised Deutsch–Märk model for electron impact K-shell ionization cross-sections of atoms at relativistic energies. *International Journal of Quantum Chemistry*, 109(7):1442–1450, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hamza:2009:MHA

[HSRP09] Andrea Hamza, András Stirling, Tibor András Rokob, and Imre Pápai. Mechanism of hydrogen activation by frustrated Lewis pairs: A molecular orbital approach. *International Journal of Quantum Chemistry*, 109(11):2416–2425, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Halim:2009:TMA

[HSS09] W. S. Abdel Halim, A. S. Shalabi, and K. A. Soliman. Transition metal atoms on oxide supports density functional calculations. *International Journal of Quantum Chemistry*, 109 (5):1094–1102, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ho:2000:SEC

[HSW+00] Minhhuy Hô, Hartmut L. Schmider, Donald F. Weaver, Vedene H. Smith, Jr., Robin P. Sagar, and Rodolfo O. Esquivel. Shannon entropy of chemical changes: S_{N2} displacement reactions. *International Journal of Quantum Chemistry*, 77 (1):376–382, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004280/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004280/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004280&PLACEBO=IE.pdf`.

Herges:2004:EFE

[HSW04] T. Herges, A. Schug, and W. Wenzel. Exploration of the free-energy surface of a three-helix peptide with stochastic optimization methods. *International Journal of Quantum Chem-*

istry, 99(5):854–863, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hopkins:2004:EOI

[HT04] Brian W. Hopkins and Gregory S. Tschumper. Extending the ONIOM integrated MO/MO approach to hydrogen bonding in biologic systems: Serine–water and threonine–water dimers. *International Journal of Quantum Chemistry*, 96(4):294–302, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hagedorn:2005:EAQ

[HT05a] George A. Hagedorn and Julio H. Toloza. Exponentially accurate quasimodes for the time-independent Born–Oppenheimer approximation on a one-dimensional molecular system. *International Journal of Quantum Chemistry*, 105(5):463–477, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hart:2005:MEM

[HT05b] James R. Hart and Ajit J. Thakkar. Moments of the electron momentum density: Requirements for ab initio and density functional theory calculations. *International Journal of Quantum Chemistry*, 102(5):673–683, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hardman:2007:FTA

[HT07] Samantha J. O. Hardman and Katherine C. Thompson. The fluorescence transition of 2-aminopurine in double- and single-stranded DNA. *International Journal of Quantum Chemistry*, 107(11):2092–2099, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hoshino:2007:DAE

[HTN07] Minoru Hoshino, Yasuhiro Tsukamoto, and Hiromi Nakai. Development of analytic energy gradient method in nuclear orbital plus molecular orbital theory. *International Journal of Quantum Chemistry*, 107(14):2575–2585, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2004:IST

[Hua04a] Ming-Ju Huang. Ab initio studies of tamoxifen and related compounds. *International Journal of Quantum Chemistry*, 96

(4):374–379, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2004:TSH

[Hua04b] Ming-Ju Huang. Theoretical study of the hydrophobic character of the dimerization of dexanabinol. *International Journal of Quantum Chemistry*, 96(4):426–431, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Halasz:2003:CIC

[HV03] G. J. Halász and Á. Vibók. Comparison of the imaginary and complex absorbing potentials using multistep potential method. *International Journal of Quantum Chemistry*, 92 (2):168–173, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hofto:2008:MIT

[HVC08] Laura R. Hofto, Karina Van Sickle, and Mauricio Cafiero. Modeling intercalation through the sandwich-type interactions between benzene and 14 polyaromatic molecules: DFT and ab initio results. *International Journal of Quantum Chemistry*, 108(1):112–118, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Havenith:2009:DVB

[HvL09] R. W. A. Havenith and J. H. van Lenthe. Delocalization in valence bond—Hyperconjugation. *International Journal of Quantum Chemistry*, 109(11):2426–2429, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Havenith:2001:MAS

[HvLJ01] Remco W. A. Havenith, Joop H. van Lenthe, and Leonardus W. Jenneskens. Möbius aromaticity in small [*n*] *trans*-annulenes? *International Journal of Quantum Chemistry*, 85(1):52–60, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502595/START;` `http://www3.interscience.wiley.com/cgi-bin/fulltext/84502595/FILE?TPL=ftx_start;` `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502595&PLACEBO=IE.pdf`.

Halasz:2002:TBF

[HVSM02] G. J. Halász, Á. Vibók, S. Suhai, and I. Mayer. Toward a BSSE-free description of strongly interacting systems. *International Journal of Quantum Chemistry*, 89(4):190–197, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hofinger:2002:MBS

[HW02] Siegfried Höfinger and Martin Wendland. Method/basis set dependence of the traceless quadrupole moment calculation for N_2, CO_2, SO_2, HCl, CO, NH_3, PH_3, HF, and H_2O. *International Journal of Quantum Chemistry*, 86(2):199–217, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85514354/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85514354/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85514354&PLACEBO=IE.pdf`.

Hoggan:2004:MHW

[HW04] Philip E. Hoggan and Charles A. Weatherford. In memory of Herbert W. Jones (1927–2002). *International Journal of Quantum Chemistry*, 100(2):67–68, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2006:SPR

[HW06] Zhi-Xiang Huang and Xian-Liang Wu. Symplectic partitioned Runge–Kutta scheme for Maxwell's equations. *International Journal of Quantum Chemistry*, 106(4):839–842, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hussein:2001:CEP

[HWPIM01] Wedad Hussein, Christopher G. Walker, Zenaida Peralta-Inga, and Jane S. Murray. Computed electrostatic potentials and average local ionization energies on the molecular surfaces of some tetracyclines. *International Journal of Quantum Chemistry*, 82(4):160–169, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/78503193/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/78503193/FILE?TPL=ftx_start;`

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=78503193&PLACEBO=IE.pdf.

Hinchley:2005:STE

[HWR05] Sarah L. Hinchley, Derek A. Wann, and David W. H. Rankin. Structure by theory and experiment: One nationality, two languages. *International Journal of Quantum Chemistry*, 101 (6):878–884, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2007:IHB

[HWY+07] Mingqiang Huang, Zhenya Wang, Yong Yang, Liqing Hao, Wenwu Zhao, Xiaoming Gao, Li Fang, and Weijun Zhang. Intramolecular hydrogen bond in the hydroxycyclohexadienyl peroxy radicals. *International Journal of Quantum Chemistry*, 107(5):1092–1098, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2004:TAS

[HY04] Ming-Ju Huang and Manyin Yi. Theoretical AM1 studies of inclusion complexes of heptakis(2-O-hydroxypropyl)-β-cyclodextrins with alkylated phenols. *International Journal of Quantum Chemistry*, 100(5):771–778, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hayashi:2000:ADM

[HYC+00] M. Hayashi, T.-S. Yang, C. H. Chang, K. K. Liang, R.-L. Chang, and S. H. Lin. Application of the density matrix method to spectroscopy and dynamics of photosynthetic reaction centers. *International Journal of Quantum Chemistry*, 80(4–5):1043–1054, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505403/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505403/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505403&PLACEBO=IE.pdf.

Hydon:2006:ISM

[Hyd06] Peter E. Hydon. Introduction to symmetry methods in the solution of differential equations that occur in chemistry and chemical biology. *International Journal of Quantum Chem-*

istry, 106(1):266–277, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hao:2007:GVF

[HZJ+07] Feng-You Hao, Yong-Fang Zhao, Xiao-Gong Jing, Xin-Ying Li, and Feng-Li Liu. Geometries, vibrational frequencies, and electron affinities of X_2Cl (X = C, Si, Ge) clusters. *International Journal of Quantum Chemistry*, 107(6):1502–1507, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hanwei:2003:CQS

[HZPY03] Yi Hanwei, Zhou Zhongyuan, Ding Peizhu, and L. H. Yu. Computation of quantum system by second-order matrix symplectic scheme. *International Journal of Quantum Chemistry*, 91(5):591–596, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2008:TID

[HZW+08] Mingqiang Huang, Weijun Zhang, Zhenya Wang, Liqing Hao, Wenwu Zhao, Xianyun Liu, Bo Long, and Li Fang. Theoretical investigation on the detailed mechanism of the OH-initiated atmospheric photooxidation of o-xylene. *International Journal of Quantum Chemistry*, 108(5):954–966, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Imamura:2006:MDC

[IA06] Akira Imamura and Yuriko Aoki. Molecular design of a π-conjugated single-chain electronically conductive polymer. *International Journal of Quantum Chemistry*, 106(8):1924–1933, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Irgibaeva:2008:SSP

[IABS08] Irina Irgibaeva, Anuar Aldongarov, Nikolay Barashkov, and Thomas Schmedake. Study of spectral properties of bis(1,10-phenanthroline) silicon hexacoordinated complexes by density functional theory. *International Journal of Quantum Chemistry*, 108(14):2641–2647, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ivanov:2006:DFM

[IAL06] Vladimir V. Ivanov, Ludwik Adamowicz, and Dmitry I. Lyakh. Dissociation of the fluorine molecule: CASCCSD method and other many-particle models. *International Journal of Quantum Chemistry*, 106(14):2875–2880, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ijjaali:2002:HLI

[IAMY02] Fatima Ijjaali, Manuel Alcamí, Otilia Mó, and Manuel Yáñez. High-level ab initio study of the N^+ (^3P) + SH_2 reactions in the gas phase: Role of spin-forbidden pathways. *International Journal of Quantum Chemistry*, 86(1):130–137, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85011806/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85011806/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85011806&PLACEBO=IE.pdf`.

Irgibaeva:2008:REA

[IBB08] I. S. Irgibaeva, D. A. Birimzhanova, and N. N. Barashkov. Research of electronic absorption spectra of benzazols derivatives by ab initio calculations. *International Journal of Quantum Chemistry*, 108(14):2700–2710, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Imamura:2008:NBO

[IBN08] Yutaka Imamura, Takeshi Baba, and Hiromi Nakai. Natural bond orbital-based energy density analysis for correlated methods: Second-order Møller–Plesset perturbation and coupled-cluster singles and doubles. *International Journal of Quantum Chemistry*, 108(8):1316–1325, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Iglesias:2008:TDD

[ICRS08] Rodrigo Sebastian Iglesias, Leandra Franciscato Campo, Fabiano Severo Rodembusch, and Valter Stefani. Time-dependent DFT-PCM investigation of the photophysics of ESIPT-exhibiting benzazole dyes. *International Journal of Quantum Chemistry*, 108(13):2334–2339, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ionescu:2006:TSS

[IDH06] Sorana Ionescu, Carmen C. Diaconu, and Mihaela Hillebrand. Theoretical study of some verapamil derivatives. *International Journal of Quantum Chemistry*, 106(6):1457–1464, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Iordanov:2009:SBC

[IDM+09] Tzvetelin D. Iordanov, Jesse L. Davis, Artëm E. Masunov, Andrew Levenson, Olga V. Przhonska, and Alexei D. Kachkovski. Symmetry breaking in cationic polymethine dyes, part 1: Ground state potential energy surfaces and solvent effects on electronic spectra of streptocyanines. *International Journal of Quantum Chemistry*, 109(15):3592–3601, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Iung:2006:PPA

[IG06] Christophe Iung and Fabien Gatti. Polyspherical parametrization of an N-atom system: Principles and applications. *International Journal of Quantum Chemistry*, 106(1):130–151, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ishikawa:2000:MOAa

[IK00a] Youichi Ishikawa and Kiyoshi Kishi. Molecular orbital approach to odor molecules: Normal fatty acids and cyclamenaldehydes. *International Journal of Quantum Chemistry*, 79(2):101–108, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72508333/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72508333/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72508333&PLACEBO=IE.pdf`.

Ishikawa:2000:MOAb

[IK00b] Youichi Ishikawa and Kiyoshi Kishi. Molecular orbital approach to possible discrimination of musk odor intensity. *International Journal of Quantum Chemistry*, 79(2):109–119, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72508332/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72508332/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72508332&PLACEBO=IE.pdf`.

Ivashin:2004:DNL

[IKL04] A. P. Ivashin, M. Y. Kovalevsky, and L. V. Logvinova. Dynamics of nematic liquid crystals with conformational degrees of freedom. *International Journal of Quantum Chemistry*, 100 (4):636–644, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Isaev:2008:PPC

[IKS08] Alexander Isaev, Tapas Kar, and Steve Scheiner. Periodicity in proton conduction along a H-bonded chain. Application to biomolecules. *International Journal of Quantum Chemistry*, 108(3):607–616, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [IKS10].

Isaev:2010:EPP

[IKS10] Alexander Isaev, Tapas Kar, and Steve Scheiner. Erratum: Periodicity in proton conduction along a H-bonded chain. Application to biomolecules. *International Journal of Quantum Chemistry*, 110(5):1136, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [IKS08].

Ilcin:2008:DCS

[ILB+08] Michal Ilčin, Vladimír Lukeš, Lukáš Bučinský, Viliam Laurinc, and Stanislav Biskupič. On the diffusion coefficients and stability of van der Waals complex Hg ... N_2. *International Journal of Quantum Chemistry*, 108(12):2150–2158, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ilarraza-Lomeli:2002:CME

[ILVMSB+02] A. C. Ilarraza-Lomelí, M. N. Valdés-Martínez, A. L. Salas-Brito, R. P. Martínez y Romero, and H. N. Núñez-Yépez. Calculation of matrix elements in relativistic quantum mechanics. *International Journal of Quantum Chemistry*, 90(1):195–201, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [ILVMSB+03].

Ilarraza-Lomeli:2003:ECM

[ILVMSB+03] A. C. Ilarraza-Lomelí, M. N. Valdés-Martínez, A. L. Salas-Brito, R. P. Martínez y Romero, and H. N. Núñez-Yépez. Erratum: Calculation of matrix elements in relativistic quantum mechanics. *International Journal of Quantum Chemistry*, 93 (1):47, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [ILVMSB+02].

Isaev:2002:GMC

[IMT+02] T. A. Isaev, N. S. Mosyagin, A. V. Titov, A. B. Alekseyev, and R. J. Buenker. GRECP/5e-MRD-CI calculation of the electronic structure of PbH. *International Journal of Quantum Chemistry*, 88(5):687–690, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ivanova:2006:ESI

[IMTG06] A. Ivanova, G. Madjarova, A. Tadjer, and N. Gospodinova. Effect of solvation and intermolecular interactions on the structure and optical properties of PANI oligomers. *International Journal of Quantum Chemistry*, 106(6):1383–1395, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Imamura:2007:ASI

[IN07] Yutaka Imamura and Hiromi Nakai. Analysis of self-interaction correction for describing core excited states. *International Journal of Quantum Chemistry*, 107(1):23–29, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ishikawa:2009:RHF

[IN09] Sascha T. Ishikawa and Takahito Nakajima. The reaction of N_2O_5 with H_3O^+: A first-principles direct molecular dynamics study of acid-catalyzed reactive uptake of N_2O_5. *International Journal of Quantum Chemistry*, 109(10):2143–2148, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Isobe:2008:EHF

[INS+08] Hiroshi Isobe, Satomichi Nishihara, Mitsuo Shoji, Shusuke Yamanaka, Jiro Shimada, Masayuki Hagiwara, and Kizashi

Yamaguchi. Extended Hartree–Fock theory of chemical reactions. VIII. Hydroxylation reactions by P450. *International Journal of Quantum Chemistry*, 108(15):2991–3009, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ishii:2004:FPA

[IOA+04] Takugo Ishii, Kazuyoshi Ogasawara, Hirohiko Adachi, Philipp Burmester, and Günter Huber. First-principles analysis for the optical absorption spectra of metal ions in solids. *International Journal of Quantum Chemistry*, 99(4):488–494, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Injan:2005:PAH

[IPPL05] Natcha Injan, Narong Pannorad, Michael Probst, and Jumras Limtrakul. Pyridine adsorbed on H-Faujasite zeolite: Electrostatic effect of the infinite crystal lattice calculated from a point charge representation. *International Journal of Quantum Chemistry*, 105(6):898–905, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Irgibaeva:2004:DPM

[Irg04] I. S. Irgibaeva. Determination of the parameters of multidimension vibration Hamiltonian of CH_3NH_2 from quantum chemical data. *International Journal of Quantum Chemistry*, 96(3):210–218, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Irgibaeva:2006:IMR

[Irg06] I. S. Irgibaeva. Ab initio modeling of reaction of primary aliphatic diamines with CS_2 in alkaline medium. *International Journal of Quantum Chemistry*, 106(10):2214–2221, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Issaoui:2009:AET

[IROW09] Noureddine Issaoui, Najeh Rekik, Brahim Oujia, and Marek J. Wójcik. Anharmonic effects on theoretical IR line shapes of medium strong H(D) bonds. *International Journal of Quantum Chemistry*, 109(3):483–499, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ichikawa:2002:AAC

[IS02] Hiroshi Ichikawa and Ken Sakata. Aromaticity/antiaromaticity in cyclic conjugated hydrocarbons. *International Journal of Quantum Chemistry*, 87(3):135–144, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89013455/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89013455/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89013455&PLACEBO=IE.pdf`.

Iftimie:2003:SQC

[IS03] Radu Iftimie and Jeremy Schofield. Separation of quantum and classical behavior in proton transfer reactions: Implications from studies of secondary kinetic isotope effects. *International Journal of Quantum Chemistry*, 91(3):404–413, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Isobe:2001:ETC

[ISK+01] H. Isobe, T. Soda, Y. Kitagawa, Y. Takano, T. Kawakami, Y. Yoshioka, and K. Yamaguchi. EHF theory of chemical reactions V. Nature of manganese-oxygen bonds by hybrid density functional theory (DFT) and coupled-cluster (CC) methods. *International Journal of Quantum Chemistry*, 85(1): 34–43, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85004196/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85004196/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85004196&PLACEBO=IE.pdf`.

Iyengar:2000:BEC

[ISS00] Srinivasan S. Iyengar, Gustavo E. Scuseria, and Andreas Savin. Bounding the extrapolated correlation energy using Padé approximants. *International Journal of Quantum Chemistry*, 79(4):222–234, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72512058/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72512058/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72512058&PLACEBO=IE.pdf`.

Ishimoto:2006:AEV

[ITN06] Takayoshi Ishimoto, Masanori Tachikawa, and Umpei Nagashima. Analysis of exponent values in Gaussian-type functions for development of protonic and deuteronic basis functions. *International Journal of Quantum Chemistry*, 106(7): 1465–1476, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ishimoto:2008:AOE

[ITN08] Takayoshi Ishimoto, Masanori Tachikawa, and Umpei Nagashima. Analytical optimization of exponent values in protonic and deuteronic Gaussian-type functions by elimination of translational and rotational motions from multi-component molecular orbital scheme. *International Journal of Quantum Chemistry*, 108(3):472–481, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ishimoto:2009:RMM

[ITN09] Takayoshi Ishimoto, Masanori Tachikawa, and Umpei Nagashima. Review of multicomponent molecular orbital method for direct treatment of nuclear quantum effect. *International Journal of Quantum Chemistry*, 109(12):2677–2694, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ivanova:2002:TSI

[ITR02] A. Ivanova, A. Tadjer, and B. Radoev. Theoretical study of insoluble polymer monolayers. *International Journal of Quantum Chemistry*, 89(4):397–404, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ishii:2009:SSM

[ITY+09] Tomohiko Ishii, Shino Tsuboi, Shohei Yukinari, Genta Sakane, Masahiro Yamashita, and Brian K. Breedlove. 2D spectrochemical series of ML_6 metal complexes for controlling the ligand field splitting. *International Journal of Quantum Chemistry*, 109(12):2734–2743, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ishikawa:2002:ELP

[IV02] Yasuyuki Ishikawa and Marius J. Vilkas. Energy levels of the 4 s^2 4 p^2 states of germanium and germaniumlike ions.

International Journal of Quantum Chemistry, 90(1):410–418, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ivanova:2005:ISR

[Iva05] Nina M. Ivanova. Ab initio study of reactions of 1-halogen-3-methoxy-1-propynes with Grignard reagent. *International Journal of Quantum Chemistry*, 101(1):90–96, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ishikawa:2000:RMM

[IVK00] Yasuyuki Ishikawa, Marius Jonas Vilkas, and Konrad Koc. Relativistic multireference Møller–Plesset perturbation theory calculations for siliconlike ions. *International Journal of Quantum Chemistry*, 77(1):433–445, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004287/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004287/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004287&PLACEBO=IE.pdf`.

Iyengar:2009:CVP

[Iye09] Srinivasan S. Iyengar. Computing vibrational properties in hydrogen-bonded systems using quantum wavepacket ab initio molecular dynamics. *International Journal of Quantum Chemistry*, 109(15):3798–3810, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ito:2004:FNA

[IYO+04] T. Ito, T. Yoshimoto, Y. Ohta, H. Kawabe, H. Nagao, and K. Nishikawa. Formulation and numerical approach to molecular systems by the Green function method without Born–Oppenheimer approximation II: Nucleus–electron correlation. *International Journal of Quantum Chemistry*, 100(6):918–926, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ikeda:2007:SEI

[IYSS07] Atsushi Ikeda, Daisuke Yokogawa, Hirofumi Sato, and Shigeyoshi Sakaki. Solvation effect on the interaction between sodium and chloride ions in aqueous solution: An analysis

based on the new resonance theory. *International Journal of Quantum Chemistry*, 107(15):3132–3136, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Isobe:2003:UCI

[IYY03] Hiroshi Isobe, Shusuke Yamanaka, and Kizashi Yamaguchi. Utility of chemical indices for transition structures of pericyclic reactions: Case study of the cope rearrangement. *International Journal of Quantum Chemistry*, 95(4–5):532–545, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Izmailov:2004:MMB

[IZ04] Arthur Izmailov and Andréi Zaitsevskii. Multireference many-body perturbation theory calculations on negative ions with small electron detachment energies. *International Journal of Quantum Chemistry*, 96(3):202–209, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2002:HLI

[Jal02] Abraham F. Jalbout. High level ab initio and density functional theory calculations of the dissociation energies, ionization energies, geometrical variations, and vibrational modes of ground and excited CO_2, CO_2^+, and CO_2^{2+}. *International Journal of Quantum Chemistry*, 86(6):541–568, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/88511887/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88511887/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88511887&PLACEBO=IE.pdf`.

Jalbout:2007:EPD

[Jal07a] Abraham F. Jalbout. Electrostatic potential–density relationships in molecules. *International Journal of Quantum Chemistry*, 107(10):1935–1942, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2007:SEE

[Jal07b] Abraham F. Jalbout. Stabilization of an excess electron on molecular surfaces by a pair of HF molecules. *International Journal of Quantum Chemistry*, 107(6):1532–1539, ???? 2007.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2008:ASE

[Jal08a] Abraham F. Jalbout. Ammoniated solvation of excess electrons on molecular surfaces. *International Journal of Quantum Chemistry*, 108(3):532–537, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2008:LET

[Jal08b] Abraham F. Jalbout. Localized electron traps on extended molecular surfaces. *International Journal of Quantum Chemistry*, 108(3):584–588, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2008:TEE

[Jal08c] Abraham F. Jalbout. Trapping excess electrons in charge pockets on molecular surfaces in an argon matrix. *International Journal of Quantum Chemistry*, 108(3):576–583, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jensen:2001:ACP

[JÅM01] Lasse Jensen, Per-Olof Åstrand, and Kurt V. Mikkelsen. An atomic capacitance-polarizability model for the calculation of molecular dipole moments and polarizabilities. *International Journal of Quantum Chemistry*, 84(5):513–522, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/82003578/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/82003578/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=82003578&PLACEBO=IE.pdf`.

Jeon:2005:SIN

[JAP+05] In-Sun Jeon, Doo-Sik Ahn, Sung-Woo Park, Sungyul Lee, and Bongsoo Kim. Structures and isomerization of neutral and zwitterion serine–water clusters: Computational study. *International Journal of Quantum Chemistry*, 101(1):55–66, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jantschi:2007:MOW

[JB07] Lorentz Jäntschi and Sorana-Daniela Bolboacă. Modeling the octanol–water partition coefficient of substituted phenols by the use of structure information. *International Journal of Quantum Chemistry*, 107(8):1736–1744, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jin:2003:CPR

[JBMP03] Ping Jin, Tore Brinck, Jane S. Murray, and Peter Politzer. Computational prediction of relative group polarizabilities. *International Journal of Quantum Chemistry*, 95(4–5):632–637, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jaskolski:2002:AM

[JBPZ02] W. Jaskólski, G. W. Bryant, J. Planelles, and M. Zieliński. Artificial molecules. *International Journal of Quantum Chemistry*, 90(3):1075–1082, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jacquemin:2000:OGS

[JC00] Denis Jacquemin and Benoît Champagne. Optimizing the geometry of stereoregular polymers. III. Polyyne and the basis set quasi-linear dependence. *International Journal of Quantum Chemistry*, 80(4–5):863–870, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505386/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505386/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505386&PLACEBO=IE.pdf`.

Jacquemin:2001:LRE

[JC01] Denis Jacquemin and Benoît Champagne. Long-range effects in optimizing the geometry of stereoregular polymers — IV: Explicit determination of the helical angle. *International Journal of Quantum Chemistry*, 85(4–5):539–545, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jeziorska:2008:CBS

[JCP+08] Małgorzata Jeziorska, Wojciech Cencek, Konrad Patkowski, Bogumił Jeziorski, and Krzysztof Szalewicz. Complete basis set extrapolations of dispersion, exchange, and coupled-clusters contributions to the interaction energy: a helium dimer study. *International Journal of Quantum Chemistry*, 108(12):2053–2075, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2008:HCO

[JCTA08] Abraham F. Jalbout, Flavio F. Contreras-Torres, and L. Adamowicz. The hydroxyacetone (CH_3COCH_2 (OH)) torsional potential and isomerization: A theoretical study. *International Journal of Quantum Chemistry*, 108(2):279–288, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2008:SEE

[JCTD08a] Abraham F. Jalbout, Flavio Contreras-Torres, and R. Del Castillo. Solvation of excess electrons trapped in charge pockets on hydrated molecular surfaces. *International Journal of Quantum Chemistry*, 108(3):567–575, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2008:FSO

[JCTD08b] Abraham F. Jalbout, Flavio F. Contreras-Torres, and Aned De Leon. Formation of simple organic molecules in the interstellar medium. *International Journal of Quantum Chemistry*, 108(3):598–606, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2008:CTS

[JdL08] Abraham F. Jalbout and Aned de Leon. Charge transfer stabilization of an excess electron on a molecular surface. *International Journal of Quantum Chemistry*, 108(4):808–813, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jacquemin:2002:CEL

[JFC02] Denis Jacquemin, Joseph G. Fripiat, and Benoît Champagne. Convergence of exchange lattice summations in direct-space polymer calculations. *International Journal of Quantum*

Chemistry, 89(5):452–463, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jimenez-Fabian:2008:AIA

[JFJMR08a] Isaac Jimenez-Fabian, Abraham F. Jalbout, Effat Moshfeghi, and Heidar Raissi. β-aminoacrolein: An ab initio, AIM and NBO study. *International Journal of Quantum Chemistry*, 108(2):383–390, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [JFJMR08b].

Jimenez-Fabian:2008:EAI

[JFJMR08b] Isaac Jimenez-Fabian, Abraham F. Jalbout, Effat Moshfeghi, and Heidar Raissi. Erratum for "β-Aminoacrolein: An Ab initio, AIM and NBO Study". *International Journal of Quantum Chemistry*, 108(6):1207, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [JFJMR08a].

Jia:2009:TSM

[JFS+09] Zhongfeng Jia, Shengyu Feng, Enfeng Song, Wenyan Sun, and Lixiao Cong. Theoretical study on the mechanism for the thermal rearrangement reactions of 2-silylethyl acetate $H_3SiCH_2CH_2OCOCH_3$. *International Journal of Quantum Chemistry*, 109(2):342–348, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jug:2000:QSR

[JG00] Karl Jug and Heiko Gerwens. QCMEE study of the reductive half-reaction of glucose oxidase. *International Journal of Quantum Chemistry*, 77(1):71–81, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004296/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004296/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004296&PLACEBO=IE.pdf`.

Jose:2009:ISC

[JG09] K. V. Jovan Jose and Shridhar R. Gadre. Ab initio study on $(CO_2)_n$ clusters via electrostatics- and molecular tailoring-based algorithm. *International Journal of Quantum Chemistry*, 109(10):2238–2247, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2009:DFS

[JHLC09a] Zhen-Yi Jiang, Yu-Qin Hou, Kuo-Hsing Lee, and San-Yan Chu. Density functional study of structural and electronic properties of maximum-spin $^{n+1}$ Au_{n-1} Ag clusters. *International Journal of Quantum Chemistry*, 109(6):1348–1356, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2009:SSH

[JHLC09b] Zhen-Yi Jiang, Yu-Qing Hou, Kuo-Hsing Lee, and San-Yan Chu. Structure and stability of high-spin Au_n ($n = 2--8$) clusters. *International Journal of Quantum Chemistry*, 109 (4):861–869, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2000:TSO

[JHR+00] Hua Liang Jiang, Xiao Qin Huang, Suo Bao Rong, Xiao Min Luo, Jian Zhong Chen, Yun Tang, Kai Xian Chen, You Cheng Zhu, Wen Qiao Jin, Zhi Qiang Chi, Ru Yun Ji, and Yang Cao. Theoretical studies on opioid receptors and ligands. I. Molecular modeling and QSAR studies on the interaction mechanism of fentanyl analogs binding toμ-opioid receptor. *International Journal of Quantum Chemistry*, 78(4):285–293, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72000073/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72000073/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72000073&PLACEBO=IE.pdf`.

Jones:2000:EAP

[JJ00] H. W. Jones and J. L. Jain. Eigenvalues to arbitrary precision for one-dimensional Schrödinger equations by the shooting method using integer arithmetic. *International Journal of Quantum Chemistry*, 80(4–5):842–847, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505414/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505414/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505414&PLACEBO=IE.pdf`.

Janowski:2002:ICN

[JJ02] Tomasz Janowski and Michał Jaszuński. Ab initio calculations of the NMR properties of the $NH_3 \ldots HH_2$ O complex. *International Journal of Quantum Chemistry*, 90(3):1083–1090, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalkanen:2006:UVS

[JJC+06] K. J. Jalkanen, V. Würtz Jürgensen, A. Claussen, A. Rahim, G. M. Jensen, R. C. Wade, F. Nardi, C. Jung, I. M. Degtyarenko, R. M. Nieminen, F. Herrmann, M. Knapp-Mohammady, T. A. Niehaus, K. Frimand, and S. Suhai. Use of vibrational spectroscopy to study protein and DNA structure, hydration, and binding of biomolecules: A combined theoretical and experimental approach. *International Journal of Quantum Chemistry*, 106(5):1160–1198, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2008:IME

[JJFdL08] Abraham F. Jalbout, Isaac Jiménez-Fabián, and Aned de Leon. Interactions of metal-encapsulated fullerenes with solvents. *International Journal of Quantum Chemistry*, 108 (6):1076–1082, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jain:2004:CFS

[JJWH04] J. L. Jain, H. W. Jones, C. A. Weatherford, and P. E. Hoggan. Closed formulae for (1s—1s), Slater two-center integrals, using the three-center nuclear attraction integral program in spherical coordinates. *International Journal of Quantum Chemistry*, 100(2):199–205, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jayakumar:2000:SIS

[JK00] N. Jayakumar and P. Kolandaivel. Studies of isomer stability using the maximum hardness principle (MHP). *International Journal of Quantum Chemistry*, 76(5):648–655, February 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000586/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000586/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000586&PLACEBO=IE.pdf`.

Jansik:2002:DMC

[JKU02] Branislav Jansík, Vladimír Kellö, and Miroslav Urban. Dipole moments calculations of transition metal mononitrides: ScN, TiN, VN, and CrN: Limits of the CCSD(T) method. *International Journal of Quantum Chemistry*, 90(3):1240–1248, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2007:APE

[JLAR07] Abraham F. Jalbout, Xin-Hua Li, and Hakima Abou-Rachid. Analytical potential energy functions and theoretical spectroscopic constants for MX/MX^- (M = Ge, Sn, Pb; X O, S, Se, Te, Po) and LuA (A = H, F) systems: Density functional theory calculations. *International Journal of Quantum Chemistry*, 107(3):522–539, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jia:2009:RCR

[JLC+09] Gui-Xiao Jia, Jun-Qian Li, Lin-Gang Chen, Yi Li, Kai-Ning Ding, and Yong-Fan Zhang. A reasonable criterion of reactivities at the defective region of single-walled carbon nanotubes. *International Journal of Quantum Chemistry*, 109(4): 668–678, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Janvier:2001:SSS

[JLI+01] P. Janvier, J.-Y. Le Questel, B. Illien, S. Suresh, E. Blart, J.-P. Quintard, and F. Odobel. Semiempirical and spectroscopic study of a novel porphyrin dyad. *International Journal of Quantum Chemistry*, 84(2):259–263, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502335/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502335/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502335&PLACEBO=IE.pdf`.

Jayasekera:2008:FPS

[JLM08] Thushari Jayasekera, B. A. Landis, and J. W. Mintmire. First-principles simulations of chiral double-wall carbon nanotubes. *International Journal of Quantum Chemistry*, 108(15):2943–

2949, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jacquemin:2009:ISU

[JLPA09] Denis Jacquemin, Adèle D. Laurent, Eric A. Perpète, and Jean-Marie André. An ab initio simulation of the UV/visible spectra of N-benzylideneaniline dyes. *International Journal of Quantum Chemistry*, 109(15):3506–3515, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jia:2009:PSS

[JLZY09] Cangzhi Jia, Tian Liu, Xiangde Zhang, and Shijun Yan. Protein secondary structure class assignment on the basis of a new graphic representation. *International Journal of Quantum Chemistry*, 109(4):819–825, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jorgensen:2000:PTR

[JM00] Solvejg Jørgensen and Kurt V. Mikkelsen. Proton transfer reactions in solution. *International Journal of Quantum Chemistry*, 77(1):221–239, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004263/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004263/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004263&PLACEBO=IE.pdf`.

Jayasekera:2007:LVE

[JM07] Thushari Jayasekera and J. W. Mintmire. Lattice vacancy effects on electron transport in multiterminal graphene nanodevices. *International Journal of Quantum Chemistry*, 107 (15):3071–3076, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jayasekera:2007:FPP

[JMEM07] T. Jayasekera, M. S. Monigold, S. L. Elizondo, and J. W. Mintmire. First-principles properties of organic polymer photovoltaic materials. *International Journal of Quantum Chemistry*, 107(15):3120–3125, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jin:2004:LIE

[JMP04] Ping Jin, Jane S. Murray, and Peter Politzer. Local ionization energy and local polarizability. *International Journal of Quantum Chemistry*, 96(4):394–401, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jacquemin:2005:LPB

[JMP05] Denis Jacquemin, Miroslav Medved', and Eric A. Perpète. Linear phosphorus–boron chains: model system with huge electronic first hyperpolarizability. *International Journal of Quantum Chemistry*, 103(2):226–234, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jin:2006:CDR

[JMP06] Ping Jin, Jane S. Murray, and Peter Politzer. Computational determination of the relative polarizabilities of molecular components. *International Journal of Quantum Chemistry*, 106 (11):2347–2355, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2009:MSV

[JNF+09] A. F. Jalbout, M. Ali Naseri, M. Fazli, H. Raissi, M. Rezaei, A. Nowroozi, and A. de Leon. Molecular structure and vibrational assignment of α-chloro acetylacetone: A density functional theory study. *International Journal of Quantum Chemistry*, 109(7):1481–1496, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalkanen:2003:VAV

[JNKMS03] K. J. Jalkanen, R. M. Nieminen, M. Knapp-Mohammady, and S. Suhai. Vibrational analysis of various isotopomers of L-Alanyl-L-Alanine in aqueous solution: Vibrational absorption, vibrational circular dichroism, Raman, and Raman optical activity spectra. *International Journal of Quantum Chemistry*, 92(2):239–259, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jankowski:2004:AAM

[JNSF04] K. Jankowski, K. Nowakowski, R. Słupski, and J. R. Flores. Application of accurate MP2 energies for closed-shell atoms in examinations of density functionals for $3d^{10}$ electron ions. *International Journal of Quantum Chemistry*, 99(4):277–287,

???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Janezic:2001:SMD

[JP01] Dušanka Janežič and Matej Praprotnik. Symplectic molecular dynamics integration using normal mode analysis. *International Journal of Quantum Chemistry*, 84(1):2–12, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84002436/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002436/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002436&PLACEBO=IE.pdf`.

Jaskolski:2008:CNS

[JP08] W. Jaskólski and M. Pelc. Carbon nanotube superlattices in a magnetic field. *International Journal of Quantum Chemistry*, 108(12):2261–2266, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jemmis:2003:EMC

[JPA03] Eluvathingal D. Jemmis, Pattiyil Parameswaran, and Anakuthil Anoop. Effect of metal complexation on ring opening of bowl-shaped hydrocarbons: Theoretical study. *International Journal of Quantum Chemistry*, 95(6):810–815, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jacquemin:2005:NRP

[JPA05] Denis Jacquemin, Eric A. Perpète, and Jean-Marie André. NLO response of polymethineimine and polymethineimine/polyacetylene conformers: Assessment of electron correlation effects. *International Journal of Quantum Chemistry*, 105 (6):553–563, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2007:WMR

[JPA07] Abraham F. Jalbout, Michele Pavanello, and Ludwik Adamowicz. The water mediated ring closing in the formose reaction. *International Journal of Quantum Chemistry*, 107 (10):2024–2031, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jayasekera:2008:EPB

[JPMM08] Thushari Jayasekera, Pavan K. Pillalamarri, J. W. Mintmire, and V. Meunier. Effect of phase-breaking events on electron transport in mesoscopic and nanodevices. *International Journal of Quantum Chemistry*, 108(15):2896–2905, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jankowski:2002:MSI

[JR02] K. Jankowski and K. Rubiniec. Model study of the impact of orbital choice on the accuracy of coupled-cluster energies. IV. Single-reference-state methods in applications to excited states. *International Journal of Quantum Chemistry*, 90(1): 250–261, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2008:DFC

[JRSA08] Abraham F. Jalbout, Amlan K. Roy, Abul Haider Shipar, and M. Samsuddin Ahmed. Density functional computational studies on the glucose and glycine Maillard reaction: Formation of the Amadori rearrangement products. *International Journal of Quantum Chemistry*, 108(3):589–597, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jeziorski:2008:IPK

[JS08] Bogumit Jeziorski and Andrzej J. Sadlej. Introduction: Professor Karol Jankowski turned 70. *International Journal of Quantum Chemistry*, 108(12):2041–2042, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Johnson:2001:MPS

[JSC01] William T. G. Johnson, Michael B. Sullivan, and Christopher J. Cramer. meta and para substitution effects on the electronic state energies and ring-expansion reactivities of phenylnitrenes. *International Journal of Quantum Chemistry*, 85(4–5):492–508, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jensen:2006:CDS

[JSvDA06] L. Jensen, Marcel Swart, Piet Th. van Duijnen, and J. Autschbach. Circular dichroism spectrum of $[Co(en)_3]^{3+}$

in water: A discrete solvent reaction field study. *International Journal of Quantum Chemistry*, 106(12):2479–2488, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Junkermeier:2009:AIA

[JTB09] Chad Junkermeier, Mark Transtrum, and Manuel Berrondo. An analytic iterative approach to solving the time-independent Schrödinger equation. *International Journal of Quantum Chemistry*, 109(5):982–998, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2003:PGD

[JTC+03] Yang Jiang, Bo Tan, Zhong-Zhou Chen, Tong Liu, Ru-Gang Zhong, Yan-Mei Li, David Jeremy Stewart, Yu-Fen Zhao, and Hua-Liang Jiang. Phosphoryl group differentiating α-amino acids from β- and γ-amino acids in prebiotic peptide formation. *International Journal of Quantum Chemistry*, 94(4): 232–241, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2007:EAG

[JTC+07] A. F. Jalbout, B. Trzaskowski, E. C. M. Chen, E. S. Chen, and Ludwik Adamowicz. Electron affinities, gas phase acidities, and potential energy curves: Benzene. *International Journal of Quantum Chemistry*, 107(5):1115–1125, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jensen:2002:BQS

[JTH02] Morten Østergaard Jensen, Thorstein Thorsteinsson, and Aage E. Hansen. Benzocyclobutadiene: The question of structures, magnetic shieldings, and aromatic character. *International Journal of Quantum Chemistry*, 90(2):616–628, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jensen:2005:RIT

[JV05] L. Jensen and Piet Th. Van Duijnen. Refractive index and third-order nonlinear susceptibility of C_{60} in the condensed phase calculated with the discrete solvent reaction field model. *International Journal of Quantum Chemistry*, 102(5):612–

619, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jishi:2000:ESC

[JWM00] R. A. Jishi, C. T. White, and J. W. Mintmire. Endohedral selenium chains in carbon, boron nitride, and BC_2 N nanotubes. *International Journal of Quantum Chemistry*, 80(3):480–485, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501021/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501021/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501021&PLACEBO=IE.pdf`.

Jiang:2008:TSB

[JWZ+08] Yanke Jiang, Jun Wu, Jianwei Zou, Yunxiang Lu, Guixiang Hu, and Qingsen Yu. Theoretical studies on the binding models of tetramethylammonium with phenol: Cation-π and hydrogen-bond interactions. *International Journal of Quantum Chemistry*, 108(7):1294–1303, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ju:2005:PDA

[JXC05] Xue-Hai Ju, He-Ming Xiao, and Li-Tao Chen. Periodic DFT approach to benzotrifuroxan crystal. *International Journal of Quantum Chemistry*, 102(2):224–229, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2004:FPS

[JXW+04] Zhen-Yi Jiang, Xiao-Hong Xu, Hai-Shun Wu, Fu-Qiang Zhang, and Zhi-Hao Jin. First principles study of the structure, electronic state, and stability of C_mN_2 clusters. *International Journal of Quantum Chemistry*, 97(4):876–882, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ji:2005:RTS

[JXZ+05] Yanju Ji, Yueyuan Xia, Mingwen Zhao, Feng Li, and Boda Huang. Reactions of ·OH with thymine studied using density functional theory. *International Journal of Quantum Chemistry*, 101(2):211–218, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jug:2002:GPB

[JZK02] Karl Jug, Bernd Zimmermann, and Andreas M. Köster. Growth pattern and bonding of copper clusters. *International Journal of Quantum Chemistry*, 90(2):594–602, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jian:2008:CCE

[JZL+08] Fang-Fang Jian, Pu-Su Zhao, Yu-Feng Li, Xian Wang, and Qing Yu. A combined computational and experimental approach for investigating a hydrogen-bonded supermolecular compound comprising benzimidazole and malonic acid. *International Journal of Quantum Chemistry*, 108(3):521–531, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2009:MDS

[JZW+09] Yan-Ke Jiang, Jian-Wei Zou, Yu-Qian Wu, Na Zhang, Qing-Sen Yu, and Yong-Jun Jiang. Molecular dynamics simulation on HP1 protein binding by histone H3 tail methylation and phosphorylation. *International Journal of Quantum Chemistry*, 109(4):746–755, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jia:2008:NMA

[JZZ+08] Zhao-Kun Jia, Shu-Fang Zhang, Zheng-Yu Zhou, An-Guo Zhang, and Rui-Yan Hou. A new method of accurate p K_b determinations for some organic amines. *International Journal of Quantum Chemistry*, 108(2):265–271, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2009:DSF

[JZZ+09] Yanke Jiang, Jianwei Zou, Min Zeng, Na Zhang, and Qingsen Yu. Dynamics simulation on the flexibility and backbone motions of HP1 chromodomain bound to free and lysine 9-methylated histone H3 tails. *International Journal of Quantum Chemistry*, 109(5):1135–1147, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karabiyik:2005:GFQ

[KA05] Hasan Karabiyik and Muhíttín Aygün. Generalized formulation of quantum and classical crystallography using Green's

functions. *International Journal of Quantum Chemistry*, 103 (6):781–791, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kapshai:2003:NDC

[KAE03] Valery Kapshai, Tatjana Alferova, and Nils Elander. Numerical determination of complex resonance energies by using a superposition of δ-potentials. *International Journal of Quantum Chemistry*, 91(4):533–540, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kapshai:2007:IEC

[KAE07] V. Kapshai, Tatjana Alferova, and Nils Elander. Integral equations and complex resonance energies for analytical potentials. *International Journal of Quantum Chemistry*, 107 (5):1029–1039, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kassaee:2008:NSN

[KAG08] M. Z. Kassaee, H. Arefrad, and M. Ghambarian. Novel silicon nanorings: Persilacyclacenes at DFT. *International Journal of Quantum Chemistry*, 108(4):696–707, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaijser:2009:WQC

[Kai09] Per Kaijser. Will quantum chemistry benefit from quantum computers? *International Journal of Quantum Chemistry*, 109(13):3003–3007, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kakkar:2003:CDF

[Kak03] Rita Kakkar. C_3H_4: Density functional study of interconversion of isomers. *International Journal of Quantum Chemistry*, 94(2):93–104, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kantorovich:2000:AGF

[Kan00a] L. N. Kantorovich. Application of the group function theory to infinite systems. *International Journal of Quantum Chemistry*, 76(4):511–534, February 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.`

wiley.com/cgi-bin/abstract/70000682/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000682/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000682&PLACEBO=IE.pdf.

Kantorovich:2000:DAM

[Kan00b] L. N. Kantorovich. Derivation of atomistic models for lattices consisting of weakly overlapping structural elements. *International Journal of Quantum Chemistry*, 78(5):306–330, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72001891/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72001891/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72001891&PLACEBO=IE.pdf.

Kina:2009:IQM

[KAN+09] Daisuke Kina, Pooja Arora, Akira Nakayama, Takeshi Noro, Mark S. Gordon, and Tetsuya Taketsugu. Ab initio QM/MM excited-state molecular dynamics study of coumarin 151 in water solution. *International Journal of Quantum Chemistry*, 109(10):2308–2318, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kurita:2000:DFS

[KANK00] Noriyuki Kurita, Masahiro Araki, Kenji Nakao, and Kinya Kobayashi. Density functional study for stacking energy of cytosine dimer: Ab initio MO calculations based on Slater-type basis set. *International Journal of Quantum Chemistry*, 76(6):677–685, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70001603/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70001603/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70001603&PLACEBO=IE.pdf.

Kaplan:2002:PEP

[Kap02] I. G. Kaplan. Is the Pauli exclusive principle an independent quantum mechanical postulate? *International Journal of Quantum Chemistry*, 89(4):268–276, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaplan:2006:IIP

[Kap06] I. G. (Ilya Grigorievich) Kaplan. *Intermolecular interactions: physical picture, computational methods, model potentials*. John Wiley, New York, NY, USA, 2006. ISBN 0-470-86332-3 (hardcover). xii + 367 pp. LCCN QD461 .K29713 2006. URL `http://www.loc.gov/catdir/enhancements/fy0622/2005021486-d.html; http://www.loc.gov/catdir/toc/ecip0516/2005021486.html`.

Kaplan:2007:PDT

[Kap07] I. G. Kaplan. Problems in DFT with the total spin and degenerate states. *International Journal of Quantum Chemistry*, 107(14):2595–2603, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karlsson:2001:BR

[Kar01] Erik B. Karlsson. Book review. *International Journal of Quantum Chemistry*, 82(4):207–208, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/78503190/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/78503190/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=78503190&PLACEBO=IE.pdf`.

Karagodova:2004:IOS

[Kar04] Tamara Ya. Karagodova. The influence of orientation and strength of external magnetic field on the time dependences of populations of atomic levels for Lamda systems. *International Journal of Quantum Chemistry*, 99(4):475–483, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karwowski:2008:SMI

[Kar08] Jacek Karwowski. A separable model of N interacting Particles. *International Journal of Quantum Chemistry*, 108(12): 2253–2260, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karwowski:2009:IPQ

[Kar09] Jacek Karwowski. Inverse problems in quantum chemistry. *International Journal of Quantum Chemistry*, 109(11):2456–

2463, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Kar10].

Karwowski:2010:EIP

[Kar10] Jacek Karwowski. Erratum: Inverse problems in quantum chemistry. *International Journal of Quantum Chemistry*, 110 (10):2004, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Kar09].

Katriel:2000:MPD

[Kat00] Jacob Katriel. Many-particle Dirac identities for arbitrary elementary spins. *International Journal of Quantum Chemistry*, 78(6):407–411, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72502335/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72502335/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72502335&PLACEBO=IE.pdf`.

Kleinman:2000:FPC

[KB00] Leonard Kleinman and D. M. Bylander. Full potential calculations of the spiral spin density wave ground state of γ-Fe. *International Journal of Quantum Chemistry*, 77(6):940–950, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000976/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000976/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000976&PLACEBO=IE.pdf`.

Kwapien:2008:IFC

[KB08] Karolina Kwapien and Ewa Broclawik. Interaction of FeO^+ cation with benzene, aniline, and 3-methylaniline: DFT study of oxygen insertion mechanism. *International Journal of Quantum Chemistry*, 108(11):2016–2022, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kysel:2008:MDD

[KBMM08] Ondrej Kysel, Šimon Budzák, Miroslav Medveď, and Pavel Mach. MP2, DFT-D, and PCM study of the HMB–TCNE complex: Thermodynamics, electric properties, and solvent effects. *International Journal of Quantum Chemistry*, 108(9):

1533–1545, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kozmutza:2007:SEM

[KBUV07] C. Kozmutza, F. Bartha, L. Udvardi, and I. Varga. Study of the effect of metal ions on hydroxyl–containing molecules. *International Journal of Quantum Chemistry*, 107(14):2730–2740, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kenney:2005:TMC

[KBV05] John W. Kenney III, Jerry A. Boatz, and Heidi A. Terrill Vosbein. Theory of Monte Carlo simulations of the magnetic circular dichroism spectra of alkali metal/rare gas systems. *International Journal of Quantum Chemistry*, 103(6):854–865, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karadakov:2009:CBP

[KC09] Peter B. Karadakov and David L. Cooper. Comparison between the performances of the spin-projected Hartree–Fock, generalized valence-bond, and spin-coupled approaches. *International Journal of Quantum Chemistry*, 109(11):2447–2455, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kirtman:2002:CPH

[KCGB02] Bernard Kirtman, Benoît Champagne, Feng Long Gu, and David M. Bishop. Coupled-perturbed Hartree–Fock treatment of infinite periodic systems: Application to static polarizabilities and hyperpolarizabilities of polydiacetylene, polybutatriene, and interacting pairs of polyacetylene chains. *International Journal of Quantum Chemistry*, 90(2):709–718, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kieninger:2007:CLB

[KCOV07] Martina Kieninger, Raúl E. Cachau, Heinz Oberhammer, and Oscar N. Ventura. Comparison of large basis set DFT and MP2 calculations in the study of the barrier for internal rotation of 2,3,5,6-tetrafluoroanisole. *International Journal of Quantum Chemistry*, 107(2):403–417, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Klos:2002:ICM

[KCS02] Jacek Kłos, Grzegorz Chałasiński, and M. M. Szcześniak. Ab initio calculations and modeling of three-dimensional adiabatic and diabatic potential energy surfaces of $F(^2P)\cdots H_2$ $(^1\Sigma^+)$ van der Waals complex. *International Journal of Quantum Chemistry*, 90(3):1038–1048, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karadakov:2009:MVB

[KCU09] Peter B. Karadakov, David L. Cooper, and Andreas Uhe. Modern valence bond description of the electronic mechanism of a [1,3] sigmatropic rearrangement linking bicyclo[3.2.0]hept-2-ene and bicyclo[2.2.1]hept-2-ene (norbornene). *International Journal of Quantum Chemistry*, 109 (9):1807–1811, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaplan:2005:CSE

[KD05] I. G. Kaplan and C. C. Díaz. Comparative study of the electron affinities of beryllium and magnesium dimers and trimers. *International Journal of Quantum Chemistry*, 104 (4):468–474, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kharat:2009:TMM

[KDC09] Bhagwat Kharat, S. B. Deshmukh, and Ajay Chaudhari. 4d transition metal monoxides, monocarbides, monoborides, mononitrides, and monofluorides: A quantum chemical study. *International Journal of Quantum Chemistry*, 109(5):1103–1115, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kwasniewski:2000:OPT

[KDF00] S. P. Kwasniewski, M. S. Deleuze, and J. P. François. Optical properties of *trans*-stilbene using semiempirical and time-dependent density functional theory: A comparative study. *International Journal of Quantum Chemistry*, 80(4–5):672–680, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505367/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505367/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505367&PLACEBO=IE.pdf`.

Kaczmarek:2007:ETL

[KDŁL07] Anna Kaczmarek, T. C. Dinadayalane, Jerzy Łukaszewicz, and Jerzy Leszczynski. Effect of tube length on the chemisorptions of one and two hydrogen atoms on the sidewalls of (3,3) and (4,4) single-walled carbon nanotubes: A theoretical study. *International Journal of Quantum Chemistry*, 107(12):2211–2219, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koppel:2000:FWD

[KDM00] H. Köppel, M. Döscher, and S. Mahapatra. Femtosecond wavepacket dynamics on strongly coupled potential energy surfaces. *International Journal of Quantum Chemistry*, 80(4–5):942–949, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505405/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505405/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505405&PLACEBO=IE.pdf`.

Kuleff:2002:FSM

[KDY+02] A. I. Kuleff, Y. I. Delchev, P. Tz. Yotov, Tz. Mineva, and J. Maruani. Formulation of Strutinsky's method for atomic systems in the extended Kohn–Sham scheme. *International Journal of Quantum Chemistry*, 89(4):217–226, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kelley:2005:RRH

[Kel05] Anne Myers Kelley. Resonance Raman and hyper-Raman spectroscopy of organic chromophores for second-order nonlinear optics. *International Journal of Quantum Chemistry*, 104 (5):602–615, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kumar:2003:SDD

[KES03] Anil Kumar, Marcus Elstner, and Sándor Suhai. SCC-DFTB-D study of intercalating carcinogens: Benzo(a)pyrene and its metabolites complexed with the G–C base pair. *International Journal of Quantum Chemistry*, 95(1):44–59, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karwowski:2002:RBP

[KF02] Jacek Karwowski and Norbert Flocke. Relations between Pariser–Parr–Pople and Heisenberg models. *International Journal of Quantum Chemistry*, 90(3):1091–1098, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kiralj:2003:CCC

[KF03a] Rudolf Kiralj and Márcia M. C. Ferreira. Combined computational and chemometric study of 1 H-indole-3-acetic acid. *International Journal of Quantum Chemistry*, 95(3):237–251, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ko:2003:DCS

[KF03b] Gwon Hee Ko and William H. Fink. Determination of the crystalline structure of nonlinear molecules in a combined quantum chemical and classic lattice potential description. *International Journal of Quantum Chemistry*, 95(6):830–836, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kairys:2007:SBS

[KF07] Visvaldas Kairys and Miguel X. Fernandes. SitCon: Binding site residue conservation visualization and protein sequence-to-function tool. *International Journal of Quantum Chemistry*, 107(11):2100–2110, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Korek:2009:TCE

[KF09] M. Korek and O. Fawwaz. Theoretical calculation of the electronic states with spin-orbit effects of the molecule NaRb. *International Journal of Quantum Chemistry*, 109(5):938–947, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kwasniewski:2001:TEU

[KFD01] S. P. Kwasniewski, J. P. François, and M. S. Deleuze. Temperature effects on the UV–Vis electronic spectrum of *trans*-stilbene. *International Journal of Quantum Chemistry*, 85 (4–5):557–568, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kunikeev:2009:NSA

[KFD09] Sharif Kunikeev, David L. Freeman, and J. D. Doll. A numerical study of the asymptotic convergence characteristics of partial averaged and reweighted Fourier path integral methods. *International Journal of Quantum Chemistry*, 109(13):2916–2925, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kang:2002:CSF

[KFQ+02] Congmin Kang, Dacheng Feng, Chuansong Qi, Weian Zhao, and Zhengting Cai. Comparative study of folate cofactor models. *International Journal of Quantum Chemistry*, 87(3):152–157, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89010611/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89010611/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89010611&PLACEBO=IE.pdf`.

Kolczewski:2000:ICM

[KFS00] Ch. Kolczewski, K. Fink, and V. Staemmler. Ab initio calculation of the magnetic exchange coupling in linear oxo-bridged heterobinuclear complexes of titanium (III), vanadium (III), and chromium (III). *International Journal of Quantum Chemistry*, 76(2):137–147, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503167/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503167/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503167&PLACEBO=IE.pdf`.

Kurunczi:2007:AMP

[KFTBS07] Ludovic Kurunczi, Simona Funar-Timofei, Alina Bora, and Edward Seclaman. Application of the MTD-PLS method to heterocyclic dye–cellulose interactions. *International Journal of Quantum Chemistry*, 107(11):2057–2065, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kotsos:2002:VPN

[KG02] B. A. Kotsos and M. E. Grypeos. Variation of the $\hbar\omega$ with the particle number and the appearance of

"kinks" for atomic clusters. *International Journal of Quantum Chemistry*, 86(5):426–432, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86511022/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86511022/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86511022&PLACEBO=IE.pdf`.

Kuganathan:2008:MTC

[KG08] Navaratnarajah Kuganathan and Jennifer C. Green. Mercury telluride crystals encapsulated within single walled carbon nanotubes: A density functional study. *International Journal of Quantum Chemistry*, 108(4):797–807, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kuganathan:2009:LIC

[KG09] Navaratnarajah Kuganathan and Jennifer C. Green. 1D lead iodide crystals encapsulated within single walled carbon nanotubes. *International Journal of Quantum Chemistry*, 109 (2):171–175, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Korchowiec:2005:EMR

[KGA05] Jacek Korchowiec, Feng Long Gu, and Yuriko Aoki. Elongation method at restricted open-shell Hartree–Fock level of theory. *International Journal of Quantum Chemistry*, 105 (6):875–882, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Korchowiec:2005:EMC

[KGI+05] Jacek Korchowiec, Feng Long Gu, Akira Imamura, Bernard Kirtman, and Yuriko Aoki. Elongation method with cutoff technique for linear SCF scaling. *International Journal of Quantum Chemistry*, 102(5):785–794, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khait:2001:PUG

[KH01] Yuriy G. Khait and Mark R. Hoffmann. Possible use of genealogical spin-adapted functions in the table-CI method. *International Journal of Quantum Chemistry*, 81(2):130–134, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76500929/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76500929/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76500929&PLACEBO=IE.pdf`.

Khait:2005:TCM

[KH05] Yuriy G. Khait and Mark R. Hoffmann. Table-CI with macroconfiguration approach for describing electronic states of molecules in intense radiation fields. *International Journal of Quantum Chemistry*, 105(6):921–928, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kar:2006:BSH

[KH06] Sabyasachi Kar and Y. K. Ho. Bound states of helium atom in dense plasmas. *International Journal of Quantum Chemistry*, 106(4):814–822, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kar:2007:BDS

[KH07] Sabyasachi Kar and Y. K. Ho. Bound D-states of helium atom under Debye screening. *International Journal of Quantum Chemistry*, 107(2):353–358, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kar:2008:UPS

[KH08a] Sabyasachi Kar and Y. K. Ho. Unnatural parity states of helium with screened Coulomb potentials. *International Journal of Quantum Chemistry*, 108(9):1491–1504, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Korek:2008:TES

[KH08b] M. Korek and A. Hamdan. Theoretical electronic structure of the molecule ScBr. *International Journal of Quantum Chemistry*, 108(3):456–461, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khetselius:2009:RPT

[Khe09] O. Yu Khetselius. Relativistic perturbation theory calculation of the hyperfine structure parameters for some heavy-element isotopes. *International Journal of Quantum Chemistry*, 109

(14):3330–3335, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kobryn:2009:TDS

[KIK09] Alexander E. Kobryn, Kengo Ichiki, and Andriy Kovalenko. Thermodynamic dependences of slip length for nanofluidic flows over crystalline surfaces: Predictions of molecular theory of solvation. *International Journal of Quantum Chemistry*, 109(8):1666–1671, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kikuchi:2009:OBE

[KIN09] Yasuaki Kikuchi, Yutaka Imamura, and Hiromi Nakai. One-body energy decomposition schemes revisited: Assessment of Mulliken-, Grid-, and conventional energy density analyses. *International Journal of Quantum Chemistry*, 109(11):2464–2473, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kirkpatrick:2008:AMC

[Kir08] James Kirkpatrick. An approximate method for calculating transfer integrals based on the ZINDO Hamiltonian. *International Journal of Quantum Chemistry*, 108(1):51–56, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kiselyov:2004:SAW

[Kis04] A. A. Kiselyov. Semiclassic approach within the He atom sphere model. *International Journal of Quantum Chemistry*, 96(5):507–511, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khait:2009:TOG

[KJH09] Yuriy G. Khait, Wanyi Jiang, and Mark R. Hoffmann. Third-order generalized Van Vleck perturbation theory variant of multireference perturbation theory for electron correlation. *International Journal of Quantum Chemistry*, 109(9):1855–1873, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kimani:2008:CSW

[KJW08] Peter Kimani, Preston Jones, and Peter Winkler. Correlation studies in weakly confining quantum dot potentials. *Inter-*

national Journal of Quantum Chemistry, 108(15):2763–2769, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kabanov:2002:PHB

[KK02a] Artem V. Kabanov and Vladislav M. Komarov. Polymorphism of hydrogen bonding in the short double helixes of oligonucleotides: Semiempirical quantum chemical study. *International Journal of Quantum Chemistry*, 88(5):579–587, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khrustov:2002:MGF

[KK02b] V. F. Khrustov and D. E. Kostychev. Multiconfigurational Green's function approach with quasidegenerate perturbation theory. *International Journal of Quantum Chemistry*, 88(4): 507–518, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karagodova:2004:NRM

[KK04] T. Ya. Karagodova and A. V. Kuptsova. Nonlinear resonant magneto-optical effects in alkaline metal vapors in the strong bichromatic laser radiation field. *International Journal of Quantum Chemistry*, 99(4):467–474, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karabulut:2005:DGD

[KK05] Hasan Karabulut and Mestan Kalay. Distributed Gaussian discrete variable representation. *International Journal of Quantum Chemistry*, 104(1):16–28, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Keshtova:2007:IIE

[KK07] Svetlana V. Keshtova and Fatima M. Keshtova. Investigation of influence of electrical induction on electrostatic interaction of atoms and molecules in solution. 1. Dependence of atomic charges in molecule from environment based on the model of FQ theory. *International Journal of Quantum Chemistry*, 107 (5):1126–1141, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaur:2008:IIH

[KK08] Damanjit Kaur and Ruchi Kohli. Intra and intermolecular hydrogen bonding in formohydroxamic acid. *International Journal of Quantum Chemistry*, 108(1):119–134, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaur:2009:SEH

[KKK09] Damanjit Kaur, Rupinder Preet Kaur, and Ruchi Kohli. Substituent effect on N H bond dissociation enthalpies of amines and amides: A theoretical study. *International Journal of Quantum Chemistry*, 109(3):559–568, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kawakami:2001:PMM

[KKM+01] Takashi Kawakami, Yasutaka Kitagawa, Fumitake Matsuoka, Yoshifumi Yamashita, Hiroshi Isobe, Hidemi Nagao, and Kizashi Yamaguchi. Possibilities of molecular magnetic metals and high T_c superconductors in field effect transistor configurations. *International Journal of Quantum Chemistry*, 85(4–5):619–635, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kolandaivel:2004:SSC

[KKMS04] P. Kolandaivel, Michaela Knapp-Mohammady, and Sandor Suhai. Studies on structure and conformational stability of free canonical 2′-deoxyribonucleosides: Approximate SCC-DFTB and LMP2 methods. *International Journal of Quantum Chemistry*, 99(1):28–38, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2003:ISI

[KKS+03] Seong-Gon Kim, Sungho Kim, Jun Shen, B. Z. Nosho, S. C. Erwin, and L. J. Whitman. Interface structures of III–V semiconductor heterostructures. *International Journal of Quantum Chemistry*, 95(4–5):561–571, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kochikov:2009:NAC

[KKS09] I. V. Kochikov, G. M. Kuramshina, and A. V. Stepanova. New approach for the correction of Ab initio molecular force fields in cartesian coordinates. *International Journal of Quantum*

Chemistry, 109(1):28–33, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Korek:2009:TES

[KKTMA09] M. Korek, S. Kontar, F. Taher-Mansour, and A. R. Allouche. Theoretical electronic structure of the molecule ScI. *International Journal of Quantum Chemistry*, 109(2):236–242, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kabanov:2004:LFI

[KKYT04] Artem V. Kabanov, Vladislav M. Komarov, Ludmila V. Yakushevich, and Alexander V. Teplukhin. Low-frequency intra- and intermolecular vibration modes of H-bonded nucleobases in oligonucleotide double helixes and hydrated nucleotide duplex: Application of the PM3 method. *International Journal of Quantum Chemistry*, 100(4):595–609, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Klimkans:2000:VME

[KL00] Agris Klimkāns and Sven Larsson. Vibrational model for electron transfer in the limit of small activation barriers. *International Journal of Quantum Chemistry*, 77(1):211–220, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004262/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004262/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004262&PLACEBO=IE.pdf`.

Ketrat:2003:TSA

[KL03] Sombat Ketrat and Jumras Limtrakul. Theoretical study of the adsorption of ethylene on alkali-exchanged zeolites. *International Journal of Quantum Chemistry*, 94(6):333–340, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khohlova:2005:ESL

[KLB+05] S. S. Khohlova, N. G. Lebedev, S. L. Bondarev, V. N. Knyukshto, A. A. Turban, V. A. Mikhailova, and A. I. Ivanov. Electronic structure of laser dye DCM and its derivatives. *International Journal of Quantum Chemistry*, 104(2):189–196, ????

2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Klein:2003:QDR

[Kle03] D. J. Klein. Quasilocal defects in regular planar networks: Categorization for molecular cones. *International Journal of Quantum Chemistry*, 95(4–5):600–616, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2007:DFI

[KLI07] Joonghan Kim, Yoon Sup Lee, and Hyotcherl Ihee. Density functional and ab initio studies on structures and energies of the ground state of CrCO. *International Journal of Quantum Chemistry*, 107(2):458–463, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khamatgalimov:2008:UPH

[KLK08] Ayrat R. Khamatgalimov, Andrey V. Luzhetskii, and Valeri I. Kovalenko. Unusual pentagon and hexagon geometry of three isomers (no 1, 20, and 23) of fullerene C_{84}. *International Journal of Quantum Chemistry*, 108(8):1334–1339, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Keffer:2000:EPA

[KM00a] D. J. Keffer and J. W. Mintmire. Efficient parallel algorithms for molecular dynamics simulations using variable charge transfer electrostatic potentials. *International Journal of Quantum Chemistry*, 80(4–5):733–742, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505420/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505420/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505420&PLACEBO=IE.pdf`.

King:2000:MSI

[KM00b] James W. King and Stephen P. Molnar. Molecular structural index control in property-directed clustering and correlation. *International Journal of Quantum Chemistry*, 80(6):1164–1171, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/75502058/START; http:`

//www3.interscience.wiley.com/cgi-bin/fulltext/75502058/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502058&PLACEBO=IE.pdf.

Kushwaha:2000:RHB

[KM00c] P. S. Kushwaha and P. C. Mishra. Relationship of hydrogen bonding energy with electrostatic and polarization energies and molecular electrostatic potentials for amino acids: An evaluation of the lock and key model. *International Journal of Quantum Chemistry*, 76(6):700–713, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70001597/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70001597/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70001597&PLACEBO=IE.pdf.

Klein:2001:MMR

[KM01] D. J. Klein and N. H. March. Molecular magnetism via resonating valence bonds for conjugated radicals and selected transition metal complexes. *International Journal of Quantum Chemistry*, 85(4–5):327–344, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karamanis:2002:EQH

[KM02] Panaghiotis Karamanis and George Maroulis. Electric quadrupole and hexadecapole moments for X_2 C CX_2, X = H, F, Cl, Br, and I. *International Journal of Quantum Chemistry*, 90(2):483–490, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

King:2003:ECA

[KM03a] James W. King and Stephen P. Molnar. Electronic and charge aspects of potential endocrine disruptors: Applications to pharmacological clustering. *International Journal of Quantum Chemistry*, 95(4–5):365–371, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

King:2003:MSP

[KM03b] James W. King and Stephen P. Molnar. Molecular similarity of potential endocrine disruptors: Structural index control of pharmacological clustering. *International Journal of*

Quantum Chemistry, 92(1):85–91, March 5, 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

King:2004:SRS

[KM04] James W. King and Stephen P. Molnar. A study of ring-substituent influence on pharmacological activity in a series of phenethylamine-type psychedelics. *International Journal of Quantum Chemistry*, 100(6):1114–1121, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

King:2005:SCB

[KM05a] James W. King and Stephen P. Molnar. Structural connotations of bioactivity in a series of organophosphinates. *International Journal of Quantum Chemistry*, 105(6):809–816, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kushwaha:2005:BSO

[KM05b] P. S. Kushwaha and P. C. Mishra. Binding of singlet oxygen with a stacked guanine dimer. *International Journal of Quantum Chemistry*, 102(4):435–442, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kushwaha:2006:BDU

[KM06] P. S. Kushwaha and P. C. Mishra. Binding of $^3O_2$ and $^1O_2$ to dyes used in photodynamic therapy in gas phase and aqueous media. *International Journal of Quantum Chemistry*, 106(7): 1683–1696, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kawamura:2005:EID

[KMK+05] Minaru Kawamura, Takuji Morimoto, Takashi Kumaya, Ryuichi Sawae, Kenichi Takarabe, and Yoshinori Manmoto. Experimental investigation of decoherence in maximally entangled mixed states. *International Journal of Quantum Chemistry*, 105(6):750–757, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kawamura:2006:DGH

[KMM+06] Minaru Kawamura, Takuji Morimoto, Yoshiyuki Mori, Ryuichi Sawae, Kenichi Takarabe, and Yoshinori Manmoto. Decoherence of a Greenberger–Horne–Zeilinger state in a five-qubit NMR quantum computer. *International Journal of*

Quantum Chemistry, 106(15):3108–3112, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kawamura:2007:EEC

[KMM+07] Minaru Kawamura, Takuji Morimoto, Yoshiyuki Mori, Ryuichi Sawae, Kenichi Takarabe, Yoshinori Manmoto, and Toshio Sakata. Effective error correction method for quantum information processing. *International Journal of Quantum Chemistry*, 107(15):3067–3070, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kedzuch:2005:AFM

[KMN05] Stanislav Kedžuch, Matúš Milko, and Jozef Noga. Alternative formulation of the matrix elements in MP2-R12 theory. *International Journal of Quantum Chemistry*, 105(6):929–936, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kolandaivel:2002:PCH

[KMS02] P. Kolandaivel, T. Mahalingam, and K. Sugandhi. Polarizability and chemical hardness — A combined study of wave function and density functional theory approach. *International Journal of Quantum Chemistry*, 86(4):368–375, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86011217/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86011217/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86011217&PLACEBO=IE.pdf`.

Kalogiratou:2006:CEO

[KMS06] Z. Kalogiratou, Th. Monovasilis, and T. E. Simos. Computation of the eigenvalues of the one-dimensional Schrödinger equation by symplectic methods. *International Journal of Quantum Chemistry*, 106(4):795–802, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kumar:2005:DFS

[KMVR05] Anil Kumar, P. C. Mishra, C. S. Verma, and V. Renugopalakrishnan. Density functional study of the heme moiety of cytochrome c. *International Journal of Quantum Chemistry*, 102 (5):1002–1009, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kong:2008:SEE

[KN08] Liguo Kong and Marcel Nooijen. Study of energetics of end-on and side-on peroxide coordination in ligated Cu_2O_2 models with state-specific equation of Motion Coupled Cluster Method. *International Journal of Quantum Chemistry*, 108 (12):2097–2107, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Katouda:2009:EPA

[KN09a] Michio Katouda and Shigeru Nagase. Efficient parallel algorithm of second-order Møller–Plesset perturbation theory with resolution-of-identity approximation (RI-MP2). *International Journal of Quantum Chemistry*, 109(10):2121–2130, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kobayashi:2009:DLH

[KN09b] Masato Kobayashi and Hiromi Nakai. Dual-level hierarchical scheme for linear-scaling divide-and-conquer correlation theory. *International Journal of Quantum Chemistry*, 109(10): 2227–2237, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kato:2004:PSI

[KNN+04] Nobuhiko Kato, Hidemi Nagao, Kiyoshi Nishikawa, Kazume Nishidate, and Kazunaka Endo. Possibility of superconductivity in intercalation compound related to MgB_2. *International Journal of Quantum Chemistry*, 96(5):457–462, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kowada:2009:TCE

[KNO09a] Y. Kowada, W. Nishitani, and K. Ogasawara. Total cluster energy calculation of lithium ion conductors by the DV-X_α method. *International Journal of Quantum Chemistry*, 109 (12):2658–2663, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kowada:2009:FSP

[KNO09b] Y. Kowada, S. Noma, and K. Ogasawara. Fluorescence spectra of Pr^{3+} ions in phosphate materials calculated by the

DVME method. *International Journal of Quantum Chemistry*, 109(12):2753–2757, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kallrot:2005:TSS

[KNRR05] Niklas Källrot, Kristina Nilsson, Torben Rasmussen, and Ulf Ryde. Theoretical study of structure of catalytic copper site in nitrite reductase. *International Journal of Quantum Chemistry*, 102(5):520–541, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kitagawa:2009:BDB

[KNS+09] Yasutaka Kitagawa, Yasuyuki Nakanishi, Toru Saito, Takashi Kawakami, Mitsutaka Okumura, and Kizashi Yamaguchi. BS DFT and BS HDFT studies of Cr Cr sextuple bond from the viewpoint of electron correlation effects. *International Journal of Quantum Chemistry*, 109(14):3315–3324, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Komorowski:2003:DAF

[KO03] Ludwik Komorowski and Piotr Ordon. DFT analysis of fluctuations in electronegativity and hardness of a molecular oscillator. *International Journal of Quantum Chemistry*, 91(3):398–403, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Komorowski:2004:AMO

[KO04] Ludwik Komorowski and Piotr Ordon. Anharmonicity of a molecular oscillator. *International Journal of Quantum Chemistry*, 99(3):153–160, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koch:2000:RIA

[Koc00] Wolfhard Koch. On Rüdenberg's integral approximations and their unrestricted and combined use in molecular orbital theories of Hartree–Fock type. *International Journal of Quantum Chemistry*, 76(2):148–160, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503168/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503168/`

FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503168&PLACEBO=IE.pdf.

Kohout:2001:ONA

[Koh01] M. Kohout. Occupation numbers for atomic shells in direct space bounded by the maxima of the one-electron potential. *International Journal of Quantum Chemistry*, 83(6):324–331, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/81501978/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/81501978/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=81501978&PLACEBO=IE.pdf.

Kohout:2002:RBO

[Koh02] M. Kohout. On the relationship between the one-electron and Bohm's quantum potential. *International Journal of Quantum Chemistry*, 87(1):12–14, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/88011403/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88011403/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88011403&PLACEBO=IE.pdf.

Kawamoto:2003:ASM

[KOH03] Syuhei Kawamoto, Tatsuki Oda, and Ikutaro Hamada. Association simulation by a metallic Car–Parrinello dynamics. *International Journal of Quantum Chemistry*, 91(2):165–170, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kohout:2004:MEL

[Koh04] M. Kohout. A measure of electron localizability. *International Journal of Quantum Chemistry*, 97(1):651–658, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kondepudi:2004:SGP

[Kon04] Dilip K. Kondepudi. Spontaneous generation and propagation of chiral asymmetry. *International Journal of Quantum Chemistry*, 98(2):222–227, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kong:2009:CBF

[Kon09] Liguo Kong. Connection between a few Jeziorski-Monkhorst ansatz-based methods. *International Journal of Quantum Chemistry*, 109(3):441–447, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karpov:2004:ME

[KOPP04] E. Karpov, G. Ordonez, T. Petrosky, and I. Prigogine. Microscopic entropy. *International Journal of Quantum Chemistry*, 98(2):69–77, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Korchowiec:2005:RCT

[Kor05] Jacek Korchowiec. Role of charge-transfer effects in regioselectivity. *International Journal of Quantum Chemistry*, 101 (6):714–721, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kuchitsu:2009:EMI

[KOT09] T. Kuchitsu, J. Okuda, and M. Tachikawa. Evaluation of molecular integral of Cartesian Gaussian type basis function with complex-valued center coordinates and exponent via the McMurchie–Davidson recursion formula, and its application to electron dynamics. *International Journal of Quantum Chemistry*, 109(3):540–548, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koziol:2001:NNM

[Koz01] J. Kozioł. Neural network modeling of physical properties of chemical compounds. *International Journal of Quantum Chemistry*, 84(1):117–126, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84002447/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002447/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002447&PLACEBO=IE.pdf`.

Kozlov:2004:PCA

[Koz04] M. G. Kozlov. Precision calculations of atoms with few valence electrons. *International Journal of Quantum Chemistry*, 100

(4):336–342, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kowalski:2000:CSS

[KP00a] K. Kowalski and P. Piecuch. Complete set of solutions of the generalized Bloch equation. *International Journal of Quantum Chemistry*, 80(4–5):757–781, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505389/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505389/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505389&PLACEBO=IE.pdf`.

Kurth:2000:REC

[KP00b] Stefan Kurth and John P. Perdew. Role of the exchange-correlation energy: Nature's glue. *International Journal of Quantum Chemistry*, 77(5):814–818, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000344/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000344/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000344&PLACEBO=IE.pdf`.

Kalninsh:2002:EEA

[KP02] K. K. Kalninsh and A. F. Podolsky. Electronic excitation in anionic polymerization of butadiene: Nonempirical calculations of reaction complexes. *International Journal of Quantum Chemistry*, 88(5):624–633, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kalninsh:2005:SCT

[KP05] K. K. Kalninsh and A. F. Podolsky. Structure of charge-transfer reaction complexes in anionic polymerization of isoprene: Quantum chemical calculations. *International Journal of Quantum Chemistry*, 104(2):114–125, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karwowski:2009:EDS

[KP09] Jacek Karwowski and Grzegorz Pestka. Energy-dependent scaling of the Dirac equation. *International Journal of Quantum Chemistry*, 109(13):2903–2908, November 5, 2009. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kakkar:2005:TSU

[KPC05] Rita Kakkar, Mallika Pathak, and Preeti Chadha. Theoretical study of unimolecular rearrangements of vinylidenes to acetylenes. *International Journal of Quantum Chemistry*, 102 (2):189–199, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kardahakis:2005:MCI

[KPČM05] Stavros Kardahakis, Jiří Pittner, Petr Čársky, and Aristides Mavridis. Multireference configuration interaction and coupled-cluster calculations on the $X\,^3\Sigma^-$, $a\,^1\Delta$, and $b\,^1\Sigma^+$ states of the NF molecule. *International Journal of Quantum Chemistry*, 104(4):458–467, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kunitsyn:2001:ACV

[KPP01] V. G. Kunitsyn, L. E. Panin, and L. M. Polyakov. Anomalous change of viscosity and conductivity in blood plasma lipoproteins in the physiological temperature range. *International Journal of Quantum Chemistry*, 81(5):348–369, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76507290/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76507290/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76507290&PLACEBO=IE.pdf`.

Karwowski:2006:RDE

[KPSH06] J. Karwowski, G. Pestka, M. Stanke, and F. E. Harris. Representation of the Dirac equation and the variational principle. *International Journal of Quantum Chemistry*, 106(15):3129–3139, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kolezynski:2003:ECP

[KPTŚ03] Andrzej Koleżyński, Wiesław S. Ptak, and Katarzyna Tkacz-Śamiech. Effective crystal potential from electronegativity viewpoint. *International Journal of Quantum Chemistry*, 91 (3):311–316, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2007:MGC

[KR07] E. S. Kryachko and F. Remacle. The magic gold cluster Au_{20}. *International Journal of Quantum Chemistry*, 107(14):2922–2934, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Krauss:2000:ISM

[Kra00] Morris Krauss. Ab initio structures of metalloenzyme active sites: Application to metalloglutathione transferase. *International Journal of Quantum Chemistry*, 76(3):331–340, January 20, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000277/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000277/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000277&PLACEBO=IE.pdf`.

Kamel:2008:CSO

[KRR08] Karol Kamel and Danuta Rusinska-Roszak. A computational study of open-chain epothilone analogue. *International Journal of Quantum Chemistry*, 108(5):967–973, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kruger:2006:PUS

[Krü06] Thomas Krüger. Periodane—an unexpectedly stable molecule of unique composition. *International Journal of Quantum Chemistry*, 106(8):1865–1869, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2000:EEL

[Kry00] Eugene S. Kryachko. Explicit expression for the leaky aquifer function. *International Journal of Quantum Chemistry*, 78 (5):303–305, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72001890/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72001890/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72001890&PLACEBO=IE.pdf`.

Kryachko:2002:OSP

[Kry02] Eugene S. Kryachko. The origin of spontaneous point mutations in DNA via Löwdin mechanism of proton tunneling in DNA base pairs: Cure with covalent base pairing. *International Journal of Quantum Chemistry*, 90(2):910–923, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2005:OPR

[Kry05] Eugene S. Kryachko. On the original proof by reductio ad absurdum of the Hohenberg–Kohn theorem for many-electron Coulomb systems. *International Journal of Quantum Chemistry*, 103(6):818–823, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [SDW07].

Kryachko:2006:PRA

[Kry06] Eugene S. Kryachko. On the proof by reductio ad absurdum of the Hohenberg–Kohn theorem for ensembles of fractionally occupied states of Coulomb systems. *International Journal of Quantum Chemistry*, 106(8):1795–1798, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2007:DSB

[Kry07a] Eugene S. Kryachko. Dicationic states of benzene dimer: Benzene dimer cation and benzene dication parenthood patterns. *International Journal of Quantum Chemistry*, 107(14):2741–2755, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2007:FAN

[Kry07b] Eugene S. Kryachko. Formula that accounts a number of atoms within a period of the periodic table. *International Journal of Quantum Chemistry*, 107(2):372–373, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2008:BRB

[Kry08a] Eugene S. Kryachko. Book review: *Intermolecular Interactions: Physical Picture, Computational Methods and Model Potentials*. By Ilya G. Kaplan, John Wiley & Sons, Ltd,

Chichester, England, 2006. ISBN-13: 978-0-470-86332-9. *International Journal of Quantum Chemistry*, 108(1):198–201, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Kap06].

Kryachko:2008:FFP

[Kry08b] Eugene S. Kryachko. The force field picture of molecular shape response. *International Journal of Quantum Chemistry*, 108 (11):1930–1938, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2009:FSC

[Kry09] Eugene S. Kryachko. Few sketches on connections between the Riccati and Ermakov–Milne–Pinney equations. *International Journal of Quantum Chemistry*, 109(13):2897–2902, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaplan:2000:CZD

[KS00] I. G. Kaplan and J. Soullard. Calculation of Zn-doped Y ceramics by the electron-correlated embedded-cluster method. *International Journal of Quantum Chemistry*, 80(3):320–326, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501017/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501017/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501017&PLACEBO=IE.pdf`.

Kakkar:2002:TSE

[KS02a] Rita Kakkar and Bhupendra K. Sarma. Theoretical study of the excited singlet and triplet states of alloxan. *International Journal of Quantum Chemistry*, 86(5):502–509, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85515908/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85515908/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85515908&PLACEBO=IE.pdf`.

Korolkov:2002:ESA

[KS02b] Dimitry V. Korolkov and Olga V. Sizova. Electronic structure of adamantane. *International Journal of Quantum Chemistry*,

88(5):606–613, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2003:QCS

[KS03a] Eugene S. Kryachko and John R. Sabin. Quantum chemical study of the hydrogen-bonded patterns in A · T base pair of DNA: Origins of tautomeric mispairs, base flipping, and Watson–Crick → Hoogsteen conversion. *International Journal of Quantum Chemistry*, 91(6):695–710, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kurita:2003:IDS

[KS03b] Noriyuki Kurita and Hideo Sekino. Ab initio and DFT studies for accurate description of van der Waals interaction between rare-gas atoms. *International Journal of Quantum Chemistry*, 91(3):355–362, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karafiloglou:2004:TET

[KS04a] P. Karafiloglou and G. Surpateanu. Three-electron two-center bonding in cycloimmonium ylides. *International Journal of Quantum Chemistry*, 98(5):456–464, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Krasilnikov:2004:FNT

[KS04b] Vladimir V. Krasilnikov and Serge E. Savotchenko. Formation of new types of inhomogeneous spatial structures in the chemical reaction in imperfect systems. *International Journal of Quantum Chemistry*, 100(4):426–434, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kar:2006:CCU

[KS06] Tapas Kar and Steve Scheiner. Cooperativity of conventional and unconventional hydrogen bonds involving imidazole. *International Journal of Quantum Chemistry*, 106(4):843–851, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kumar:2007:BSO

[KS07] Santosh Kumar and Patrick K. Schelling. Basis-set optimization for first-principles simulation of liquid water. *International Journal of Quantum Chemistry*, 107(3):556–566, ????

2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kadantsev:2008:ACB

[KS08] Eugene S. Kadantsev and Hartmut L. Schmider. Analysis of chemical bonding in electronic excited states using parity function. *International Journal of Quantum Chemistry*, 108(1):1–14, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kreye:2009:CBQ

[KS09] W. C. Kreye and Paul G. Seybold. Correlations between quantum chemical indices and the pK_a s of a diverse set of organic phenols. *International Journal of Quantum Chemistry*, 109 (15):3679–3684, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaur:2008:UST

[KSBK08] Damanjit Kaur, Punita Sharma, Prasad V. Bharatam, and Mondeep Kaur. Understanding selenocysteine through conformational analysis, proton affinities, acidities and bond dissociation energies. *International Journal of Quantum Chemistry*, 108(5):983–991, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2003:OES

[KSG03] Yong-Hoon Kim, Martin Städele, and Andreas Görling. Optical excitations of Si by time-dependent density functional theory based on exact-exchange Kohn–Sham band structure. *International Journal of Quantum Chemistry*, 91(2):257–262, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khait:2004:MME

[KSH04] Yuriy G. Khait, Jie Song, and Mark R. Hoffmann. Macroconfigurations in molecular electronic structure theory. *International Journal of Quantum Chemistry*, 99(4):210–220, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kitagawa:2007:GOM

[KSI+07] Yasutaka Kitagawa, Toru Saito, Masahide Ito, Yasuyuki Nakanishi, Mitsuo Shoji, Kenichi Koizumi, Shusuke Ya-

manaka, Takashi Kawakami, Mitsutaka Okumura, and Kizashi Yamaguchi. Geometry optimization method based on approximate spin projection and its application to F_2, CH_2, $CH_2O{\cdot}O$, and active site of urease. *International Journal of Quantum Chemistry*, 107(15):3094–3102, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Korambath:2000:IMO

[KSK00] Prakashan P. Korambath, "Babu" B. K. Singaraju, and Shashi P. Karna. Ab initio molecular orbital theory study of GaAs clusters: The geometry. *International Journal of Quantum Chemistry*, 77(2):563–573, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70002216/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70002216/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70002216&PLACEBO=IE.pdf`.

Kawamura:2004:FPM

[KSK+04] Minaru Kawamura, Ryuichi Sawae, Takashi Kumaya, Kenichi Takarabe, Yoshinori Manmoto, and Toshio Sakata. Fast preparation method of effective pure states for NMR-quantum computer with controlled-not gates. *International Journal of Quantum Chemistry*, 100(6):1033–1037, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koizumi:2004:ESM

[KSN+04] K. Koizumi, M. Shoji, Y. Nishiyama, Y. Maruno, Y. Kitagawa, K. Soda, S. Yamanaka, M. Okumura, and K. Yamaguchi. The electronic structure and magnetic property of metal-oxo, porphyrin manganese-oxo, and μ-oxo-bridged manganese porphyrin dimer. *International Journal of Quantum Chemistry*, 100(6):943–956, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Krasilnikov:2005:CNS

[KSN05] Vladimir V. Krasilnikov, Serge E. Savotchenko, and Alexander N. Nemtsev. Conditions and numerical simulation of dissipative structure formation in imperfect double-component reaction-diffusion systems. *International Journal of Quantum Chemistry*, 104(2):148–156, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kitagawa:2009:ASP

[KSN+09] Yasutaka Kitagawa, Toru Saito, Yasuyuki Nakanishi, Yusuke Kataoka, Mitsuo Shoji, Kenichi Koizumi, Takashi Kawakami, Mitsutaka Okumura, and Kizashi Yamaguchi. Approximately spin-projected Hessian for broken symmetry method and stretching frequencies of F_2 and singlet O_2. *International Journal of Quantum Chemistry*, 109(15):3641–3648, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kolandaivel:2000:SCB

[KSS00] P. Kolandaivel, N. Suba, and K. Senthilkumar. Study of chemical bonding in H_2 and HF molecules: Wave function and density functional theory (DFT) parameters approach. *International Journal of Quantum Chemistry*, 76(5):662–669, February 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000588/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000588/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000588&PLACEBO=IE.pdf`.

Kitagawa:2001:IHD

[KSS+01] Y. Kitagawa, T. Soda, Y. Shigeta, S. Yamanaka, Y. Yoshioka, and K. Yamaguchi. Improvement of the hybrid density functional method from the viewpoint of effective exchange integrals. *International Journal of Quantum Chemistry*, 84 (5):592–600, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/82003605/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/82003605/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=82003605&PLACEBO=IE.pdf`.

Kitagawa:2008:TSE

[KSS+08] Y. Kitagawa, M. Shoji, T. Saito, Y. Nakanishi, K. Koizumi, T. Kawakami, M. Okumura, and K. Yamaguchi. Theoretical studies on effects of hydrogen bonds attaching to cysteine ligands on 4Fe-4S clusters. *International Journal of Quantum Chemistry*, 108(15):2881–2887, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kohn:2004:HKT

[KSU04] Walter Kohn, Andreas Savin, and Carsten A. Ullrich. Hohenberg–Kohn theory including spin magnetism and magnetic fields. *International Journal of Quantum Chemistry*, 100(1):20–21, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kohn:2005:HKT

[KSU05] Walter Kohn, Andreas Savin, and Carsten A. Ullrich. Hohenberg–Kohn theory including spin magnetism and magnetic fields. *International Journal of Quantum Chemistry*, 101(5):20–21, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kruger:2000:PIC

[KSWR00] Sven Krüger, Thomas J. Seemüller, Alexander Wörndle, and Notker Rösch. Properties of isomers of the cluster Ni_8 from density functional studies. *International Journal of Quantum Chemistry*, 80(4–5):567–574, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505382/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505382/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505382&PLACEBO=IE.pdf`.

Kalhous:2004:NVR

[KSZČ04] Miloš Kalhous, L. Skála, J. Zamastil, and J. Čížek. New version of the Rayleigh–Schrödinger perturbation theory: Examples. *International Journal of Quantum Chemistry*, 99(4):325–335, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kozmutza:2005:TIW

[KT05] Cornelia Kozmutza and Ernő Tfirst. Theoretical investigation of weakly interacting molecular systems using the virial theorem. *International Journal of Quantum Chemistry*, 104 (4):578–585, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kawakami:2005:PMB

[KTH+05] Takashi Kawakami, Takeshi Taniguchi, Tomohiro Hamamoto, Yasutaka Kitagawa, Mitsutaka Okumura, and Kizashi Yamaguchi. Possibilities of molecule-based spintoronics of DNA wires, sheets, and related materials. *International Journal of Quantum Chemistry*, 105(6):655–671, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kawakami:2004:TSM

[KTK+04] Takashi Kawakami, Takeshi Taniguchi, Yasutaka Kitagawa, Takuya Matsumoto, Yohsuke Kamada, Toyonari Sugimoto, Mitsutaka Okumura, and Kizashi Yamaguchi. Theoretical studies on magnetic interaction in one-dimensional spin chains of hydrogen atoms (H_n) and copper bromide (Cu_nBr_m). *International Journal of Quantum Chemistry*, 100(6):907–917, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2002:MOR

[KTN02] Eugene S. Kryachko, Oksana Tishchenko, and Minh Tho Nguyen. Mechanism of the oxidation reaction of Cu with N_2O via nonadiabatic electron transfer. *International Journal of Quantum Chemistry*, 89(4):329–340, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khakimov:2003:TBM

[KUS+03] Z. M. Khakimov, F. T. Umarova, N. T. Sulaymonov, A. E. Kiv, and A. A. Levin. Tight-binding molecular dynamics simulation of Si H bond dissociation in silicon clusters. *International Journal of Quantum Chemistry*, 93(5):351–359, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kutzelnigg:2003:EPF

[Kut03] Werner Kutzelnigg. n-Electron problem and its formulation in terms of k-particle density cumulants. *International Journal of Quantum Chemistry*, 95(4–5):404–423, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kutzelnigg:2008:RCP

[Kut08] Werner Kutzelnigg. Relativistic corrections to the partial wave expansion of two-electron atoms. *International Jour-*

nal of Quantum Chemistry, 108(12):2280–2290, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kutzelnigg:2009:HMB

[Kut09] Werner Kutzelnigg. How many-body perturbation theory (MBPT) has changed quantum chemistry. *International Journal of Quantum Chemistry*, 109(15):3858–3884, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2001:PDB

[KV01] Eugene S. Kryachko and Sergey N. Volkov. Preopening of the DNA base pairs. *International Journal of Quantum Chemistry*, 82(4):193–204, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/78503194/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/78503194/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=78503194&PLACEBO=IE.pdf`.

Kryachko:2002:ESD

[KV02] Eugene S. Kryachko and António J. C. Varandas. Existence of strictly diabatic basis sets for the two-state problem. *International Journal of Quantum Chemistry*, 89(4):255–259, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kavitha:2005:LLS

[KV05] K. Kavitha and P. Venuvanalingam. Low-lying stepwise paths for ethylene 1,3-dipolar cycloadditions: A DFT study. *International Journal of Quantum Chemistry*, 104(1):64–78, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kalaiselvan:2007:ROB

[KV07] Anbarasan Kalaiselvan and Ponnambalam Venuvanalingam. Ring opening of boriranes vis-à-vis aziridines: An ab initio and DFT probe on the mechanisms. *International Journal of Quantum Chemistry*, 107(7):1590–1597, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kowalski:2008:NCE

[KV08] Karol Kowalski and Marat Valiev. Noniterative corrections to equation-of-motion coupled-cluster excited state energies based on the reduced method of moments of coupled cluster equations. *International Journal of Quantum Chemistry*, 108 (12):2178–2190, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kiametis:2008:RES

[KVF+08] Alessandra S. Kiametis, Fábio M. Vieira, A. L. A. Fonseca, Geraldo M.e Silva, and Ricardo Gargano. Rovibrational energies and spectroscopic constants of the H system in the electronic states 1S σ, 7 i σ, 5 f π, 5 g π, 6 i π, and 6 i φ. *International Journal of Quantum Chemistry*, 108(13):2398–2402, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kalaiselvan:2005:IDM

[KVPS05] Anbarasan Kalaiselvan, Ponnambalam Venuvanalingam, Jordi Poater, and Miquel Solà. Ab initio and DFT modeling of stereoselective deamination of aziridines by nitrosyl chloride. *International Journal of Quantum Chemistry*, 102 (2):139–146, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kilshtain-Vardi:2002:MAZ

[KVSG02] Alexandra Kilshtain-Vardi, Gil Shoham, and Amiram Goldblum. Mechanism of action of zinc proteinases: A MNDO/d/H study of alternative general-acid general-base catalytic pathways for carboxypeptidase-A. *International Journal of Quantum Chemistry*, 88(1):87–98, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90511925/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90511925/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90511925&PLACEBO=IE.pdf`.

Kolev:2005:DES

[KVSS05] Tsonko M. Kolev, Evelina A. Velcheva, Bistra A. Stamboliyska, and Michael Spiteller. DFT and experimental studies of the structure and vibrational spectra of curcumin. *International Journal of Quantum Chemistry*, 102(6):1069–1079,

???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kobychev:2004:TSD

[KVT04] Vladimir B. Kobychev, Nadezhda M. Vitkovskaya, and Boris A. Trofimov. Theoretical study of the double bond migration mechanism with participation of hydroxide ion. *International Journal of Quantum Chemistry*, 100(4):367–374, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kobychev:2002:TAP

[KVZ+02] Vladimir B. Kobychev, Nadezhda M. Vitkovskaya, Irina L. Zaytseva, Elena Yu. Larionova, and Boris A. Trofimov. Theoretical analysis of pyrrole anions addition to carbon disulfide and carbon dioxide. *International Journal of Quantum Chemistry*, 88(5):542–548, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kobychev:2004:PAA

[KVZT04] Vladimir B. Kobychev, Nadezhda M. Vitkovskaya, Irina L. Zaytseva, and Boris A. Trofimov. Pyrrole anion addition to carbon disulfide: An ab initio study. *International Journal of Quantum Chemistry*, 100(4):360–366, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2003:GSS

[KW03] Eugene S. Kryachko and Stephen Wilson. Generation of systematic sequences of even-tempered basis sets: Empirical generating formulae. *International Journal of Quantum Chemistry*, 93(2):112–120, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kvamme:2009:RBS

[KWC09] Brandon Kvamme, Matthew C. F. Wander, and Aurora E. Clark. The role of basis set superposition error in water addition reactions to Ln(III) cations. *International Journal of Quantum Chemistry*, 109(11):2474–2481, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kohout:2006:ASE

[KWG06] M. Kohout, F. R. Wagner, and Y. Grin. Atomic shells from the electron localizability in momentum space. *International*

Journal of Quantum Chemistry, 106(7):1499–1507, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kondov:2006:CST

[KWT06] Ivan Kondov, Haobin Wang, and Michael Thoss. Computational study of titanium (IV) complexes with organic chromophores. *International Journal of Quantum Chemistry*, 106 (6):1291–1303, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kan:2004:DSB

[KWWQ04] Ying Kan, Guo-Shi Wu, Li-Duo Wang, and Yong Qiu. DFT study of bridge atom dependence of absorption and emitting wavelength of tridentate ligand chelates of aluminum. *International Journal of Quantum Chemistry*, 98(3):325–334, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2000:DBM

[KY00] Eugene S. Kryachko and David R. Yarkony. Diabatic bases and molecular properties. *International Journal of Quantum Chemistry*, 76(2):235–243, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503175/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503175/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503175&PLACEBO=IE.pdf`.

Korek:2005:ETM

[KY05] M. Korek and G. Younes. Electronic transition moment with spin-orbit coupling of the molecular ion KRb^+. *International Journal of Quantum Chemistry*, 101(1):84–89, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Korek:2003:TSL

[KYA03] M. Korek, G. Younes, and A. R. Allouche. Theoretical study of the low-lying electronic states of the molecular ion KRb^+. *International Journal of Quantum Chemistry*, 92(4):376–380, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kitagawa:2004:TSE

[KYT+04] Y. Kitagawa, S. Yamanaka, R. Takeda, M. Shoji, K. Koizumi, Y. Nishiyama, Y. Maruno, T. Kawakami, M. Okumura, and K. Yamaguchi. Theoretical studies on effective exchange integrals using spin correlation function analysis and magnetic effective density functional (MEDF) method. *International Journal of Quantum Chemistry*, 100(6):927–936, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kyvala:2009:CTM

[Kýv09] Mojmír Kývala. Calculation of transition matrix elements by nonsingular orbital transformations. *International Journal of Quantum Chemistry*, 109(6):1200–1227, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2008:IRI

[KZ08] Hae-Won Kim and Daniel Zeroka. Internal-rotation and inversion potential energy surfaces for methylamine and methylphosphine. *International Journal of Quantum Chemistry*, 108(5):974–982, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Krykunov:2009:UEE

[KZ09] Mykhaylo Krykunov and Tom Ziegler. On the use of the exact exchange optimized effective potential method for static response properties. *International Journal of Quantum Chemistry*, 109(14):3246–3258, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Katriel:2001:SDD

[KZB01] Jacob Katriel, Federico Zahariev, and Kieron Burke. Symmetry and degeneracy in density functional theory. *International Journal of Quantum Chemistry*, 85(4–5):432–435, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kakkar:2009:CRS

[KZG09] Rita Kakkar, Sheza Zaidi, and Rajni Grover. The Curtius rearrangement of some organic azides: A DFT mechanistic study. *International Journal of Quantum Chemistry*, 109(5):

1058–1069, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kusmin:2007:SHG

[KZS07] Ilya V. Kusmin, Georgy M. Zhidomirov, and Vitaly N. Solkan. Swift hopping gallium over $[AlO_4]^-$ tetrahedra in Ga/ZSM-5: A DFT study. *International Journal of Quantum Chemistry*, 107(13):2434–2441, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Krykunov:2009:HDF

[KZvL09] Mykhaylo Krykunov, Tom Ziegler, and Erik van Lenthe. Hybrid density functional calculations of nuclear magnetic shieldings using Slater-type orbitals and the zeroth-order regular approximation. *International Journal of Quantum Chemistry*, 109(8):1676–1683, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lampman:2006:GDD

[LA06] Gary M. Lampman and James C. Aumiller. Geometry of 1,3-dihalocyclobutanes by dipole moment analysis. *International Journal of Quantum Chemistry*, 106(1):211–214, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Loos:2007:CIC

[LA07] Pierre-François Loos and Xavier Assfeld. Core-ionized and core-excited states of macromolecules. *International Journal of Quantum Chemistry*, 107(12):2243–2252, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lefebvre:2009:ULI

[LA09] R. Lefebvre and O. Atabek. Unusual low-intensity regime in laser-induced molecular photodissociation. *International Journal of Quantum Chemistry*, 109(14):3423–3429, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ladik:2000:TCO

[Lad00] Janos J. Ladik. Theoretical considerations on oncogene activation by chemical carcinogens and antioncogene in-

activation by ionizing radiations: possibilities of hindrance of the initiation of cancer in the cell. *International Journal of Quantum Chemistry*, 78(6):450–458, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72502340/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72502340/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72502340&PLACEBO=IE.pdf`.

Ladik:2006:NCL

[Lad06] Janos Ladik. The normal and cancerous living cell. *International Journal of Quantum Chemistry*, 106(14):2827–2832, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Louis-Achille:2000:ESM

[LADD00] Vanina Louis-Achille, Laurent De Windt, and Mireille Defranceschi. Electronic structure of minerals: The apatite group as a relevant example. *International Journal of Quantum Chemistry*, 77(6):991–1006, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000981/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000981/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000981&PLACEBO=IE.pdf`.

Lagana:2004:I

[Lag04] Antonio Laganà. Introduction. *International Journal of Quantum Chemistry*, 96(6):519, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lakhno:2008:DN

[Lak08] V. D. Lakhno. DNA nanobioelectronics. *International Journal of Quantum Chemistry*, 108(11):1970–1981, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lee:2009:STT

[LAK09] Han Myoung Lee, David J. Anick, and Kwang S. Kim. Structures of tri-, tetra-, and hexahydrated hydride anion clusters.

International Journal of Quantum Chemistry, 109(9):1820–1826, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2008:EMG

[LAL+08] Qingzhong Li, Xiulin An, Feng Luan, Wenzou Li, Baoan Gong, Jianbo Cheng, and Jiazhong Sun. The effect of methyl group on the cooperativity between three types of hydrogen bond: OH$\cdots$O, CH$\cdots$O, and OH$\cdots\pi$. *International Journal of Quantum Chemistry*, 108(3):558–566, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lammert:2007:DLF

[Lam07] Paul E. Lammert. Differentiability of Lieb functional in electronic density functional theory. *International Journal of Quantum Chemistry*, 107(10):1943–1953, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2009:SAN

[LAQ+09] Yun Li, Hongqi Ai, Zhongnan Qi, Wei He, and Liang Zhang. Stability analysis of the neutral noble gas molecules FNgX and their anions $FNgX^-$ (Ng = He, Ar, Kr; X = O, S). *International Journal of Quantum Chemistry*, 109(4):782–789, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larsson:2001:BR

[Lar01] Sven Larsson. Book review. *International Journal of Quantum Chemistry*, 82(4):205–206, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/78503192/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/78503192/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=78503192&PLACEBO=IE.pdf`.

Larsson:2002:CMS

[Lar02] Sven Larsson. Chemical model for superconductivity. *International Journal of Quantum Chemistry*, 90(4-5):1457–1469, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lexa:2007:SLE

[LAS+07] Katrina W. Lexa, Katherine A. Alser, Amanda M. Salisburg, Damien J. Ellens, Lorena Hernandez, Sam J. Bono, Heather C. Michael, Jennifer R. Derby, Jaime G. Skiba, Steven Feldgus, Karl N. Kirschner, and George C. Shields. The search for low energy conformational families of small peptides: Searching for active conformations of small peptides in the absence of a known receptor. *International Journal of Quantum Chemistry*, 107(15):3001–3012, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Latosinska:2003:NPE

[Lat03a] J. N. Latosińska. NQR parameters: Electric field gradient tensor and asymmetry parameter studied in terms of density functional theory. *International Journal of Quantum Chemistry*, 91(3):284–296, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Latosinska:2003:STC

[Lat03b] J. N. Latosińska. Studies of thiazide compounds in terms of density functional theory. *International Journal of Quantum Chemistry*, 91(3):339–349, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lavarda:2003:RBA

[Lav03a] F. C. Lavarda. Relation between antioxidant activity and electronic structure of phenols. *International Journal of Quantum Chemistry*, 95(3):219–223, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lavor:2003:DAG

[Lav03b] Carlile Lavor. A deterministic approach for global minimization of molecular potential energy functions. *International Journal of Quantum Chemistry*, 95(3):336–343, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lazzeretti:2002:NES

[Laz02] Paolo Lazzeretti. Nuclear electromagnetic shieldings via charge and current density functions. *International Journal of Quantum Chemistry*, 90(1):464–471, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lohr:2002:MLT

[LB02] Lawrence L. Lohr and S. M. Blinder. Models for low-temperature helium dimers and trimers. *International Journal of Quantum Chemistry*, 90(1):419–423, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Laug:2003:GFE

[LB03] P. Laug and H. Borouchaki. Generation of finite element meshes on molecular surfaces. *International Journal of Quantum Chemistry*, 93(2):131–138, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lohr:2006:SHM

[LB06] Lawrence L. Lohr and S. M. Blinder. Semiempirical hyperspherical model for $^4\mathrm{He}_N$ clusters. *International Journal of Quantum Chemistry*, 106(4):981–985, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Losada:2002:FMA

[LBAB02] J. C. Losada, R. M. Benito, F. J. Arranz, and F. Borondo. Frequency map analysis and scars in molecular vibrations. *International Journal of Quantum Chemistry*, 86(2):167–174, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85011804/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85011804/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85011804&PLACEBO=IE.pdf`.

Lasorne:2006:QDS

[LBMVDL06] B. Lasorne, M. C. Bacchus-Montabonel, N. Vaeck, and M. Desouter-Lecomte. Quantum dynamics simulations of photodissociation reactions. *International Journal of Quantum Chemistry*, 106(3):670–675, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ladik:2004:CHH

[LBP04] J. Ladik, F. Bogar, and B. Penke. Comparison of HF, HF + MP2, LDA, BLYP, and B3LYP band structures of the homopolypeptides. *International Journal of Quantum Chemistry*, 98(6):522–527, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lemes:2008:PEF

[LBSB08] N. H. T. Lemes, E. Borges, R. V. Sousa, and J. P. Braga. Potential energy function from differential cross-section data: An inverse quantum scattering theory approach. *International Journal of Quantum Chemistry*, 108(13):2623–2627, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liao:2002:SSS

[LC02] Hsin-Yi Liao and San-Yan Chu. Structural symmetry study of some bis-adduct of an acceptor with two donors. *International Journal of Quantum Chemistry*, 90(2):507–515, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lin:2005:DSS

[LC05] Jyh Shing Lin and Wen-Chi Chou. DFT study of surface reactivity of CX_3I (X = H and F) with CH_2I_2 to form CH_2CX_2 on the Ag(111) surface. *International Journal of Quantum Chemistry*, 102(5):858–865, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ludwig:2003:EPB

[LCBC03] Valdemir Ludwig, Kaline Coutinho, Antonio Carlos Borin, and Sylvio Canuto. Electronic polarization of 1H-benzotriazole in water: Ground and first excited-state dipole moments. *International Journal of Quantum Chemistry*, 95(4–5):572–579, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2008:KDP

[LCCC08] Min-Hsien Liu, Sou-Ro Cheng, Ken-Fa Cheng, and Cheng Chen. Kinetics of decomposition pathways of an energetic GZT molecule. *International Journal of Quantum Chemistry*, 108(3):482–486, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2009:CST

[LCCH09a] Min-Hsien Liu, Ken-Fa Cheng, Cheng Chen, and Yaw-Sun Hong. Computational study of TNT synthesis in solvated nitration reaction systems. *International Journal of Quantum*

Chemistry, 109(5):1009–1023, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2009:GSR

[LCCH09b] Min-Hsien Liu, Ken-Fa Cheng, Cheng Chen, and Yaw-Sun Hong. A guiding simulation research on developing promising energetic materials. *International Journal of Quantum Chemistry*, 109(8):1618–1625, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2005:TSA

[LCH05a] Min-Hsien Liu, Cheng Chen, and Yaw-Shun Hong. Theoretical study of ANTO molecular systems: Causes of insensitivity of the energetic compound NTO. *International Journal of Quantum Chemistry*, 102(3):239–249, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2005:TSU

[LCH05b] Min-Hsien Liu, Cheng Chen, and Yaw-Shun Hong. Theoretical study of the unimolecular decomposition mechanisms of energetic TNAD and TNAZ explosives. *International Journal of Quantum Chemistry*, 102(4):398–408, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luis:2000:CSZ

[LCK00] Josep M. Luis, Benoît Champagne, and Bernard Kirtman. Calculation of static zero-point vibrational averaging corrections and other vibrational curvature contributions to polarizabilities and hyperpolarizabilities using field-induced coordinates. *International Journal of Quantum Chemistry*, 80(3):471–479, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501015/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501015/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501015&PLACEBO=IE.pdf`.

Li:2009:CSN

[LCL+09a] Qingzhong Li, Jianbo Cheng, Wenzuo Li, Baoan Gong, and Jiazhong Sun. Comparative study on the nonadditivity of methyl group in lithium bonding and hydrogen bonding.

International Journal of Quantum Chemistry, 109(5):1127–1134, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2009:TSH

[LCL+09b] Wen-Zuo Li, Jian-Bo Cheng, Qing-Zhong Li, Bao-An Gong, and Jia-Zhong Sun. Theoretical study on HBC^- and HCB^- anions using multiconfiguration second-order perturbation theory. *International Journal of Quantum Chemistry*, 109(5): 1074–1079, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liebman:2001:DBP

[LČM01] Joel F. Liebman, Ivan Černušák, and Andrea Miková. Dicoordinate boron and phosphorus. $HBCN^-$ and $HPCN^-$ case study. *International Journal of Quantum Chemistry*, 84 (1):140–148, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84002450/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002450/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002450&PLACEBO=IE.pdf`.

Lavor:2005:UIB

[LCN05] Carlile C. Lavor, Thiago Messias Cardozo, and Marco Antonio Chaer Nascimento. Using an interval branch-and-bound algorithm in the Hartree–Fock method. *International Journal of Quantum Chemistry*, 103(5):500–504, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Largo:2001:TSC

[LCRB01] Antonio Largo, Alvaro Cimas, Pilar Redondo, and Carmen Barrientos. Theoretical study of C_nCl, C_nCl^+, C_nCl^- ($n = 1--7$) clusters. *International Journal of Quantum Chemistry*, 84(1):127–135, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84002448/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002448/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002448&PLACEBO=IE.pdf`.

Li:2000:TRT

[LCT00] Jiabo Li, Christopher J. Cramer, and Donald G. Truhlar. Two-response-time model based on CM2/INDO/S2 electrostatic potentials for the dielectric polarization component of solvatochromic shifts on vertical excitation energies. *International Journal of Quantum Chemistry*, 77(1):264–280, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004266/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004266/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004266&PLACEBO=IE.pdf`.

Liu:2005:NMB

[LD05] Xue-Shen Liu and Pei-Zhu Ding. Numerical method based on Magnus expansion and a new shooting method for eigenvalues of Schrödinger equation. *International Journal of Quantum Chemistry*, 103(2):149–156, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2006:DST

[LDG+06] Feng-Ling Liu, Ai-Ming Du, Wei-Ling Guo, Yu-Qing Zhai, Shuai Feng, and Su-Jing Wang. DFT study of three $C_{22}H_{14}$ isomers of tripentaprismane. *International Journal of Quantum Chemistry*, 106(7):1508–1515, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lopes:2009:RSQ

[LDM09] Pedro E. M. Lopes, Eugene Demchuk, and Alexander D. Mackerell, Jr. Reconstruction of the (011) surface on α-quartz: A semiclassical Ab initio molecular dynamics study. *International Journal of Quantum Chemistry*, 109(1):50–64, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lacaze-Dufour:2001:DFS

[LDMR01] Corinne Lacaze-Dufour, Tzonka Mineva, and Nino Russo. Density functional study of the structural, electronic, and magnetic properties of neutral and charged rhodium clusters up to tetramer. *International Journal of Quantum Chemistry*, 85(3):162–170, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.`

interscience.wiley.com/cgi-bin/abstract/85510947/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85510947/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85510947&PLACEBO=IE.pdf.

Lau:2005:TSV

[LDP05] Kah Chun Lau, Mrinalini Deshpande, and Ravindra Pandey. A theoretical study of vibrational properties of neutral and cationic B_{12} clusters. *International Journal of Quantum Chemistry*, 102(5):656–664, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lau:2005:TSE

[LDPP05] Kah Chun Lau, Mrinalini Deshpande, Ranjit Pati, and Ravindra Pandey. A theoretical study of electronic and vibrational properties of neutral, cationic, and anionic B_{24} clusters. *International Journal of Quantum Chemistry*, 103(6):866–874, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Langreth:2005:VWD

[LDR+05] D. C. Langreth, M. Dion, H. Rydberg, E. Schröder, P. Hyldgaard, and B. I. Lundqvist. Van der Waals density functional theory with applications. *International Journal of Quantum Chemistry*, 101(5):599–610, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2008:TMA

[LDR+08] Qiang-Gen Li, Chao Deng, Yi Ren, Ning-Bew Wong, San-Yan Chu, and Xin Wang. Tautomerism of monochalcogenosilanoic acids $CH_3Si(O)XH$ (X = S, Se, Te) in the gas phase and in the polar and aprotic solution: An ab initio computational investigation. *International Journal of Quantum Chemistry*, 108(1):142–150, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2004:TSR

[LDXW04] Lai-Cai Li, Ping Deng, Ming-Hou Xu, and Ning-Bew Wong. Theoretical study of reaction mechanism for CH_2CHX (X = H, F, Cl) with ozone. *International Journal of Quantum Chemistry*, 98(3):309–316, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2005:TSR

[LDZ+05] Lai-Cai Li, Ping Deng, Yuan-Qiang Zhu, Dong Zha, An-Min Tian, Ming-Hou Xu, and Ning-Bew Wong. Theoretical study on the reaction mechanism and thermodynamics of tin oxidation by oxygen species and chlorine species. *International Journal of Quantum Chemistry*, 104(3):367–372, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lundin:2001:NMS

[LE01] Urban Lundin and Olle Eriksson. Novel method of self-interaction corrections in density functional calculations. *International Journal of Quantum Chemistry*, 81(4):247–252, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76505741/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76505741/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76505741&PLACEBO=IE.pdf`.

Lefebvre:2000:RTP

[Lef00] R. Lefebvre. Resonant tunneling in the presence of two electric fields: One static and the other oscillating. *International Journal of Quantum Chemistry*, 80(2):110–116, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001277/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001277/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001277&PLACEBO=IE.pdf`.

Lefebvre:2005:TDQ

[Lef05] R. Lefebvre. Transmissivity and degeneracy of quasi-energies. *International Journal of Quantum Chemistry*, 104(4):411–417, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lefebvre:2006:FVN

[Lef06] Roland Lefebvre. Floquet versus non-Floquet solutions for a periodic Hamiltonian. *International Journal of Quantum Chemistry*, 106(14):2848–2853, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lefebvre:2007:STB

[Lef07] Roland Lefebvre. Scattering by a triangular barrier. *International Journal of Quantum Chemistry*, 107(14):2643–2649, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lesk:2003:EPB

[Les03] Arthur M. Lesk. From electrons to proteins and back again. *International Journal of Quantum Chemistry*, 95(6):678–682, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leszczynski:2004:Pa

[Les04a] Jerzy Leszczynski. Preface. *International Journal of Quantum Chemistry*, 96(4):293, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leszczynski:2004:Pb

[Les04b] Jerzy Leszczynski. Preface. *International Journal of Quantum Chemistry*, 100(5):709, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leszczynski:2005:P

[Les05] Jerzy Leszczynski. Preface. *International Journal of Quantum Chemistry*, 105(4):301, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leszczynski:2006:P

[Les06] Jerzy Leszczynski. Preface. *International Journal of Quantum Chemistry*, 106(11):2305, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leszczynski:2007:P

[Les07] Jerzy Leszczynski. Preface. *International Journal of Quantum Chemistry*, 107(12):2185, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leszczynski:2009:P

[Les09] Jerzy Leszczynski. Preface. *International Journal of Quantum Chemistry*, 109(1):1–2, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Latino:2007:NNA

[LFADSF07] Diogo A. R. S. Latino, Filomena F. M. Freitas, João Aires-De-Sousa, and Fernando M. S. Silva Fernandes. Neural networks to approach potential energy surfaces: Application to a molecular dynamics simulation. *International Journal of Quantum Chemistry*, 107(11):2120–2132, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Labello:2006:CRB

[LFK06] Nicholas P. Labello, Antonio M. Ferreira, and Henry A. Kurtz. Correlated, relativistic, and basis set limit molecular polarizability calculations to evaluate an augmented effective core potential basis set. *International Journal of Quantum Chemistry*, 106(15):3140–3148, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lopes:2008:EWF

[LFR+08] Kelson C. Lopes, Wallace D. Fragoso, Mozart N. Ramos, Arquimedes M. Pereira, and Regiane C. M. U. Araújo. Effects of wave function modifications on calculated H C and C C stretching frequencies. *International Journal of Quantum Chemistry*, 108(13):2374–2385, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2007:QCS

[LFZ07] Rui Li, Dacheng Feng, and Feng Zhu. Quantum chemical study of penicillin: Reactions after acylation. *International Journal of Quantum Chemistry*, 107(10):2032–2039, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lordeiro:2003:DMS

[LGBJ03] R. A. Lordeiro, F. F. Guimarães, J. C. Belchior, and R. L. Johnston. Determination of main structural compositions of nanoalloy clusters of Cu_xAu_y ($x + y \leq 30$) using a genetic algorithm approach. *International Journal of Quantum Chemistry*, 95(2):112–125, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lecomte:2005:FEE

[LGJP05] C. Lecomte, B. Guillot, C. Jelsch, and A. Podjarny. Frontier example in experimental charge density research: Experimen-

tal electrostatics of proteins. *International Journal of Quantum Chemistry*, 101(5):624–634, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ludena:2004:EAT

[LGKN04] Eduardo V. Ludeña, Daniel Gómez, Valentin Karasiev, and Pedro Nieto. Exact analytic total energy functional for Hooke's atom generated by local-scaling transformations. *International Journal of Quantum Chemistry*, 99(4):297–307, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Low:2000:BCT

[LH00] Arthur A. Low and Michael B. Hall. Benzene chromium tricarbonyl revisited: Theoretical study of the structure and dynamics of $(\eta^6\text{-}C_6H_6)Cr(CO)_3$. *International Journal of Quantum Chemistry*, 77(1):152–160, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004255/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004255/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004255&PLACEBO=IE.pdf`.

Lin:2003:TSI

[LH03] Ching-Yeh Lin and Jia-Jen Ho. Theoretical studies of isomerization barriers of 2-pentoxy radical and its products. *International Journal of Quantum Chemistry*, 91(3):461–466, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liebman:2005:WAA

[LH05] Joel F. Liebman and Zelek S. Herman. Where are the angles? Angular dependence (and independence) of orbitals and functions. *International Journal of Quantum Chemistry*, 101 (3):283–286, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2007:HBS

[LH07a] Quan Li and Fang-Qian Huang. Hydrogen bonding structure and many-body interactions in 1,3,5-triazine–$(water)_3$ and 1,2,4-triazine–$(water)_3$ complexes. *International Journal*

of Quantum Chemistry, 107(3):567–573, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2007:IIE

[LH07b] Dan Liu and Frank Hagelberg. Impact of internal electron transfer on the structure of C_{74} encapsulating Sc and La metal atom impurities. *International Journal of Quantum Chemistry*, 107(12):2253–2260, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luo:2007:MCC

[LH07c] Yi Luo and Zhaomin Hou. Modeling η^5-$C_5Me_4SiMe_3$ with η^3-C_3H_5 for DFT study of a tetranuclear yttrium polyhydrido complex $[(\eta^5\text{-}C_5Me_4SiMe_3)YH_2]_4$. *International Journal of Quantum Chemistry*, 107(2):374–381, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lee:2000:EPA

[LHG00] Michael S. Lee and Martin Head-Gordon. Extracting polarized atomic orbitals from molecular orbital calculations. *International Journal of Quantum Chemistry*, 76(2):169–184, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503170/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503170/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503170&PLACEBO=IE.pdf`.

Lauenstein:2000:MDS

[LHL+00] Albert Lauenstein, Kersti Hermansson, Jan Lindgren, Michael Probst, and Philippe A. Bopp. Molecular dynamics simulation of an aqueous aluminium(III) chloride solution with three-body interactions. *International Journal of Quantum Chemistry*, 80(4–5):892–906, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505425/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505425/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505425&PLACEBO=IE.pdf`.

Larin:2005:EEF

[LHTV05] A. V. Larin, C. Hansenne, D. N. Trubnikov, and D. P. Vercauteren. Evaluation of electric field within pores of aluminophosphate sieves. *International Journal of Quantum Chemistry*, 105(6):839–856, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Levi:2009:NIC

[LHV+09] C. Levi, G. J. Halász, Á. Vibók, I. Bar, Y. Zeiri, R. Kosloff, and M. Baer. A novel intraline of conical intersections for methylamine: A theoretical study. *International Journal of Quantum Chemistry*, 109(11):2482–2489, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2009:CMS

[Li09] Yumin Li. CCSD(T) and MRCI studies on the ground and excited states of BrOClO and ClOBrO. *International Journal of Quantum Chemistry*, 109(3):516–525, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liao:2008:CSF

[Lia08] Hsin-Yi Liao. Computational study of the fluorination effect on nitrogen–boron bond. *International Journal of Quantum Chemistry*, 108(1):84–89, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lee:2003:ERE

[LIBM03] M.-T. Lee, I. Iga, L. M. Brescansin, and L. E. Machado. Elastic and rotational excitation cross sections for electron–nitrous oxide collisions. *International Journal of Quantum Chemistry*, 95(3):260–266, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Linderberg:2001:BR

[Lin01] Jan Linderberg. Book review. *International Journal of Quantum Chemistry*, 83(6):348, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/81501980/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/81501980/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=81501980&PLACEBO=IE.pdf`.

Lindgren:2006:HFS

[Lin06] Ingvar Lindgren. Helium fine structure: Unsolved many-body-QED Problem. *International Journal of Quantum Chemistry*, 106(14):2833–2835, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Linderberg:2009:SRC

[Lin09] Jan Linderberg. Separable representations of the Coulomb interaction. *International Journal of Quantum Chemistry*, 109 (13):2866–2871, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2002:RGA

[Liu02] Shubin Liu. Recurrent generation of approximate functionals in density functional theory. *International Journal of Quantum Chemistry*, 90(1):282–290, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2006:CAD

[Liu06] Shubin Liu. Conditions for accurate description of the electron density of atoms and molecules. *International Journal of Quantum Chemistry*, 106(8):1762–1768, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2008:HBC

[Liu08] Ying Liu. Hydrogen bonding characterization of $XH_2NH_2 \cdots HNO$ (X = B, Al, Ga) complexes: A theoretical investigation. *International Journal of Quantum Chemistry*, 108(6): 1123–1129, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liverts:2002:UCS

[Liv02] E. Z. Liverts. Unconventional consideration of the symmetry properties — new techniques and computer codes: Application for high-temperature superconductors. *International Journal of Quantum Chemistry*, 88(4):519–524, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Librelon:2003:HAG

[LJ03] P. R. Librelon and F. E. Jorge. Highly accurate Gaussian basis sets for the atoms from H through Xe. *International Journal*

of Quantum Chemistry, 95(2):190–193, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2003:SSB

[LJL+03] Qian Shu Li, Qiao Jin, Qiong Luo, Au Chin Tang, Jian Kang Yu, and Hong Xing Zhang. Structure and stability of B_6, B_6^+, and B_6^- clusters. *International Journal of Quantum Chemistry*, 94(5):269–278, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lee:2009:TCC

[LJL09a] Dong-Ki Lee, Gwang-Hi Jeung, and Yoon Sup Lee. Two component calculations of Pt_2 with relativistic effective core potential including spin-orbit operator. *International Journal of Quantum Chemistry*, 109(9):1975–1983, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Long:2009:DSH

[LJL09b] Qingping Long, Hongbing Ji, and Shushen Lv. DFT study on the hydrogen bonds of phenol–cyclohexanone and phenol–H_2O_2 in the Baeyer–Villiger oxidation. *International Journal of Quantum Chemistry*, 109(3):448–458, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2009:ETS

[LJMM09] Junwen Li, Thushari Jayasekera, Vincent Meunier, and John W. Mintmire. Electronic transport of silicon nanowires with surface defects. *International Journal of Quantum Chemistry*, 109(15):3705–3710, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ladadwa:2000:CBE

[LK00a] Imad Ladadwa and Sabre Kais. Critical behavior of electron impact ionization of atoms. *International Journal of Quantum Chemistry*, 80(4–5):575–581, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505423/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505423/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505423&PLACEBO=IE.pdf`.

Larsson:2000:LCS

[LK00b] Sven Larsson and Agris Klimkāns. Localization, conductivity, and superconductivity. *International Journal of Quantum Chemistry*, 80(4–5):713–720, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505388/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505388/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505388&PLACEBO=IE.pdf`.

Lovallo:2002:IMC

[LK02] Christopher C. Lovallo and Mariusz Klobukowski. Improved model core potentials: Application to the thermochemistry of organoxenon complexes. *International Journal of Quantum Chemistry*, 90(3):1099–1107, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ludena:2003:RNK

[LKE03] Eduardo V. Ludeña, Valentin V. Karasiev, and Lorenzo Echevarría. Realizations of the noninteracting kinetic energy functional enhancement factor through local-scaling transformations: Atoms. *International Journal of Quantum Chemistry*, 91(2):94–104, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ley-Koo:2009:CGF

[LKG09] Eugenio Ley-Koo and Araceli Góngora. Common generating function for three-dimensional hydrogen atom complete wave functions. *International Journal of Quantum Chemistry*, 109 (4):790–800, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2001:SEA

[LL01] An Yong Li and Mu Zhen Liao. Symmetrization of eigenfunctions of angular momentum in point groups. *International Journal of Quantum Chemistry*, 83(5):286–302, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/81002390/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/81002390/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=81002390&PLACEBO=IE.pdf`.

Lin:2004:DFS

[LL04] Jyh Shing Lin and Lien-Feng Lee. Density functional study of XH_4 (X = Si and Ge) reactivity upon dissociative adsorption onto the Si(100) surface. *International Journal of Quantum Chemistry*, 97(2):736–746, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larsson:2001:PSW

[LLB01] B. Larsson, T. Levitina, and E. J. Brändas. On prolate spheroidal wave functions for signal processing. *International Journal of Quantum Chemistry*, 85(4–5):392–397, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2007:IIS

[LLL+07] Ying Liu, Wenqing Liu, Haiyang Li, Yong Yang, and Shuang Cheng. Interaction of the important species HNO and $HFSO_2$ in the atmosphere: Theoretical study of the N H and S H blue-shifted hydrogen bonds. *International Journal of Quantum Chemistry*, 107(2):396–402, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liao:2006:RSS

[LLLZ06] Bo Liao, Jiawei Luo, Renfa Li, and Wen Zhu. RNA secondary structure 2D graphical representation without degeneracy. *International Journal of Quantum Chemistry*, 106(8): 1749–1755, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liao:2007:NMA

[LLLZ07] Bo Liao, Jiawei Luo, Renfa Li, and Wen Zhu. Novel method for analyzing proteome. *International Journal of Quantum Chemistry*, 107(6):1295–1300, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2005:AAM

[LLP05] Daoming Lu, Liping Lu, and Jialun Ping. Application of algebraic method to the high overtones of C_6H_6 and C_6D_6. *International Journal of Quantum Chemistry*, 101(2):174–185, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lee:2000:HEB

[LLR+00] Jooyoung Lee, Adam Liwo, Daniel R. Ripoll, Jaroslaw Pillardy, Jeffrey A. Saunders, Kenneth D. Gibson, and Harold A. Scheraga. Hierarchical energy-based approach to protein-structure prediction: Blind-test evaluation with CASP3 targets. *International Journal of Quantum Chemistry*, 77(1):90–117, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004251/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004251/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004251&PLACEBO=IE.pdf`.

Lago:2004:QVS

[LLR04] N. Faginas Lago, A. Laganà, and A. Riganelli. Quantum vs. semiclassic initial value representation probabilities for nonreactive systems. *International Journal of Quantum Chemistry*, 96(6):547–553, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lin:2005:PIC

[LLSY05] Xi Lin, Ju Li, Elisabeth Smela, and Sidney Yip. Polaron-induced conformation change in single polypyrrole chain: An intrinsic actuation mechanism. *International Journal of Quantum Chemistry*, 102(5):980–985, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2005:LRTa

[LLW+05a] Rui Yan Li, Zhi Ru Li, Di Wu, Xi Yun Hao, Ru Jiao Li, and Chia Chung Sun. Long-range π-type hydrogen bond in dimers CH_2HF, CH_2OH_2O, and CH_2ONH_3. *International Journal of Quantum Chemistry*, 103(2):157–166, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2005:LRTb

[LLW+05b] Ruiyan Li, Zhiru Li, Di Wu, Xiyun Hao, Rujiao Li, and Chiachung Sun. Long-range π-type hydrogen bond in the dimers CH_2O HF, CH_2OH_2O, and CH_2ONH_3. *International Journal of Quantum Chemistry*, 103(3):299–307, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2007:ICM

[LLW+07] Qiang-Gen Li, Guo-Ming Liang, Xin Wang, San-Yan Chu, and Yi Ren. Ab initio computational modeling on the tautomerism of monochalcogenocarboxylic acids $CH_3C(O)XH$ (X = S, Se, and Te) in the polar and aprotic solution. *International Journal of Quantum Chemistry*, 107(4):921–929, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2003:MST

[LLX+03] Qianshu Li, Shunfeng Lü, Yaoming Xie, Paul V. R. Schleyer, and Henry F. Schaefer III. Molecular structures, thermochemistry, and electron affinities for the dichlorine oxides: Cl_2O_n / Cl_2O ($n = 1--4$). *International Journal of Quantum Chemistry*, 95(6):731–757, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2009:STE

[LLYJ09] Xiao-Jun Li, Chun-Ping Li, Ju-Cai Yang, and Abraham F. Jalbout. The structures, thermochemistry, and electron affinities of hydrogenated silicon clusters Si_6H_n /Si_6H ($n = 3--14$). *International Journal of Quantum Chemistry*, 109 (6):1283–1301, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2006:TSR

[LLYL06] Ying Liu, Wenqing Liu, Yong Yang, and Jianguo Liu. Theoretical study of the red- and blue-shifted hydrogen bonds of nitroxyl and acetylene dimers. *International Journal of Quantum Chemistry*, 106(9):2122–2128, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2000:NSO

[LLZ+00] Xue-Shen Liu, Xiao-Yan Liu, Zhong-Yuan Zhou, Pei-Zhu Ding, and Shou-Fu Pan. Numerical solution of one-dimensional time-independent Schrödinger equation by using symplectic schemes. *International Journal of Quantum Chemistry*, 79(6):343–349, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72515272/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72515272/FILE?TPL=ftx_start; http://www3.`

interscience.wiley.com/cgi-bin/fulltext?ID=72515272&PLACEBO=IE.pdf.

Liu:2004:ISH

[LLZ04] Ji-Feng Liu, Xiang-Yuan Li, and Quan Zhu. Ab initio study of hydrogen bonding interaction and photoinduced electron transfer between 4-nitroquinoline-1-oxide and tryptophan. *International Journal of Quantum Chemistry*, 98(1):33–43, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2009:GRD

[LLZH09] Zanbo Liu, Bo Liao, Wen Zhu, and Guohua Huang. A 2D graphical representation of DNA sequence based on dual nucleotides and its application. *International Journal of Quantum Chemistry*, 109(5):948–958, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2002:VPV

[LM02a] Jiabo Li and Roy McWeeny. VB2000: Pushing valence bond theory to new limits. *International Journal of Quantum Chemistry*, 89(4):208–216, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lo:2002:CFR

[LM02b] Shun S. Lo and Daniel A. Morales. Closed-form rectangular atomic wave functions of an N-dimensional atom. *International Journal of Quantum Chemistry*, 88(2):263–274, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Loock:2004:BR

[LM04] H.-P. Loock and S. Manzhos. Book review. *International Journal of Quantum Chemistry*, 98(6):528–529, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2009:OSN

[LMDW09] Aixiao Li, François Maurel, Michel Delamar, and Baoshan Wang. ONIOM study of the nonbonding interaction of the 2PU inhibitor with the CDK2 and CDK4 cyclin-dependant kinases. *International Journal of Quantum Chemistry*, 109

(5):1148–1157, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Laschuk:2003:IPW

[LME03] Eduardo F. Laschuk, Márcio M. Martins, and Stefano Evangelisti. Ab initio potentials for weakly interacting systems: Homonuclear rare gas dimers. *International Journal of Quantum Chemistry*, 95(3):303–312, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lopez:2002:ATA

[LMGM02] Jos Luis López, Marcos Mandado, Ana M. Graña, and Ricardo A. Mosquera. Approximate transferability in alkanenitriles. *International Journal of Quantum Chemistry*, 86 (2):190–198, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86510679/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86510679/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86510679&PLACEBO=IE.pdf`.

Li:2000:PCC

[LMJ00] Shuhua Li, Jing Ma, and Yuansheng Jiang. Pair-correlated configuration interaction method and its approximate version for solving the electron correlation problem in molecules. *International Journal of Quantum Chemistry*, 78(3):153–167, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71007684/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71007684/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71007684&PLACEBO=IE.pdf`.

Lee:2002:IRR

[LML02] H. Y. Lee, A. M. Mebel, and S. H. Lin. An ab initio/Rice–Ramsperger–Kassel–Marcus study of photodissociation of carbonyl cyanide. *International Journal of Quantum Chemistry*, 90(2):566–574, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lathiotakis:2004:DFT

[LML+04] N. N. Lathiotakis, M. A. L. Marques, M. Lüders, L. Fast, and E. K. U. Gross. Density functional theory for superconductors. *International Journal of Quantum Chemistry*, 99(5):790–797, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lambin:2003:CSI

[LMMB03] P. Lambin, G. I. Márk, V. Meunier, and L. P. Biró. Computation of STM images of carbon nanotubes. *International Journal of Quantum Chemistry*, 95(4–5):493–503, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leopoldini:2008:BMU

[LMRT08] M. Leopoldini, T. Marino, N. Russo, and M. Toscano. On the binding mode of urease active site inhibitors: A density functional study. *International Journal of Quantum Chemistry*, 108(11):2023–2029, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lopez-Moraza:2000:SSC

[LMSB00] Sara López-Moraza, Luis Seijo, and Zoila Barandiarán. Structure and spectroscopy of Cr^{3+} defects in $KMgF_3$, $KZnF_3$, and $CsCaF_3$ crystals. An ab initio model potential embedded cluster study. *International Journal of Quantum Chemistry*, 77(6):961–972, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000978/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000978/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000978&PLACEBO=IE.pdf`.

Liu:2005:SMC

[LMX+05] Yufang Liu, Heng Ma, Houju Xu, Jinfeng Sun, and Keli Han. Study of the molecular configuration and the dipole moment in fluorinated liquid crystals. *International Journal of Quantum Chemistry*, 102(4):415–421, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2003:NGD

[LN03] Chao-Ping Liu and J. J. Soares Neto. Numerically generated DVR and generator coordinate approximation for calculating rotational energies of H and H_2O. *International Journal of Quantum Chemistry*, 95(2):103–111, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lundqvist:2006:DSB

[LNPL06] Maria J. Lundqvist, Mattias Nilsing, Petter Persson, and Sten Lunell. DFT study of bare and dye-sensitized TiO_2 clusters and nanocrystals. *International Journal of Quantum Chemistry*, 106(15):3214–3234, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lizarraga:2002:NMD

[LNSE02] R. Lizárraga, L. Nordström, E. Sjöstedt, and O. Eriksson. Noncollinear magnetization density in VAu_4. *International Journal of Quantum Chemistry*, 90(6):1610–1613, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Loew:2000:SSF

[Loe00] Gilda Loew. Structure, spectra, and function of heme sites. *International Journal of Quantum Chemistry*, 77(1):54–70, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004295/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004295/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004295&PLACEBO=IE.pdf`.

Lorquet:2008:ADR

[Lor08] J. C. Lorquet. Adiabatic decoupling of the reaction coordinate. *International Journal of Quantum Chemistry*, 108(10):1629–1636, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2000:ESC

[LP00a] Xiangzhu Li and Josef Paldus. Effect of spin contamination on the prediction of barrier heights by coupled-cluster theory: $F + H_2 \rightarrow HF + H$ reaction. *International Journal of Quantum Chemistry*, 77(1):281–290,

???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004267/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004267/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004267&PLACEBO=IE.pdf`.

Li:2000:TVR

[LP00b] Xiangzhu Li and Josef Paldus. Truncated version of the reduced multireference coupled-cluster method with perturbation selection of higher than pair clusters. *International Journal of Quantum Chemistry*, 80(4–5):743–756, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505413/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505413/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505413&PLACEBO=IE.pdf`.

Li:2004:SEG

[LP04a] Xiangzhu Li and Josef Paldus. Size extensivity of a general-model-space state-universal coupled-cluster method. *International Journal of Quantum Chemistry*, 99(6):914–924, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luzanov:2004:WRP

[LP04b] A. V. Luzanov and O. V. Prezhdo. Weyl representation of the permutation operators and exchange interaction. *International Journal of Quantum Chemistry*, 96(5):474–482, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2005:RGN

[LP05a] Xiangzhu Li and Josef Paldus. Recursive generation of natural orbitals in a truncated orbital space. *International Journal of Quantum Chemistry*, 105(6):672–678, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luzanov:2005:ICD

[LP05b] A. V. Luzanov and O. V. Prezhdo. Irreducible charge density matrices for analysis of many-electron wave functions. *International Journal of Quantum Chemistry*, 102(5):582–601,

???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leiva:2007:DHS

[LP07] P. Leiva and M. Piris. Description of high-spin restricted open-shell molecules with the Piris natural orbital functional. *International Journal of Quantum Chemistry*, 107(1):1–11, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2008:CCA

[LP08] Xiangzhu Li and Josef Paldus. Coupled-cluster approach to spontaneous symmetry breaking in molecules: The linear N_3 radical. *International Journal of Quantum Chemistry*, 108 (12):2117–2127, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2009:EDP

[LP09a] Xiangzhu Li and Josef Paldus. Energetics of 1,n-didehydropolyene diradicals and performance of reduced multireference coupled-cluster method. *International Journal of Quantum Chemistry*, 109(14):3305–3314, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2009:SBS

[LP09b] Xiangzhu Li and Josef Paldus. Symmetry breaking in spin-restricted, open-shell Hartree–Fock wave functions. *International Journal of Quantum Chemistry*, 109(8):1756–1765, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lebedev:2004:OSC

[LPC04] N. G. Lebedev, I. V. Ponomareva, and L. A. Chernozatonskii. Orbital-stoichiometric cluster model of carbon nanotube generation on quantum dots of diamond surface. *International Journal of Quantum Chemistry*, 96(2):155–166, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liem:2004:SLW

[LPL04] S. Y. Liem, P. L. A. Popelier, and M. Leslie. Simulation of liquid water using a high-rank quantum topological electrostatic

potential. *International Journal of Quantum Chemistry*, 99 (5):685–694, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Llorens:2002:ISE

[LPV02] Oriol Llorens, Juan J. Perez, and Hugo O. Villar. Investigation of structural and electronic biases in mutagenic compounds. *International Journal of Quantum Chemistry*, 88(1):107–117, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90010559/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90010559/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90010559&PLACEBO=IE.pdf`.

Larin:2005:CCT

[LPV05] A. V. Larin, V. S. Parbuzin, and D. P. Vercauteren. Cumulative coordinate technique for approximation of high atomic multipole moments of aluminophosphate sieves on the basis of electron densities calculated with DFT methods. *International Journal of Quantum Chemistry*, 101(6):807–818, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Litinsky:2007:PSS

[LPV07] A. O. Litinsky, V. N. Perminov, and G. Y. Vasiljeva. Peculiarities of the silica surface center structure in rigid dehydroxidation conditions. *International Journal of Quantum Chemistry*, 107(2):326–329, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2005:TSTb

[LPZW05] Feng-Ling Liu, Ling Peng, Jian-Xia Zhao, and Shou-Qing Wang. Theoretical study of two $C_{50}H_{40}$ isomers with three dodecahedrane cages sharing two pentagons. *International Journal of Quantum Chemistry*, 103(2):167–175, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liegeois:2006:IPH

[LQC06] Vincent Liégeois, Olivier Quinet, and Benoît Champagne. Investigation of polyethylene helical conformations: Theoretical study by vibrational Raman optical activity. *Inter-*

national Journal of Quantum Chemistry, 106(15):3097–3107, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liao:2008:QSA

[LQC+08] Si Yan Liao, Li Qian, Jin Can Chen, Hai Liang Lu, and Kang Cheng Zheng. 2D and 3D-QSAR studies on antiproliferative thiazolidine analogs. *International Journal of Quantum Chemistry*, 108(8):1380–1390, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liao:2009:TSQ

[LQM+09] Si Yan Liao, Li Qian, Ti Fang Miao, Hai Liang Lu, and Kang Cheng Zheng. Theoretical studies on QSAR and mechanism of 2-indolinone derivatives as tubulin inhibitors. *International Journal of Quantum Chemistry*, 109(5):999–1008, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Laszlo:2001:TSF

[LR01] István László and André Rassat. Toroidal and spherical fullerene-like molecules with only pentagonal and heptagonal faces. *International Journal of Quantum Chemistry*, 84 (1):136–139, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84002449/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002449/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002449&PLACEBO=IE.pdf`.

Largo:2004:TSP

[LRB04] Antonio Largo, Pilar Redondo, and Carmen Barrientos. Theoretical study of possible ion-molecule reactions leading to precursors of glycine in the interstellar medium. *International Journal of Quantum Chemistry*, 98(4):355–360, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Licona:2005:IDF

[LRS05] R. Licona and J. F. Rivas-Silva. Ab initio density functional study of MgO (001) surface with topological defects. *International Journal of Quantum Chemistry*, 104(6):919–928, ????

2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lefebvre:2001:PRH

[LS01a] R. Lefebvre and B. Stern. Partial rates in the high-frequency regime of intense-field photoionization of hydrogen. *International Journal of Quantum Chemistry*, 84(5):552–558, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502594/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502594/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502594&PLACEBO=IE.pdf`.

Liptak:2001:EDT

[LS01b] Matthew D. Liptak and George C. Shields. Experimentation with different thermodynamic cycles used for pK_a calculations on carboxylic acids using complete basis set and Gaussian-n models combined with CPCM continuum solvation methods. *International Journal of Quantum Chemistry*, 85(6):727–741, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85512108/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85512108/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85512108&PLACEBO=IE.pdf`.

Lindgren:2002:BOD

[LS02] Ingvar Lindgren and Sten Salomonson. Brueckner orbitals and density-functional theory. *International Journal of Quantum Chemistry*, 90(1):294–308, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liptak:2005:CDF

[LS05] Matthew D. Liptak and George C. Shields. Comparison of density functional theory predictions of gas-phase deprotonation data. *International Journal of Quantum Chemistry*, 105 (6):580–587, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lakhno:2008:BLE

[LS08] V. D. Lakhno and V. B. Sultanov. Baseline logical elements on the basis of DNA. *International Journal of Quantum Chem-*

istry, 108(11):1913–1920, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larsson:2002:QRC

[LSBDL02] Per-Erik Larsson, Nessima Salhi-Benachenhou, Xicheng Dong, and Sten Lunell. Quadricyclane radical cation isomerization reactions: a theoretical study. *International Journal of Quantum Chemistry*, 90(4-5):1388–1395, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lai:2001:SVS

[LSC01] Chin-Hung Lai, Ming-Der Su, and San-Yan Chu. Structures, vibrational spectra, and relative energies of HXSiS (X = H, F, and Cl) isomers. *International Journal of Quantum Chemistry*, 82(1):14–25, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76510763/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76510763/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76510763&PLACEBO=IE.pdf`.

Liao:2002:ESE

[LSC02] Hsin-Yi Liao, Ming-Der Su, and San-Yan Chu. An examination of substituent effects on the stabilization of a silicon–selenium double bond. *International Journal of Quantum Chemistry*, 90(2):663–668, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liao:2001:DFS

[LSCC01] Hsin-Yi Liao, Ming-Der Su, Wen-Sheng Chung, and San-Yan Chu. Density functional study of the relative reactivity in the concerted 1,3-dipolar cycloaddition of nitrile ylide to disubstituted ethylenes. *International Journal of Quantum Chemistry*, 83(6):318–323, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/81501977/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/81501977/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=81501977&PLACEBO=IE.pdf`.

Liu:2002:SAU

[LSD02] Xue-Shen Liu, Li-Wei Su, and Pei-Zhu Ding. Symplectic algorithm for use in computing the time-independent Schrödinger equation. *International Journal of Quantum Chemistry*, 87(1):1–11, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/88510572/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88510572/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88510572&PLACEBO=IE.pdf`.

Lundin:2005:TSC

[LSE05] U. Lundin, I. Sandalov, and O. Eriksson. Theory of strongly correlated electron systems. II. Including correlation effects into electronic structure calculations. *International Journal of Quantum Chemistry*, 102(6):1046–1055, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lindgren:2008:NPC

[LSH08] Ingvar Lindgren, Sten Salomonson, and Daniel Hedendahl. A numerical procedure for combined many-body-QED calculations. *International Journal of Quantum Chemistry*, 108(12): 2272–2279, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liao:2006:EWZ

[LSK+06] Yi Liao, Zhong-Min Su, Yu-He Kan, Shu-Mei Yue, Jian-Fang Ma, and Ji-Hua Yang. Effect of water on zinc (II), cadmium (II) complexes with pyridylimidazole: Theoretical study of stability and electronic spectrum. *International Journal of Quantum Chemistry*, 106(2):490–500, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lei:2008:IET

[LSL+08] Yibo Lei, Bingbing Suo, Anyang Li, Yusheng Dou, Yubin Wang, and Zhenyi Wen. Involvement of excited triplet state in the photodissociation of cyclobutane. *International Journal of Quantum Chemistry*, 108(4):788–796, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2001:NST

[LSLD01] Xue-Shen Liu, Li-Wei Su, Xiao-Yan Liu, and Pei-Zhu Ding. Numerical solution of a two-dimensional time-independent Schrödinger equation by using symplectic schemes. *International Journal of Quantum Chemistry*, 83(5):303–309, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/81002393/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/81002393/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=81002393&PLACEBO=IE.pdf`.

Lindgren:2005:CAK

[LSM05] I. Lindgren, S. Salomonson, and F. Möller. Construction of accurate Kohn–Sham potentials for the lowest states of the helium atom: Accurate test of the ionization-potential theorem. *International Journal of Quantum Chemistry*, 102(5): 1010–1017, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leblanc:2006:FAR

[LSM+06] Marie Leblanc, Didier Siri, Sylvain R. A. Marque, Sandra Grimaldi, Denis Bertin, and Paul Tordo. β-fragmentation of alkoxyl radicals: Natural bond orbital analysis. *International Journal of Quantum Chemistry*, 106(3):676–685, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lazar:2001:EHM

[LSPS01] Armand Lázár, Péter R. Surján, Magnus Paulsson, and Sven Stafström. An effective hopping model for weakly interacting π systems: Electronic structure of stacked polyaromatic hydrocarbons. *International Journal of Quantum Chemistry*, 84(2):216–225, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502340/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502340/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502340&PLACEBO=IE.pdf`.

Lendvay:2009:P

[LSS09] György Lendvay, Péter R. Surján, and Péter G. Szalay. Preface. *International Journal of Quantum Chemistry*, 109(11): 2329–2330, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lawrenz:2005:MMS

[LSWT05] Morgan E. Lawrenz, E. A. Salter, Andrzej Wierzbicki, and W. J. Thompson. Molecular modeling study of binding to the catalytic site of PDE4 enzymes by a novel class of inhibitors. *International Journal of Quantum Chemistry*, 105 (4):410–415, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lejeune:2004:VSS

[LTL04] Olivier Lejeune, Mustapha Tlidi, and René Lefever. Vegetation spots and stripes: Dissipative structures in arid landscapes. *International Journal of Quantum Chemistry*, 98(2): 261–271, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lin:2005:TSG

[LTL05a] Wen-Hsin Lin, Chih-Chiang Tu, and Shyi-Long Lee. Theoretical studies of growth mechanism of small fullerene cage $C_2 4 (D_{6d})^+$. *International Journal of Quantum Chemistry*, 103 (4):355–368, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luo:2005:CIE

[LTL05b] Xiaoling Luo, Dianyong Tang, and Ming Li. Computational investigation of enantio- and regioselectivity of rhodium-catalyzed asymmetric hydroformylation of vinyl formate with CHIRAPHOS-type ligand. *International Journal of Quantum Chemistry*, 105(2):108–123, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luo:2006:RMR

[LTL06] Xiaoling Luo, Dianyong Tang, and Ming Li. Revealing the mechanism of Rh(I)-catalyzed hydroformylation of 4-pyridylethene derivatives: DFT study. *International Journal of Quantum Chemistry*, 106(8):1844–1852, ???? 2006.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2005:MAH

[LTLS05] Ming Li, Dianyong Tang, Xiaoling Luo, and Wei Shen. Mechanism of asymmetric hydrogenation of enamides with $[Rh(BisP^*)]^+$ catalyst: Model DFT study. *International Journal of Quantum Chemistry*, 102(1):53–63, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larin:2002:DBC

[LTV02] Alexander V. Larin, Dmitrii N. Trubnikov, and Daniel P. Vercauteren. Differences between the CO and NO properties for stability of alkali metal complexes $Me(XO)_n^+$, X = C or N. *International Journal of Quantum Chemistry*, 90(2):541–548, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larin:2003:IHB

[LTV03] A. V. Larin, D. N. Trubnikov, and D. P. Vercauteren. Influence of hydrogen bonding on the properties of water molecules adsorbed in zeolite frameworks. *International Journal of Quantum Chemistry*, 92(1):71–84, March 5, 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larin:2005:IXR

[LTV05] A. V. Larin, D. N. Trubnikov, and D. P. Vercauteren. Improvement of X-ray diffraction geometries of water physisorbed in zeolites on the basis of periodic Hartree–Fock calculations. *International Journal of Quantum Chemistry*, 102(5):971–979, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larin:2007:IQC

[LTV07] A. V. Larin, D. N. Trubnikov, and D. P. Vercauteren. Ab initio QM calculation of the electric field convergence versus atomic basis sets in periodic models of proton-substituted zeolites. *International Journal of Quantum Chemistry*, 107(15):3137–3150, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2009:ISV

[LTW09] Lei Vincent Liu, Wei Quan Tian, and Yan Alexander Wang. Ab initio studies of vacancy-defected fullerenes and single-walled carbon nanotubes. *International Journal of Quantum Chemistry*, 109(14):3441–3456, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2000:TMW

[LTY00] Shu-Chung Liu, Li-Da Tong, and Yeong-Nan Yeh. Trees with the minimum Wiener number. *International Journal of Quantum Chemistry*, 78(5):331–340, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72001892/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72001892/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72001892&PLACEBO=IE.pdf`.

Li:2009:PSS

[LTY09] Xiao-Hong Li, Zheng-Xin Tang, and Xiang-Dong Yang. PCM study of the solvent and substituent effects on bond dissociation energies of the C NO bond. *International Journal of Quantum Chemistry*, 109(6):1403–1409, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2006:TSE

[Lu06] Shen-Zhuang Lu. Theoretical study of electric field-induced intramolecular electron transfer in donor–acceptor pairs via the rigid space and their suitability as molecular electronic devices. *International Journal of Quantum Chemistry*, 106 (7):1664–1671, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lucas:2002:RSG

[Luc02] Amand A. Lucas. Rosetta Stone of the genetic language. *International Journal of Quantum Chemistry*, 90(4-5):1491–1504, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lund:2004:BR

[Lun04] Anders Lund. Book Review. *International Journal of Quantum Chemistry*, 97(4):889, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luzanov:2008:MCR

[Luz08] Anatoliy V. Luzanov. Matrix-covariant representation of high-order configuration interaction and coupled cluster theories. *International Journal of Quantum Chemistry*, 108(4):671–695, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larin:2001:CCA

[LV01a] A. V. Larin and D. P. Vercauteren. Cumulative coordinates for approximations of high-order atomic multipole moments in aluminosilicate and aluminophosphate sieves. *International Journal of Quantum Chemistry*, 83(2):70–85, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002389/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002389/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002389&PLACEBO=IE.pdf`.

Larin:2001:QCC

[LV01b] A. V. Larin and D. P. Vercauteren. Quadrupole coupling constants C_{QQ} for ^{2}H, ^{27}Al, and ^{17}O atoms calculated at the periodic Hartree–Fock level for understanding the geometry of H-form aluminosilicates. *International Journal of Quantum Chemistry*, 82(4):182–192, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/78503196/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/78503196/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=78503196&PLACEBO=IE.pdf`.

Lavin:2001:SPN

[LVM01] C. Lavín, A. M. Velasco, and I. Martín. Spectral properties of neutral selenium and tellurium. A relativistic treatment. *International Journal of Quantum Chemistry*, 84(6):694–704, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/82502287/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/82502287/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=82502287&PLACEBO=IE.pdf.

Loverix:2006:QCS

[LVSG06] Stefan Loverix, Wim Versees, Jan Steyaert, and Paul Geerlings. Quantum chemical study of leaving group activation in *T. vivax* nucleoside hydrolase. *International Journal of Quantum Chemistry*, 106(3):565–570, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Langhoff:2005:SPM

[LW05] P. W. Langhoff and C. L. Winstead. Spectral properties of minimal-basis-set orbitals: Implications for molecular electronic continuum states. *International Journal of Quantum Chemistry*, 102(5):948–955, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2007:NCF

[LW07] Liwei Liu and Tianming Wang. Novel characterization of the folding of proteins. *International Journal of Quantum Chemistry*, 107(10):1970–1974, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2008:TIC

[LW08] Zhi-Ming Li and Quan-Rui Wang. A theoretical investigation on the cycloaddition reaction between azocarbenium ions and nitriles. *International Journal of Quantum Chemistry*, 108 (6):1067–1075, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lee:2001:BTM

[LWC01] H. Y. Lee, S. P. Wang, and T. C. Chang. Bond types of molecular orbitals and the photoelectron spectrum. *International Journal of Quantum Chemistry*, 81(1):53–65, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/75502170/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75502170/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502170&PLACEBO=IE.pdf.

Li:2009:TSI

[LWC+09] Qingzhong Li, Xilin Wang, Jianbo Cheng, Wenzuo Li, Baoan Gong, and Jiazhong Sun. Theoretical study on the interlay of hydrogen bonds in the trimers involving HCN and water. *International Journal of Quantum Chemistry*, 109(6):1396–1402, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2008:TSP

[LWCF08] Xi Lu, Huayang Wang, Zhengting Cai, and Dacheng Feng. Theoretical study on the partial potential energy surface and formation mechanism of the reactive resonance state of HO + $CH_4 \rightarrow H_2O + CH_3$ system. *International Journal of Quantum Chemistry*, 108(2):334–338, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2008:SPB

[LWL+08] Rui-Yan Li, Bing-Qiang Wang, Zhi-Ru Li, Di Wu, and Ying Li. Structures and properties of π Br-bond in complexes $C_2H_{4-n}F_nBrF$ ($n = 0--2$). *International Journal of Quantum Chemistry*, 108(1):151–160, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2002:QCS

[LWW+02] Lai-Cai Li, Jing Wang, Xin Wang, An-Min Tian, and Ning-Bew Wong. Quantum chemical study of the reaction mechanism of ozone and methane with fluorine and chlorine atoms. *International Journal of Quantum Chemistry*, 87(5):288–292, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90513427/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90513427/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90513427&PLACEBO=IE.pdf`.

Liu:2005:TSH

[LWZ+05] Shu-Zhen Liu, Hong-Qi Wang, Zheng-Yu Zhou, Xiu-Li Dong, and Xiao-Li Gong. Theoretical study of helical structure caused by chirality of cysteine dimer. *International Journal of Quantum Chemistry*, 105(1):66–73, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2009:RSC

[LWZ+09] Jiaye Li, Jinping Wu, Chenggang Zhou, Bo Han, Xinjian Lei, Roy Gordon, and Hansong Cheng. On the relative stability of cobalt- and nickel-based amidinate complexes against β-migration. *International Journal of Quantum Chemistry*, 109 (4):756–763, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2000:TSI

[LXD00] Jinshan Li, Heming Xiao, and Haishan Dong. Theoretical study on intermolecular interaction of epoxyethane dimer. *International Journal of Quantum Chemistry*, 78(2):94–98, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71005516/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71005516/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71005516&PLACEBO=IE.pdf`.

Li:2000:QCSa

[LXH+00] Ming Li, Rugang Xie, Changwei Hu, Xin Wang, and Anmin Tian. Quantum chemical study on enantioselective reduction of aromatic ketones catalyzed by chiral cyclic sulfur-containing oxazaborolidines. Part 1. Structures and properties of catalysts. *International Journal of Quantum Chemistry*, 78(4):245–251, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72000078/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72000078/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72000078&PLACEBO=IE.pdf`.

Li:2000:QCSc

[LXHT00] Ming Li, Rugang Xie, Xairong Hu, and Anmin Tian. Quantum chemical study on enantioselective reduction of aromatic ketones catalyzed by chiral cyclic sulfur-containing oxazaborolidines. Part 3. Structures of catalyst-alkoxyborane adducts. *International Journal of Quantum Chemistry*, 78(4):261–268, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72000080/START; http:`

//www3.interscience.wiley.com/cgi-bin/fulltext/72000080/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72000080&PLACEBO=IE.pdf.

Li:2000:QCSb

[LXTT00] Ming Li, Rugang Xie, Shuanghe Tian, and Anmin Tian. Quantum chemical study on enantioselective reduction of aromatic ketones catalyzed by chiral cyclic sulfur-containing oxazaborolidines. Part 2. Structures of catalyst-borane-ketone adducts. *International Journal of Quantum Chemistry*, 78 (4):252–260, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72000079/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72000079/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72000079&PLACEBO=IE.pdf.

Lu:2008:TSMa

[LXXC08] Xiu Hui Lu, Yue Hua Xu, Ping Ping Xiang, and Xin Che. Theoretical studies of mechanism of cycloaddition reaction between germylidene and formaldehyde. *International Journal of Quantum Chemistry*, 108(1):75–83, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2000:PES

[LXY00] Yuhui Lu, Daiqian Xie, and Guosen Yan. A potential energy surface for the electronic ground state of CO_2. *International Journal of Quantum Chemistry*, 78(4):269–280, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72000081/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72000081/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72000081&PLACEBO=IE.pdf.

Ladik:2002:HCN

[LY02] J. Ladik and Y.-J. Ye. Hopping conductivity in nucleotide base stacks. *International Journal of Quantum Chemistry*, 90 (2):838–847, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lankau:2009:NHB

[LY09] Timm Lankau and Chin-Hui Yu. The NHN^+ hydrogen bridge between 4,5-dihydro-1 H-imidazole and various amines. *International Journal of Quantum Chemistry*, 109(10):2286–2296, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2008:TSMb

[LYCX08] Xiu Hui Lu, Hai Bin Yu, Xin Che, and Ping Ping Xiang. Theoretical study of mechanism of cycloaddition reaction between dimethylmethylenesilylene and formaldehyde. *International Journal of Quantum Chemistry*, 108(6):1114–1122, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lopez:2002:TSH

[LYDK02] Xabier Lopez, Darrin M. York, Annick Dejaegere, and Martin Karplus. Theoretical studies on the hydrolysis of phosphate diesters in the gas phase, solution, and RNase A. *International Journal of Quantum Chemistry*, 86(1):10–26, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85008605/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85008605/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85008605&PLACEBO=IE.pdf`.

Lin:2006:SME

[LYP+06] Ping Lin, Weitao Yang, Lars C. Pedersen, Masa Negishi, and Lee G. Pedersen. Searching for the minimum energy path in the sulfuryl transfer reaction catalyzed by human estrogen sulfotransferase: Role of enzyme dynamics. *International Journal of Quantum Chemistry*, 106(14):2981–2998, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2007:TSM

[LYWX07] Xiu Hui Lu, Hai Bin Yu, Wei Rong Wu, and Yue Hua Xu. Theoretical studies of mechanisms of cycloaddition reaction between difluoromethylene carbene and acetone. *International Journal of Quantum Chemistry*, 107(2):451–457, ???? 2007.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luzanov:2005:CSO

[LZ05] A. V. Luzanov and O. A. Zhikol. Collectivity, shell openness indices, and complexity measures of multiconfigurational states: Computations within full CI scheme. *International Journal of Quantum Chemistry*, 104(2):167–180, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2009:NMG

[LZA+09] Qingzhong Li, Hongjie Zhu, Xiulin An, Baoan Gong, and Jianbo Cheng. Nonadditivity of methyl group in single-electron hydrogen bond of methyl radical-water complex. *International Journal of Quantum Chemistry*, 109(3):605–611, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lebedev:2004:FCN

[LZC04a] N. G. Lebedev, I. V. Zaporotskova, and L. A. Chernozatonskii. Fluorination of carbon nanotubes: Quantum chemical investigation within MNDO approximation. *International Journal of Quantum Chemistry*, 96(2):142–148, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lebedev:2004:HES

[LZC04b] N. G. Lebedev, I. V. Zaporotskova, and L. A. Chernozatonskii. Hiral effects of single-wall carbon nanotube fluorination and hydrogenation. *International Journal of Quantum Chemistry*, 100(4):548–558, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2003:QCSa

[LZHT03] Ming Li, Wenxu Zheng, Rongxing He, and Anmin Tian. Quantum chemical study on enantioselective reduction of keto oxime ether with borane catalyzed by oxazaborolidine. Part 2. Structures of catalyst-alkoxyborane adduct with a four-membered ring and succeeding reaction intermediates. *International Journal of Quantum Chemistry*, 93(4):294–306, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2006:ISR

[LZJ+06] X. Li, Y. Zhao, X. Jing, F. Liu, and F. Hao. Ab initio study of Rg_2I^- (Rg = Ar, Kr, Xe). *International Journal of Quantum Chemistry*, 106(5):1086–1092, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2003:QCSb

[LZT03] Ming Li, Wenxu Zheng, and Anmin Tian. Quantum chemical study on enantioselective reduction of keto oxime ether with borane catalyzed by oxazaborolidine. Part 3. Properties of intermediates during hydride transfer. *International Journal of Quantum Chemistry*, 93(4):307–316, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luo:2007:FPS

[LZW+07] Chen Luo, Chenggang Zhou, Jinping Wu, T. J. Dhilip Kumar, Naduvalath Balakrishnan, Robert C. Forrey, and Hansong Cheng. First principles study of small palladium cluster growth and isomerization. *International Journal of Quantum Chemistry*, 107(7):1632–1641, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2007:SEN

[LZWY07] Yun-Xiang Lu, Jian-Wei Zou, Yan-Hua Wang, and Qing-Sen Yu. Substituent effects on noncovalent halogen/π interactions: Theoretical study. *International Journal of Quantum Chemistry*, 107(6):1479–1486, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2005:TSTa

[LZXD05] Feng-Ling Liu, Jian-Xia Zhao, Ying Xie, and Lian-Hua Dai. Theoretical study of two $C_{30}H_{20}$ isomers with a dodecahedrane cage and two pentaprismane cages sharing two pentagons. *International Journal of Quantum Chemistry*, 102 (3):275–281, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2005:SSB

[LZXL05] Qianshu Li, Yi Zhao, Wenguo Xu, and Nan Li. Structure and stability of B_8 clusters. *International Journal of Quantum Chemistry*, 101(2):219–229, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2001:QCS

[LZYT01] Ming Li, Wenxu Zheng, Feng Yang, and Anmin Tian. Quantum chemical study on enantioselective reduction of keto oxime ether with borane catalyzed by oxazaborolidine. Part 1. Structures of catalyst-borane-keto oxime ether adducts. *International Journal of Quantum Chemistry*, 81(4):291–304, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76505739/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76505739/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76505739&PLACEBO=IE.pdf`.

Li:2006:TSR

[LZZ+06a] Lai-Cai Li, Yan Zheng, Dong Zha, An-Min Tian, and Ming-Hou Xu. Theoretical studies on the reaction mechanism of CH_2CH radical with HNCO. *International Journal of Quantum Chemistry*, 106(7):1672–1682, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2006:DCI

[LZZ+06b] Jinfeng Lu, Songling Zhu, Zhengyu Zhou, Qunyan Wu, and Gang Zhao. DFT calculations of the ionization potentials and electron affinities of serinamide. *International Journal of Quantum Chemistry*, 106(9):2073–2081, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2007:TSM

[LZZ+07] Lai-Cai Li, Dong Zha, Yan Zheng, Xin Wang, An-Min Tian, and Ning-Bew Wong. Theoretical study of molecular interaction between tirapazamine enzymatic catalysis metabolites and water. *International Journal of Quantum Chemistry*, 107 (2):507–514, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maniero:2005:FCI

[MA05] Angelo M. Maniero and Paulo H. Acioli. Full configuration interaction pseudopotential determination of the ground-state potential energy curves of Li_2 and LiH. *International Journal of Quantum Chemistry*, 103(5):711–717, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mokrousov:2006:MAE

[MABB06] Yuriy Mokrousov, Nicolae Atodiresei, Gustav Bihlmayer, and Stefan Blügel. Magnetic anisotropy energies of metal–benzene sandwiches. *International Journal of Quantum Chemistry*, 106(15):3208–3213, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marques:2008:COA

[MAFR08] Alexandra T. Marques, Agostinho Antunes, Pedro A. Fernandes, and Maria J. Ramos. Computational optimization of AG18051 inhibitor for amyloid-β binding alcohol dehydrogenase enzyme. *International Journal of Quantum Chemistry*, 108(11):1982–1991, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maitra:2005:MFP

[Mai05] Neepa T. Maitra. Memory formulas for perturbations in time-dependent density functional theory. *International Journal of Quantum Chemistry*, 102(5):573–581, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maiti:2008:ETE

[Mai08a] Santanu K. Maiti. Erratum: Tuning of electron transport through molecular bridge systems: A study of shot noise. *International Journal of Quantum Chemistry*, 108(9):1615, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Mai08b].

Maiti:2008:TET

[Mai08b] Santanu K. Maiti. Tuning of electron transport through molecular bridge systems: A study of shot noise. *International Journal of Quantum Chemistry*, 108(1):135–141, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Mai08a].

Makowski:2007:SYP

[Mak07] Marcin Makowski. Simple yet powerful techniques for optimization of horizontal recursion steps in Gaussian-type two-electron integral evaluation algorithms. *International Journal of Quantum Chemistry*, 107(1):30–36, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malli:2002:PER

[Mal02] Gulzari L. Malli. Prediction of the existence of radon carbonyl: RnCO. *International Journal of Quantum Chemistry*, 90(2):611–615, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malinovskaya:2005:PFC

[Mal05a] S. A. Malinovskaya. Pulse function for control of the coherent excitation in stimulated Raman spectroscopy. *International Journal of Quantum Chemistry*, 102(3):313–317, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malinovskaya:2005:CLE

[Mal05b] Svetlana V. Malinovskaya. Cooperative laser–electron–nuclear processes: QED calculation of a spectrum of electron–nuclear γ-transitions of a nucleus in the neutral atom. *International Journal of Quantum Chemistry*, 104(4):486–490, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malinovskaya:2007:CPC

[Mal07] Svetlana Malinovskaya. Chirped pulse control methods for imaging of biological structure and dynamics. *International Journal of Quantum Chemistry*, 107(15):3151–3158, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mandal:2005:GTP

[Man05] Bholanath Mandal. Graph theoretical procedure for obtaining analytical expressions of eigenspectra of linear chains and cycles with alternant vertex weights and same edge weight: Application to some complicated graphs. *International Journal of Quantum Chemistry*, 103(2):140–148, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:1987:EPD

[Mar87a] N. H. March. Effective potential determining one-dimensional Slater sum in independent-particle theory. *Journal of Mathematical Physics*, 28(12):2973–2974, December 1987. CODEN JMAPAQ. ISSN 0022-2488 (print), 1089-7658 (electronic), 1527-2427.

March:1987:EDS

[Mar87b] N. H. March. Electron density and Slater sum of a semi-infinite electron gas in d dimensions. *Journal of Mathematical Physics*, 28(12):2975–2976, December 1987. CODEN JMAPAQ. ISSN 0022-2488 (print), 1089-7658 (electronic), 1527-2427.

March:2000:BSE

[Mar00a] N. H. March. Bond stretching and electronic correlation in relation to mechanical and tribological properties of solids. *International Journal of Quantum Chemistry*, 80(2):193–200, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73001278/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001278/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001278&PLACEBO=IE.pdf.

March:2000:ETR

[Mar00b] N. H. March. Electron theory related to mechanical properties of condensed phases. *International Journal of Quantum Chemistry*, 77(6):1049–1059, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/71000975/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000975/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000975&PLACEBO=IE.pdf.

March:2000:PTI

[Mar00c] N. H. March. Phase transitions in insulating molecular fluids and in assemblies of charged particles. *International Journal of Quantum Chemistry*, 80(4–5):692–700, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505387/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505387/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505387&PLACEBO=IE.pdf.

March:2003:CIC

[Mar03a] N. H. March. Classic ionic crystals and quantal Wigner electron solids: Role of electron correlation. *International Journal*

of Quantum Chemistry, 92(1):11–21, March 5, 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:2003:NED

[Mar03b] N. H. March. Nonlocal energy density functionals: Models plus some exact general results. *International Journal of Quantum Chemistry*, 92(1):1–10, March 5, 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:2004:GSG

[Mar04a] N. H. March. Ground-state geometry and electronic structure of light atom clusters, especially H isotopes, Li, B, and C. *International Journal of Quantum Chemistry*, 100(6):877–886, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maruani:2004:OIP

[Mar04b] Jean Maruani. Obituary: Ilya Prigogine (1917–2003). *International Journal of Quantum Chemistry*, 99(4):183–184, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:2005:NGI

[Mar05a] N. H. March. Next generation of ab initio energy density functionals: Thoughts and facts from solvable models. *International Journal of Quantum Chemistry*, 101(5):494–505, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:2005:RDF

[Mar05b] N. H. March. Relativistic density functional theory posed in terms of difference equations. *International Journal of Quantum Chemistry*, 105(6):701–708, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marmorino:2005:LBW

[Mar05c] M. G. Marmorino. Lower bounds to the Weizsäcker energy. *International Journal of Quantum Chemistry*, 104(6):880–884, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:2006:QSC

[Mar06a] N. H. March. Quantum statistics of charged particles and fingerprints of Wigner crystallization in D dimensions. *International Journal of Quantum Chemistry*, 106(15):3032–3042, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maroulis:2006:CBD

[Mar06b] George Maroulis. Comment on "B3LYP density functional study on spectroscopic properties of CuO^- and CuS^-". *International Journal of Quantum Chemistry*, 106(7):1721, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [MBD05].

March:2007:IDD

[Mar07a] N. H. March. The idempotent Dirac density matrix as a functional of the diagonal ground-state electron density obtained from diffraction experiments. *International Journal of Quantum Chemistry*, 107(15):3266–3271, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marmorino:2007:NLB

[Mar07b] M. G. Marmorino. New lower bound formula from the local energy. *International Journal of Quantum Chemistry*, 107(7): 1543–1547, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marmorino:2008:CCM

[Mar08] M. G. Marmorino. Comment on the connected-moments polynomial approach. *International Journal of Quantum Chemistry*, 108(7):1304–1307, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:2009:RBM

[Mar09] N. H. March. The relation between magnetization and internal energy for ferromagnets Fe, Ni, and electron-doped In_2O_3 : Cr, antiferromagnetically ordered $ZnCu_3$ $(OH)_6Cl_2$, and the layered material κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl. *International Journal of Quantum Chemistry*, 109(15):3819–3826, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marrouni:2008:TSI

[MARK08] Karim El Marrouni, Hakima Abou-Rachid, and Serge Kaliaguine. Theoretical study of ignition reactions of linear symmetrical monoethers as potential diesel fuel additives: DFT calculations. *International Journal of Quantum Chemistry*, 108(1):40–50, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Massa:2002:NSA

[Mas02] Lou Massa. A note suggesting an approximation for the Hohenberg and Kohn functional. *International Journal of Quantum Chemistry*, 90(1):291–293, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Masamura:2004:IIE

[Mas04] M. Masamura. Intermolecular interaction energies for deprotonated complexes. *International Journal of Quantum Chemistry*, 100(1):28–40, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Montgomery:2007:DCD

[MAS07] H. E. Montgomery, Jr., N. A. Aquino, and K. D. Sen. Degeneracy of confined D-dimensional harmonic oscillator. *International Journal of Quantum Chemistry*, 107(4):798–806, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mizuno:2009:ILD

[MAS09] Masataka Mizuno, Hideki Araki, and Yasuharu Shirai. Investigation of lattice defects in $LaNi_5$ by positron annihilation spectroscopy and first-principles calculations. *International Journal of Quantum Chemistry*, 109(12):2758–2763, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matar:2000:LSD

[Mat00] S. F. Matar. Local spin density functional investigations of the chemical bonding and of the magnetism in some uranium ternary intermetallic systems: How physics and chemistry can meet in the solid state. *International Journal of Quantum Chemistry*, 77(5):911–926, ????

2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/71000342/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000342/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000342&PLACEBO=IE.pdf.

Matamala:2002:DCQ

[Mat02a] Adelio R. Matamala. Discrete and continuum quantum states for the Kratzer oscillator. *International Journal of Quantum Chemistry*, 89(3):129–134, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mathar:2002:MCT

[Mat02b] Richard J. Mathar. Mutual conversion of three flavors of Gaussian type orbitals. *International Journal of Quantum Chemistry*, 90(1):227–243, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Mat10].

Mathar:2007:TFD

[Mat07] Richard J. Mathar. Table of Feynman diagrams of the interacting Fermion Green's function. *International Journal of Quantum Chemistry*, 107(10):1975–1984, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mathar:2010:EMC

[Mat10] Richard J. Mathar. Erratum: Mutual conversion of three flavors of Gaussian type orbitals. *International Journal of Quantum Chemistry*, 110(4):962, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Mat02b].

Mavridis:2005:P

[Mav05] Aristides Mavridis. Preface. *International Journal of Quantum Chemistry*, 104(4):381, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mayer:2002:HFM

[May02a] I. Mayer. Hermitian Fock matrix in the chemical Hamiltonian approach: Fulfilling Löwdin's prediction. *International Journal of Quantum Chemistry*, 90(1):89–91, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mayer:2002:LMS

[May02b] I. Mayer. On Löwdin's method of symmetric orthogonalization. *International Journal of Quantum Chemistry*, 90(1): 63–65, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mayer:2004:IBP

[May04] I. Mayer. Interrelations between the a priori and a posteriori BSSE correction schemes. *International Journal of Quantum Chemistry*, 100(4):559–566, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

May:2006:OSD

[May06] Volkhard May. Open system dynamics approach to polyatomic molecules: Excitons in chromophore complexes. *International Journal of Quantum Chemistry*, 106(15):3056–3070, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mondal:2000:PDC

[MB00] Chandan Kumar Mondal and S. P. Bhattacharyya. Photodetachment dynamics of closed-shell anions: Effects of perturbation by a strong neighboring dipole. *International Journal of Quantum Chemistry*, 79(3):178–189, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72508369/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72508369/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72508369&PLACEBO=IE.pdf`.

Mainardi:2001:SSB

[MB01a] Daniela S. Mainardi and Perla B. Balbuena. Surface segregation in bimetallic nanoclusters: Geometric and thermodynamic effects. *International Journal of Quantum Chemistry*, 85(4–5):580–591, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mondal:2001:QHL

[MB01b] Chandan Kumar Mondal and S. P. Bhattacharyya. Quantum hysteresis loops in coupled two-dimensional microscopic systems: Loop area and energy dissipation. *In-*

ternational Journal of Quantum Chemistry, 83(1):11–21, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/79502658/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/79502658/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=79502658&PLACEBO=IE.pdf`.

Modal:2002:TDF

[MB02a] Chandan Kumar Modal and S. P. Bhattacharyya. Time-dependent Fourier grid Hamiltonian method for studying the curve crossing dynamics: Dynamics of predissociation of NaI. *International Journal of Quantum Chemistry*, 88(3):310–316, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mukhopadhyay:2002:BSO

[MB02b] S. Mukhopadhyay and K. Bhattacharyya. Bound states of oscillators in infinite and finite domains: A semiclassical study. *International Journal of Quantum Chemistry*, 86(4):330–341, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86510684/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86510684/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86510684&PLACEBO=IE.pdf`.

Mukhopadhyay:2004:EAW

[MB04] S. Mukhopadhyay and K. Bhattacharyya. Error in an approximate wave function and an error minimization scheme. *International Journal of Quantum Chemistry*, 96(5):492–500, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maji:2005:QDS

[MB05a] Kaushik Maji and S. P. Bhattacharyya. Quantum dynamics of a system of coupled nonlinear oscillators: Spectral and information entropy-based analysis. *International Journal of Quantum Chemistry*, 105(2):101–107, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maji:2005:QDR

[MB05b] Kaushik Maji and S. P. Bhattacharyya. Quantum dynamics of relaxation of a pair of coupled Morse oscillators: Effects of mass and electrical asymmetries. *International Journal of Quantum Chemistry*, 104(6):894–902, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mukhopadhyay:2005:CSM

[MB05c] S. Mukhopadhyay and K. Bhattacharyya. Confined systems and the modified virial theorem from semiclassical considerations. *International Journal of Quantum Chemistry*, 101(1): 27–32, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marenich:2006:EMC

[MB06] Aleksandr V. Marenich and James E. Boggs. Equation-of-motion coupled-cluster study of Jahn–Teller effect in X^2E $CF_3O^{\cdot}$ and $CF_3S^{\cdot}$. *International Journal of Quantum Chemistry*, 106(13):2609–2616, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marmorino:2007:ALB

[MB07a] M. G. Marmorino and Ryan W. Bauernfeind. Approximate lower bounds of the Weinstein and Temple variety. *International Journal of Quantum Chemistry*, 107(6):1405–1414, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maruani:2007:ECR

[MB07b] Jean Maruani and Christiane Bonnelle. Electron cross relaxation as a function of single relaxation contributions in double-core ionization energies and spin–orbit splitting of atoms from Ar to Ba. I. $1s^-$ $2p^-$ double-core holes. *International Journal of Quantum Chemistry*, 107(14):2716–2729, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martinez:2004:TSB

[MBA+04] Ramón Martínez, Felipe Brito, Mary Lorena Araujo, Fernando Ruette, and Aníbal Sierraalta. Theoretical study of beryllium (II) complexes using CATIVIC: New parametric method. *International Journal of Quantum Chemistry*, 97

(4):854–864, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moreira:2008:CST

[MBA+08] Rafael Y. O. Moreira, Davi S. B. Brasil, Cláudio N. Alves, Giselle M. S. P. Guilhon, Lourivaldo S. Santos, Mara S. P. Arruda, Adolfo H. Müller, Patrícia S. Barbosa, Alcicley S. Abreu, Edilene O. Silva, Victor M. Rumjanek, Jaime Souza, Jr., Albérico B. F. da Silva, and Regina H. de A. Santos. Crystal structure and theoretical calculations of Julocrotine, a natural product with antileishmanial activity. *International Journal of Quantum Chemistry*, 108(3):513–520, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Midda:2005:BDF

[MBD05] S. Midda, N. C. Bera, and A. K. Das. B3LYP density functional study on spectroscopic properties of CuO^- and CuS^-. *International Journal of Quantum Chemistry*, 105(1):43–47, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [Mar06b].

Mondal:2009:SSC

[MBD09] Bhaskar Mondal, Narayan C. Bera, and Abhijit K. Das. Stability, spectroscopic constants, and dissociation of CO^{2+}: A theoretical study. *International Journal of Quantum Chemistry*, 109(3):469–476, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Molder:2001:QCC

[MBK01] U. Mölder, P. Burk, and I. A. Koppel. Quantum chemical calculations of geometries and gas-phase deprotonation energies of linear polyyne chains. *International Journal of Quantum Chemistry*, 82(2):73–85, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/77502750/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/77502750/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=77502750&PLACEBO=IE.pdf`.

Mandal:2004:CRG

[MBM04] Bholanath Mandal, Manas Banerjee, and Asok K. Mukherjee. Cardinalities of reciprocal graphs. *International Journal of Quantum Chemistry*, 99(3):119–126, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mandal:2005:CCP

[MBM05] Bholanath Mandal, Manas Banerjee, and Asok K. Mukherjee. Construction of characteristic polynomial of reciprocal graphs from the number of pendant vertices. *International Journal of Quantum Chemistry*, 101(2):119–126, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mendizabal:2009:TSE

[MBOA09] Fernando Mendizabal, Darwin Burgos, and Claudio Olea-Azar. Theoretical study of electronic spectra of [Pt_3 (μ-CO)$_3$ (CO)$_3$] ($n = 3--5$) complexes. *International Journal of Quantum Chemistry*, 109(3):477–482, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martinez:2004:ESE

[MBOL04] A. Martinez, F. Bogar, P. Otto, and J. Ladik. Effect of static electric field on the HF band structure of a guanine stack. *International Journal of Quantum Chemistry*, 99(5):833–840, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mukhopadhyay:2001:WSQ

[MBP01] S. Mukhopadhyay, K. Bhattacharyya, and R. K. Pathak. Wilson–Sommerfeld quantization rule revisited. *International Journal of Quantum Chemistry*, 82(3):113–125, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/77004284/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/77004284/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=77004284&PLACEBO=IE.pdf`.

Mankovsky:2003:TDI

[MBP03] S. V. Man'kovsky, D. Baldomir, and M. Pereiro. Thickness-dependent interface magnetism of Fe/Cr/Fe trilayers. *International Journal of Quantum Chemistry*, 91(2):234–238, ????

2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mitroy:2007:CWC

[MBR07] J. Mitroy, M. W. J. Bromley, and K. Ratnavelu. Convergence of an s-wave calculation of the He ground state. *International Journal of Quantum Chemistry*, 107(4):907–920, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maciel:2007:APE

[MBRA07] Glauciete S. Maciel, Ana Carla P. Bitencourt, Mirco Ragni, and Vincenzo Aquilanti. Alkyl peroxides: Effect of substituent groups on the torsional mode around the O — O bond. *International Journal of Quantum Chemistry*, 107(14):2697–2707, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mota:2005:AAZ

[MBRS05] Claudio J. A. Mota, Daniel L. Bhering, and Alejandro Ramírez-Solís. Activation of alkanes on zeolites: A DFT study of hydride abstraction and dehydrogenation on extra-framework aluminum species. *International Journal of Quantum Chemistry*, 105(2):174–185, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malinovskaya:2000:RCT

[MC00] S. A. Malinovskaya and L. S. Cederbaum. The role of coherence and time in the mechanism of dynamical symmetry breaking and localization. *International Journal of Quantum Chemistry*, 80(4–5):950–957, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505379/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505379/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505379&PLACEBO=IE.pdf`.

Mennucci:2003:IMP

[MC03] Benedetta Mennucci and Roberto Cammi. Ab initio model to predict NMR shielding tensors for solutes in liquid crystals. *International Journal of Quantum Chemistry*, 93(2):121–130,

???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martin:2006:DTN

[MC06a] Bodo Martin and Timothy Clark. Dispersion treatment for NDDO-based semiempirical MO techniques. *International Journal of Quantum Chemistry*, 106(5):1208–1216, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mota:2006:AEC

[MC06b] G. V. S. Mota and F. L. P. Costa. Application of the equivalent-core calculation to the Cl in core level on condensed $SiCl_4$. *International Journal of Quantum Chemistry*, 106(13): 2747–2751, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morbec:2008:OPT

[MC08] J. M. Morbec and K. Capelle. Orbital-polarization terms: From a phenomenological to a first-principles description of orbital magnetism in density-functional theory. *International Journal of Quantum Chemistry*, 108(13):2433–2441, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mora:2008:IDC

[MCC08] Jose R. Mora, Tania Cordova, and Gabriel Chuchani. Ab initio and DFT calculations of benzaldoxime elimination kinetics in the gas phase. *International Journal of Quantum Chemistry*, 108(10):1735–1741, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mu:2008:TMV

[MCF08] Wei-Hua Mu, Gregory Adam Chasse, and De-Cai Fang. Test and modification of the van der Waals' radii employed in the default PCM model. *International Journal of Quantum Chemistry*, 108(9):1422–1434, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malaspina:2009:IAM

[MCF09] Thaciana Malaspina, Luciano T. Costa, and Eudes E. Fileti. Ab initio analysis of monomers and dimers of trialkylphos-

phine oxides: Structural and thermodynamic stability. *International Journal of Quantum Chemistry*, 109(2):250–258, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Molawi:2002:LRD

[MCH02] Kian Molawi, Aron J. Cohen, and Nicholas C. Handy. Left–right and dynamic correlation. *International Journal of Quantum Chemistry*, 89(2):86–93, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

McKinney:2004:TDI

[McK04] Paul Caylor McKinney. Two deltons: An inseparable Schrödinger equation. *International Journal of Quantum Chemistry*, 98(3):291–298, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mateos-Cortes:2002:HMI

[MCLKC02] S. Mateos-Cortés, E. Ley-Koo, and S. A. Cruz. Hydrogen molecular ion inside penetrable prolate spheroidal boxes: Electronic and vibrational properties. *International Journal of Quantum Chemistry*, 86(4):376–389, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/88011408/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88011408/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88011408&PLACEBO=IE.pdf`.

Mora:2005:ABM

[MCN+05] M. Mora, M. E. Castro, A. Niño, F. J. Melendez, and C. Muñoz-Caro. Analysis of B3LYP and MP2 conformational population distributions in *trans*-nicotine, acetylcholine, and ABT-594. *International Journal of Quantum Chemistry*, 103 (1):25–33, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marin:2003:SMS

[MCR03] J. L. Marin, G. Campoy, and R. Riera. Simple model to study some properties of H trapped in solids. *International Journal of Quantum Chemistry*, 93(4):271–274, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Montanari:2006:IEC

[MCZWD06] B. Montanari, B. Civalleri, C. M. Zicovich-Wilson, and R. Dovesi. Influence of the exchange-correlation functional in all-electron calculations of the vibrational frequencies of corundum (α-Al_2O_3). *International Journal of Quantum Chemistry*, 106(7):1703–1714, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morozov:2002:MVI

[MD02] V. A. Morozov and Y. M. Dubina. Modeling of vibronic interaction and chaotic dynamics in electronic and nuclear subsystems of molecules. *International Journal of Quantum Chemistry*, 88(5):564–569, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Midda:2004:SCM

[MD04] S. Midda and A. K. Das. Spectroscopic constants and molecular properties of CN^-, SiH^-, PO^-, SO^-, SF^-, and SiS^-: Density functional study. *International Journal of Quantum Chemistry*, 98(5):447–455, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matanovic:2006:AVS

[MD06] I. Matanović and N. Došlić. Anharmonic vibrational spectra of acetylacetone. *International Journal of Quantum Chemistry*, 106(6):1367–1374, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mborong:2008:POD

[MD08] V. B. Mborong and A. M. Dikandé. Polarons in one-dimensional molecular chains with intermolecular and intramolecular vibrations. *International Journal of Quantum Chemistry*, 108(1):189–197, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mandal:2005:CUP

[MDBM05] Bholanath Mandal, Kakali Datta, Manas Banerjee, and Asok K. Mukherjee. Construction and utilisation of planar graphs of two series of IPR fullerenes through the use of threefold rotational symmetry. *International Journal of Quantum Chemistry*, 105(3):201–208, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Motiu:2007:RPH

[MDG07] Stefan Motiu, Daniela Dogaru, and Valentin Gogonea. Reactivation pathway of the hydrogenase H-cluster: Density functional theory study. *International Journal of Quantum Chemistry*, 107(5):1248–1252, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Michelini:2001:DFS

[MDJ01] M. C. Michelini, R. Pis Diez, and A. H. Jubert. Density functional study of small Ni_n clusters, with $n = 2 - 6, 8$, using the generalized gradient approximation. *International Journal of Quantum Chemistry*, 85(1):22–33, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/83002310/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/83002310/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=83002310&PLACEBO=IE.pdf`.

Miguel:2003:DSE

[MdlV03] Beatriz Miguel and José Manuel García de la Vega. DFT study of the electronic structure and Jahn–Teller effect of tetrabromomethane cation. *International Journal of Quantum Chemistry*, 91(3):414–417, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morozov:2004:MQC

[MDS04] V. A. Morozov, Y. M. Dubina, and P. P. Shorygin. Mixed quantum–classic intramolecular dynamics at light transformation by molecules. *International Journal of Quantum Chemistry*, 96(3):226–233, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martins:2009:TIC

[MDS+09] João B. L. Martins, Jussara A. Durães, Maria J. A. Sales, Alessandra F. A. Vilela, Geraldo Magela e Silva, and Ricardo Gargano. Theoretical investigation of carotenoid ultraviolet spectra. *International Journal of Quantum Chemistry*, 109(4):739–745, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mintz:2007:TCC

[MDSW07] Benjamin Mintz, Sage Driskell, Amy Shah, and Angela K. Wilson. Truncation of the correlation consistent basis sets: Application to extended systems. *International Journal of Quantum Chemistry*, 107(15):3077–3088, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meissner:2008:CCC

[Mei08] Leszek Meissner. Coupled-cluster corrected MR-CISD method with noniterative evaluation of connected triples. *International Journal of Quantum Chemistry*, 108(12):2199–2210, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mendizabal:2008:TSE

[Men08a] Fernando Mendizabal. Theoretical study of the electronic spectra of bi- and tri-heteronuclear platinum complexes. *International Journal of Quantum Chemistry*, 108(6):1164–1172, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Molina:2008:QSA

[MEN+08b] Enrique Molina, Ernesto Estrada, Delvin Nodarse, Luis A. Torres, Humberto González, and Eugenio Uriarte. Quantitative structure-antibacterial activity relationship modeling using a combination of piecewise linear regression-discriminant analysis (I): Quantum chemical, topographic, and topological descriptors. *International Journal of Quantum Chemistry*, 108(10):1856–1871, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Merzel:2004:MES

[Mer04] Franci Merzel. Molecular electronic structure problem solved by numerical one-electron Green's functions. *International Journal of Quantum Chemistry*, 96(6):554–561, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moustafa:2002:ESS

[MESH02] H. Moustafa, K. M. El-Sawy, and Rifaat Hilal. Electronic structure of some adenosine receptor antagonists: I. Equilibrium geometries, charge density distributions, and sub-

stituent effects. *International Journal of Quantum Chemistry*, 87(6):389–399, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/91015780/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91015780/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91015780&PLACEBO=IE.pdf.

Mohanty:2000:PRL

[MET00] D. Mohanty, R. Elber, and D. Thirumalai. Probing the role of local propensity in peptide turn formation. *International Journal of Quantum Chemistry*, 80(4–5):1125–1128, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505427/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505427/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505427&PLACEBO=IE.pdf.

Metropoulos:2005:GCI

[Met05] Aristophanes Metropoulos. Generation of the $C_2H_3O^+$ ion in reactions of $O(^3P)$ with 2-butyne. *International Journal of Quantum Chemistry*, 104(4):482–485, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moustafa:2002:EGG

[METSH02] H. Moustafa, S. El-Taher, M. F. Shibl, and Rifaat Hilal. Equilibrium geometry and gas-phase proton affinity of 2-thiouracil derivatives. *International Journal of Quantum Chemistry*, 87(6):378–388, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/91015490/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91015490/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91015490&PLACEBO=IE.pdf.

Meyer:2000:ISF

[Mey00] Michael Meyer. Ab initio study of flavonoids. *International Journal of Quantum Chemistry*, 76(6):724–732, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70001598/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70001598/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70001598&PLACEBO=IE.pdf.

Melin:2003:AEL

[MF03] Junia Melin and P. Fuentealba. Application of the electron localization function to radical systems. *International Journal of Quantum Chemistry*, 92(4):381–390, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mezey:2000:TSD

[MFA00] Paul G. Mezey, Kenichi Fukui, and Shigeru Arimoto. Treatment of small deformations of polyhedral shapes of functional group distributions in biomolecules. *International Journal of Quantum Chemistry*, 76(6):756–761, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70001601/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70001601/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70001601&PLACEBO=IE.pdf.

Moreira:2007:HSC

[MFR07] I. S. Moreira, P. A. Fernandes, and M. J. Ramos. Hot spot computational identification: Application to the complex formed between the hen egg white lysozyme (HEL) and the antibody HyHEL-10. *International Journal of Quantum Chemistry*, 107(2):299–310, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Makarewicz:2005:EGD

[MG05] J. Makarewicz and V. N. Glushkov. Efficient generation of distributed spherical Gaussian basis sets for molecules. *International Journal of Quantum Chemistry*, 102(4):353–367, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohri:2008:MOE

[MG08] Fumihito Mohri and Alexander A. Granovsky. A molecular orbital explanation for the B N bond shortening in H_3BNH_3 on going from the gaseous to the solid state. *International*

Journal of Quantum Chemistry, 108(3):544–557, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Munoz-Garcia:2009:FPS

[MGAS09] Ana Belén Muñoz-García, Eduardo Anglada, and Luis Seijo. First-principles study of the structure and the electronic structure of yttrium aluminum garnet $Y_3Al_5O_{12}$. *International Journal of Quantum Chemistry*, 109(9):1991–1998, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mihaylov:2006:TSS

[MGB+06] Tzvetan Mihaylov, Ivelina Georgieva, Günther Bauer, Irena Kostova, Ilia Manolov, and Natasha Trendafilova. Theoretical study of the substituent effect on the intramolecular hydrogen bonds in di(4-hydroxycoumarin) derivatives. *International Journal of Quantum Chemistry*, 106(6):1304–1315, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martin:2000:ANB

[MGC00] Bodo Martin, Peter Gedeck, and Timothy Clark. Additive NDDO-based atomic polarizability model. *International Journal of Quantum Chemistry*, 77(1):473–497, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004291/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004291/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004291&PLACEBO=IE.pdf`.

Machado:2001:ICX

[MGCD01] Francisco B. C. Machado, Tapan K. Ghanty, Subhas Chakravorty, and Ernest R. Davidson. Ab initio calculations on XF_n^q (X = I, Xe, Cs, and Ba; $n = 1, 2, 4,$ and6; $q = -1, 0, +1,$ and + 2) molecules. *International Journal of Quantum Chemistry*, 81(3):238–245, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76504672/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76504672/`

FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76504672&PLACEBO=IE.pdf.

MagelaeSilva:2008:QMC

[MGdS+08] Geraldo Magela e Silva, Ricardo Gargano, Washington B. da Silva, Luiz F. Roncaratti, and Paulo H. Acioli. Quantum Monte Carlo and genetic algorithm study of the potential energy surface of the H molecule. *International Journal of Quantum Chemistry*, 108(13):2318–2325, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meza:2005:LHP

[MGG05] Rocío Meza, Bárbara Gordillo, and Marcelo Galván. Local HSAB principle in the conjugate addition of *p*-substituted thiophenols to cyclohexenone. *International Journal of Quantum Chemistry*, 104(1):29–37, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malinovskaya:2009:OPT

[MGK+09] S. V. Malinovskaya, A. V. Glushkov, O. Yu. Khetselius, A. A. Svinarenko, E. V. Mischenko, and T. A. Florko. Optimized perturbation theory scheme for calculating the interatomic potentials and hyperfine lines shift for heavy atoms in the buffer inert gas. *International Journal of Quantum Chemistry*, 109(14):3325–3329, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morales-Guzman:2001:HFQ

[MGMP01] J. D. Morales-Guzmán, J. Morales, and J. J. Peña. Hamiltonian factorization on the quantum phase space. *International Journal of Quantum Chemistry*, 85(4–5):239–243, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mora:2004:OPA

[MGMR04] M. A. Mora, Laura Galicia, and M. A. Mora-Ramirez. Oxidative polymerization of 5 amino,1,10-phenanthroline: A theoretical study. *International Journal of Quantum Chemistry*, 97(6):983–991, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mora:2000:ESC

[MGV00] M. A. Mora, Laura Galicia, and Humberto Vázquez. Electronic structure and conformation of aniline and metachloroaniline dimers. *International Journal of Quantum Chemistry*, 78(2):99–111, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71005517/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71005517/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71005517&PLACEBO=IE.pdf`.

Michalkova:2004:TSA

[MGZL04] A. Michalkova, L. Gorb, O. A. Zhikol, and J. Leszczynski. Theoretical study of adsorption of methyl tert-butyl ether on the substituted tetrahedral surface of dickite. *International Journal of Quantum Chemistry*, 100(5):818–831, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mayer:2003:IEE

[MH03] I. Mayer and A. Hamza. Interatomic exchange energy components. *International Journal of Quantum Chemistry*, 92 (2):174–180, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mayer:2005:ADI

[MH05] I. Mayer and A. Hamza. Atomic decomposition of identity: General formalism for population analysis and energy decomposition. *International Journal of Quantum Chemistry*, 103 (6):798–807, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mineva:2006:OHT

[MH06] Tzonka Mineva and Thomas Heine. Orbital hardness tensors from hydrogen through xenon from Kohn–Sham perturbed orbitals. *International Journal of Quantum Chemistry*, 106 (6):1396–1405, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

McBride:2009:DIM

[MH09] Kendra L. McBride and John D. Head. DFT investigation of MoS_2 nanoclusters used as desulfurization catalysts. *International Journal of Quantum Chemistry*, 109(15):3570–3582, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

McClellan:2005:ATH

[MHB05] Joshua J. McClellan, Thomas F. Hughes, and Rodney J. Bartlett. Application of the transfer Hamiltonian formalism to high-energy model systems. *International Journal of Quantum Chemistry*, 105(6):914–920, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mazurkiewicz:2007:CEE

[MHGR07] Kamil Mazurkiewicz, Maciej Harańczyk, Maciej Gutowski, and Janusz Rak. Can an excess electron localize on a purine moiety in the adenine–thymine Watson–Crick base pair? A computational study. *International Journal of Quantum Chemistry*, 107(12):2224–2232, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matsumoto:2007:TDW

[MHI+07] D. Matsumoto, K. Hayashi, T. Ida, M. Mizuno, K. Endo, and K. Nishikawa. Two-dimensional wavepacket dynamics with quantum hydrodynamics. *International Journal of Quantum Chemistry*, 107(15):3169–3177, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Muhlhauser:2004:ESL

[MHP04] Max Mühlhäuser, Jan Haubrich, and Sigrid D. Peyerimhoff. The electronic spectrum of linear HC_9H^+. *International Journal of Quantum Chemistry*, 100(1):53–58, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maruyama:2008:IIH

[MHT+08] Youhei Maruyama, Kenta Hongo, Masanori Tachikawa, Yoshiyuki Kawazoe, and Hiroshi Yasuhara. Ab initio interpretation of Hund's rule for the methylene molecule: Variational optimization of its molecular geometries and energy component analysis. *International Journal of Quantum Chemistry*,

108(4):731–743, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mayer:2000:QMT

[MHV00] Alexandre Mayer, Mark J. Hagmann, and Jean-Pol Vigneron. Quantum mechanical theory of electronic photon-stimulated field emission by transfer matrices and Green's functions. *International Journal of Quantum Chemistry*, 80(4–5):816–823, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505390/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505390/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505390&PLACEBO=IE.pdf`.

March:2003:RPC

[MHV03] N. H. March, I. A. Howard, and V. E. Van Doren. Recent progress in constructing nonlocal energy density functionals. *International Journal of Quantum Chemistry*, 92(2):192–204, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Micha:2000:DMT

[Mic00] David A. Micha. Density matrix theory and computational aspects of quantum dynamics in active medium. *International Journal of Quantum Chemistry*, 80(3):394–405, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501018/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501018/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501018&PLACEBO=IE.pdf`.

Micha:2006:DMC

[Mic06a] David A. Micha. Density matrix calculations of gaseous and adsorbate dynamics in electronically excited molecular systems. *International Journal of Quantum Chemistry*, 106(15):3371–3382, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Micha:2006:QDT

[Mic06b] David A. Micha. Quantum dynamics with trajectories. Introduction to quantum hydrodynamics. *International Journal*

of Quantum Chemistry, 106(7):1720, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Micha:2009:CRG

[Mic09] David A. Micha. Chemical reactions in the gas phase and in condensed matter: From wavefunctions to density operators. *International Journal of Quantum Chemistry*, 109(13):2937–2942, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Minikis:2000:TGT

[MJ00] Ryan M. Minikis and Jan H. Jensen. Toward a general theory of hydrogen bonding: A study of hydrogen bonds involving H_2 O and HF. *International Journal of Quantum Chemistry*, 76(3):341–358, January 20, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000278/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000278/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000278&PLACEBO=IE.pdf`.

Muniz:2006:HMC

[MJ06] E. P. Muniz and F. E. Jorge. HF and MP2 calculations on CN^-, N_2, AlF, SiO, PN, SC, ClB, and P_2 using correlated molecular wave functions. *International Journal of Quantum Chemistry*, 106(4):943–951, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Michalkova:2005:TSA

[MJG+05] A. Michalkova, L. D. Johnson, L. Gorb, O. A. Zhikol, O. V. Shishkin, and J. Leszczynski. Theoretical study of adsorption of methyl tert-butyl ether on broken clay minerals surfaces. *International Journal of Quantum Chemistry*, 105(4):325–340, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mahlmann:2000:ZFS

[MK00] Jürgen Mählmann and Martin Klessinger. Zero-field splitting calculations based on semiempirical MR-CI wave functions. *International Journal of Quantum Chemistry*, 77(1):446–453, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70004288/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004288/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004288&PLACEBO=IE.pdf.

Molnar:2001:TAI

[MK01] Stephen P. Molnar and James W. King. Theory and applications of the integrated molecular transform and the normalized molecular moment structure descriptors: QSAR and QSPR paradigms. *International Journal of Quantum Chemistry*, 85(6):662–675, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85010144/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85010144/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85010144&PLACEBO=IE.pdf.

Molski:2002:GEP

[MK02] Marcin Molski and Jerzy Konarski. A generalized expansion of the potential energy of diatomic molecules. *International Journal of Quantum Chemistry*, 90(1):183–187, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mammino:2008:CSI

[MK08] Liliana Mammino and Mwadham M. Kabanda. A computational study of the interactions of the caespitate molecule with water. *International Journal of Quantum Chemistry*, 108(10):1772–1791, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maruani:2005:AER

[MKCB05] J. Maruani, A. I. Kuleff, D. P. Chong, and C. Bonnelle. Ansatz for the evaluation of the relativistic contributions to core ionization energies in complex molecules involving heavy atoms. *International Journal of Quantum Chemistry*, 104(4):397–410, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malde:2005:GTS

[MKCS05] Alpeshkumar Malde, Santosh Khedkar, Evans Coutinho, and Anil Saran. Geometry, transition states, and vibrational spectra of boron isostere of N-methylacetamide by ab initio calculations. *International Journal of Quantum Chemistry*, 102 (5):734–742, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Misra:2003:IEM

[MKDM03] Anirban Misra, D. J. Klein, Sambhu N. Datta, and N. H. March. Internal energy and magnetic moment of three-dimensional ferromagnets. *International Journal of Quantum Chemistry*, 95(4–5):451–454, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mallick:2009:LDE

[MKHP09] Govind Mallick, Shashi P. Karna, Haiying He, and Ravindra Pandey. Length-dependence of electron transfer coupling matrix in polyene wires: Ab initio molecular orbital theory study. *International Journal of Quantum Chemistry*, 109(6): 1302–1310, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Magnuson:2002:MHC

[MKLP02] Eric C. Magnuson, Jessica Koehler, Gene Lamm, and George R. Pack. $Mg(H_2O)_6^{2+}$–π (cytosine) interactions in a DNA dodecamer. *International Journal of Quantum Chemistry*, 88(1):236–243, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89016143/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89016143/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89016143&PLACEBO=IE.pdf`.

Maximov:2004:LEA

[MKZ04a] S. G. Maximov, L. S. Kuzmenkov, and J. L. Guardado Zavala. Local equilibrium approach for Fermi systems and quantum hydrodynamics. *International Journal of Quantum Chemistry*, 100(4):311–323, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maximov:2004:NOM

[MKZ04b] S. G. Maximov, L. S. Kuzmenkov, and J. L. Guardado Zavala. Nonlinear oscillations in the molecular dimer: Asymptotic solutions. *International Journal of Quantum Chemistry*, 100 (4):324–335, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mitnik:2001:LND

[ML01] Daniel Glossman Mitnik and Alfredo Márquez Lucero. Local and nonlocal density functional calculations of the molecular structure of isomeric thiadiazole monoxides. *International Journal of Quantum Chemistry*, 81(1):105–115, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/75502158/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75502158/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502158&PLACEBO=IE.pdf`.

Marcal:2003:IMT

[ML03] Nei Marçal and Bernardo Laks. Insulator-to-metal transition on polyselenophene. *International Journal of Quantum Chemistry*, 95(3):230–236, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marcal:2005:TIO

[ML05] Nei Marçal and Bernardo Laks. Theoretical investigation of optical properties in oligo(trans-1,2-di(2-thienyl) ethylene). *International Journal of Quantum Chemistry*, 103(5):617–624, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marcal:2008:EOP

[ML08] Nei Marçal and Bernardo Laks. The electronic and optical properties of oligo(trans-1,2-di(2-thienyl)-1,3-butadiene): A theoretical study. *International Journal of Quantum Chemistry*, 108(13):2499–2506, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mladenov:2002:QCS

[Mla02] Ivaïlo M. Mladenov. Quantization on curved surfaces. *International Journal of Quantum Chemistry*, 89(4):248–254, ????

2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maruani:2004:Pa

[MLB04a] Jean Maruani, Roland Lefebvre, and Erkki Brandas. Preface. *International Journal of Quantum Chemistry*, 99(4):179–180, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maruani:2004:Pb

[MLB04b] Jean Maruani, Roland Lefebvre, and Erkki Brandas. Preface. *International Journal of Quantum Chemistry*, 99(5):567–568, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marcal:2006:TCS

[MLD06] Nei Marçal, Bernardo Laks, and Ricardo Paupitz Barbosa Dos Santos. Theoretical conformational study of poly(trans-1, 2-di(2-thienyl) ethylene): Effects on the electronic structure and optical properties. *International Journal of Quantum Chemistry*, 106(13):2723–2730, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mishra:2000:NOS

[MLL00] Rama K. Mishra, Ying-Ting Lin, and Shyi-Long Lee. Nonlinear optical study of the five IPR isomers of C_{78} generated by capping C_{72} through C_6. *International Journal of Quantum Chemistry*, 77(2):574–579, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70002217/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70002217/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70002217&PLACEBO=IE.pdf`.

Mishra:2001:CDF

[MLL01] Rama K. Mishra, Ying-Ting Lin, and Shyi-Long Lee. C_{28} (D_2): Fullerene growth mechanism. *International Journal of Quantum Chemistry*, 84(6):642–648, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85008258/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85008258/FILE?TPL=ftx_start;`

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85008258&PLACEBO=IE.pdf.

Murray:2007:PNT

[MLP07] Jane S. Murray, Pat Lane, and Peter Politzer. A predicted new type of directional noncovalent interaction. *International Journal of Quantum Chemistry*, 107(12):2286–2292, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Murray:2008:SHH

[MLP08] Jane S. Murray, Pat Lane, and Peter Politzer. Simultaneous σ-hole and hydrogen bonding by sulfur- and selenium-containing heterocycles. *International Journal of Quantum Chemistry*, 108(15):2770–2781, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meunier:2006:DFT

[MLSB06] Vincent Meunier, Wenchang Lu, Bobby G. Sumpter, and Jerry Bernholc. Density functional theory studies of quantum transport in molecular systems. *International Journal of Quantum Chemistry*, 106(15):3334–3342, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mignon:2004:FAV

[MLSG04] Pierre Mignon, Stefan Loverix, Jan Steyaert, and Paul Geerlings. Functional assessment of "in vivo" and "in silico" mutations in the guanine binding site of RNase T_1: A DFT study. *International Journal of Quantum Chemistry*, 99(1): 53–58, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malolepsza:2009:CGE

[MLW+09] Edyta Małolepsza, Yuan-Pern Lee, Henryk A. Witek, Stephan Irle, Chun-Fu Lin, and Horng-Ming Hsieh. Comparison of geometric, electronic, and vibrational properties for all pentagon/hexagon-bearing isomers of fullerenes C_{38}, C_{40}, and C_{42}. *International Journal of Quantum Chemistry*, 109(9): 1999–2011, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meng:2006:DFS

[MLZS06] Qingxi Meng, Ming Li, Jinsheng Zhang, and Wei Shen. Density function studies on the $PtCl_2$-catalyzed asymmetric cycloisomerization reaction of hydroxylated enynes. *International Journal of Quantum Chemistry*, 106(7):1569–1579, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Markovits:2002:TIZ

[MM02] A. Markovits and C. Minot. Theoretical investigation of the Ziegler–Natta catalysis in heterogeneous conditions. *International Journal of Quantum Chemistry*, 89(4):389–396, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mitin:2007:IBS

[MM07] Alexander V. Mitin and Kenneth M. Merz, Jr. An improved 6-31G basis set for atoms Ga through Kr. *International Journal of Quantum Chemistry*, 107(15):3028–3038, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [MM09].

Mitin:2009:EIB

[MM09] Alexander V. Mitin and Kenneth M. Merz, Jr. Erratum: An improved 6-31G* basis set for atoms Ga through Kr. *International Journal of Quantum Chemistry*, 109(5):1158, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [MM07].

Mondal:2003:SAC

[MMB03] Chandan Kumar Mondal, Kaushik Maji, and S. P. Bhattacharyya. Simple approach to computing tunneling time: Test cases. *International Journal of Quantum Chemistry*, 94 (2):57–64, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martinez-Magadan:2002:EQM

[MMCC02] J. M. Martínez-Magadán, A. Cuán, and M. Castro. An embedded QM/MM study for different SiO_2 /Al_2O_3 ratios of the HZSM-5 zeolite and for their interaction with *n*-heptane. *International Journal of Quantum Chemistry*, 88(6):750–766,

???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Minaev:2009:QCS

[MME09] Boris F. Minaev, Valentina A. Minaeva, and Yurij V. Evtuhov. Quantum-chemical study of the singlet oxygen emission. *International Journal of Quantum Chemistry*, 109(3):500–515, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Montero:2000:MMH

[MMF00] Luis A. Montero, José Molina, and Jürgen Fabian. Multiple minima hypersurfaces of water clusters for calculations of association energy. *International Journal of Quantum Chemistry*, 79(1):8–16, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72504316/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72504316/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72504316&PLACEBO=IE.pdf`.

Mercero:2002:AII

[MML+02] Jose M. Mercero, Jon M. Matxain, Xabier Lopez, Joseph E. Fowler, and Jesus M. Ugalde. Aluminum (III) interactions with the side chains of aromatic aminoacids. *International Journal of Quantum Chemistry*, 90(2):859–881, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malbouisson:2006:OEP

[MMM06] L. A. C. Malbouisson, M. G. R. Martins, and N. Makiuchi. One-electron properties using a CI method based on multiple Hartree–Fock solutions. *International Journal of Quantum Chemistry*, 106(13):2772–2778, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morishita:2009:P

[MMOM09] Masao Morishita, Yasuji Muramatsu, Kazuyoshi Ogasawara, and Masahiko Morinaga. Preface. *International Journal of Quantum Chemistry*, 109(12):2639, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mercero:2004:FSS

[MMR+04] Jose M. Mercero, Jon M. Matxain, Elixabete Rezabal, Xabier Lopez, and Jesus M. Ugalde. The first solvation shell of aluminum (III) and magnesium (II) cations in a protein model environment. *International Journal of Quantum Chemistry*, 98(4):409–424, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Minicozzi:2008:RMA

[MMR+08] V. Minicozzi, S. Morante, G. C. Rossi, F. Stellato, N. Christian, and K. Jansen. The role of metals in amyloid aggregation—Experiments and ab initio simulations. *International Journal of Quantum Chemistry*, 108(11):1992–2015, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maiti:2009:DDF

[MMS+09] Buddhadev Maiti, Patrick M. McLaurin, Raymond Sadeghi, S. Ajith Perera, and Jorge A. Morales. Dynamics for the dynamic Frank Harris: Exploring $H^+ + CF_4$ at $E_{lab} = 20$ and 30 eV. *International Journal of Quantum Chemistry*, 109 (13):3026–3035, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marino:2007:GPI

[MMT+07] T. Marino, D. Mazzuca, M. Toscano, N. Russo, and A. Grand. Gas phase interaction of zinc ion with purine and pyrimidine DNA and RNA bases. *International Journal of Quantum Chemistry*, 107(2):311–317, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martin:2004:ASI

[MMV04] I. Martín, E. Mayor, and A. M. Velasco. Application of spectral intensities through a model potential approach to the prediction of photodissociation rate constants of CFC molecules in the ionosphere. *International Journal of Quantum Chemistry*, 100(6):1003–1013, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martin:2005:MQD

[MMV05a] I. Martín, E. Mayor, and A. M. Velasco. Molecular quantum defect orbital (MQDO) calculation of the photoionization of

CF_3X (X = Br, I): Study of ligand substitution effects. *International Journal of Quantum Chemistry*, 104(4):522–529, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Menendez:2005:SEA

[MMV05b] J. M. Menéndez, I. Martín, and A. M. Velasco. The Stark effect in atomic Rydberg states through a quantum defect approach. *International Journal of Quantum Chemistry*, 102 (5):956–960, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Miric:2002:TSM

[MMZ02] Aleksandra Mirić, Miloš Milčić, and Snežana D. Zarić. Theoretical study of metal ligand aromatic cation-π interactions of $[Co(NH_3)_6]^{3+}$ with benzene. *International Journal of Quantum Chemistry*, 87(6):354–359, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/91015781/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91015781/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91015781&PLACEBO=IE.pdf`.

March:1999:SSC

[MNA+99] N. H. March, L. M. Nieto, C. Amovilli, L. C. Balbás, and M. L. Glasser. Slater sum for central field problems characterized by its s-wave component alone. *Journal of Mathematical Physics*, 40(6):2671–2679, June 1999. CODEN JMAPAQ. ISSN 0022-2488 (print), 1089-7658 (electronic), 1527-2427. URL `http://jmp.aip.org/resource/1/jmapaq/v40/i6/p2671_s1`.

Medved:2005:LNP

[MNJP05] Miroslav Medveď, Jozef Noga, Denis Jacquemin, and Eric A. Perpète. Longitudinal NLO properties of C_2H_2, HCCF, and C_2F_2: Electron correlation and vibration effects. *International Journal of Quantum Chemistry*, 102(2):209–223, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maniero:2002:PTP

[MNMV02] A. M. Maniero, J. F. Rocha Neto, L. A. C. Malbouisson, and J. D. M. Vianna. Partitioning technique proce-

dure revisited: Application to many-electron systems using the Møller–Plesset Hamiltonian. *International Journal of Quantum Chemistry*, 90(6):1586–1595, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matveev:2007:LRF

[MNR07] Alexei V. Matveev, Vladimir A. Nasluzov, and Notker Rösch. Linear response formalism for the Douglas–Kroll–Hess approach to the Dirac–Kohn–Sham problem: First- and second-order nuclear displacement derivatives of the energy. *International Journal of Quantum Chemistry*, 107(15):3236–3249, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Milko:2007:ADF

[MNV07] Matúš Milko, Jozef Noga, and Štefan Varga. Accuracy of density fitting in calculation of two-electron repulsion integrals in periodic systems. *International Journal of Quantum Chemistry*, 107(11):2158–2168, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matos:2006:OEA

[MO06] M. Matos and R. B. Oliveira. One-electron approach to describe charge and orbital order in Mn_2OBO_3. *International Journal of Quantum Chemistry*, 106(13):2737–2746, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mendizabal:2002:MMC

[MOA02] Fernando Mendizabal and Claudio Olea-Azar. Metallomacrocycle (MacM) complex with cyanide as bridged ligand: Electronic structures of $[MacMCN]_n$. *International Journal of Quantum Chemistry*, 87(2):89–100, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89014733/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89014733/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89014733&PLACEBO=IE.pdf`.

Mendizabal:2005:TSE

[MOA05] Fernando Mendizabal and Claudio Olea-Azar. Theoretical study of the electronic spectrum of binuclear gold(I) com-

plexes. *International Journal of Quantum Chemistry*, 103(1): 34–44, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mendizabal:2007:TSC

[MOA07] Fernando Mendizabal and Claudio Olea-Azar. Theoretical study in $[C_2H_4–Tl]^+$ and $[C_2H_2–Tl]^+$ complexes. *International Journal of Quantum Chemistry*, 107(1):232–239, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mendizabal:2001:PCB

[MOAB01] Fernando Mendizabal, Claudio Olea-Azar, and Rodolfo Briones. Phthalocyanoiron complex with bridged ligands. Electronic structure of monomers and polymers. *International Journal of Quantum Chemistry*, 82(4):170–181, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/78503191/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/78503191/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=78503191&PLACEBO=IE.pdf`.

Mendizabal:2007:TSI

[MOAM07] Fernando Mendizábal, Claudio Olea-Azar, and Sebastian Miranda. Theoretical study of the interaction d^{10}-d^8 between Pt(0) and M(I) on the $[Pt(PH_3)_3MPH_3]$ complexes (M = Cu, Ag, Au). *International Journal of Quantum Chemistry*, 107 (6):1454–1458, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohamed:2000:CRB

[Moh00] Adel A. Mohamed. Conformations and rotational barriers of 2,2′-bithiazole and 4,4′-dimethyl-2,2′-bithiazole semiemperical, ab initio, and density functional theory calculations. *International Journal of Quantum Chemistry*, 79(6):367–377, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72515275/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72515275/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72515275&PLACEBO=IE.pdf`.

Martinez:2003:CPH

[MOL03] A. Martinez, P. Otto, and J. Ladik. Coupled-perturbed Hartree–Fock theory for quasi–one-dimensional periodic systems: Calculation of static and dynamic nonlinear optical properties of model systems. *International Journal of Quantum Chemistry*, 94(5):251–268, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monkhorst:2000:WQC

[Mon00] Hendrik J. Monkhorst. On the wanderings of a quantum chemist in the world of fusion power and politics. *International Journal of Quantum Chemistry*, 77(1):468–472, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004290/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004290/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004290&PLACEBO=IE.pdf`.

Mondal:2005:PDC

[Mon05] Chandan Kumar Mondal. Photodetachment dynamics from closed-shell anions in the presence of a bichromatic field. *International Journal of Quantum Chemistry*, 103(3):258–266, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mondal:2008:DIP

[Mon08] Chandan Kumar Mondal. Dipole induced photodetachment dynamics of halide anions. *International Journal of Quantum Chemistry*, 108(1):15–24, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monkhorst:2009:MAF

[Mon09] Hendrik J. Monkhorst. My association with Frank Harris: An arc of forty-four years. *International Journal of Quantum Chemistry*, 109(13):2821–2825, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morales:2009:IPS

[MOPdP09] J. Morales, G. Ovando, J. J. Peña, and G. Ares de Parga. Isospectral potentials for the Schrödinger equation with a

position-dependent mass: Free-particle potential model. *International Journal of Quantum Chemistry*, 109(14):3171–3177, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morales:2002:BTE

[Mor02] Daniel A. Morales. Bounds for the total π-electron energy. *International Journal of Quantum Chemistry*, 88(3):317–330, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morales:2003:SSB

[Mor03] Daniel A. Morales. Systematic search of bounds for total π-electron energy. *International Journal of Quantum Chemistry*, 93(1):20–31, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moriwake:2004:FPC

[Mor04] Hiroki Moriwake. First-principles calculation of formation energy of neutral point defects in perovskite-type $BaTiO_3$. *International Journal of Quantum Chemistry*, 99(5):824–827, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morgon:2006:CPA

[Mor06] Nelson H. Morgon. Calculation of proton affinity using the CR-CCSD[T]/ECP method. *International Journal of Quantum Chemistry*, 106(13):2658–2663, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morgon:2008:ACS

[Mor08] Nelson H. Morgon. Application of CCSD(T)/(ECP + GCM) for studying gas-phase electron and proton affinities. *International Journal of Quantum Chemistry*, 108(13):2454–2458, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meissner:2000:DIS

[MP00] Holger Meissner and Josef Paldus. Direct iterative solution of the generalized Bloch equation. V. Application to N_2. *International Journal of Quantum Chemistry*, 80(4–5):782–798, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505401/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505401/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505401&PLACEBO=IE.pdf`.

Makowski:2005:FCJ

[MP05] Marcin Makowski and Marek T. Pawlikowski. Franck–Condon and Jahn–Teller effects in the E state of (CO) molecule. Resonance and preresonance Raman study in terms of time-dependent density functional theory: New insight into an old story. *International Journal of Quantum Chemistry*, 104 (5):589–601, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Makowski:2006:ARN

[MP06] Marcin Makowski and Marek T. Pawlikowski. Absorption, resonance, and near-resonance Raman studies of the tetracyanoquinodimethane neutral and its monoanion in terms of density functional theory and complete active space self-consistent field methods. *International Journal of Quantum Chemistry*, 106(8):1736–1748, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Montero:2008:F

[MP08] Luis A. Montero and Carlos Pérez. Foreword. *International Journal of Quantum Chemistry*, 108(10):1617–1720, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohazab:2009:SAU

[MP09] Ali R. Mohazab and Steven S. Plotkin. Structural alignment using the generalized Euclidean distance between conformations. *International Journal of Quantum Chemistry*, 109(14): 3217–3228, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mracec:2007:NPI

[MPBM07] Maria Mracec, Aurelia Pascariu, Stefan Berger, and Mircea Mracec. New possible ionic structures in Wittig reaction: Analysis of stability and rotation barriers by semiempirical PM3 method. *International Journal of Quantum Chemistry*,

107(8):1782–1793, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Murray:2000:CMS

[MPIP00] Jane S. Murray, Zenaida Peralta-Inga, and Peter Politzer. Computed molecular surface electrostatic potentials of the nonionic and zwitterionic forms of glycine, histidine, and tetracycline. *International Journal of Quantum Chemistry*, 80(6):1216–1223, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/75501736/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75501736/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75501736&PLACEBO=IE.pdf`.

Murray:2001:CCN

[MPIP+01] Jane S. Murray, Zenaida Peralta-Inga, Peter Politzer, Kaushalya Ekanayake, and Pierre LeBreton. Computational characterization of nucleotide bases: Molecular surface electrostatic potentials and local ionization energies, and local polarization energies. *International Journal of Quantum Chemistry*, 83(3-4):245–254, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002593/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002593/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002593&PLACEBO=IE.pdf`.

McEwen:2006:HKF

[MPKB06] J.-S. McEwen, S. H. Payne, H. J. Kreuzer, and C. Bracher. Hopping kinetics on a finite 1D chain: An exact analysis. *International Journal of Quantum Chemistry*, 106(14):2889–2903, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monard:2003:DER

[MPRGLL03] Gérald Monard, Xavier Prat-Resina, Angels González-Lafont, and José M. Lluch. Determination of enzymatic reaction pathways using QM/MM methods. *International Journal of Quantum Chemistry*, 93(3):229–244, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martins:2002:TIS

[MPS+02] Jão B. L. Martins, Marco A. Perez, Carlos H. T. P. Silva, C. A. Taft, M. Arissawa, Elson Longo, P. C. Mello, Fulvia M. L. G. Stamato, and J. G. R. Tostes. Theoretical ab initio study of ranitidine. *International Journal of Quantum Chemistry*, 90 (2):575–586, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Magnasco:2000:NTM

[MR00] Valerio Magnasco and Arnaldo Rapallo. New translation method for STOs and its application to calculation of two-center two-electron integrals. *International Journal of Quantum Chemistry*, 79(2):91–100, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72508335/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72508335/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72508335&PLACEBO=IE.pdf`.

Mujica:2002:PTT

[MRG02] Vladimiro Mujica, Mark A. Ratner, and Osvaldo Goscinski. Partitioning technique and transport across molecular interfaces: Many-body effects. *International Journal of Quantum Chemistry*, 90(1):14–19, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mora:2002:IQM

[MRMR02] M. A. Mora, A. Raya, and M. A. Mora-Ramirez. Ab initio quantum mechanical characterization of platinum, palladium, and nickel complexes of L-ascorbic acid. *International Journal of Quantum Chemistry*, 90(2):882–887, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mendizabal:2006:CSA

[MROA06] Fernando Mendizabal, Dana Reyes, and Claudio Olea-Azar. Complexes self-associate by hydrogen bonding and metallophilic attraction: Theoretical study. *International Journal of Quantum Chemistry*, 106(4):906–912, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marino:2001:TET

[MRST01] T. Marino, N. Russo, E. Sicilia, and M. Toscano. Tautomeric equilibria of 2- and 4-thiouracil in gas phase and in solvent: A density functional study. *International Journal of Quantum Chemistry*, 82(1):44–52, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76510760/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76510760/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76510760&PLACEBO=IE.pdf`.

Mineva:2000:OEA

[MRT00] Tzonka Mineva, Nino Russo, and Marirosa Toscano. Odd-even alternation of global hardnesses in the Na_n ($n = 2--9$) clusters. *International Journal of Quantum Chemistry*, 80(2):105–109, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001280/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001280/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001280&PLACEBO=IE.pdf`.

Marino:2001:GPA

[MRTT01] T. Marino, N. Russo, E. Tocci, and M. Toscano. Gas-phase acidity of proline from density functional computations. *International Journal of Quantum Chemistry*, 84(2):264–268, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502325/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502325/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502325&PLACEBO=IE.pdf`.

Molina:2000:ESG

[MS00] B. Molina and L. E. Sansores. Electronic structure of Ge_3 N_4 possible structures. *International Journal of Quantum Chemistry*, 80(2):249–257, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001290/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001290/FILE?TPL=ftx_start;`

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001290&PLACEBO=IE.pdf.

March:2003:MMC

[MS03] Norman H. March and R. H. Squire. Microscopic mechanism for C_{60} superconductivity. *International Journal of Quantum Chemistry*, 92(3):261–275, April 5, 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matos:2005:ESA

[MS05] Maria Matos and Anivaldo X. Souza. Electronic structure analysis of two crystalline phases of $Fe_3O_2BO_3$. *International Journal of Quantum Chemistry*, 103(5):562–571, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Montgomery:2009:EDD

[MS09] H. E. Montgomery, Jr. and K. D. Sen. Electron density and its derivatives at the nucleus for spherically confined hydrogen atom. *International Journal of Quantum Chemistry*, 109(4):688–692, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marmorino:2000:LBP

[MSB00] M. G. Marmorino, J. C. Schug, and C. A. Beattie. Lower bound problems and bounds to atomic ionization energies. *International Journal of Quantum Chemistry*, 77(4):779–784, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70500252/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70500252/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70500252&PLACEBO=IE.pdf.

Muller:2003:RPP

[MSC03] Imke B. Müller, Robin Santra, and Lorenz S. Cederbaum. Resonances and pseudoresonances in a potential with attractive Coulomb tail: A study using analytic-continuation techniques. *International Journal of Quantum Chemistry*, 94(2):75–92, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monev:2005:CDP

[MSC05] Valentin Monev, Milena Spassova, and Benoît Champagne. Charge distributions in polyacetylene chains containing a positively charged defect. *International Journal of Quantum Chemistry*, 104(3):354–366, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moayedi:2004:ESP

[MSJ04] S. K. Moayedi, M. Solimannejad, and Abraham F. Jalbout. Exact solutions for the position-dependent effective mass Schrödinger equation using the analogy with a PT-symmetric invariant anharmonic potential. *International Journal of Quantum Chemistry*, 100(1):16–19, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mori:2005:QCE

[MSK+05] Yoshiyuki Mori, Ryuichi Sawae, Minaru Kawamura, Toshio Sakata, and Kenichi Takarabe. Quantum circuits for an effective pure state in NMR quantum computer. *International Journal of Quantum Chemistry*, 105(6):758–761, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mireles:2003:TSM

[MSMS03] N. Mireles, L. E. Sansores, A. Martínez, and R. Salcedo. Theoretical study of 4-, 5-, 6-, and 7-member ring superphane cages with a metal atom inside. *International Journal of Quantum Chemistry*, 94(1):51–56, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mishra:2005:ISO

[MSS05] P. C. Mishra, A. K. Singh, and S. Suhai. Interaction of singlet oxygen and superoxide radical anion with guanine and formation of its mutagenic modification 8-oxoguanine. *International Journal of Quantum Chemistry*, 102(3):282–301, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matsui:2009:SDP

[MSS09] Toru Matsui, Takeshi Sato, and Yasuteru Shigeta. Sequence dependent proton-transfer reaction in stacked GC pair I: The

possibility of proton-transfer reactions. *International Journal of Quantum Chemistry*, 109(10):2168–2177, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mireles:2000:TDA

[MSSM00] N. Mireles, R. Salcedo, L. E. Sansores, and A. Martínez. Theoretical description of aromaticity in superphane cages. *International Journal of Quantum Chemistry*, 80(2):258–263, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001288/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001288/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001288&PLACEBO=IE.pdf`.

Malli:2004:REC

[MST04] Gulzari L. Malli, Martin Siegert, and David P. Turner. Relativistic and electron correlation effects for molecules of heavy elements: Ab initio fully relativistic coupled-cluster calculations for PbH_4. *International Journal of Quantum Chemistry*, 99(6):940–949, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malli:2008:AEA

[MST08] Gulzari L. Malli, Martin Siegert, and David P. Turner. All-electron all-virtual spinor space relativistic coupled-cluster calculations for molecules of heavy elements using contracted basis set: Prediction of atomization energy of PbH_4 *. *International Journal of Quantum Chemistry*, 108(12):2299–2304, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Micha:2002:DDM

[MT02] David A. Micha and Brian Thorndyke. Dissipative dynamics in many-atom systems: A density matrix treatment. *International Journal of Quantum Chemistry*, 90(2):759–771, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maday:2003:PTA

[MT03] Yvon Maday and Gabriel Turinici. Parallel in time algorithms for quantum control: Parareal time discretization scheme. *In-*

ternational Journal of Quantum Chemistry, 93(3):223–228, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Minkov:2004:MIN

[MT04] I. Minkov and A. Tadjer. Magnetic interactions in nonalternant mixed molecular radical crystals and mixed ion radical crystals. *International Journal of Quantum Chemistry*, 99 (5):667–676, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mosyagin:2002:GMC

[MTB+02] N. S. Mosyagin, A. V. Titov, R. J. Buenker, H.-P. Liebermann, and A. B. Alekseyev. GRECP/MRD-CI calculations on the Hg atom and HgH molecule. *International Journal of Quantum Chemistry*, 88(5):681–686, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matos:2009:SES

[MTE09] Maria Matos, Joice Terra, and D. E. Ellis. Semiempirical electronic structure calculation on Ca and Pb apatites. *International Journal of Quantum Chemistry*, 109(4):849–860, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moriwake:2003:FPC

[MTO+03] Hiroki Moriwake, Isao Tanaka, Fumiyasu Oba, Yukinori Koyama, and Hirohiko Adachi. First principles calculations of the formation energy of Cr/Al vacancies in spinel-type $MgCr_2O_4$ and $MgAl_2O_4$. *International Journal of Quantum Chemistry*, 91(2):208–210, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mallik:2004:ATH

[MTRD04] Aditi Mallik, DeCarlos E. Taylor, Keith Runge, and James W. Dufty. Application of transfer Hamiltonian quantum mechanics to multi-scale modeling. *International Journal of Quantum Chemistry*, 100(6):1019–1025, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marino:2004:GPI

[MTRG04] T. Marino, M. Toscano, N. Russo, and A. Grand. Gas-phase interaction between DNA and RNA bases and copper (II) ion:

A density functional study. *International Journal of Quantum Chemistry*, 98(4):347–354, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moriyama:2009:MSS

[MTWN09] Hiroko Moriyama, Hiroshi Tatewaki, Yoshihiro Watanabe, and Haruyuki Nakano. Molecular spinors suitable for four-component relativistic correlation calculations: Studies of LaF^+ and LaF using multiconfigurational quasi-degenerate perturbation theory. *International Journal of Quantum Chemistry*, 109(9):1898–1904, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mukhopadhyay:2000:SCA

[Muk00] Atri Mukhopadhyay. On the structure of the Clifford algebra unitary group adapted states in the many-electron correlation problem. *International Journal of Quantum Chemistry*, 77(3):607–614, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004056/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004056/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004056&PLACEBO=IE.pdf`.

Mach:2002:ISE

[MUL02] P. Mach, J. Urban, and J. Leszczynski. *Ab initio* study of electronic spectra of merocyanine 540 and its photoproducts. *International Journal of Quantum Chemistry*, 87(5):265–269, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/91012970/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91012970/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91012970&PLACEBO=IE.pdf`.

Munoz:2002:TKD

[Muñ02] Victor Muñoz. Thermodynamics and kinetics of downhill protein folding investigated with a simple statistical mechanical model. *International Journal of Quantum Chemistry*, 90(4-5):1522–1528, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mishra:2002:TSA

[MV02] Manoj K. Mishra and Arun Venkatnathan. Treatment of shape and Auger resonances using the dilated electron propagator. *International Journal of Quantum Chemistry*, 90(4-5): 1334–1347, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mikheikin:2002:RMO

[MVA02] I. D. Mikheikin, I. K. Vorontsova, and I. A. Abronin. Reactivity of molecular oxygen on the surface of ionic crystals. *International Journal of Quantum Chemistry*, 88(4):489–495, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martin:2000:SEE

[MVdCD00] Graça M. B. Martin, Maria Domingues Vargas, Carlos Jorge da Cunha, and Joaquim Delphino Da Motta Neto. Solvent effects on the electronic absorption spectrum and evaluation of nonlinear optical (NLO) properties of $[Co_2\mu\text{-}\eta^2\text{-}(C_6H_5)CC(C_6H_4NO_2)(CO)_6]$. *International Journal of Quantum Chemistry*, 80(4–5):1055–1061, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505407/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505407/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505407&PLACEBO=IE.pdf`.

Moskovsky:2004:NUW

[MVG+04] Alexander A. Moskovsky, Vitaly V. Vanovsky, Alexander A. Granovsky, Denis A. Firsov, and Alexander V. Nemukhin. A new universal Web interface to quantum chemistry programs. *International Journal of Quantum Chemistry*, 100 (4):645–648, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matamala-Vasquez:2000:CPM

[MVK00] Adelio Matamala-Vásquez and Jacek Karwowski. Commutator perturbation method in the study of vibrational-rotational spectra of diatomic molecules. *International Journal of Quantum Chemistry*, 77(4):721–726, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (elec-

tronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70500248/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70500248/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70500248&PLACEBO=IE.pdf.

Moskovsky:2006:IRE

[MVKN06] A. A. Moskovsky, V. V. Vanovschi, S. S. Konyukhov, and A. V. Nemukhin. Implementation of the replica-exchange molecular dynamics method for rigid bodies. *International Journal of Quantum Chemistry*, 106(10):2208–2213, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martin:2001:PPN

[MVL+01] I. Martín, A. M. Velasco, C. Lavín, E. Olalla, and E. Bustos. Photoabsorption processes in nitrous oxide and formaldehyde. *International Journal of Quantum Chemistry*, 85(4–5):345–353, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martin:2002:TSR

[MVL02] I. Martín, A. M. Velasco, and C. Lavín. Theoretical study of the Rydberg spectra of chemically relevant isovalent radicals. *International Journal of Quantum Chemistry*, 86(1):59–66, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/86511423/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86511423/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86511423&PLACEBO=IE.pdf.

Mesquita:2005:LSQ

[MVLM05] Marcus V. Mesquita, Áurea R. Vasconcellos, Roberto Luzzi, and Sergio Mascarenhas. Large-scale quantum effects in biological systems. *International Journal of Quantum Chemistry*, 102(6):1116–1130, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matamala-Vasquez:2000:AAA

[MVP00] Adelio Matamala-Vásquez and Josep Planelles. Algebraic approach to the asymmetric rigid rotor. *International Journal of Quantum Chemistry*, 77(4):704–709,

???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70500245/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70500245/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70500245&PLACEBO=IE.pdf`.

Moncrieff:2005:CLD

[MW05] D. Moncrieff and S. Wilson. Computational linear dependence in molecular electronic structure calculations using universal basis sets. *International Journal of Quantum Chemistry*, 101 (4):363–371, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mang:2006:FHV

[MW06a] Chaoyong Mang and Kechen Wu. First hyperpolarizabilities of vinylogue organometallic sesquifulvalene chromophores: A DFT study. *International Journal of Quantum Chemistry*, 106(12):2529–2535, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Muhandiramge:2006:SAS

[MW06b] R. D. Muhandiramge and J. B. Wang. Spin-adapted states: A basis for quantum dot structure calculation. *International Journal of Quantum Chemistry*, 106(1):27–53, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mei:2006:THB

[MWHZ06] Ye Mei, Emilia L. Wu, K. L. Han, and J. Z. H. Zhang. Treating hydrogen bonding in ab initio calculation of biopolymers. *International Journal of Quantum Chemistry*, 106(5):1267–1276, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meng:2008:DFC

[MWL08] Qingxi Meng, Fen Wang, and Ming Li. Density functional computations of alkynylation of ethanimine catalyzed by chiral zinc(II)-complexes. *International Journal of Quantum Chemistry*, 108(2):362–369, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Milman:2000:ESP

[MWW+00] V. Milman, B. Winkler, J. A. White, C. J. Pickard, M. C. Payne, E. V. Akhmatskaya, and R. H. Nobes. Electronic structure, properties, and phase stability of inorganic crystals: A pseudopotential plane-wave study. *International Journal of Quantum Chemistry*, 77(5):895–910, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000341/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000341/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000341&PLACEBO=IE.pdf`.

Meng:2005:SEL

[MWXL05] Fancui Meng, Huanjie Wang, Weiren Xu, and Chengbu Liu. Substituent effect of large conjugate groups on the DNA base pair derivatives: Density functional study. *International Journal of Quantum Chemistry*, 104(1):79–86, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Micha:2000:MPM

[MY00] David A. Micha and Zhigang Yi. Molecular photoexcitation in a medium: Density operator approach. *International Journal of Quantum Chemistry*, 77(1):367–375, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004279/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004279/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004279&PLACEBO=IE.pdf`.

Ma:2008:AMO

[MY08a] Dongxia Ma and Danny L. Yeager. Approximate MCSCF optimization for multiconfigurational spin-tensor electron propagator method (MCSTEP): The vertical ionization potentials of CO, HCN, HNC, H_2CO, and O_3. *International Journal of Quantum Chemistry*, 108(1):100–111, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ma:2008:EOM

[MY08b] Dongxia Ma and Danny L. Yeager. Equivalent orbitals for multiconfigurational spin-tensor electron propagator method

(MCSTEP): The vertical ionization potentials of B, NO, CF, and OF. *International Journal of Quantum Chemistry*, 108 (6):1130–1136, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mishima:2008:EAM

[MY08c] K. Mishima and K. Yamashita. Entanglement of angular momenta of atoms and molecules. *International Journal of Quantum Chemistry*, 108(8):1352–1357, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mishima:2009:DIV

[MY09] K. Mishima and K. Yamashita. Decoherence of intramolecular vibrational entanglement in polyatomic molecules. *International Journal of Quantum Chemistry*, 109(9):1827–1833, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meng:2001:LGM

[MYGD01] Qingtian Meng, Xizhang Yi, Daren Guan, and Shiliang Ding. A Lie group method for molecular rovibrational spectra via the broken symmetry of $U^{(r)}(2) \otimes U^{(v)}(4)$. *International Journal of Quantum Chemistry*, 83(2):53–59, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002392/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002392/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002392&PLACEBO=IE.pdf`.

Meng:2003:TDW

[MYH03] Qing-Tian Meng, Guang-Hui Yang, and Ke-Li Han. Time-dependent wave packet approach to Rabi oscillation in strong laser field. *International Journal of Quantum Chemistry*, 95 (1):30–36, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martinez-Y-Romero:2007:AAR

[MYRNYSB07] R. P. Martínez-Y-Romero, H. N. Núñez-Yépez, and A. L. Salas-Brito. Algebraic approach to radial ladder operators in the hydrogen atom. *International Journal of Quantum Chemistry*, 107(7):1608–1613, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morishita:2009:FEI

[MYS+09] M. Morishita, H. Yamamoto, S. Shikada, M. Kusumoto, Y. Matsumoto, A. Onoue, N. Nishimura, and H. Ohtani. Formation energies of the intermetallic compounds at the ground and thermally excited states determined by the ab initio energetic calculation and calorimetric measurement. *International Journal of Quantum Chemistry*, 109(12):2695–2705, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monaco:2009:ASO

[MZ09] Guglielmo Monaco and Riccardo Zanasi. On the analysis of some orbital contributions to the current density in circulenes. *International Journal of Quantum Chemistry*, 109 (2):243–249, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meng:2001:LAA

[MZD01] Qingtian Meng, Yujun Zheng, and Shiliang Ding. Lie algebraic approach to Fermi resonance levels of CS_2 and CO_2. *International Journal of Quantum Chemistry*, 81(2):154–161, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76500930/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76500930/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76500930&PLACEBO=IE.pdf`.

Mebel:2005:PES

[MZD+05] A. M. Mebel, T. S. Zyubina, Y. A. Dyakov, A. D. Bandrauk, and S. H. Lin. Potential energy surfaces in Coulomb explosion of polyatomic molecules: Benzene and cyclohexane trications and acetylene dication. *International Journal of Quantum Chemistry*, 102(5):506–519, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ma:2005:VTE

[MZF05] Dong-Xia Ma, Neng-Wu Zheng, and Jing Fan. Variational treatment on the energy of the He-sequence ground state with weakest bound electron potential model theory. *International Journal of Quantum Chemistry*, 105(1):12–17, ????

2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mitoraj:2009:OTI

[MZMZ09] Mariusz P. Mitoraj, Hongjuan Zhu, Artur Michalak, and Tom Ziegler. On the origin of the *trans*-influence in square planar d^8-complexes: A theoretical study. *International Journal of Quantum Chemistry*, 109(14):3379–3386, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mahavadi:2003:SEP

[MZN+03] Madhavi Mahavadi, Diana N. Zeiger, Dahlia Naqib, Maria Victoria Roux, Rafael Notario, and Joel F. Liebman. The strain energy of perchlorocyclopropane is small: It might even be negative. A density functional theory study of perhalocycloalkanes. *International Journal of Quantum Chemistry*, 95 (6):784–790, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nesterenko:2006:FSC

[NAE06] N. S. Nesterenko, A. V. Avdey, and A. Yu Ermilov. FTIR study of the CO adsorption over Pt/MFI catalysts: Ab initio interpretation. *International Journal of Quantum Chemistry*, 106(10):2281–2289, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2003:EEE

[Nag03a] Á. Nagy. Exact expressions for energy functional in the time-dependent density functional theory. *International Journal of Quantum Chemistry*, 92(2):229–233, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2003:I

[Nag03b] Á Nagy. Introduction. *International Journal of Quantum Chemistry*, 92(2):95, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2003:PPT

[Nag03c] Á Nagy. Preface: Proceedings of the Third Research Workshop and Graduate School on Physics and Chemistry of Quantum Systems. *International Journal of Quantum Chemistry*,

92(2):93–94, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagao:2004:TSM

[Nag04a] Hidemi Nagao. Theoretical studies on many-band effects in superconductivity and magnetism. *International Journal of Quantum Chemistry*, 100(6):867–876, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2004:TIE

[Nag04b] Á. Nagy. Theories for individual excited states. *International Journal of Quantum Chemistry*, 99(4):256–264, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2006:HEG

[Nag06] Á. Nagy. Hierarchy of equations in the generalized density functional theory. *International Journal of Quantum Chemistry*, 106(5):1043–1051, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakai:2002:SDN

[Nak02] Hiromi Nakai. Simultaneous determination of nuclear and electronic wave functions without Born–Oppenheimer approximation: Ab initio NO+MO/HF theory. *International Journal of Quantum Chemistry*, 86(6):511–517, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86513256/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86513256/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86513256&PLACEBO=IE.pdf`.

Nakai:2007:NOP

[Nak07] Hiromi Nakai. Nuclear orbital plus molecular orbital theory: Simultaneous determination of nuclear and electronic wave functions without Born–Oppenheimer approximation. *International Journal of Quantum Chemistry*, 107(14):2849–2869, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nalewajski:2000:CSE

[Nal00a] Roman F. Nalewajski. Charge sensitivities of the externally interacting open reactants. *International Journal of Quantum Chemistry*, 78(3):168–178, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71007685/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71007685/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71007685&PLACEBO=IE.pdf`.

Nalewajski:2000:ICD

[Nal00b] Roman F. Nalewajski. Integral constraint on the density functional for nonadditive kinetic energy in Kohn–Sham theory for subsystems. *International Journal of Quantum Chemistry*, 76(2):252–258, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503177/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503177/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503177&PLACEBO=IE.pdf`.

Nalewajski:2008:UFI

[Nal08] Roman F. Nalewajski. Use of Fisher information in quantum chemistry. *International Journal of Quantum Chemistry*, 108 (12):2230–2252, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nalewajski:2009:CBD

[Nal09a] Roman F. Nalewajski. Chemical bond descriptors from molecular information channels in orbital resolution. *International Journal of Quantum Chemistry*, 109(3):425–440, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nalewajski:2009:IOC

[Nal09b] Roman F. Nalewajski. Information origins of the chemical bond: Bond descriptors from molecular communication channels in orbital resolution. *International Journal of Quantum Chemistry*, 109(11):2495–2506, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Navrotsky:2009:EON

[Nav09] Alexandra Navrotsky. Energetics of oxide nanoparticles. *International Journal of Quantum Chemistry*, 109(12):2647–2657, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nalewajski:2005:EII

[NB05] Roman F. Nalewajski and Elżbieta Broniatowska. Entropy/information indices of the "stockholder" atoms-in-molecules. *International Journal of Quantum Chemistry*, 101(4):349–362, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Novakovskaya:2004:NIF

[NBS04] Yu. V. Novakovskaya, D. S. Bezrukov, and N. F. Stepanov. Nitrite ion formation: Nonempirical simulation in terms of cluster model. *International Journal of Quantum Chemistry*, 100(4):460–468, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nandy:2002:SDH

[NCB02] Subhajit Nandy, Pinaki Chaudhury, and S. P. Bhattacharyya. Stochastic diagonalization of Hamiltonian: A genetic algorithm-based approach. *International Journal of Quantum Chemistry*, 90(1):188–194, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nikolaev:2002:SPP

[ND02] A. V. Nikolaev and P. N. Dyachkov. Solution of periodic Poisson's equation and the Hartree–Fock approach for solids with extended electron states: Application to linear augmented plane wave method. *International Journal of Quantum Chemistry*, 89(2):57–85, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [ND03].

Nikolaev:2003:ESP

[ND03] A. V. Nikolaev and P. N. Dyachkov. Erratum: Solution of periodic Poisson's equation and the Hartree–Fock approach for solids with extended electron states: Application to linear augmented plane wave method, International Journal of Quantum Chemistry, Volume 89, Number 2, 2002, pages 57–85. *International Journal of Quantum Chemistry*, 93(5):375–

376, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [ND02].

Neese:2001:CIC

[Nee01] Frank Neese. Configuration interaction calculation of electronic g tensors in transition metal complexes. *International Journal of Quantum Chemistry*, 83(3-4):104–114, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002590/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002590/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002590&PLACEBO=IE.pdf`.

Negadi:2000:PPT

[Nég00] Tidjani Négadi. On the planar periodic table. *International Journal of Quantum Chemistry*, 78(4):206–211, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72000074/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72000074/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72000074&PLACEBO=IE.pdf`.

Negadi:2003:CGC

[Nég03a] Tidjani Négadi. Cracking the genetic code(s) with a modular determinative degree: An algebraic approach. *International Journal of Quantum Chemistry*, 91(6):651–662, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Negadi:2003:RTB

[Nég03b] Tidjani Négadi. Rumer's transformation, in biology, as the negation, in classical logic. *International Journal of Quantum Chemistry*, 94(2):65–74, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nesbet:2000:ECE

[Nes00] R. K. Nesbet. Exchange and correlation energy in density functional theory. *International Journal of Quantum Chemistry*, 77(2):521–525, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70002211/`

START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70002211/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70002211&PLACEBO=IE.pdf.

Nesbet:2001:CIE

[Nes01a] R. K. Nesbet. Can an independent-electron model be exact for an N-electron system? *International Journal of Quantum Chemistry*, 85(4–5):405–410, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nesbet:2001:LPI

[Nes01b] R. K. Nesbet. Local potentials in independent-electron models. *International Journal of Quantum Chemistry*, 81(6):384–388, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/76509321/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76509321/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76509321&PLACEBO=IE.pdf.

Nesbet:2002:OFT

[Nes02a] R. K. Nesbet. Orbital functional theory of linear response and excitation. *International Journal of Quantum Chemistry*, 86(4):342–346, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/86011220/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86011220/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86011220&PLACEBO=IE.pdf.

Nesbet:2002:TFT

[Nes02b] R. K. Nesbet. Thomas–Fermi theory revisited. *International Journal of Quantum Chemistry*, 90(1):262–265, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nesbet:2003:ELV

[Nes03a] R. K. Nesbet. Energy-linearized variational cellular method for large molecules and solids. *International Journal of Quantum Chemistry*, 91(1):46–50, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nesbet:2003:NPI

[Nes03b] R. K. Nesbet. Nonlocal potentials in independent-electron models. *International Journal of Quantum Chemistry*, 95 (6):816–820, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nesbet:2004:EPI

[Nes04a] R. K. Nesbet. The exclusion principle for interacting electrons: Kohn–Sham versus Thomas–Fermi. *International Journal of Quantum Chemistry*, 100(6):937–942, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nesbet:2004:NPS

[Nes04b] R. K. Nesbet. Nonlocal potentials for short-range electronic correlation in atoms, molecules, and solids. *International Journal of Quantum Chemistry*, 100(2):114–120, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nesbet:2005:UHF

[Nes05] R. K. Nesbet. Unrestricted Hartree–Fock then and now. *International Journal of Quantum Chemistry*, 102(5):602–605, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Newton:2000:MDA

[New00] Marshall D. Newton. Modeling donor/acceptor interactions: Combined roles of theory and computation. *International Journal of Quantum Chemistry*, 77(1):255–263, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004265/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004265/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004265&PLACEBO=IE.pdf`.

Nikiforov:2002:CPS

[NF02] I. S. Nikiforov and D. A. Filippov. Calculation of a power spectrum and definition of wave functions of an ion Cr^{3+} in antiferromagnetic crystal Cr_2O_3 in the model of a crystalline field. *International Journal of Quantum Chemistry*, 88(5):

676–680, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nascimento:2003:RMG

[NF03] D. L. Nascimento and A. L. A. Fonseca. Relativistic method to get analytic solutions for many-body problems: Application to the H molecule. *International Journal of Quantum Chemistry*, 95(3):274–280, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nascimento:2006:NAU

[NF06] D. L. Nascimento and A. L. A. Fonseca. New approach using the relativistic Hamilton–Jacobi equation to evaluate the correct energy levels for the hydrogen atom. *International Journal of Quantum Chemistry*, 106(13):2779–2789, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nabais:2004:PRS

[NFFA04] Catarina Nabais, Rui P. S. Fartaria, Fernando M. S. Silva Fernandes, and Luísa M. Abrantes. Prediction of reactive sites for the electropolymerization of *p*-benzenesulfonic acid derivatives: Ab initio and experimental study. *International Journal of Quantum Chemistry*, 99(1):11–27, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Niquet:2005:AAD

[NFG05] Y. M. Niquet, M. Fuchs, and X. Gonze. Avoiding asymptotic divergence of the potential from orbital- and energy-dependent exchange-correlation functionals. *International Journal of Quantum Chemistry*, 101(6):635–644, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Niedwieski:2002:SIC

[NFL+02] Antonio Carlos Niedwieski, Jaísa Fernandes Soares, George Jeffery Leigh, Fábio Souza Nunes, and Joaquim Delphino Da Motta Neto. Semiempirical INDO/S calculations on the absorption spectrum of mono- and trinuclear vanadium(II) complexes. *International Journal of Quantum Chemistry*, 88(2): 245–251, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nascimento:2005:DHA

[NFP05] D. L. Nascimento, A. L. A. Fonseca, and O. Portilho. Determination of the helium atom ground state through the Hamilton–Jacobi equation. *International Journal of Quantum Chemistry*, 103(5):505–508, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakano:2001:TON

[NFT+01] M. Nakano, H. Fujita, M. Takahata, S. Kiribayashi, and K. Yamaguchi. Third-order nonlinear optical properties of dendritic molecular aggregates: Effects of fractal architecture. *International Journal of Quantum Chemistry*, 84(6):649–659, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85008257/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85008257/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85008257&PLACEBO=IE.pdf`.

Neyman:2002:HBE

[NGRR02] Konstantin M. Neyman, Dmitri I. Ganyushin, Žilvinas Rinkevičius, and Notker Rösch. Hydrogen-bonding effects on electronic g-tensors of semiquinone anion radicals: Relativistic density functional investigation. *International Journal of Quantum Chemistry*, 90(4-5):1404–1413, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nemukhin:2006:MDB

[NGTB06] A. V. Nemukhin, B. L. Grigorenko, I. A. Topol, and S. K. Burt. Modeling dioxygen binding to the non-heme iron-containing enzymes. *International Journal of Quantum Chemistry*, 106(10):2184–2190, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakatsuji:2000:MMS

[NH00] Hiroshi Nakatsuji and Zhen-Ming Hu. Mechanism of methanol synthesis on Cu(100) and Zn/Cu(100) surfaces: Comparative dipped adcluster model study. *International Journal of Quantum Chemistry*, 77(1):341–349, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004276/START; http:`

//www3.interscience.wiley.com/cgi-bin/fulltext/70004276/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004276&PLACEBO=IE.pdf.

Nicolaides:2002:TAN

[Nic02] Cleanthes A. Nicolaides. Time asymmetry, nonexponential decay, and complex eigenvalues in the theory and computation of resonance states. *International Journal of Quantum Chemistry*, 89(2):94–105, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nicolaides:2005:EHS

[Nic05a] Athanassios Nicolaides. Effect of halogen substitution on p- phenylenebiscarbene. *International Journal of Quantum Chemistry*, 104(4):475–481, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nicolaides:2005:CCW

[Nic05b] Cleanthes A. Nicolaides. On calculations of correlated wave functions with heavy configurational mixing. *International Journal of Quantum Chemistry*, 102(3):250–264, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Natsume:2006:DSE

[NID+06] Takayuki Natsume, Yasuyuki Ishikawa, Kenichi Dedachi, Takayuki Tsukamoto, and Noriyuki Kurita. DFT study of the electronic properties of DNA–DNA and PNA–DNA double strands. *International Journal of Quantum Chemistry*, 106(15):3278–3287, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nishikawa:2005:LCP

[NIS+05] K. Nishikawa, T. Ito, K. Sugimori, Y. Ohta, and H. Nagao. Laser control of proton motion in porphyrin derivative. *International Journal of Quantum Chemistry*, 102(5):665–672, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Neto:2002:HAG

[NJC02] A. Canal Neto, F. E. Jorge, and R. Centoducatte. Highly accurate Gaussian basis sets for some 14-electron diatomic

systems. *International Journal of Quantum Chemistry*, 90 (1):244–249, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Neto:2002:IGC

[NJD02] A. Canal Neto, F. E. Jorge, and M. De Castro. Improved generator coordinate Hartree–Fock method applied to generate Gaussian basis sets for the isoelectronic series of the atoms He to Ne. *International Journal of Quantum Chemistry*, 88 (2):252–262, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nowroozi:2009:HBA

[NJR+09] A. Nowroozi, A. F. Jalbout, H. Roohi, E. Khalilinia, M. Sadeghi, A. de Leon, and H. Raissi. Hydrogen bonding in acetylacetaldehyde: Theoretical insights from the theory of atoms in molecules. *International Journal of Quantum Chemistry*, 109(7):1505–1514, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagao:2005:TSE

[NK05a] Hidemi Nagao and Hiroyuki Kawabe. Theoretical studies on effective interactions in two-band system. *International Journal of Quantum Chemistry*, 105(6):571–579, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nirmala:2005:DFS

[NK05b] V. Nirmala and P. Kolandaivel. Density functional studies on hydrogen-bonded clusters of hydrogen halides and the interaction on halide anions. *International Journal of Quantum Chemistry*, 103(3):322–331, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagao:2006:TSE

[NK06] Hidemi Nagao and Hiroyuki Kawabe. Theoretical studies of the effect of pair scattering process on two-gap superconductivity in Eliashberg theory. *International Journal of Quantum Chemistry*, 106(15):3048–3055, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagao:2001:TSF

[NKK+01] Hidemi Nagao, Yasutaka Kitagawa, Takashi Kawakami, Takashi Yoshimoto, Hiroaki Saito, and Kizashi Yamaguchi. Theoretical studies on field-induced superconductivity in molecular crystals. *International Journal of Quantum Chemistry*, 85(4–5):608–618, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakano:2005:HDA

[NKN+05] Masayoshi Nakano, Ryohei Kishi, Tomoshige Nitta, Benoît Champagne, Edith Botek, and Kizashi Yamaguchi. Hyperpolarizability density analysis of the enhancement of second hyperpolarizability of π-conjugated oligomers by intermolecular interaction. *International Journal of Quantum Chemistry*, 102(5):702–710, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Needs:2002:QMC

[NKP+02] R. J. Needs, P. R. C. Kent, A. R. Porter, M. D. Towler, and G. Rajagopal. Quantum Monte Carlo calculations for ground and excited states. *International Journal of Quantum Chemistry*, 86(2):218–225, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85006581/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85006581/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85006581&PLACEBO=IE.pdf`.

Nakanishi:2009:EEE

[NKS+09] Yasuyuki Nakanishi, Yasutaka Kitagawa, Toru Saito, Yusuke Kataoka, Toru Matsui, Takashi Kawakami, Mitsutaka Okumura, and Kizashi Yamaguchi. Estimation of effective exchange integral value of polyradical systems based on the band calculation. *International Journal of Quantum Chemistry*, 109(15):3632–3640, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Norberg:2004:BRC

[NLD+04] Daniel Norberg, Per-Erik Larsson, Xi-Cheng Dong, Nessima Salhi-Benachenhou, and Sten Lunell. Bicyclopropylidene radical cation: A rehybridization ring opening to tetramethyle-

neethane. *International Journal of Quantum Chemistry*, 98 (5):473–483, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2001:LTN

[NM01] Á. Nagy and N. H. March. Legendre transform of the noninteracting kinetic energy: Especially from March-Murray perturbation theory based on plane waves. *International Journal of Quantum Chemistry*, 82(3):138–142, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/77004283/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/77004283/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=77004283&PLACEBO=IE.pdf`.

Nathaniel:2006:DFS

[NMNB06] Rachel Nathaniel, Tzonka Mineva, Rositca Nikolova, and Anka Bojilova. Density functional study of the interaction of 3-(ω-bromoacetyl)coumarin with phosphites. *International Journal of Quantum Chemistry*, 106(6):1357–1366, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakatsuji:2009:HDF

[NN09] Hiroshi Nakatsuji and Hiroyuki Nakashima. How does the free complement wave function become accurate and exact finally for the hydrogen atom starting from the Slater and Gaussian initial functions and for the helium atom on the cusp conditions? *International Journal of Quantum Chemistry*, 109(10):2248–2262, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagao:2001:TSQ

[NNNY01] Hidemi Nagao, Masayoshi Nakano, Kiyoshi Nishikawa, and Kizashi Yamaguchi. Theoretical study on quantum dynamics of Bose system interacting with photon field. *International Journal of Quantum Chemistry*, 84(4):401–408, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85004219/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85004219/`

FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85004219&PLACEBO=IE.pdf.

Nagao:2000:TSS

[NNS+00] Hidemi Nagao, Masamichi Nishino, Yasuteru Shigeta, Yasunori Yoshioka, and Kizashi Yamaguchi. Theoretical studies on superconducting and other phases: Triplet superconductivity, ferromagnetism, and ferromagnetic metal. *International Journal of Quantum Chemistry*, 80(4–5):721–732, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505377/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505377/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505377&PLACEBO=IE.pdf.

Nowak:2002:DFS

[NOHN02] W. Nowak, Y. Ohtsuka, J. Hasegawa, and H. Nakatsuji. Density functional study on geometry and electronic structure of nitrile hydratase active site model. *International Journal of Quantum Chemistry*, 90(3):1174–1187, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagaoka:2000:ITC

[NOM00] Masataka Nagaoka, Takuya Okamoto, and Yutaka Maruyama. Internal temperature concept for fast-transient dynamics of chemical species in solution. *International Journal of Quantum Chemistry*, 80(2):117–124, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73001273/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001273/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001273&PLACEBO=IE.pdf.

Nooijen:2003:FPS

[Noo03] Marcel Nooijen. First-principles simulation of the UV absorption spectrum of ketene. *International Journal of Quantum Chemistry*, 95(6):768–783, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nooijen:2006:IHT

[Noo06] Marcel Nooijen. Investigation of Herzberg–Teller Franck–Condon approaches and classical simulations to include effects due to vibronic coupling in circular dichroism spectra: The case of dimethyloxirane continued. *International Journal of Quantum Chemistry*, 106(12):2489–2510, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Novakovskaya:2007:DWC

[Nov07] Yulia V. Novakovskaya. Dynamics of water clusters upon UV-excitation leading to ionization: Nonempirical study. *International Journal of Quantum Chemistry*, 107(14):2763–2780, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nowak:2001:CSR

[Now01] Grażyna Nowak. Common-sense reasoning cast over D-U model in simulation of chemical reactions. *International Journal of Quantum Chemistry*, 84(2):282–289, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502342/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502342/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502342&PLACEBO=IE.pdf`.

Nagao:2001:TSD

[NOY+01] Hidemi Nagao, Yasuhito Ohta, Takashi Yoshimoto, Hiroaki Saito, Jun Maki, Hiroyuki Kawabe, Koji Ohta, and Kiyoshi Nishikawa. Theoretical study on dependence of hyperpolarizability of one-dimensional ring system on the delocalization transition. *International Journal of Quantum Chemistry*, 84(6):686–693, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502392/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502392/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502392&PLACEBO=IE.pdf`.

Nagy:2001:MAD

[NP01] Szilvia Nagy and János Pipek. Multiresolution analysis of density operators, electron density, and energy functionals.

International Journal of Quantum Chemistry, 84(5):523–529, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/82003579/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/82003579/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=82003579&PLACEBO=IE.pdf`.

Nivesanond:2005:ICI

[NPLV05] Kanda Nivesanond, Anik Peeters, Dirk Lamoen, and Christian Van Alsenoy. Ab initio calculation of the interaction energy in the P2 binding pocket of HIV-1 protease. *International Journal of Quantum Chemistry*, 105(3):292–299, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2009:RRE

[NR09] Á. Nagy and E. Romera. Relative Rényi entropy for atoms. *International Journal of Quantum Chemistry*, 109(11):2490–2494, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Neto:2003:GBS

[NRJD03] A. Canal Neto, B. L. Rodrigues, F. E. Jorge, and E. V. R. De Castro. Gaussian basis sets for low-lying excited states of the atoms from He to Kr. *International Journal of Quantum Chemistry*, 95(2):184–189, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nemukhin:2005:QMM

[NRK+05] A. V. Nemukhin, A. Yu. Rogachev, S. V. Konyukhov, A. V. Bochenkova, and A. A. Granovsky. QM/MM modeling of the structures and properties of the β-diketonate–based lanthanide complexes. *International Journal of Quantum Chemistry*, 104(2):203–213, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nasluzov:2002:DFE

[NRS+02] Vladimir A. Nasluzov, Vladimir V. Rivanenkov, Alexey M. Shor, Konstantin M. Neyman, Uwe Birkenheuer, and Notker Rösch. Density functional embedded cluster calculations on Lewis acid centers of the α-$Al_2O_3(0001)$ surface: Adsorption

of a CO probe. *International Journal of Quantum Chemistry*, 90(1):386–402, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Novakovskaya:2002:HEN

[NS02] Yulia V. Novakovskaya and Nikolai F. Stepanov. Hydrated electron: Nonempirical cluster approach. *International Journal of Quantum Chemistry*, 88(4):496–506, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Naidu:2004:LCO

[NS04] A. Ramesh Naidu and Vipin Srivastava. Löwdin's canonical orthogonalization: Getting round the restriction of linear independence. *International Journal of Quantum Chemistry*, 99 (6):882–888, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nasertayoob:2008:RFQ

[NS08] Payam Nasertayoob and Shant Shahbazian. Revisiting the foundations of quantum theory of atoms in molecules (QTAIM): The variational procedure and the zero-flux conditions. *International Journal of Quantum Chemistry*, 108 (9):1477–1484, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nasertayoob:2009:RFQ

[NS09] Payam Nasertayoob and Shant Shahbazian. Revisiting the foundations of the quantum theory of atoms in molecules: Toward a rigorous definition of topological atoms. *International Journal of Quantum Chemistry*, 109(4):726–732, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nikitina:2006:MIE

[NSG+06] E. Nikitina, V. Sulimov, F. Grigoriev, O. Kondakova, and S. Luschekina. Mixed implicit/explicit solvation models in quantum mechanical calculations of binding enthalpy for protein–ligand complexes. *International Journal of Quantum Chemistry*, 106(8):1943–1963, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ndip:2004:TSG

[NSLR04] Edmund Moses N. Ndip, Manoj K. Shukla, Jerzy Leszczynski, and Richard L. Redington. Theoretical study of the ground-state gas-phase unimolecular decomposition channels of propynoic acid. *International Journal of Quantum Chemistry*, 100(5):779–787, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nalewajski:2002:IDA

[NŚM02] Roman F. Nalewajski, Elžbieta Świtka, and Artur Michalak. Information distance analysis of molecular electron densities. *International Journal of Quantum Chemistry*, 87(4):198–213, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90011258/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90011258/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90011258&PLACEBO=IE.pdf`.

Nakao:2009:TIB

[NSS09] Yoshihide Nakao, Ken Saito, and Shigeyoshi Sakaki. Theoretical investigation of μ-O-bridged dinuclear Re complexes: Electronic structure, bonding nature, and absorption spectra. *International Journal of Quantum Chemistry*, 109(10):2319–2327, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nikitina:2004:SCB

[NSZZ04] E. Nikitina, V. Sulimov, V. Zayets, and N. Zaitseva. Semiempirical calculations of binding enthalpy for protein–ligand complexes. *International Journal of Quantum Chemistry*, 97 (2):747–763, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nemukhin:2002:EPR

[NTB02] Alexander V. Nemukhin, Igor A. Topol, and Stanley K. Burt. Energy profiles for the rate-limiting stage of the serine protease prototype reaction. *International Journal of Quantum Chemistry*, 88(1):34–40, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89010614/START; http://www3.interscience.`

wiley.com/cgi-bin/fulltext/89010614/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89010614&PLACEBO=IE.pdf.

Nooijen:2009:MCC

[NU09] Marcel Nooijen and Debajyoti Upadhyay. On a manifestly covariant classical mechanics or ruminations on "The Computable Universe" and the role of mathematical physics in solving the natural resource problems of the future. *International Journal of Quantum Chemistry*, 109(8):1684–1698, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakata:2006:CVD

[NUY+06] K. Nakata, T. Ukai, S. Yamanaka, T. Takada, and K. Yamaguchi. CASSCF version of density functional theory. *International Journal of Quantum Chemistry*, 106(15):3325–3333, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nicolas:2003:TSS

[NVA+03] Inés Nicolás, Martha Vilchis, Nidia Aragón, René Miranda, Germund Hojer, and Miguel Castro. Theoretical study of the structure and antimicrobial activity of horminone. *International Journal of Quantum Chemistry*, 93(6):411–421, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Na:2001:QTR

[NW01] Kyungsun Na and Robert E. Wyatt. Quantum trajectories for resonant scattering. *International Journal of Quantum Chemistry*, 81(3):206–213, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/76504662/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76504662/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76504662&PLACEBO=IE.pdf.

Niu:2008:PPL

[NWSC08] Ying-Yu Niu, Rong Wang, Qian-Zhen Su, and Shu-Lin Cong. The photoassociation and photodissociation in laser-assisted collision reaction H + Cl^+. *International Journal of Quantum*

Chemistry, 108(2):289–295, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nie:2007:SES

[NWZ+07a] Aihua Nie, Jinping Wu, Chenggang Zhou, Shujuan Yao, Chen Luo, Robert C. Forrey, and Hansong Cheng. Structural evolution of subnano platinum clusters. *International Journal of Quantum Chemistry*, 107(1):219–224, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ning:2007:ISL

[NWZ+07b] Liancai Ning, Jinping Wu, Chenggang Zhou, Shujuan Yao, Zhenbang Pi, and Hansong Cheng. Influence of sequential lithium insertions on the physical properties of spinel manganese oxide. *International Journal of Quantum Chemistry*, 107(1):225–231, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakano:2001:QPI

[NY01] M. Nakano and K. Yamaguchi. Quantum-phase and information-entropy dynamics of dimers interacting with a single-mode coherent field: The difference between one- and two-exciton models. *International Journal of Quantum Chemistry*, 84(5):530–545, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84501973/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84501973/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84501973&PLACEBO=IE.pdf`.

Nakano:2003:MCW

[NY03] Masayoshi Nakano and Kizashi Yamaguchi. Monte Carlo Wave Function (MCWF) approach to dissipative quantum systems interacting with a single-mode quantized field. *International Journal of Quantum Chemistry*, 95(4–5):461–471, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakano:2004:QPD

[NY04] M. Nakano and K. Yamaguchi. Quantum-phase dynamics of molecular systems interacting with a two-mode squeezed vacuum field: Detuning effects. *International Journal of Quan-*

tum Chemistry, 99(4):421–430, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nishihara:2008:RBS

[NYU+08] S. Nishihara, S. Yamanaka, T. Ukai, K. Nakata, K. Kusakabe, Y. Yonezawa, H. Nakamura, T. Takada, and K. Yamaguchi. Resonating broken symmetry CI approach for ion-radical systems: Comparison with UHF, hybrid-DFT, and CASSCF-DFT. *International Journal of Quantum Chemistry*, 108(15): 2966–2977, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Orimoto:2002:ITS

[OA02] Yuuichi Orimoto and Yuriko Aoki. Ab initio through-space/bond interaction analysis of the long C-C bonds in Bi(anthracene-9,10-dimethylene) photoisomers. *International Journal of Quantum Chemistry*, 86(5):456–467, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86510686/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86510686/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86510686&PLACEBO=IE.pdf`.

Orimoto:2003:PTB

[OA03] Yuuichi Orimoto and Yuriko Aoki. Pure through-bond state in organic molecules for analysis of the relationship between intramolecular interactions and total energy. *International Journal of Quantum Chemistry*, 92(4):355–366, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Orgaz:2005:BPN

[OA05] Emilio Orgaz and Andrea Aburto. Bonding properties of the new zintl-phase hydrides. *International Journal of Quantum Chemistry*, 101(6):783–792, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olszewski:2002:MER

[OB02] S. Olszewski and M. Baszczak. Magnetoresistance effect, Runge–Lenz vector, and the torque vector due to anisotropy of electron orbits in cubic lattices submitted to the action of a constant magnetic field. *Inter-*

national Journal of Quantum Chemistry, 87(6):366–377, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/91015782/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91015782/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91015782&PLACEBO=IE.pdf.

Obermayr:2000:MPL

[Obe00] Werner Obermayr. Method for performing LCAO band structure calculations in crystalline solids: Application to rubidium. *International Journal of Quantum Chemistry*, 78(4):212–225, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72000075/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72000075/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72000075&PLACEBO=IE.pdf.

Olszewski:2000:EDCa

[OBK00a] S. Olszewski, M. Baszczak, and T. Kwiatkowski. Effect of dimensionality of a crystal lattice on the properties of a localized impurity. *International Journal of Quantum Chemistry*, 79(2):57–74, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72508334/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72508334/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72508334&PLACEBO=IE.pdf.

Olszewski:2000:EDCb

[OBK00b] S. Olszewski, M. Baszczak, and T. Kwiatkowski. Effect of dimensionality of a crystal lattice on the properties of a localized impurity. *International Journal of Quantum Chemistry*, 80(1):61–78, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72515500/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72515500/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72515500&PLACEBO=IE.pdf.

Ogurtsov:2006:MMP

[OBM06] I. Ya. Ogurtsov, I. Balan, and G. Munteanu. Multipole moments and polarizability of molecular systems with D_{3h} symmetry in orbitally degenerate states. *International Journal of Quantum Chemistry*, 106(6):1413–1418, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Odashima:2008:EAL

[OC08] Mariana M. Odashima and K. Capelle. Empirical analysis of the Lieb–Oxford bound in ions and molecules. *International Journal of Quantum Chemistry*, 108(13):2428–2432, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ortega-Castro:2007:SCH

[OCAMOHL07] J. Ortega-Castro, L. Alfonso-Méndez, P. Otto, and A. Hernández-Laguna. Soft Coulomb hole method applied to molecules. *International Journal of Quantum Chemistry*, 107(5):1046–1059, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Oh:2007:ISU

[OCK07] Chang Young Oh, Heechol Choi, and Hong Lae Kim. Ab initio study of the unimolecular decomposition of 2-butenenitrile: Molecular elimination channels. *International Journal of Quantum Chemistry*, 107(1):92–104, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ogasawara:2009:FPC

[OCWY09] K. Ogasawara, A. Chaya, S. Watanabe, and H. Yoshida. First-principles calculation of magnetic circular dichroism of transition-metal $L_{2,3}$-edge X-ray absorption near-edge structures. *International Journal of Quantum Chemistry*, 109(12):2672–2676, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

OBrien:2003:SLS

[OD03] Ted A. O'Brien and Ernest R. Davidson. Semiempirical local spin: Theory and implementation of the ZILSH method for predicting Heisenberg exchange constants of polynuclear transition metal complexes. *International Journal of Quantum*

Chemistry, 92(3):294–325, April 5, 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Orestes:2005:ELC

[OdSC05] E. Orestes, A. B. F. da Silva, and K. Capelle. Energy lowering of current-carrying single-particle states in open-shell atoms due to an exchange-correlation vector potential. *International Journal of Quantum Chemistry*, 103(5):516–522, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Orgaz:2000:CBF

[OG00] Emilio Orgaz and Michèle Gupta. Chemical bonding features of the ternary alkali metal platinum and palladium hydrides. *International Journal of Quantum Chemistry*, 80(2):141–152, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001283/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001283/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001283&PLACEBO=IE.pdf`.

Omar:2003:CSV

[OGJdlV03] Salama Omar, Raúl Gonzalez-Jonte, and José Manuel Garciá de la Vega. Conformational study of the vinylphosphonic acid and derivatives. *International Journal of Quantum Chemistry*, 91(3):333–338, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Orgaz:2003:CBT

[OHT03] Emilio Orgaz and Jesús Hernández-Trujillo. Chemical bonding in ternary magnesium hydrides. *International Journal of Quantum Chemistry*, 94(3):150–164, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ordonez:2004:DPF

[OK04] Gonzalo Ordonez and Sungyun Kim. Dressed-particle formulation of Brownian motion. *International Journal of Quantum Chemistry*, 98(2):87–102, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ordon:2005:DED

[OK05] Piotr Ordon and Ludwik Komorowski. DFT energy derivatives and their renormalization in molecular vibrations. *International Journal of Quantum Chemistry*, 101(6):703–713, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ozmen:2003:CTC

[ÖKAY03] Ayhan Özmen, Asli Karakaş, Ülfet Atav, and Yusuf Yakar. Computation of two-center Coulomb integrals over Slater-type orbitals using elliptical coordinates. *International Journal of Quantum Chemistry*, 91(1):13–19, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [Har03].

Okuno:2000:ESR

[Oku00] Yoshishige Okuno. Extension of solution-reaction-surface description to examination of nonequilibrium solvation effect for microsolvated reaction. *International Journal of Quantum Chemistry*, 77(4):791–796, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70500243/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70500243/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70500243&PLACEBO=IE.pdf`.

Okuno:2001:EKE

[Oku01] Yoshishige Okuno. Expressing kinetic-energy for vibration-rotation motions in general rotating systems of axes and introducing quasirectilinear vibrational coordinates to simplify Hamiltonian forms. *International Journal of Quantum Chemistry*, 83(1):22–29, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/79502659/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/79502659/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=79502659&PLACEBO=IE.pdf`.

Okumura:2008:DSH

[OKY+08] Mitsutaka Okumura, Masahiro Kinoshita, Hirotaka Yabushita, Yasutaka Kitagawa, Takashi Kawakami, and Kizashi Yamaguchi. DFT study for the heterojunction effect in the precious metal clusters. *International Journal of Quantum Chemistry*, 108(15):2888–2895, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olszewski:2004:CAR

[Ols04] S. Olszewski. Combinatorical analysis of the Rayleigh–Schrödinger perturbation theory based on a circular scale of time. *International Journal of Quantum Chemistry*, 97(3): 784–801, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Okuno:2002:TEE

[OM02] Yoshishige Okuno and Shinro Mashiko. A theory of excitation–energy transfer regarded as nonadiabatic transition and its comparison to Förster's theory. *International Journal of Quantum Chemistry*, 90(2):772–777, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Okuno:2003:TEE

[OM03] Yoshishige Okuno and Shinro Mashiko. Theory of excitation energy transfer regarded as nonadiabatic transition 2: Calculational evidence of nonadiabatic interaction causing intermolecular excitation energy transfer. *International Journal of Quantum Chemistry*, 94(1):36–43, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olalla:2004:TSV

[OM04] E. Olalla and I. Martín. Theoretical study of the valence and K-shell spectra of atmospherically relevant CO_2. *International Journal of Quantum Chemistry*, 99(4):502–510, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Okuno:2005:CER

[OM05] Yoshishige Okuno and Shinro Mashiko. Convenient expression of the rate constant for nonadiabatic transition. *International Journal of Quantum Chemistry*, 102(1):8–18, ????

2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

ORourke:2004:MQC

[OMC04] S. F. C. O'Rourke, D. M. McSherry, and D. S. F. Crothers. Magnetically quantized continuum distorted-wave theory in atomic and molecular collisions. *International Journal of Quantum Chemistry*, 99(5):569–576, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ostopovici:2007:EBS

[OMMB07] Liliana Ostopovici, Maria Mracec, Mircea Mracec, and Ana Borota. Exploring the binding site of the human muscarinic M3 receptor: Homology modeling and docking study. *International Journal of Quantum Chemistry*, 107(8):1794–1802, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olbert-Majkut:2002:MID

[OMMWL02] Adriana Olbert-Majkut, Zofia Mielke, Robert Wieczorek, and Zdzisław Latajka. Matrix isolation and DFT studies of nitrous acid complexes with nitrogen dioxide. *International Journal of Quantum Chemistry*, 90(3):1140–1150, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohta:2003:DTN

[OMN+03] Y. Ohta, J. Maki, H. Nagao, H. Kono, and Y. Fujimura. Dual transformation for non-Born–Oppenheimer time-dependent density functional theory. *International Journal of Quantum Chemistry*, 91(2):105–112, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohta:2004:IPH

[OMNN04] Yasuhito Ohta, J. Maki, Hidemi Nagao, and Kiyoshi Nishikawa. Ionization process of the hydrogen atom in intense laser fields: Non–Born–Oppenheimer 1D model calculations. *International Journal of Quantum Chemistry*, 97(5):891–895, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohta:2001:CQE

[OMY+01] Y. Ohta, J. Maki, T. Yoshimoto, Y. Shigeta, H. Nagao, and K. Nishikawa. Calculation of quasiparticle en-

ergy of molecular systems by the GW method. *International Journal of Quantum Chemistry*, 84(3):348–353, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/83002308/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/83002308/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=83002308&PLACEBO=IE.pdf`.

Orimoto:2005:NBC

[ONA05] Yuuichi Orimoto, Kazunari Naka, and Yuriko Aoki. NBO-based CI/MP through-space/bond interaction analysis and its application to stereoelectronic effects in S_N 2 reactions. *International Journal of Quantum Chemistry*, 104(6):911–918, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Onishi:2007:CMP

[Oni07] Taku Onishi. The changes of magnetic properties of the perovskite-type titanium oxides by the structural distortions: In the case of $LaTiO_3$ and $YTiO_3$. *International Journal of Quantum Chemistry*, 107(15):3089–3093, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Onishi:2008:HDS

[Oni08] Taku Onishi. The hybrid-DFT study on bandgap estimation for the perovskite-type titanium oxide of $SrTiO_3$. *International Journal of Quantum Chemistry*, 108(15):2856–2861, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Onishi:2009:TSE

[Oni09] Taku Onishi. Theoretical study on the effects of oxygen doping on the lithium ion conductive perovskite-type manganese fluoride of $K_xBa_{(1-x)/2}MnF_3$. *International Journal of Quantum Chemistry*, 109(15):3659–3665, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Oda:2000:TSM

[ONK+00] Akifumi Oda, Hidemi Nagao, Yasutaka Kitagawa, Yasuteru Shigeta, and Kizashi Yamaguchi. Theoretical studies on magnetic behavior in clusters by the genetic algorithms. *International Journal of Quantum Chemistry*, 80(4–5):646–656,

???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505376/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505376/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505376&PLACEBO=IE.pdf.

Oda:2005:SGS

[ONK+05] Akifumi Oda, Hidemi Nagao, Yasutaka Kitagawa, Yasuteru Shigeta, Mitsuo Shoji, Hiroya Nitta, Mitsutaka Okumura, and Kizashi Yamaguchi. Search for the ground states of Ising spin clusters by using the genetic algorithms. *International Journal of Quantum Chemistry*, 105(6):645–654, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ozdogan:2002:ETC

[ÖO02] T. Özdoğan and M. Orbay. Evaluation of two-center overlap and nuclear attraction integrals over Slater-type orbitals with integer and noninteger principal quantum numbers. *International Journal of Quantum Chemistry*, 87(1):15–22, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/88011400/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88011400/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88011400&PLACEBO=IE.pdf. See comment [Gus03].

Ortiz:2005:SDS

[OOD+05] R. Ponce Ortiz, R. Malavé Osuna, M. C. Ruiz Delgado, J. Casado, S. A. Jenekhe, V. Hernandez, and J. T. Lopez Navarrete. Spectroscopic and DFT studies of donor–acceptor molecules containing phenylquinoline and phenothiazine moieties in various redox states. *International Journal of Quantum Chemistry*, 104(5):635–644, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohta:2003:UQM

[OOK03] Yasuhito Ohta, Koji Ohta, and Kenichi Kinugawa. Unified quantum molecular dynamics method based on centroid molecular dynamics and semiempirical molecular orbital theory. *International Journal of Quantum Chemistry*, 95(4–5):

372–379, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Oztekin:2002:CNA

[ÖÖOY02] E. Öztekin, S. Özcan, M. Orbay, and M. Yavuz. Calculation of nuclear-attraction and modified overlap integrals using Gegenbauer coefficients. *International Journal of Quantum Chemistry*, 90(1):136–143, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olszewski:2007:DES

[OR07] S. Olszewski and T. Roliński. Density of electron states in crystalline systems calculated in the presence and absence of the magnetic field. *International Journal of Quantum Chemistry*, 107(5):1223–1240, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olszewski:2009:DBM

[OR09] S. Olszewski and T. Rolińnski. Dupré–blundell model for the Landau diamagnetism applied to electrons gyrating in a crystalline solid. *International Journal of Quantum Chemistry*, 109(5):1045–1057, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Orlikowski:2002:EWR

[Orl02] Tadeusz Orlikowski. Energies and widths of the resonance states of the He ion. *International Journal of Quantum Chemistry*, 90(3):1188–1190, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Orlenko:2007:UHE

[Orl07] Elena Orlenko. The universal Hamiltonian of the exchange interaction for the system of particles with an arbitrary spin j. *International Journal of Quantum Chemistry*, 107(14):2838–2843, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ortiz:2003:QAE

[Ort03] J. V. Ortiz. Quasiparticle approximations and electron propagator theory. *International Journal of Quantum Chemistry*, 95(4–5):593–599, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ortiz:2004:BR

[Ort04a] J. V. Ortiz. Book review. *International Journal of Quantum Chemistry*, 100(1):59, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ortiz:2004:BOD

[Ort04b] J. V. Ortiz. Brueckner orbitals, Dyson orbitals, and correlation potentials. *International Journal of Quantum Chemistry*, 100(6):1131–1135, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ortiz:2005:ERS

[Ort05] J. V. Ortiz. An efficient, renormalized self-energy for calculating the electron binding energies of closed-shell molecules and anions. *International Journal of Quantum Chemistry*, 105 (6):803–808, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohrn:2000:Ia

[ÖS00a] N. Y. Öhrn and J. R. Sabin. Introduction. *International Journal of Quantum Chemistry*, 80(4–5):507, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505381/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505381/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505381&PLACEBO=IE.pdf`.

Ohrn:2000:Ib

[ÖS00b] N. Y. Öhrn and J. R. Sabin. Introduction. *International Journal of Quantum Chemistry*, 80(6):1137, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/75501738/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75501738/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75501738&PLACEBO=IE.pdf`.

Ohrn:2000:MCZ

[ÖS00c] Yngve Öhrn and John R. Sabin. Michael Charles Zerner. *International Journal of Quantum Chemistry*, 78(4):205, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72000082/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72000082/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72000082&PLACEBO=IE.pdf.

Ohrn:2001:Ia

[ÖS01a] N. Y. Öhrn and J. R. Sabin. Introduction. *International Journal of Quantum Chemistry*, 85(4–5):171, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohrn:2001:Ib

[ÖS01b] N. Y. Öhrn and J. R. Sabin. Introduction. *International Journal of Quantum Chemistry*, 85(6):637, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85515913/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85515913/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85515913&PLACEBO=IE.pdf.

Ohrn:2002:I

[ÖS02] N. Yngve Öhrn and John R. Sabin. Introduction. *International Journal of Quantum Chemistry*, 90(1):12–13, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohrn:2003:Ia

[ÖS03] N. Y. Öhrn and J. R. Sabin. Introduction. *International Journal of Quantum Chemistry*, 95(4–5):345, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohrn:2004:I

[ÖS04] N. Y. Öhrn and J. R. Sabin. Introduction. *International Journal of Quantum Chemistry*, 100(6):833, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohrn:2005:I

[ÖS05a] N. Y. Öhrn and J. R. Sabin. Introduction. *International Journal of Quantum Chemistry*, 105(6):533, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohrn:2005:MJP

[ÖS05b] N. Yngve Öhrn and John R. Sabin. In memory of John A. Pople (1925–2004). *International Journal of Quantum Chemistry*, 102(5):471–472, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohrn:2006:I

[ÖS06] N. Y. Öhrn and J. R. Sabin. Introduction. *International Journal of Quantum Chemistry*, 106(15):3001, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohrn:2007:I

[ÖS07] N. Y. Öhrn and J. R. Sabin. Introduction. *International Journal of Quantum Chemistry*, 107(15):2987, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohrn:2008:Ib

[ÖS08] N. Y. Öhrn and J. R. Sabin. Introduction. *International Journal of Quantum Chemistry*, 108(15):2745, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohrn:2009:I

[ÖS09] N. Y. Öhrn and J. R. Sabin. Introduction. *International Journal of Quantum Chemistry*, 109(15):3505, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohrn:2001:POL

[ÖSB01] Yngve Öhrn, John R. Sabin, and Erkki Brändas. Per-Olov Löwdin 1916–2000. *International Journal of Quantum Chemistry*, 81(1):i–ii, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/75502160/START;` `http://www3.interscience.wiley.com/cgi-bin/fulltext/75502160/FILE?TPL=ftx_start;` `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502160&PLACEBO=IE.pdf`.

Obolensky:2007:IEV

[OSSG07] O. I. Obolensky, V. V. Semenikhina, A. V. Solov'yov, and W. Greiner. Interplay of electrostatic and van der Waals forces

in coronene dimer. *International Journal of Quantum Chemistry*, 107(6):1335–1343, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

OBrien:2007:OQC

[OSW07] Kerrie A. O'Brien, E. A. Salter, and A. Wierzbicki. ONIOM quantum chemistry study of cyclic nucleotide recognition in phosphodiesterase 5. *International Journal of Quantum Chemistry*, 107(12):2197–2203, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Otto:2004:D

[Ott04] Peter Otto. Dedication. *International Journal of Quantum Chemistry*, 99(4):181–182, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ou:2006:CCT

[Ou06] Jianping Ou. Conjugated chemical trees with minimal energy and prescribed diameter. *International Journal of Quantum Chemistry*, 106(8):1782–1785, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohsaku:2001:QSM

[OY01] Tadafumi Ohsaku and Kizashi Yamaguchi. QED-SCF, MC-SCF, and coupled-cluster methods in quantum chemistry. *International Journal of Quantum Chemistry*, 85(4–5):272–280, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohta:2000:AAP

[OYB+00] Y. Ohta, T. Yoshimoto, T. Bando, H. Kizu, H. Nagao, and K. Nishikawa. Analysis of adiabatic population transfer in multilevel systems by Hückel model. *International Journal of Quantum Chemistry*, 80(4–5):1068–1075, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505422/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505422/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505422&PLACEBO=IE.pdf`.

Ohsaku:2002:QED

[OYYY02] Tadafumi Ohsaku, Shusuke Yamanaka, Daisuke Yamaki, and Kizashi Yamaguchi. Quantum electrodynamical density-matrix functional theory and group theoretical consideration of its solution. *International Journal of Quantum Chemistry*, 90(1):273–281, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ozdogan:2003:UTE

[Özd03] T. Özdoğan. Unified treatment for the evaluation of arbitrary multielectron multicenter molecular integrals over Slater-type orbitals with noninteger principal quantum numbers. *International Journal of Quantum Chemistry*, 92(5):419–427, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ozdogan:2004:FSA

[Özd04] Telhat Özdoğan. Fast and stable algorithm for analytical evaluation of two-center overlap integrals over Slater-type orbitals with integer and noninteger principal quantum numbers. *International Journal of Quantum Chemistry*, 100(2): 69–79, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Oztekin:2004:OIR

[Özt04] Emin Öztekin. Overlap integrals with respect to quantum numbers over Slater-type orbitals via the Fourier-transform method. *International Journal of Quantum Chemistry*, 100 (2):236–243, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paikeday:2002:PPA

[PA02] Joseph M. Paikeday and Jason Alexander. Polarization potential for e-argon scattering by differential scattering minimization at intermediate energies. *International Journal of Quantum Chemistry*, 90(2):778–785, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paikeday:2004:CAE

[PA04a] Joseph M. Paikeday and Brad T. Ashley. Critical angle and energy of DCS surface for *e*-argon scattering. *International*

Journal of Quantum Chemistry, 100(6):1079–1085, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Puzari:2004:SCF

[PA04b] Panchanan Puzari and Satrajit Adhikari. Semi-classical formulation of time-dependent discrete variable representation method. *International Journal of Quantum Chemistry*, 98 (5):434–446, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pakiari:2008:CSR

[PA08] A. H. Pakiari and S. M. Azami. Coherent superposition of resonance wave function in terms of weighted orthogonalized natural localized configurations. *International Journal of Quantum Chemistry*, 108(2):219–228, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paikeday:2000:PPA

[Pai00] Joseph M. Paikeday. Polarization potential for e-atom scattering by DCS minimization at intermediate energies. *International Journal of Quantum Chemistry*, 80(4–5):989–998, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505406/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505406/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505406&PLACEBO=IE.pdf`.

Palafox:2000:SFP

[Pal00] Mauricio Alcolea Palafox. Scaling factors for the prediction of vibrational spectra. I. Benzene molecule. *International Journal of Quantum Chemistry*, 77(3):661–684, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004061/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004061/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004061&PLACEBO=IE.pdf`.

Palacios:2001:CFF

[Pal01a] José Luis Palacios. Closed-form formulas for Kirchhoff index. *International Journal of Quantum Chemistry*, 81(2):135–

140, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/76500936/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76500936/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76500936&PLACEBO=IE.pdf.

Palacios:2001:RDG

[Pal01b] José Luis Palacios. Resistance distance in graphs and random walks. *International Journal of Quantum Chemistry*, 81(1): 29–33, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/75502159/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75502159/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502159&PLACEBO=IE.pdf.

Panin:2001:ASR

[Pan01] A. I. Panin. Approximate solution of the representability problem. *International Journal of Quantum Chemistry*, 85(1): 1–17, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85004198/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85004198/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85004198&PLACEBO=IE.pdf.

Panin:2002:PRP

[Pan02] A. I. Panin. Pure representability problem and new models of the electronic Fock space. *International Journal of Quantum Chemistry*, 87(1):23–36, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/88511528/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88511528/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88511528&PLACEBO=IE.pdf.

Panin:2004:NRE

[Pan04] A. I. Panin. New realizations of electronic configuration interaction spaces. *International Journal of Quantum Chemistry*, 98(1):11–25, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Panin:2005:EFS

[Pan05] A. I. Panin. Electronic Fock spaces: Phase prefactors and new algebraic structure. *International Journal of Quantum Chemistry*, 105(3):246–259, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Panin:2006:EFS

[Pan06] A. I. Panin. Electronic Fock space as associative superalgebra. *International Journal of Quantum Chemistry*, 106(8):1786–1794, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Panin:2007:DOA

[Pan07] A. I. Panin. 1-density operators and algebraic version of the Hohenberg–Kohn theorem. *International Journal of Quantum Chemistry*, 107(4):858–874, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Patterson:2006:CHD

[Pat06] C. H. Patterson. Comparison of hybrid density functional, Hartree–Fock, and GW calculations on NiO. *International Journal of Quantum Chemistry*, 106(15):3383–3386, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paulus:2004:WFB

[Pau04] Beate Paulus. Wave-function-based ab initio correlation treatment for the buckminsterfullerene C_{60}. *International Journal of Quantum Chemistry*, 100(6):1026–1032, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Podeszwa:2003:COS

[PB03] Rafał Podeszwa and Rodney J. Bartlett. Crystal orbital study of polycarbonyl. *International Journal of Quantum Chemistry*, 95(4–5):638–642, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pupyshev:2004:CDM

[PB04] Vladimir I. Pupyshev and Vladimir V. Bobrikov. The confined diatomic molecule problem. *International Journal of Quan-*

tum Chemistry, 100(4):528–538, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Popelier:2009:GFH

[PB09] Paul L. A. Popelier and Éric A. G. Brémond. Geometrically faithful homeomorphisms between the electron density and the bare nuclear potential. *International Journal of Quantum Chemistry*, 109(11):2542–2553, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Poulos:2002:CCC

[PBB+02] Thomas L. Poulos, Tiffany Barrows, B. Bhaskar, Christopher A. Bonagura, and Huiying Li. Coupling crystallography and computational biochemistry in understanding heme enzyme structure and function. *International Journal of Quantum Chemistry*, 88(1):211–219, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90513474/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90513474/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90513474&PLACEBO=IE.pdf`.

Pereiro:2001:MPD

[PBI+01] M. Pereiro, D. Baldomir, M. Iglesias, C. Rosales, and M. Castro. Model potential density functional study of small cobalt clusters, Co_n, $n \leq 3$. *International Journal of Quantum Chemistry*, 81(6):422–430, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76509304/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76509304/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76509304&PLACEBO=IE.pdf`.

Popelier:2003:FGE

[PBM03] Paul L. A. Popelier, James Burke, and Nathaniel O. J. Malcolm. Functional groups expressed as graphs extracted from the Laplacian of the electron density. *International Journal of Quantum Chemistry*, 92(3):326–336, April 5, 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pereiro:2003:ICM

[PBMA03] M. Pereiro, D. Baldomir, S. Man'kovsky, and J. Arias. Ab initio calculations of magnetic properties of Fe–Cr trilayer as a function of ferromagnetic slab thickness. *International Journal of Quantum Chemistry*, 91(2):245–251, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pascual:2002:NGS

[PBS02] José Luis Pascual, Zoila Barandiarán, and Luis Seijo. On the nature of the ground state of Cr(V) defects in YVO_4: An ab initio model potential embedded-cluster study. *International Journal of Quantum Chemistry*, 90(2):751–758, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Panina:2004:DSR

[PBSC04] Natalia S. Panina, Alexander N. Beljaev, Svetlana A. Simanova, and Mario Calligaris. DFT study of the role of intermolecular interactions in the formation of stable halogeno– and ammineaqua– platinum(II) coordination compounds. *International Journal of Quantum Chemistry*, 96(2):80–88, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pinto-Bazurco:2006:QQI

[PBTP06] Mariano Pinto-Bazurco, Ivanka Tsakovska, and Ilza Pajeva. QSAR and 3D QSAR of inhibitors of the epidermal growth factor receptor. *International Journal of Quantum Chemistry*, 106(6):1432–1444, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paldus:2004:PPS

[PČ04a] Josef Paldus and Jiří Čížek. Preface: Proceedings of the Seventh European Workshop on Quantum Systems in Chemistry and Physics. *International Journal of Quantum Chemistry*, 99(6):877–878, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ponec:2004:GPA

[PC04b] Robert Ponec and David L. Cooper. Generalized population analysis of three-center two-electron bonding. *International*

Journal of Quantum Chemistry, 97(6):1002–1011, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palmeiro:2007:NVR

[PC07] R. Palmeiro and O. Castaño. New valley ridge inflection point associated to the bifurcation of a valley on potential energy surfaces. *International Journal of Quantum Chemistry*, 107 (14):2687–2696, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Padilla-Campos:2009:TIA

[PC09] Luis Padilla-Campos. Theoretical investigation of the adsorption of oxygen on small bimetallic Li_mCu_n $(m, n \leq 4)$ clusters. *International Journal of Quantum Chemistry*, 109(6): 1357–1367, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pavanello:2008:ABO

[PCBA08] Michele Pavanello, Mauricio Cafiero, Sergiy Bubin, and Ludwik Adamowicz. Accurate Born–Oppenheimer calculations of the low-lying $c\,^3\Sigma$ and $a\,^3\Sigma$ excited states of helium dimer. *International Journal of Quantum Chemistry*, 108(12):2291–2298, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perrine:2005:QPA

[PCF05] Trilisa M. Perrine, Rajat K. Chaudhuri, and Karl F. Freed. Quadratic Padé approximants and the intruder state problem of multireference perturbation methods. *International Journal of Quantum Chemistry*, 105(1):18–33, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pittner:2002:FRS

[PČH02] Jiří Pittner, Petr Čársky, and Ivan Hubač. Four- and 8-reference state-specific Brillouin–Wigner coupled-cluster method: Study of the singlet oxygen. *International Journal of Quantum Chemistry*, 90(3):1031–1037, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pasha:2008:QSA

[PCKC08] Farhan A. Pasha, Hwan W. Chung, Soon B. Kang, and Seung J. Cho. 3D-quantitative structure activity analysis and

quantum chemical analysis of pyrido-di-indoles. *International Journal of Quantum Chemistry*, 108(2):391–400, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pollet:2003:ECE

[PCL+03] R. Pollet, F. Colonna, T. Leininger, H. Stoll, H.-J. Werner, and A. Savin. Exchange-correlation energies and correlation holes for some two- and four-electron atoms along a nonlinear adiabatic connection in density functional theory. *International Journal of Quantum Chemistry*, 91(2):84–93, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:2000:DFS

[PCM00] Peter Politzer, Monica C. Concha, and Jane S. Murray. Density functional study of dimers of dimethylnitramine. *International Journal of Quantum Chemistry*, 80(2):184–192, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001274/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001274/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001274&PLACEBO=IE.pdf`.

Palermo:2008:RAR

[PCML08] Nicholas Y. Palermo, József Csontos, Richard F. Murphy, and Sándor Lovas. Role of aromatic residues in stabilizing the secondary and tertiary structure of avian pancreatic polypeptide. *International Journal of Quantum Chemistry*, 108(4):814–819, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pahl:2009:IAI

[PCS09] E. Pahl, F. Calvo, and P. Schwerdtfeger. The importance of accurate interaction potentials in the melting of argon nanoclusters. *International Journal of Quantum Chemistry*, 109(9):1812–1819, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perez:2004:NAE

[PCT+04] J. E. Pérez, J. C. Cesco, O. E. Taurian, F. S. Ortiz, A. E. Rosso, C. C. Denner, and G. O. Giubergia. A new algorithm

to evaluate bielectronic integrals with 1s Slater-type orbitals obtained by the integral transforms. *International Journal of Quantum Chemistry*, 99(2):70–79, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perez:2005:EBI

[PCT+05] J. E. Pérez, J. C. Cesco, O. E. Taurian, F. S. Ortiz, A. E. Rosso, C. C. Denner, and G. O. Giubergia. Evaluation of bielectronic integrals for 1s Slater orbitals by using averages. *International Journal of Quantum Chemistry*, 102(6):1056–1060, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Panda:2005:TEE

[PD05] Anirban Panda and Sambhu N. Datta. Transport of excitation energy in a molecular aggregate. VIII. Numerical simulation of exciton processes in thylakoid membrane. *International Journal of Quantum Chemistry*, 105(1):84–98, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pisani:2000:CET

[PDR+00] C. Pisani, R. Dovesi, C. Roetti, M. Causà, R. Orlando, S. Casassa, and V. R. Saunders. CRYSTAL and EMBED, two computational tools for the ab initio study of electronic properties of crystals. *International Journal of Quantum Chemistry*, 77(6):1032–1048, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000983/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000983/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000983&PLACEBO=IE.pdf`.

Poater:2004:AED

[PDS04] J. Poater, M. Duran, and M. Solà. Analysis of electronic delocalization in buckminsterfullerene (C_{60}). *International Journal of Quantum Chemistry*, 98(4):361–366, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pupyshev:2004:BSM

[PE04] Vladimir I. Pupyshev and Alexandr Y. Ermilov. Bound states of multipoles. *International Journal of Quantum Chemistry*,

96(3):185–192, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pearson:2002:IEA

[Pea02] Ralph G. Pearson. Improving the energies of approximate wave functions using the concepts of density functional theory. *International Journal of Quantum Chemistry*, 86(3):273–279, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/88011744/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88011744/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88011744&PLACEBO=IE.pdf`.

Pearson:2005:SCS

[Pea05] Ralph G. Pearson. Self-consistent shielding in atoms and molecules. *International Journal of Quantum Chemistry*, 101 (3):239–245, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pearson:2008:ACD

[Pea08] Ralph G. Pearson. Applying the concepts of density functional theory to simple systems. *International Journal of Quantum Chemistry*, 108(5):821–826, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pejov:2002:IAA

[Pej02] Ljupčo Pejov. Interaction of acetonitrile with alkaline metal cations: A density functional, coupled-cluster, and quadratic configuration interaction study. *International Journal of Quantum Chemistry*, 86(4):356–367, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85515549/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85515549/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85515549&PLACEBO=IE.pdf`.

Pejov:2003:DFS

[Pej03] Ljupčo Pejov. Density functional study of indole–pyrrole heterodimer potential energy hypersurface. *International Journal of Quantum Chemistry*, 92(6):516–527, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Penotti:2000:ESL

[Pen00a] Fabio E. Penotti. On the electronic structure of Li_2 (X^1) and its changes with internuclear distance. *International Journal of Quantum Chemistry*, 78(5):378–397, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72001895/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72001895/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72001895&PLACEBO=IE.pdf`.

Penotti:2000:ISF

[Pen00b] Fabio E. Penotti. On the identification of symmetry-forbidden spin subspaces for configurations employing nonorthogonal orbitals. *International Journal of Quantum Chemistry*, 78(1): 24–31, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71001655/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71001655/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71001655&PLACEBO=IE.pdf`.

Penotti:2006:ESB

[Pen06] Fabio E. Penotti. Electronic structure of BeH_2. *International Journal of Quantum Chemistry*, 106(5):1153–1159, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Petrie:2000:DBS

[Pet00] Simon Petrie. Do branched structures exist for cyanide-containing magnesium compounds? Computational studies on a range of mixed-ligand compounds XMg(CN) (X = F, Cl, OH, SH, NH_2, CH_3, CN). *International Journal of Quantum Chemistry*, 76(5):626–642, February 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000584/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000584/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000584&PLACEBO=IE.pdf`.

Petrosky:2004:SML

[Pet04] T. Petrosky. Stochastic Maxwell–Lorentz equation in radiation damping. *International Journal of Quantum Chemistry*, 98(2):103–111, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pavao:2006:QBM

[PF06] Antonio C. Pavão and Joacy V. Ferreira. Quark–boson molecular orbital calculations. *International Journal of Quantum Chemistry*, 106(13):2578–2580, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pakiari:2008:DDD

[PFA08] A. H. Pakiari, S. Fakhraee, and S. M. Azami. Decomposition of deformation density into orbital components. *International Journal of Quantum Chemistry*, 108(3):415–422, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palmeiro:2002:NTB

[PFC02] Raul Palmeiro, Luis Manuel Frutos, and Obis Castaño. Note on the theory of bifurcation of chemical reactions. *International Journal of Quantum Chemistry*, 86(5):422–425, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85514350/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85514350/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85514350&PLACEBO=IE.pdf`.

Pickholz:2008:DNP

[PFdP08] Mónica Pickholz, Leonardo Fernandes Fraceto, and Eneida de Paula. Distribution of neutral prilocaine in a phospholipid bilayer: Insights from molecular dynamics simulations. *International Journal of Quantum Chemistry*, 108(13):2386–2391, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pasqualoto:2006:MDS

[PFSFH06] Kerly F. M. Pasqualoto, Márcia M. C. Ferreira, Osvaldo A. Santos-Filho, and Anton J. Hopfinger. Molecular dynamics simulations of a set of isoniazid derivatives bound to InhA, the

enoyl-acp reductase from *M. tuberculosis*. *International Journal of Quantum Chemistry*, 106(13):2689–2699, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Petrov:2005:CSD

[PFSP05] Anton S. Petrov, Joni Funseth-Smotzer, and George R. Pack. Computational study of dimethyl phosphate anion and its complexes with water, magnesium, and calcium. *International Journal of Quantum Chemistry*, 102(5):645–655, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Petersilka:2000:EET

[PGB00] M. Petersilka, E. K. U. Gross, and Kieron Burke. Excitation energies from time-dependent density functional theory using exact and approximate potentials. *International Journal of Quantum Chemistry*, 80(4–5):534–554, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505399/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505399/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505399&PLACEBO=IE.pdf`.

Palusiak:2009:ECT

[PGB09] Marcin Palusiak, Célia Fonseca Guerra, and F. Matthias Bickelhaupt. π-electronic communication through mono and multinuclear gold(I) complexes. *International Journal of Quantum Chemistry*, 109(11):2507–2519, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pickard:2006:CWO

[PGF+06] Frank C. Pickard IV, Daniel R. Griffith, Skylar J. Ferrara, Matthew D. Liptak, Karl N. Kirschner, and George C. Shields. CCSD(T), W1, and other model chemistry predictions for gas-phase deprotonation reactions. *International Journal of Quantum Chemistry*, 106(15):3122–3128, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palafox:2005:SFP

[PGN+05] M. Alcolea Palafox, M. Gill, N. J. Nunez, V. K. Rastogi, Lalit Mittal, and Rekha Sharma. Scaling factors for the prediction

of vibrational spectra. II. The aniline molecule and several derivatives. *International Journal of Quantum Chemistry*, 103 (4):394–421, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palafox:2002:SPM

[PGNT02] M. Alcolea Palafox, M. Gil, J. L. Núñez, and G. Tardajos. Study of phenothiazine and *N*-methyl phenothiazine by infrared, Raman, ^{1}H-, and ^{13}C-NMR spectroscopies. *International Journal of Quantum Chemistry*, 89(3):147–171, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Popova:2007:ISS

[PGP+07] Angelina D. Popova, Miglena. K. Georgieva, Ognyan. I. Petrov, Katya. V. Petrova, and Evelina. A. Velcheva. IR spectral and structural studies of 4-aminobenzenesulfonamide (sulfanilamide)-d_0, -d_4, and -^{15}N, as well as their azanions: Combined DFT B3LYP/experimental approach. *International Journal of Quantum Chemistry*, 107(8):1752–1764, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pomogaev:2009:EMC

[PGPA09] Vladimir Pomogaev, Feng Long Gu, Anna Pomogaeva, and Yuriko Aoki. Elongation method for calculating excited states of aromatic molecules embedded in polymers. *International Journal of Quantum Chemistry*, 109(6):1328–1340, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Piecuch:2008:BMM

[PGW08] Piotr Piecuch, Jeffrey R. Gour, and Marta Włoch. Biorthogonal method of moments of coupled-cluster equations: Alternative derivation, further considerations, and application to a model magnetic system. *International Journal of Quantum Chemistry*, 108(12):2128–2149, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Piecuch:2009:LEC

[PGW09] Piotr Piecuch, Jeffrey R. Gour, and Marta Włoch. Left-eigenstate completely renormalized equation-of-motion coupled-cluster methods: Review of key concepts, extension to excited

states of open-shell systems, and comparison with electron-attached and ionized approaches. *International Journal of Quantum Chemistry*, 109(14):3268–3304, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pinchon:2007:NIF

[PH07] Didier Pinchon and Philip E. Hoggan. New index functions for storing Gaunt coefficients. *International Journal of Quantum Chemistry*, 107(12):2186–2196, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pinchon:2009:GAE

[PH09] Didier Pinchon and Philip E. Hoggan. Gaussian approximation of exponential type orbitals based on B functions. *International Journal of Quantum Chemistry*, 109(2):135–144, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pinchon:2008:NEL

[PHH08] Didier Pinchon, Philip E. Hoggan, and Frank E. Harris. A new expansion of the leaky aquifer function. *International Journal of Quantum Chemistry*, 108(15):3042–3046, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Piecuch:2006:ADP

[PHK+06] Piotr Piecuch, So Hirata, Karol Kowalski, Peng-Dong Fan, and Theresa L. Windus. Automated derivation and parallel computer implementation of renormalized and active-space coupled-cluster methods. *International Journal of Quantum Chemistry*, 106(1):79–97, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Phung:2009:ISM

[PHNN09a] T. V. B. Phung, T. Hashimoto, K. Nishikawa, and H. Nagao. Ab-initio studies of magnetic properties of small-sized and cuboctahedral aluminum nanoclusters. *International Journal of Quantum Chemistry*, 109(14):3457–3465, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Phung:2009:TSI

[PHNN09b] Thi Viet Bac Phung, Taihei Hashimoto, Kyoshi Nishikawa, and Hidemi Nagao. Theoretical studies on ionization potential of aluminum clusters. *International Journal of Quantum Chemistry*, 109(15):3602–3612, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perez:2008:SSW

[PHR08] Jhon F. Pérez, C. Z. Hadad, and Albeiro Restrepo. Structural studies of the water tetramer. *International Journal of Quantum Chemistry*, 108(10):1653–1659, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palanichamy:2002:SSA

[PI02] R. Rajeswara Palanichamy and K. Iyakutti. Structural stability analysis of Wigner crystal with Gaussian and Yukawa-type positive background. *International Journal of Quantum Chemistry*, 86(5):478–486, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86511023/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86511023/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86511023&PLACEBO=IE.pdf`.

Palafox:2002:QCS

[PIGN02] Mauricio Alcolea Palafox, Nerea Iza, Manuel Gil, and José Luís Núñez. Quantum chemical study of several monocyclic complex β-lactam C-3, C-4, and N-derivatives, and β-ring model molecules. *International Journal of Quantum Chemistry*, 89(1):25–47, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Park:2007:SSG

[PILD07] Sung-Woo Park, Suk Im, Sungyul Lee, and C. Desfrançois. Structure and stability of glycine–$(H_2O)_3$ cluster and anion: Zwitterion vs. canonical glycine. *International Journal of Quantum Chemistry*, 107(6):1316–1327, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Piris:2006:NAT

[Pir06] Mario Piris. A new approach for the two-electron cumulant in natural orbital functional theory. *International Journal of Quantum Chemistry*, 106(5):1093–1104, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pires:2003:GBS

[PJ03] José M. Pires and F. E. Jorge. Gaussian basis sets for polyatomic molecules containing first- and second-row atoms. *International Journal of Quantum Chemistry*, 95(2):144–148, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perpete:2007:IIS

[PJ07] Eric A. Perpète and Denis Jacquemin. Ab initio investigation of the solvent and electron correlation effects on the geometries and first hyperpolarizabilities of push–pull oligomers. *International Journal of Quantum Chemistry*, 107(11):2066–2074, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pulay:2009:ECE

[PJ09] Peter Pulay and Tomasz Janowski. Efficient calculation of the energy of a molecule in an arbitrary electric field. *International Journal of Quantum Chemistry*, 109(10):2113–2120, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pinheiro:2000:IGC

[PJdC00] J. C. Pinheiro, F. E. Jorge, and E. V. R. de Castro. An improved generator coordinate Hartree–Fock method applied to the choice of contracted Gaussian basis sets for first-row diatomic molecules. *International Journal of Quantum Chemistry*, 78(1):15–23, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71001654/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71001654/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71001654&PLACEBO=IE.pdf`.

Politzer:2001:I

[PJM01] Peter Politzer, William L. Jorgensen, and Jane S. Murray. Introduction. *International Journal of Quantum Chemistry*, 83(3-4):97, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002582/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002582/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002582&PLACEBO=IE.pdf`.

Preat:2008:TST

[PJP08] Julien Preat, Denis Jacquemin, and Eric A. Perpète. Tayloring standard TDDFT approaches for computing UV/Vis transitions in thiocarbonyl chromophores. *International Journal of Quantum Chemistry*, 108(4):762–773, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pratt:2009:CSS

[PJS+09a] Lawrence M. Pratt, Darrel Jones, Andrea Sease, Donta Busch, Emmanuel Faluade, Son C. Nguyen, and Bui T. Thanh. Calculation of the solvation state of organolithium compounds: Effects of basis sets and electron correlation methods. *International Journal of Quantum Chemistry*, 109(1):34–42, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Przybytek:2009:IOF

[PJS09b] Michal Przybytek, Bogumil Jeziorski, and Krzysztof Szalewicz. Infinite-order functional for nonlinear parameters optimization in explicitly correlated coupled cluster theory. *International Journal of Quantum Chemistry*, 109(13):2872–2884, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Peng:2009:IRS

[PJZ+09] Ke Peng, Lijun Jin, Weiqun Zhou, Wen Yang, and Min Li. The investigation on the relative stability of different clusters of thiourea dioxide in water using gas phase quantum chemical calculations. *International Journal of Quantum Chemistry*, 109(6):1368–1375, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palinko:2001:SMP

[PK01a] I. Pálinkó and T. Körtvélyesi. Structural motifs in α-pyridyl- and α-furylcinnamic acid assemblies — A molecular modeling study. *International Journal of Quantum Chemistry*, 84(2):269–275, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502330/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502330/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502330&PLACEBO=IE.pdf`.

Parusel:2001:IAC

[PK01b] Andreas B. J. Parusel and Gottfried Köhler. Influence of the alkyl chain length on the excited-state properties of 4-dialkyl-benzonitriles. A theoretical DFT/MRCI study. *International Journal of Quantum Chemistry*, 84(2):149–156, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502327/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502327/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502327&PLACEBO=IE.pdf`.

Pelikan:2001:ESP

[PKB+01] P. Pelikán, M. Košuth, S. Biskupič, J. Noga, M. Straka, A. Zajac, and P. Baňacký. Electron structure of polysilanes. Are these polymers one-dimensional systems? *International Journal of Quantum Chemistry*, 84(2):157–168, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502332/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502332/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502332&PLACEBO=IE.pdf`.

Pecur:2000:CES

[PKS+00] S. Pečur, L. Klasinc, K. Stettmaier, W. Bors, and S. P. McGlynn. Calculations and electron spin resonance spectra of syringic and sinapinic acid. *International Journal of Quantum Chemistry*, 80(6):1210–1215, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (elec-

tronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/75501737/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75501737/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75501737&PLACEBO=IE.pdf.

Panin:2005:EGT

[PKT05] L. E. Panin, V. G. Kunitsyn, and F. V. Tusikov. Effect of glucocorticoids and their complexes with apolipoprotein A-I on the secondary structure of eukaryotic DNA. *International Journal of Quantum Chemistry*, 101(4):450–467, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Peplowski:2008:CDS

[PKZN08] Lukasz Peplowski, Karina Kubiak, Slawomir Zelek, and Wieslaw Nowak. A comparative DFT study of substrates and products of industrial enzyme nitrile hydratase. *International Journal of Quantum Chemistry*, 108(1):161–179, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:2000:KSS

[PL00] Peter Politzer and Pat Lane. Kohn–Sham studies of oxygen systems. *International Journal of Quantum Chemistry*, 77(1):336–340, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70004275/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004275/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004275&PLACEBO=IE.pdf.

Podolyan:2009:MVT

[PL09] Yevgeniy Podolyan and Jerzy Leszczynski. MaSK: A visualization tool for teaching and research in computational chemistry. *International Journal of Quantum Chemistry*, 109(1): 8–16, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Planelles:2001:LOB

[Pla01] Josep Planelles. Ladder operators and boundary conditions. *International Journal of Quantum Chemistry*, 81(2):141–147,

???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76500934/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76500934/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76500934&PLACEBO=IE.pdf`.

Preat:2007:DTD

[PLA+07] Julien Preat, Pierre-François Loos, Xavier Assfeld, Denis Jacquemin, and Eric A. Perpète. DFT and TD-DFT investigation of IR and UV spectra of solvated molecules: Comparison of two SCRF continuum models. *International Journal of Quantum Chemistry*, 107(3):574–585, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:2002:AME

[PLC02] Peter Politzer, Pat Lane, and Monica C. Concha. Atomic and molecular energies in terms of electrostatic potentials at nuclei. *International Journal of Quantum Chemistry*, 90(1):459–463, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palting:2004:GAV

[PLC04] Pancracio Palting, Jorge Ricardo Letelier, and Ying Nan Chiu. Geminal approach to vibronic models of superconductivity in crystals. I. The Jahn–Teller effect. *International Journal of Quantum Chemistry*, 96(1):56–68, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Persson:2002:QCP

[PLO02] Petter Persson, Sten Lunell, and Lars Ojamäe. Quantum chemical prediction of the adsorption conformations and dynamics at HCOOH-covered ZnO(1010) surfaces. *International Journal of Quantum Chemistry*, 89(3):172–180, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Piris:2008:NOF

[PLU08] Mario Piris, Xabier Lopez, and Jesus M. Ugalde. Natural orbital functional description of van der Waals interactions: A case study of the effect of the basis set for the helium dimer.

International Journal of Quantum Chemistry, 108(10):1660–1663, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

PereiraDaSilva:2003:PQS

[PM03] Andre Elvas Pereira Da Silva and Geraldo Magela e Silva. Polyacetylene as a qubit system. *International Journal of Quantum Chemistry*, 95(3):224–229, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:2004:NIE

[PM04a] Peter Politzer and Yuguang Ma. Noncovalent intermolecular energetics: RDX crystal. *International Journal of Quantum Chemistry*, 100(5):733–739, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Porras:2004:AAC

[PM04b] Ignacio Porras and Andrés Moya. Approximate atomic calculations and stability of negative ions with a modified Thomas–Fermi–Dirac model. *International Journal of Quantum Chemistry*, 99(4):288–296, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

PaesLima:2006:EIP

[PM06a] Matheus Paes Lima and Geraldo Magela e Silva. Effects of impurities on polaron dynamics in conjugated polymers: Effective potentials. *International Journal of Quantum Chemistry*, 106(13):2597–2602, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

PaesLima:2006:PSU

[PM06b] Matheus Paes Lima and Geraldo Magela e Silva. Polaron stability under collision with different defects in conjugated polymers. *International Journal of Quantum Chemistry*, 106 (13):2603–2608, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:2009:CEE

[PM09] Peter Politzer and Jane S. Murray. Computed effects of electric fields upon the C — NO_2 and N — NO_2 bonds of nitromethane and dimethylnitramine. *International Journal of Quantum Chemistry*, 109(1):3–7, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:2000:PSF

[PMAA00] Peter Politzer, Jane S. Murray, and Fakher Abu-Awwad. Prediction of solvation free energies from computed properties of solute molecular surfaces. *International Journal of Quantum Chemistry*, 76(5):643–647, February 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000585/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000585/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000585&PLACEBO=IE.pdf`.

Politzer:2006:P

[PMB06] Peter Politzer, Jane Murray, and Erkki Brändas. Preface. *International Journal of Quantum Chemistry*, 106(14):2819, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pascariu:2008:DNS

[PMB08] Aurelia Pascariu, Mircea Mracec, and Stefan Berger. Dynamic NMR study of the oxaphosphetane complexation with lithium during the Wittig reaction. *International Journal of Quantum Chemistry*, 108(6):1052–1058, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Patel:2009:TSP

[PMBM09] Pansy D. Patel, Ivan A. Mikhailov, Kevin D. Belfield, and Artëm E. Masunov. Theoretical study of photochromic compounds, part 2: Thermal mechanism for byproduct formation and fatigue resistance of diarylethenes used as data storage materials. *International Journal of Quantum Chemistry*, 109 (15):3711–3722, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:2002:CRM

[PMC02] Peter Politzer, Jane S. Murray, and Monica C. Concha. The complementary roles of molecular surface electrostatic potentials and average local ionization energies with respect to electrophilic processes. *International Journal of Quantum Chemistry*, 88(1):19–27, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.`

wiley.com/cgi-bin/abstract/90010556/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90010556/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90010556&PLACEBO=IE.pdf.

Perez-Marin:2000:DFS

[PMCOSC00] L. Perez-Marín, M. Castro, E. Otazo-Sánchez, and G. A. Cisneros. Density functional study of molecular recognition and reactivity of thiourea derivatives used in sensors for heavy metal polluting cations. *International Journal of Quantum Chemistry*, 80(4–5):609–622, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505384/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505384/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505384&PLACEBO=IE.pdf.

Papp:2007:MBB

[PMHW07] P. Papp, P. Mach, I. Hubač, and S. Wilson. Many-body Brillouin–Wigner second-order perturbation theory: A robust and efficient approach to the multireference correlation problem. *International Journal of Quantum Chemistry*, 107(14): 2622–2631, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:2007:HBH

[PML07] Peter Politzer, Jane S. Murray, and Pat Lane. σ-hole bonding and hydrogen bonding: Competitive interactions. *International Journal of Quantum Chemistry*, 107(15):3046–3052, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pathak:2009:TIS

[PML09a] Biswarup Pathak, D. Majumdar, and Jerzy Leszczynski. Theoretical investigations of the structure and bonding of several transition metal complexes to probe their carbon monoxide releasing properties. *International Journal of Quantum Chemistry*, 109(10):2263–2272, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Peng:2009:CKP

[PML09b] Daoling Peng, Jianyi Ma, and Wenjian Liu. On the construction of Kramers paired double group symmetry functions. *International Journal of Quantum Chemistry*, 109(10):2149–2167, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:2009:CDE

[PML09c] Peter Politzer, Jane S. Murray, and Pat Lane. Computational determination of effects of electric fields upon "trigger linkages" of prototypical energetic molecules. *International Journal of Quantum Chemistry*, 109(3):534–539, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:2005:CPS

[PMLC05] Peter Politzer, Yuguang Ma, Pat Lane, and Monica C. Concha. Computational prediction of standard gas, liquid, and solid-phase heats of formation and heats of vaporization and sublimation. *International Journal of Quantum Chemistry*, 105(4):341–347, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:2009:EDC

[PMLC09] Peter Politzer, Jane S. Murray, Pat Lane, and Monica C. Concha. Electrostatically driven complexes of SiF_4 with amines. *International Journal of Quantum Chemistry*, 109(15):3773–3780, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:2007:NFB

[PMLTL07] Peter Politzer, Jane S. Murray, Pat Lane, and Alejandro Toro-Labbé. A noteworthy feature of bond dissociation/formation reactions. *International Journal of Quantum Chemistry*, 107 (11):2153–2157, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Piris:2004:NOF

[PMO04] Mario Piris, Alberto Martinez, and Peter Otto. Natural orbital functional approach: Calculation of dielectric properties in molecules. *International Journal of Quantum Chemistry*,

97(4):827–831, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:2001:MSE

[PMPI01] Peter Politzer, Jane S. Murray, and Zenaida Peralta-Inga. Molecular surface electrostatic potentials in relation to noncovalent interactions in biological systems. *International Journal of Quantum Chemistry*, 85(6):676–684, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85006601/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85006601/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85006601&PLACEBO=IE.pdf`.

Pena:2004:IOP

[PMZGGR04] J. J. Peña, J. Morales, E. Zamora-Gallardo, and J. García-Ravelo. Isospectral orthogonal polynomials from the Darboux transforms. *International Journal of Quantum Chemistry*, 100 (6):957–963, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Petkova:2007:IBA

[PNBV07] Nevena I. Petkova, Rositca D. Nikolova, Anka G. Bojilova, and Georgi N. Vayssilov. Influence of BH_3 and alkaline cation released from the reduction agent on a tandem reduction/acylation reaction—A computational study. *International Journal of Quantum Chemistry*, 107(8):1814–1825, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palafox:2002:TQC

[PNG02] M. Alcolea Palafox, J. L. Núñez, and M. Gil. Theoretical quantum chemical study of benzoic acid: Geometrical parameters and vibrational wavenumbers. *International Journal of Quantum Chemistry*, 89(1):1–24, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Purqon:2008:SPS

[PNN08] Acep Purqon, Hidemi Nagao, and Kiyoshi Nishikawa. Synchronization patterns in spaghetti-like nanoclusters. *International Journal of Quantum Chemistry*, 108(15):2870–2880,

???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Piris:2003:OPD

[PO03] Mario Piris and Peter Otto. One-particle density matrix functional for correlation in molecular systems. *International Journal of Quantum Chemistry*, 94(6):317–323, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Piris:2005:NOF

[PO05] Mario Piris and Peter Otto. Natural orbital functional for correlation in polymers. *International Journal of Quantum Chemistry*, 102(1):90–97, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pacheco-Ortin:2008:TSA

[POAVdlM08] Sandy Maria Pacheco-Ortín, Esther Agacino-Valdés, and Pablo de la Mora. Theoretical study of O_2 adsorption and CO_2 formation in bimetallic dimer clusters Au–M. *International Journal of Quantum Chemistry*, 108(10):1796–1801, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pogliani:2005:MPP

[Pog05] Lionello Pogliani. Model of the physical properties of halides with complete graph-based indices. *International Journal of Quantum Chemistry*, 102(1):38–52, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Polavarapu:2006:QMP

[Pol06] Prasad L. Polavarapu. Quantum mechanical predictions of chiroptical vibrational properties. *International Journal of Quantum Chemistry*, 106(8):1809–1814, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pomeau:2004:ENT

[Pom04] Yves Pomeau. Equilibrium and nonequilibrium theory of dilute Bose gases. *International Journal of Quantum Chemistry*, 98(2):118–124, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pena:2007:ESS

[POM+07] J. J. Peña, G. Ovando, J. Morales, J. García-Ravelo, and C. Pacheco-García. Exactly solvable Schrödinger equations with a position-dependent mass: Null potential. *International Journal of Quantum Chemistry*, 107(15):3039–3045, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pena:2008:ESQ

[POM+08a] J. J. Peña, G. Ovando, J. Morales, J. García-Ravelo, and J. García. Exactly solvable quantum potentials with special functions solutions. *International Journal of Quantum Chemistry*, 108(10):1750–1757, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pena:2008:PDM

[POM+08b] J. J. Peña, G. Ovando, J. Morales, J. GarcÍa-Ravelo, and C. Pacheco-García. Position-dependent mass Schrödinger equations allowing harmonic oscillator (HO) eigenvalues. *International Journal of Quantum Chemistry*, 108(15):2906–2913, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pena:2001:SQP

[POMGM01] J. J. Peña, G. Ovando, D. Morales-Guzmán, and J. Morales. Solvable quartic potentials and their isospectral partners. *International Journal of Quantum Chemistry*, 85(4–5):244–250, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Porter:2001:AEL

[Por01] L. E. Porter. Anomalous energy losses for light projectiles traversing a polyvinylformyl resin. *International Journal of Quantum Chemistry*, 85(4–5):455–462, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Porter:2002:OTV

[Por02] L. E. Porter. Observed trends in values of target mean excitation energy and Barkas-effect parameter extracted from stopping power measurements. *International Journal of Quantum Chemistry*, 90(2):684–688, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Porter:2003:FOP

[Por03] L. E. Porter. Further observations of projectile-z dependence in target parameters of modified Bethe–Bloch theory. *International Journal of Quantum Chemistry*, 95(4–5):504–511, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Porter:2004:SOT

[Por04] L. E. Porter. Studies of observed trends in values of Bethe–Bloch parameters extracted from stopping power measurements. *International Journal of Quantum Chemistry*, 100 (6):973–980, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Potz:2001:QCC

[Pöt01] Walter Pötz. Quantum coherent control of Coulomb enhancement by two-color pulseshaping. *International Journal of Quantum Chemistry*, 85(4–5):398–404, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pou:2003:ECE

[POV+03] P. Pou, R. Oszwałdowski, H. Vázquez, R. Pérez, F. Flores, and J. Ortega. Exchange correlation energy as a function of the orbital occupancies: Implementation on first principles local orbital methods. *International Journal of Quantum Chemistry*, 91(2):151–156, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Planelles:2000:RAA

[PPP00] Josep Planelles, Guillermo Peris, and Josef Paldus. Reciprocal adjustment of approximate coupled cluster and configuration interaction approaches. *International Journal of Quantum Chemistry*, 77(4):693–703, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70500241/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70500241/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70500241&PLACEBO=IE.pdf`.

Piquemal:2008:WCL

[PPP+08] J.-P. Piquemal, J. Pilmé, O. Parisel, H. Gérard, I. Fourré, J. Bergès, C. Gourlaouen, A. De La Lande, M.-C. Van Severen, and B. Silvi. What can be learnt on biologically relevant systems from the topological analysis of the electron localization function? *International Journal of Quantum Chemistry*, 108(11):1951–1969, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pecul:2005:ICV

[PR05] Magdalena Pecul and Kenneth Ruud. Ab initio calculation of vibrational Raman optical activity. *International Journal of Quantum Chemistry*, 104(5):816–829, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paulus:2009:AMI

[PR09] Beate Paulus and Krzysztof Rosciszewski. Application of the method of increments to the adsorption of H_2S on graphene. *International Journal of Quantum Chemistry*, 109(13):3055–3062, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Prat-Resina:2004:GOT

[PRBGLL04] Xavier Prat-Resina, Josep Maria Bofill, Àngels González-Lafont, and José M. Lluch. Geometry optimization and transition state search in enzymes: Different options in the microiterative method. *International Journal of Quantum Chemistry*, 98(4):367–377, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pitarch-Ruiz:2006:RCD

[PRCEM06] J. Pitarch-Ruiz, C. J. Calzado, S. Evangelisti, and D. Maynau. Reduction of the CI dimension based on the use of local orbitals: Application to conjugated systems and excited states. *International Journal of Quantum Chemistry*, 106 (3):609–622, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pitarch-Ruiz:2004:LMO

[PREM04] J. Pitarch-Ruiz, S. Evangelisti, and D. Maynau. Localized molecular orbitals for excited states of polyenals, polyendials,

and polyenones. *International Journal of Quantum Chemistry*, 97(1):688–699, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pitarch-Ruiz:2005:LOS

[PREM05] J. Pitarch-Ruiz, S. Evangelisti, and D. Maynau. Local orbitals for the study of the $\pi \rightarrow \pi$ * excitation in polyenes. *International Journal of Quantum Chemistry*, 101(3):325–333, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pavlov:2004:NME

[PRG+04] R. L. Pavlov, P. P. Raychev, V. P. Garistov, M. Dimitrova-Ivanovich, and J. Maruani. Nuclear moments and electron density matrices in atoms. *International Journal of Quantum Chemistry*, 99(4):308–316, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Price:2005:CPR

[Pri05] Harry L. Price. Correlating the positional reactivity of a masked electrophilic center to the topology of the electron density. *International Journal of Quantum Chemistry*, 102 (5):480–488, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Podolyan:2001:IPH

[PRL01] Yevgeniy Podolyan, Yury V. Rubin, and Jerzy Leszczyński. An ab initio post-Hartree–Fock study of vibrational infrared spectra of 5-azacytosine and cytosine. *International Journal of Quantum Chemistry*, 83(3-4):203–212, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002592/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002592/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002592&PLACEBO=IE.pdf`.

Porter:2002:AMS

[PRM02] L. E. Porter, J. Räisänen, and F. Munnik. Analysis of measurements of stopping powers of formvar, polyimide, polysulfone, and vyns for 3.6 to 10.5 MeV ^{7}Li ions. *International Journal of Quantum Chemistry*, 90(4-5):1368–1377,

???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palafox:2003:BST

[PRM03] M. Alcolea Palafox, V. K. Rastogi, and Lalit Mittal. Benzonitriles: Survey of their importance and scaling of their vibrational frequencies. *International Journal of Quantum Chemistry*, 94(4):189–204, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palafox:2006:IRS

[PRM+06] M. A. Palafox, V. K. Rastogi, Lalit Mittal, W. Kiefer, and H. P. Mital. IR and Raman spectra, density functional computations of vibrational spectrum, molecular geometry, atomic charges, and some molecular properties of 3-aminobenzonitrile molecule. *International Journal of Quantum Chemistry*, 106 (8):1885–1901, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pelegrini:2003:MST

[PRNM03] Marina Pelegrini, Orlando Roberto-Neto, and Francisco B. C. Machado. MRSDCI study of the two lower-lying doublet electronic states of the BeB, MgB, and CaB molecules. *International Journal of Quantum Chemistry*, 95(3):205–212, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pena:2005:ESC

[PRRMLB05] J. J. Peña, M. A. Romero-Romo, J. Morales, and J. L. López-Bonilla. Exactly solvable combined potentials and their isospectral partners from SUSY. *International Journal of Quantum Chemistry*, 105(6):731–739, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paukku:2009:SHA

[PRS+09] Yuliya Paukku, Bakhtiyor Rasulev, Vladimir Syrov, Zainab Khushbaktova, and Jerzy Leszczynski. Structure-hepatoprotective activity relationship study of sesquiterpene lactones: A QSAR analysis. *International Journal of Quantum Chemistry*, 109 (1):17–27, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palacio:2008:MDS

[PRSLA08] Juan Carlos Castro Palacio, Jesús Rubayo-Soneira, Andrea Lombardi, and Vincenzo Aquilanti. Molecular dynamics simulations and hyperspherical mode analysis of NO in Kr crystals with the use of ab initio potential energy surfaces for the Kr–NO complex. *International Journal of Quantum Chemistry*, 108(10):1821–1830, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Puente:2002:WLD

[PS02] Antonio Puente and Llorenç Serra. Wigner localization and dynamics in two-electron semiconductor rings. *International Journal of Quantum Chemistry*, 86(1):27–34, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85008604/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85008604/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85008604&PLACEBO=IE.pdf`.

Pan:2003:CHK

[PS03a] Xiao-Yin Pan and Viraht Sahni. Corollary to the Hohenberg–Kohn theorem. *International Journal of Quantum Chemistry*, 95(4–5):387–393, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Peric:2003:UNC

[PS03b] Miljenko Perić and Ljiljana Stevanović. Use of the normal coordinates in variational and perturbative ab initio handling of the vibronic and spin–orbit couplings in Π electronic states of linear tetra-atomic molecules. *International Journal of Quantum Chemistry*, 92(3):276–293, April 5, 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Polonyi:2003:DDE

[PS03c] J. Polonyi and K. Sailer. Density-dependent effective action for electron systems. *International Journal of Quantum Chemistry*, 92(2):181–191, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Peterangelo:2004:SIA

[PS04] Stephen C. Peterangelo and Paul G. Seybold. Synergistic interactions among QSAR descriptors. *International Journal of Quantum Chemistry*, 96(1):1–9, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Patil:2007:NIM

[PS07] S. H. Patil and K. D. Sen. Net information measures for modified Yukawa and Hulthén potentials. *International Journal of Quantum Chemistry*, 107(9):1864–1874, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pan:2008:NPF

[PS08] Xiao-Yin Pan and Viraht Sahni. New perspectives on the fundamental theorem of density functional theory. *International Journal of Quantum Chemistry*, 108(15):2756–2762, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Puzari:2005:QDI

[PSA05] Panchanan Puzari, Biplab Sarkar, and Satrajit Adhikari. Quantum dynamics of inelastic scattering with a moving grid. *International Journal of Quantum Chemistry*, 105(3):209–224, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Poleshchuk:2005:EAC

[PSB+05] O. Kh. Poleshchuk, E. L. Shevchenko, V. Branchadell, M. Lein, and G. Frenking. Energy analysis of the chemical bond in group IV and V complexes: A density functional theory study. *International Journal of Quantum Chemistry*, 101 (6):869–877, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palma:2007:FCF

[PSC+07] A. Palma, L. Sandoval, K. Churyumov, V. Chavushyan, and A. Berezhnoy. Franck–Condon factors for molecules observed in comets. *International Journal of Quantum Chemistry*, 107 (14):2650–2653, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pacheco-Sanchez:2007:LZT

[PSCLGN07] J. H. Pacheco-Sánchez, S. Castillo, H. Luna-García, and O. Novaro. Landau–Zener theory for avoided crossings applied to the gallium–silane reactions. *International Journal of Quantum Chemistry*, 107(15):3053–3060, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pierdominici-Sottile:2005:QSS

[PSEP05] Gustavo Pierdominici-Sottile, Julián Echave, and Juliana Palma. Quantum study of the structure of the active site of methylamine dehydrogenase. *International Journal of Quantum Chemistry*, 105(6):937–945, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pernpointner:2000:AEF

[PSH00] Markus Pernpointner, Peter Schwerdtfeger, and Bernd A. Hess. Accurate electric field gradients for the coinage metal chlorides using the PCNQM method. *International Journal of Quantum Chemistry*, 76(3):371–384, January 20, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000280/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000280/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000280&PLACEBO=IE.pdf`.

Person:2002:QME

[PSK02] Willis B. Person, Krystyna Szczepaniak, and Jozef S. Kwiatkowski. Quantum mechanical and experimental infrared and Raman studies of 1-methyluracil and its hydrogen-bonded dimer. *International Journal of Quantum Chemistry*, 90(3):995–1020, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pan:2007:NFC

[PSM07] Xiao-Yin Pan, Viraht Sahni, and Lou Massa. Normalization and Fermi–Coulomb and Coulomb hole sum rules for approximate wave functions. *International Journal of Quantum Chemistry*, 107(4):816–823, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palma:2004:SQF

[PSML04] A. Palma, L. Sandoval, M. Martin, and R. Lefebvre. Second quantization and Floquet quasienergies of the parabolic barrier. *International Journal of Quantum Chemistry*, 99(4):484–487, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pacheco-Sanchez:2008:TPF

[PSN08] Juan Horacio Pacheco-Sánchez and Octavio Novaro. Transition probabilities found for M + CH_4 reactions (M = zinc, copper). *International Journal of Quantum Chemistry*, 108 (10):1645–1652, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pasha:2005:QSE

[PSS05] F. A. Pasha, H. K. Srivastava, and P. P. Singh. QSAR study of estrogens with the help of PM3-based descriptors. *International Journal of Quantum Chemistry*, 104(1):87–100, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Panin:2000:ESC

[PT00] A. I. Panin and A. V. Tulub. Electronic structure of cations X — OH_2^+ (X = C, N, O). *International Journal of Quantum Chemistry*, 77(2):580–588, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70002208/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70002208/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70002208&PLACEBO=IE.pdf`.

Proynov:2006:CMG

[PT06] Emil I. Proynov and Ajit J. Thakkar. Is combining meta-GGA correlation functionals with the OPTX exchange functional useful? *International Journal of Quantum Chemistry*, 106 (2):436–446, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ponec:2000:MBO

[PTLB00] Robert Ponec, Alicia Torre, Luis Lain, and Roberto C. Bochicchio. Multicenter bonding in open-shell systems. A non-

linear population analysis approach. *International Journal of Quantum Chemistry*, 77(4):710–715, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70500246/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70500246/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70500246&PLACEBO=IE.pdf.

Procel:2003:MWE

[PTS03] Luis Miguel Prócel, Francisco Tipán, and Arvids Stashans. Mott–Wannier excitons in the tetragonal $BaTiO_3$ lattice. *International Journal of Quantum Chemistry*, 91(4):586–590, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pudzianowski:2002:PIB

[Pud02] Andrew T. Pudzianowski. A protoporphyrin IX-based model for cytochrome P-450 iron-binding inhibitors: SAM1 calculations of structure and complexation enthalpy. *International Journal of Quantum Chemistry*, 88(1):147–153, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/89013454/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89013454/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89013454&PLACEBO=IE.pdf.

Patoary:2008:EIK

[PUH+08a] M. A. R. Patoary, M. Alfaz Uddin, A. K. F. Haque, A. K. Basak, M. R. Talukder, K. R. Karim, and B. C. Saha. Electron impact K-shell ionization cross sections of atoms at relativistic energies. *International Journal of Quantum Chemistry*, 108 (6):1023–1035, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Patoary:2008:BEM

[PUH+08b] M. A. R. Patoary, M. Alfaz Uddin, A. K. F. Haque, M. Shahjahan, A. K. Basak, and B. C. Saha. Binary encounter model for the electron impact K-shell ionization of atoms. *International Journal of Quantum Chemistry*, 108(8):1326–1333, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Patoary:2009:EME

[PUH+09] M. A. R. Patoary, M. Alfaz Uddin, A. K. F. Haque, M. Shahjahan, A. K. Basak, M. R. Talukder, and B. C. Saha. Empirical model for the electron impact K-shell ionization cross section of atoms. *International Journal of Quantum Chemistry*, 109 (5):897–906, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pupyshev:2002:HFT

[Pup02] Vladimir I. Pupyshev. Hellmann–Feynman theorem near the threshold. *International Journal of Quantum Chemistry*, 88 (4):380–391, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pupyshev:2005:JTT

[Pup05] Vladimir I. Pupyshev. Jahn–Teller theorem and nodal points of wave functions. *International Journal of Quantum Chemistry*, 104(2):157–166, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pupyshev:2007:SPJ

[Pup07] Vladimir I. Pupyshev. Simplest proof of the Jahn–Teller theorem for molecular systems. *International Journal of Quantum Chemistry*, 107(6):1446–1453, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Putz:2003:EDS

[Put03] Mihai V. Putz. Electronic density from structure factor determination in small deformed crystals. *International Journal of Quantum Chemistry*, 94(4):222–231, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Putz:2005:MAE

[Put05] Mihai V. Putz. Markovian approach of the electron localization functions. *International Journal of Quantum Chemistry*, 105(1):1–11, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Putz:2006:SFE

[Put06] Mihai V. Putz. Systematic formulations for electronegativity and hardness and their atomic scales within density functional softness theory. *International Journal of Quantum Chemistry*,

106(2):361–389, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Putz:2009:EQO

[Put09] Mihai V. Putz. Electronegativity: Quantum observable. *International Journal of Quantum Chemistry*, 109(4):733–738, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Petrov:2009:HSB

[PV09] Klára Tarcsay Petrov and Tamás Veszprémi. Hydrogen and silyl bridges in group 13 and 14 atom containing molecules. *International Journal of Quantum Chemistry*, 109(11):2526–2541, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Peeters:2002:ICY

[PVB+02] Anik Peeters, C. Van Alsenoy, F. Bartha, F. Bogár, M.-L. Zhang, and V. E. Van Doren. *Ab initio* calculation of the Young's modulus ofα-polyamides. *International Journal of Quantum Chemistry*, 87(5):303–310, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90512106/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90512106/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90512106&PLACEBO=IE.pdf`.

Peeters:2003:IIY

[PVB+03] Anik Peeters, C. Van Alsenoy, F. Bartha, F. Bogár, M.-L. Zhang, and V. Van Doren. Ab initio investigation of the Young's modulus of polyamide-6. *International Journal of Quantum Chemistry*, 91(1):32–38, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pauwels:2004:DES

[PVV+04] Ewald Pauwels, Veronique Van Speybroeck, Gauthier Vanhaelewyn, Freddy Callens, and Michel Waroquier. DFT-EPR study of radiation-induced radicals in α-D-glucose. *International Journal of Quantum Chemistry*, 99(2):102–108, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pauwels:2003:AMC

[PVW03a] E. Pauwels, V. Van Speybroeck, and M. Waroquier. Application of molecular cluster models to study the amino acid L-α-alanine and its derived radicals in the crystalline state. *International Journal of Quantum Chemistry*, 91(3):511–516, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Peirs:2003:SCS

[PVW03b] K. Peirs, D. Van Neck, and M. Waroquier. Self-consistent solution of Dyson's equation up to second order for closed- and open-shell atomic systems. *International Journal of Quantum Chemistry*, 91(2):113–118, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Peeters:2000:USM

[PVZV00] Anik Peeters, C. Van Alsenoy, M.-L. Zhang, and V. E. Van Doren. On the use of supermolecule model for calculation of Young's modulus of crystalline polymers. *International Journal of Quantum Chemistry*, 80(3):425–431, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501010/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501010/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501010&PLACEBO=IE.pdf`.

Pettey:2007:QWP

[PW07] Lucas R. Pettey and Robert E. Wyatt. Quantum wave packet dynamics on multidimensional adaptive grids: Applications of the moving boundary truncation method. *International Journal of Quantum Chemistry*, 107(7):1566–1573, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pernal:2009:OFE

[PW09] Katarzyna Pernal and Tomasz A. Wesolowski. Orbital-free effective embedding potential: Density-matrix functional theory case. *International Journal of Quantum Chemistry*, 109 (11):2520–2525, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pang:2009:TSR

[PXZ+09] Jing-Lin Pang, Hong-Bin Xie, Shao-Wen Zhang, Yi-Hong Ding, and Ao-Qing Tang. Theoretical study on reaction mechanism of isocyanate radical NCO with ethene. *International Journal of Quantum Chemistry*, 109(4):801–810, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pye:2000:IIL

[Pye00] Cory C. Pye. An ab initio investigation of lithium ion hydration. II. Tetra- versus hexacoordination and halide complexes. *International Journal of Quantum Chemistry*, 76(1):62–76, January 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503196/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503196/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503196&PLACEBO=IE.pdf`.

Pyykko:2001:NNS

[Pyy01] Pekka Pyykkö. A note on nodal structures, partial screening, and periodic trends among alkali metals and alkaline earths. *International Journal of Quantum Chemistry*, 85(1):18–21, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85009056/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85009056/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85009056&PLACEBO=IE.pdf`.

Peng:2009:TSI

[PYZ09] Ke Peng, Wen Yang, and Weiqun Zhou. Theoretical study on interactions between thiourea S-monoxide and water. *International Journal of Quantum Chemistry*, 109(4):811–818, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qu:2005:TSE

[QBTS05] Yuhui Qu, Xiufang Bian, Hongwei Tang, and Pengchao Si. Theoretical study of energies, structures, and vibrational spectra of the carbonic acid–hydroperoxy radical complexes. *International Journal of Quantum Chemistry*, 101(4):381–388,

???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quinet:2000:HEU

[QC00] Olivier Quinet and Benoît Champagne. Hybridization effect upon the vibrational second hyperpolarizability: An ab initio study of acetylene, ethylene, and ethane. *International Journal of Quantum Chemistry*, 80(4–5):871–881, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505415/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505415/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505415&PLACEBO=IE.pdf`.

Quinet:2001:SFG

[QC01] Olivier Quinet and Benoît Champagne. Sum-frequency generation first hyperpolarizability from time-dependent Hartree–Fock method. *International Journal of Quantum Chemistry*, 85(4–5):463–468, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quinet:2002:IFD

[QC02] Olivier Quinet and Benoît Champagne. Investigation of the frequency-dispersion effects on the Raman spectra of small polyenes. *International Journal of Quantum Chemistry*, 89 (4):341–348, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quintao:2002:TSH

[QCC02] Andréa Dias Quintão, Kaline Coutinho, and Sylvio Canuto. Theoretical study of the hydrogen bond interaction between methylene blue and water and possible role on energy transfer for photodynamics. *International Journal of Quantum Chemistry*, 90(2):634–640, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quintanar:2005:ACR

[QCC05] Carlos Quintanar, Reyna Caballero, and V. M. Castaño. Adsorption of CO on the rumpled MgO(100), MgO(100):Ni, and MgO(100):Cr surfaces: A density functional approach. *International Journal of Quantum Chemistry*, 102(5):820–828,

???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qiao:2005:TSO

[QCFJ05] Qing-An Qiao, Zheng-Ting Cai, Da-Cheng Feng, and Yuan-Sheng Jiang. Theoretical study of one-carbon unit transfer between methyl-AICA and N^1-methyl-N^1-acryloyl-formamide. *International Journal of Quantum Chemistry*, 101(1):33–39, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quintanar:2004:LRI

[QCK04] Carlos Quintanar, Reyna Caballero, and Andreas M. Köster. Long-range interactions in embedded ionic cluster calculations. *International Journal of Quantum Chemistry*, 96(5): 483–491, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quinet:2006:TDD

[QCV06] Olivier Quinet, Benoît Champagne, and Stan J. A. Van Gisbergen. Time-dependent density functional theory simulation of hyper-Raman spectra. *International Journal of Quantum Chemistry*, 106(3):599–608, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qin:2004:CCB

[QD04] Changyong Qin and Steven R. Davis. Conformational conversion of the boat and chair structures of bicyclo[3.2.0]hept-6-ene. *International Journal of Quantum Chemistry*, 96(4):432–435, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quinet:2009:PCW

[QDÖ09] O. Quinet, E. Deumens, and Y. Öhrn. Proton collisions with the water dimer at keV energies. *International Journal of Quantum Chemistry*, 109(2):259–265, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qi:2004:OSO

[QFC04] C. S. Qi, D. C. Feng, and Z. T. Cai. ONIOM study of one-carbon unit transfer from imidazolidine to dUMP analogue. *International Journal of Quantum Chemistry*, 100(1):22–27,

???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quiney:2004:CUT

[QG04] Harry M. Quiney and Ian P. Grant. Conventional and unconventional techniques in quantum chemistry. *International Journal of Quantum Chemistry*, 99(4):198–209, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quintanar:2000:DFE

[QGM+00] Carlos Quintanar, Marco Garcia, Mayra Martinez, Miguel Castro, J. L. Boldu, Eduardo Muñoz, and Peter R. Taylor. Density functional embedding approach to the Mn impurities in NaBr crystals. *International Journal of Quantum Chemistry*, 79(1):34–46, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72504318/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72504318/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72504318&PLACEBO=IE.pdf`.

Quiney:2002:DEA

[QGW02] H. M. Quiney, V. N. Glushkov, and S. Wilson. The Dirac equation in the algebraic approximation: VIII. Comparison of finite basis set and finite element molecular Dirac–Hartree–Fock calculations for the H_2, LiH, and BH ground states. *International Journal of Quantum Chemistry*, 89(4):227–236, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quiney:2004:DEA

[QGW04] H. M. Quiney, V. N. Glushkov, and S. Wilson. The Dirac equation in the algebraic approximation. IX. Matrix Dirac–Hartree–Fock calculations for the HeH and BeH ground states using distributed Gaussian basis sets. *International Journal of Quantum Chemistry*, 99(6):950–962, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qi:2005:CEF

[QLD05] Yue-Ying Qi, Xue-Shen Liu, and Pei-Zhu Ding. Continuum eigen-functions of 1-D time-independent Schrödinger equa-

tion solved by symplectic algorithm. *International Journal of Quantum Chemistry*, 101(1):21–26, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qiu:2009:PDI

[QLJ+09] Ling Qiu, Jianguo Lin, Xuehai Ju, Min Yang, Shineng Luo, and Guoxian Cao. Periodic DFT investigation on the structure and properties of TNAD crystal. *International Journal of Quantum Chemistry*, 109(7):1598–1608, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qu:2006:ESS

[QMB+06] Yuhui Qu, Wanyong Ma, Xiufang Bian, Hongwei Tang, and Weixing Tian. Electronic structure and stability of BP clusters: theoretical calculations for $(BP)_n$ $(n = 2--4)$. *International Journal of Quantum Chemistry*, 106(4):960–967, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qian:2000:APK

[QS00a] Zhixin Qian and Viraht Sahni. Analytical properties of the Kohn–Sham theory exchange and correlation energy and potential via quantal density functional theory. *International Journal of Quantum Chemistry*, 80(4–5):555–566, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505410/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505410/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505410&PLACEBO=IE.pdf`.

Qian:2000:PFK

[QS00b] Zhixin Qian and Viraht Sahni. Proof of finiteness of Kohn–Sham theory electron interaction potential at the nucleus of atoms. *International Journal of Quantum Chemistry*, 79 (4):205–208, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72512062/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72512062/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72512062&PLACEBO=IE.pdf`.

Qian:2000:TDD

[QS00c] Zhixin Qian and Viraht Sahni. Time-dependent differential virial theorems. *International Journal of Quantum Chemistry*, 78(5):341–347, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72001893/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72001893/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72001893&PLACEBO=IE.pdf`.

Qian:2005:EEP

[QS05] Zhixin Qian and Viraht Sahni. Exact electronic properties in the classically forbidden region of a metal surface. *International Journal of Quantum Chemistry*, 104(6):929–945, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quan:2007:QSC

[QTT07] Wei-Long Quan, Ping-Ying Tang, and Bi-Yu Tang. Quantum scattering calculation for reaction Br + H_2 on two potential energy surfaces. *International Journal of Quantum Chemistry*, 107(3):657–664, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quinet:2005:VSD

[Qui05] Olivier Quinet. Vibrational spectroscopies: Description of general analytical TDHF schemes for their simulation. *International Journal of Quantum Chemistry*, 104(5):727–743, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quintao:2001:VBS

[QV01] A. D. Quintão and R. O. Vianna. Valence bond study of the fragmentation of C_{2v} Li_4^- cluster. *International Journal of Quantum Chemistry*, 81(1):76–89, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/75502168/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75502168/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502168&PLACEBO=IE.pdf`.

Quiney:2005:LPQ

[QW05] H. M. Quiney and S. Wilson. Literate programming in quantum chemistry: A simple example. *International Journal of Quantum Chemistry*, 104(4):430–445, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qiu:2005:TSS

[QXJG05] Ling Qiu, He Ming Xiao, Xue Hai Ju, and Xue Dong Gong. Theoretical study of the structures and properties of cyclic nitramines: Tetranitrotetraazadecalin (TNAD) and its isomers. *International Journal of Quantum Chemistry*, 105(1): 48–56, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qu:2007:TSS

[QZ07] Yuhui Qu and Youzhong Zhang. Theoretical study of structure and vibrational properties of Mg_nO_n ($n = 3--10$) clusters. *International Journal of Quantum Chemistry*, 107(4): 962–967, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rincon:2002:ATE

[RA02] Luis Rincón and Rafael Almeida. An analysis of the topology of the electron charge density and the reactant-product electronic structure variation along the intrinsic reaction coordinate. *International Journal of Quantum Chemistry*, 86 (2):151–166, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85510858/START;` `http://www3.interscience.wiley.com/cgi-bin/fulltext/85510858/FILE?TPL=ftx_start;` `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85510858&PLACEBO=IE.pdf`.

Rauk:2003:PEB

[RA03a] A. Rauk and D. A. Armstrong. Potential energy barriers for dissociative attachment to HF.HF and HCl.HCl: Ab initio study. *International Journal of Quantum Chemistry*, 95 (6):683–696, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [RA04].

Rehr:2003:TDD

[RA03b] J. J. Rehr and A. L. Ankudinov. Time-dependent density functional theory calculations of X-ray absorption. *International Journal of Quantum Chemistry*, 95(4–5):487–492, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rauk:2004:EPE

[RA04] A. Rauk and D. A. Armstrong. Erratum: Potential energy barriers for dissociative attachment to HF.HF and HCl.HCl: An ab initio study. *International Journal of Quantum Chemistry*, 96(1):69, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [RA03a].

Rincon:2005:MBE

[RAA05] Luis Rincón, Rafael Almeida, and David García Aldea. Many-body energy decomposition analysis of cooperativity in hydrogen fluoride clusters. *International Journal of Quantum Chemistry*, 102(4):443–453, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Robert:2000:QSQ

[RACD00] David Robert, Lluís Amat, and Ramon Carbó-Dorca. Quantum similarity QSAR: Study of inhibitors binding to thrombin, trypsin, and factor Xa, including a comparison with CoMFA and CoMSIA methods. *International Journal of Quantum Chemistry*, 80(3):265–282, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501016/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501016/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501016&PLACEBO=IE.pdf`.

Rosselli:2005:QCS

[RAdS05] F. P. Rosselli, C. N. Albuquerque, and A. B. F. da Silva. Quantum chemical and statistical study of megazol-derived compounds with trypanocidal activity. *International Journal of Quantum Chemistry*, 103(5):738–748, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Randic:2002:GTC

[Ran02] Milan Randić. A graph theoretical characterization of proteomics maps. *International Journal of Quantum Chemistry*, 90(2):848–858, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rashev:2002:CSA

[Ras02] Svetoslav Rashev. Complex symmetrized analysis of benzene vibrations. *International Journal of Quantum Chemistry*, 89 (4):292–298, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rashev:2004:DIS

[Ras04] Svetoslav Rashev. Determination of an improved set of harmonic force constants for benzene. *International Journal of Quantum Chemistry*, 99(6):894–902, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rusu:2006:MTS

[RB06] T. Rusu and V. Bulacovschi. Multiobjective Tabu Search method used in chemistry. *International Journal of Quantum Chemistry*, 106(6):1406–1412, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rusu:2007:CAM

[RB07] T. Rusu and V. Bulacovschi. Computer aid molecular design based on meta-heuristics techniques. *International Journal of Quantum Chemistry*, 107(8):1745–1751, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Randic:2008:RSBa

[RB08] Milan Randić and Alexandru T. Balaban. Ring signatures for benzenoids with up to seven rings, Part 1: Catacondensed systems. *International Journal of Quantum Chemistry*, 108 (5):865–897, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [RB11].

Randic:2011:ERS

[RB11] Milan Randić and Alexandru T. Balaban. Erratum: Ring signatures for benzenoids with up to seven rings, Part 1: Catacondensed systems. *International Journal of Quantum Chem-*

istry, 111(12):3252–3253, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [RB08].

Ragni:2007:OCD

[RBA07] Mirco Ragni, Ana Carla P. Bitencourt, and Vincenzo Aquilanti. Orthogonal coordinates for the dynamics of four bodies and for the representation of potentials of tetra-atomic molecules. *International Journal of Quantum Chemistry*, 107 (14):2870–2888, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Redondo:2004:TSS

[RBL04] Pilar Redondo, Carmen Barrientos, and Antonio Largo. Theoretical study of the structures and stabilities of AlC_n, AlC, and AlC ($n = 1--7$) monocyclic clusters. *International Journal of Quantum Chemistry*, 96(6):615–626, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Redondo:2008:DFS

[RBL08] Pilar Redondo, Carmen Barrientos, and Antonio Largo. A density functional study of CoC_n ($n = 1--8$) clusters: Structures and stabilities. *International Journal of Quantum Chemistry*, 108(10):1684–1695, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rhouma:2004:OEP

[RBLS04] M. Ben El Hadj Rhouma, H. Berriche, Z. Ben Lakhdar, and F. Spiegelman. One-electron pseudopotential calculations of electronic properties of $NaAr_n$: Low-energy isomers and absorption spectra. *International Journal of Quantum Chemistry*, 99(4):495–501, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rivelino:2005:TIH

[RC05] Roberto Rivelino and Sylvio Canuto. Theoretical investigation of hydrogen bonding in lactonitrile–water complexes. *International Journal of Quantum Chemistry*, 103(5):654–658, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Robert:2000:GTA

[RCD00] David Robert and Ramon Carbó-Dorca. General trends in atomic and nuclear quantum similarity measures. *International Journal of Quantum Chemistry*, 77(3):685–692, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004062/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004062/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004062&PLACEBO=IE.pdf`.

Ragazzi:2002:IMM

[RCF02] Massimo Ragazzi, Paola Carbone, and Dino R. Ferro. Ab initio molecular modeling of ^{13}C NMR chemical shifts of polymers. 1. Ethylene–norbornene copolymers. *International Journal of Quantum Chemistry*, 88(5):663–669, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Recamier:2000:GEC

[RCJF00] J. Récamier, O. Castaños, R. Jáuregui, and A. Frank. Generation and evolution of collective atomic states. *International Journal of Quantum Chemistry*, 80(4–5):1129–1135, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505374/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505374/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505374&PLACEBO=IE.pdf`.

Rocha:2000:IRP

[RD00] Willian R. Rocha and Wagner B. De Almeida. Insertion reaction of propene into Rh — H bond in $HRh(CO)(PH_3)_2$ (C_3 H_6) compound: A density functional study. *International Journal of Quantum Chemistry*, 78(1):42–51, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71001657/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71001657/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71001657&PLACEBO=IE.pdf`.

Romera:1997:ASD

[RDK97] E. Romera, J. S. Dehesa, and Toshikatsu Koga. Analytical Schwartz density applied to heavy two-electron ions. *International Journal of Quantum Chemistry*, 61 (3):525–531, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42422; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42422&PLACEBO=IE.pdf`. See erratum [RDK02].

Romera:2002:EAS

[RDK02] E. Romera, J. S. Dehesa, and T. Koga. Erratum: Analytical Schwartz density applied to heavy two-electron ions. *International Journal of Quantum Chemistry*, 87(5):322, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/91012971/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91012971/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91012971&PLACEBO=IE.pdf`. See [RDK97].

Recamier:2002:CSA

[RdLJ+02] J. Récamier, P. García de León, R. Jáuregui, A. Frank, and O. Castaños. Coherent states for anharmonic diatomic molecules. *International Journal of Quantum Chemistry*, 89 (6):494–502, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rodrigues:2008:EPS

[RdSH08] Eduardo F. F. Rodrigues, Eduardo L. de Sá, and Roberto L. A. Haiduke. Electrostatic properties of small molecules by means of atomic multipoles from the quantum theory of atoms in molecules. *International Journal of Quantum Chemistry*, 108(13):2417–2427, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roncero:2007:EQC

[RdTdLC+07] O. Roncero, R. Pérez de Tudela, M. P. de Lara-Castells, R. Prosmiti, G. Delgado-Barrio, and P. Villarreal. Exact and quantum chemistry-like calculations in helium doped clusters: The He_2Br_2 (X) example. *International Journal of Quantum*

Chemistry, 107(14):2756–2762, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rakityansky:2006:ACI

[RE06] S. A. Rakityansky and N. Elander. Analyzing the contribution of individual resonance poles of the S-matrix to two-channel scattering. *International Journal of Quantum Chemistry*, 106 (5):1105–1129, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rabaa:2007:TSR

[REHH07] Hassan Rabaâ, Bernd Engels, Thomas Hupp, and A. Stephen K. Hashmi. Theoretical study of the reaction of alkynes with furan catalyzed by $AuCl_3$ and AuCl. *International Journal of Quantum Chemistry*, 107(2):359–365, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rettrup:2006:AGR

[Ret06] Sten Rettrup. Alternative graphical representation of determinantal many-electron states. *International Journal of Quantum Chemistry*, 106(12):2511–2517, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rodrigues:2001:MDP

[RF01] Pedro C. R. Rodrigues and Fernando M. S. Silva Fernandes. Molecular dynamics of phase transitions in clusters of alkali halides. *International Journal of Quantum Chemistry*, 84(2):169–180, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502338/START;` `http://www3.interscience.wiley.com/cgi-bin/fulltext/84502338/FILE?TPL=ftx_start;` `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502338&PLACEBO=IE.pdf`.

Randazzo:2009:DSM

[RFCG09] J. M. Randazzo, A. L. Frapiccini, F. D. Colavecchia, and G. Gasaneo. Discrete sets of many-body Sturmians. *International Journal of Quantum Chemistry*, 109(2):125–134, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rico:2000:MFT

[RFE+00] J. Fernández Rico, J. J. Fernández, I. Ema, R. López, and G. Ramírez. Master formulas for two- and three-center one-electron integrals involving Cartesian GTO, STO, and BTO. *International Journal of Quantum Chemistry*, 78(2):83–93, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/71005515/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71005515/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71005515&PLACEBO=IE.pdf.

Rico:2001:FCI

[RFE+01] J. Fernández Rico, J. J. Fernández, I. Ema, R. López, and G. Ramírez. Four-center integrals for Gaussian and exponential functions. *International Journal of Quantum Chemistry*, 81(1):16–28, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/75502161/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75502161/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502161&PLACEBO=IE.pdf.

Romero:2005:HID

[RFF05] Carlos Romero, Lioudmila Fomina, and Serguei Fomine. How important is the dispersion interaction for cyclobis(paraquat-*p*-phenylene)-based molecular "shuttles"? A theoretical study. *International Journal of Quantum Chemistry*, 102(2):200–208, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rico:2000:MIG

[RFLR00] J. Fernández Rico, J. J. Fernández, R. López, and G. Ramírez. Molecular integrals for Gaussian and exponential-type functions: Shift operators. *International Journal of Quantum Chemistry*, 78(3):137–145, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/71007682/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71007682/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71007682&PLACEBO=IE.pdf.

Reyes:2005:WAC

[RFRF05] Abraham Reyes, Lioudmila Fomina, Lev Rumsh, and Serguei Fomine. Are water–aromatic complexes always stabilized due to π–H interactions? LMP2 study. *International Journal of Quantum Chemistry*, 104(3):335–341, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ren:2000:TIH

[RFS+00] Aimin Ren, Jikang Feng, Xiuyun Sun, Wei Li, Weiquan Tian, Chiachung Sun, XueHe Zheng, and Michael C. Zerner. Theoretical investigation of the heterofullerenes C_{59} N and C_{69} N and their dimers. *International Journal of Quantum Chemistry*, 78(6):422–436, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72502337/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72502337/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72502337&PLACEBO=IE.pdf`.

Roohi:2008:CNN

[RG08] H. Roohi and Y. Gholipour. Characterization of the NH$\cdots$ON and NH$\cdots$NOH-bonds in nitrosamine dimers. *International Journal of Quantum Chemistry*, 108(3):462–471, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Recamier:2006:LAM

[RGMP06] J. Récamier, M. Gorayeb, W. L. Mochán, and J. L. Paz. Lie algebraic method applied to a pulsed anharmonic oscillator. *International Journal of Quantum Chemistry*, 106(15):3160–3166, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rehaman:2007:PAC

[RGP07] Abdul Rehaman, Laura Gagliardi, and Pekka Pyykkö. Pocket and antipocket conformations for the CH_4 @C_{84} endohedral fullerene. *International Journal of Quantum Chemistry*, 107 (5):1162–1169, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rees:2002:SH

[RH02] D. Rees and G. G. Hall. Space hybrids. *International Journal of Quantum Chemistry*, 89(6):503–513, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rulisek:2003:UDM

[RH03] Lubomír Rulíšek and Zdeněk Havlas. Using DFT methods for the prediction of the structure and energetics of metal-binding sites in metalloproteins. *International Journal of Quantum Chemistry*, 91(3):504–510, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rees:2005:CG

[RH05] D. Rees and G. G. Hall. Cubature grids. *International Journal of Quantum Chemistry*, 102(1):19–30, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Reinhardt:2009:CDW

[RH09] Peter Reinhardt and Philip E. Hoggan. Cusps and derivatives for wave-functions expanded in Slater orbitals: A density study. *International Journal of Quantum Chemistry*, 109(14): 3191–3198, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ruiz:2002:MVC

[RHH+02] L. F. Ruiz, P. A. Hervieux, J. Hanssen, M. F. Politis, and F. Martín. Molecular view of charge exchange in ion-C_{60} collisions. *International Journal of Quantum Chemistry*, 86 (1):106–113, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85008595/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85008595/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85008595&PLACEBO=IE.pdf`.

Reimers:2000:NSP

[RHHH00] Jeffrey R. Reimers, Michael C. Hutter, Jason M. Hughes, and Noel S. Hush. Nature of the special-pair radical cation in bacterial photosynthesis. *International Journal of Quantum Chemistry*, 80(6):1224–1243, ????

2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/75501734/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75501734/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75501734&PLACEBO=IE.pdf.

Rodriguez-Hernandez:2005:TSP

[RHM05] P. Rodríguez-Hernández and A. Muñoz. Theoretical study of the pressure-induced structural phase transition of ScSb and YSb. *International Journal of Quantum Chemistry*, 101 (6):770–773, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rajeswarapalanichamy:2003:FVN

[RI03] R. Rajeswarapalanichamy and K. Iyakutti. Ferromagnetic vs. nonmagnetic phases of 2-D Wigner electron crystal. *International Journal of Quantum Chemistry*, 92(3):337–343, April 5, 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rajeswarapalanichamy:2005:APD

[RI05] R. Rajeswarapalanichamy and K. Iyakutti. Antiferromagnetic phase of a 2-D Wigner crystal. *International Journal of Quantum Chemistry*, 102(1):112–117, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rivail:2001:F

[Riv01] Jean-Louis Rivail. Foreword. *International Journal of Quantum Chemistry*, 84(5):441, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85008759/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85008759/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85008759&PLACEBO=IE.pdf.

Robles:2003:VSM

[RIVB03] R. Robles, J. Izquierdo, A. Vega, and L. C. Balbás. Is the vanadium(001) surface magnetic? Pseudopotential toward all-electron calculations. *International Journal of Quantum Chemistry*, 91(2):230–233, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Romanowski:2008:RKS

[RJ08] Zbigniew Romanowski and Abraham F. Jalbout. Representation of Kohn–Sham free atom eigenfunctions by Slater-type orbitals. *International Journal of Quantum Chemistry*, 108 (9):1465–1476, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Robbins:2006:EPM

[RJB+06] Adele M. Robbins, Ping Jin, Tore Brinck, Jane S. Murray, and Peter Politzer. Electrostatic potential as a measure of gas phase carbocation stability. *International Journal of Quantum Chemistry*, 106(14):2904–2909, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raissi:2009:IHBb

[RJF+09a] H. Raissi, A. F. Jalbout, H. Farsi, B. Abbasi, A. de Leon, and S. Moghiminia. Intramolecular hydrogen bonding in 3-imino-propenylamine: Theoretical investigations. *International Journal of Quantum Chemistry*, 109(7):1609–1616, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raissi:2009:IHBa

[RJF+09b] H. Raissi, A. F. Jalbout, M. Fazli, M. Yoosefian, H. Ghiassi, Z. Wang, and A. de Leon. Intramolecular hydrogen bonding in derivatives of 3-amino-propenethial. *International Journal of Quantum Chemistry*, 109(7):1497–1504, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raissi:2008:ESI

[RJN+08] H. Raissi, A. F. Jalbout, M. A. Nasseria, M. Yoosefian, H. Ghiassi, and A. J. Hameed. The effect of substitution on the intramolecular hydrogen bonding in 3-hydroxy-propenethial. *International Journal of Quantum Chemistry*, 108(9):1444–1451, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roy:2008:BSS

[RJP08] Amlan K. Roy, Abraham F. Jalbout, and Emil I. Proynov. Bound state spectra of the 3D rational potential. *International Journal of Quantum Chemistry*, 108(5):827–836, ????

2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramirez:2009:OPS

[RKM09] Jessica J. Ramirez, Dmitri S. Kilin, and David A. Micha. Optical properties of the Si(111):H surface with adsorbed Ag clusters. *International Journal of Quantum Chemistry*, 109 (15):3694–3704, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rodriguez:2006:CES

[RKR+06] Ana M. Rodríguez, Joseph C. P. Koo, Dante E. Rojas, Nélida M. Peruchena, and Ricardo D. Enriz. Conformational and electronic study of N-acetyl-L-isoleucine-N-methylamide using DFT and IPCM calculations. *International Journal of Quantum Chemistry*, 106(7):1580–1595, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Remacle:2004:EER

[RL04] F. Remacle and R. D. Levine. Electronic and electrical response of arrays of metallic quantum dots. *International Journal of Quantum Chemistry*, 99(5):743–751, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rico:2001:NPM

[RLA+01] J. Fernández Rico, R. López, A. Aguado, I. Ema, and G. Ramírez. New program for molecular calculations with Slater-type orbitals. *International Journal of Quantum Chemistry*, 81(2):148–153, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76500932/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76500932/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76500932&PLACEBO=IE.pdf`.

Rabinowitz:2002:WDM

[RLB02] James Rabinowitz, Stephen Little, and Katrina Brown. Why does 5-methylchrysene interact with DNA as both a planar and a nonplanar polycyclic aromatic hydrocarbon? Quantum mechanical studies. *International Journal of Quantum Chemistry*, 88(1):99–106, ???? 2002. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/89015695/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89015695/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89015695&PLACEBO=IE.pdf.

Rai:2003:ICC

[RLBK03] Sachchida N. Rai, Heinz-Peter Liebermann, Robert J. Buenker, and Mineo Kimura. Ab initio CI calculations of the potential curves and nonadiabatic coupling matrix elements for collisions of protons with the ethylene molecule. *International Journal of Quantum Chemistry*, 95(6):866–876, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rico:2004:AET

[RLER04] J. Fernández Rico, R. López, I. Ema, and G. Ramírez. Accuracy of the electrostatic theorem for high-quality Slater and Gaussian basis sets. *International Journal of Quantum Chemistry*, 100(2):221–230, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rico:2008:TCC

[RLER08] J. Fernández Rico, R. López, I. Ema, and G. Ramírez. Three-center Coulomb repulsion integrals with Slater functions. *International Journal of Quantum Chemistry*, 108(9): 1415–1421, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Redondo:2001:TSA

[RLGB01] Pilar Redondo, Antonio Largo, Flor García, and Carmen Barrientos. Theoretical study of AlC_3^+. *International Journal of Quantum Chemistry*, 84(6):660–669, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85008256/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85008256/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85008256&PLACEBO=IE.pdf.

Rostkowska:2002:NMA

[RLNA02] Hanna Rostkowska, Leszek Lapinski, Maciej J. Nowak, and Ludwik Adamowicz. Normal mode analysis of the vibrational spectrum of tropolone—A molecule with seven-membered ring. *International Journal of Quantum Chemistry*, 90(3): 1163–1173, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rico:2004:EFI

[RLRE04] J. Fernández Rico, R. López, G. Ramírez, and I. Ema. Electric field integrals for Slater-type orbitals. *International Journal of Quantum Chemistry*, 100(2):131–141, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roohi:2007:BSH

[RM07] H. Roohi and B. Machiabadi. Blue-shifted H-bond in aromatic sulfines: An ab initio calculation. *International Journal of Quantum Chemistry*, 107(7):1559–1565, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Randic:2000:CPP

[RMB00] Milan Randić, Denise Mills, and Subhash C. Basak. On characterization of physical properties of amino acids. *International Journal of Quantum Chemistry*, 80(6):1199–1209, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/75501733/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75501733/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75501733&PLACEBO=IE.pdf`.

Ramalho:2003:INI

[RME+03] Teodorico C. Ramalho, Tales L. C. Martins, Luiz Eduardo, Pizarro Borges, and José Daniel Figueroa-Villar. Influence of nonbonded interactions in the kinetics of formation of chalcogenol esters from chalcogenoacetylenes. *International Journal of Quantum Chemistry*, 95(3):267–273, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raissi:2007:AEE

[RMJ+07] Heidar Raissi, Effat Moshfeghi, Abraham F. Jalbout, Mohammad Saeid Hosseini, and Mustapha Fazli. An approach to estimate the energy and strength of the intramolecular hydrogen bond in different conformers of 4-methylamino-3-penten-2-one. *International Journal of Quantum Chemistry*, 107(9): 1835–1845, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ruette:2008:IPQ

[RMKS08] Fernando Ruette, Stefania A. M. Marcantognini, Valentin V. Karasiev, and Morella Sánchez. Improvements of parametric quantum methods with new elementary parametric functionals. *International Journal of Quantum Chemistry*, 108(10): 1831–1839, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Recamier:2005:NRD

[RMM05] J. Récamier, W. L. Mochán, and J. Maytorena. Nonlinear response of a deformed oscillator. *International Journal of Quantum Chemistry*, 105(6):794–802, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roberto-Neto:2005:CCS

[RNCM05] Orlando Roberto-Neto, Subhas Chakravorty, and Francisco B. C. Machado. Coupled-cluster study of the equilibrium geometry and harmonic vibrational frequencies of the methyl radical. *International Journal of Quantum Chemistry*, 103 (5):649–653, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ryabinkin:2004:PHC

[RNS04] I. G. Ryabinkin, Yu. V. Novakovskaya, and N. F. Stepanov. Photoexcited O_3 $(H_2O)_n$ cluster decay: Nonempirical simulation of model systems. *International Journal of Quantum Chemistry*, 100(4):477–488, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Randic:2009:IAC

[RNVTP09] Milan Randić, Marjana Novič, Dražen Vikić-Topić, and Dejan Plavšić. On intramolecular average ^{13}C chemical shift in nonanes. *International Journal of Quantum Chemistry*, 109

(13):3093–3102, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rosch:2000:IMC

[RÖ00] Notker Rösch and Yngve Öhrn. Introduction: Michael C. Zerner. *International Journal of Quantum Chemistry*, 77(1): 1–2, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004261/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004261/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004261&PLACEBO=IE.pdf`.

Ryde:2001:SSR

[RO01] Ulf Ryde and Mats H. M. Olsson. Structure, strain, and reorganization energy of blue copper models in the protein. *International Journal of Quantum Chemistry*, 81(5):335–347, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76507288/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76507288/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76507288&PLACEBO=IE.pdf`.

Rohlfing:2000:ESM

[Roh00] Michael Rohlfing. Excited states of molecules from Green's function perturbation techniques. *International Journal of Quantum Chemistry*, 80(4–5):807–815, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505409/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505409/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505409&PLACEBO=IE.pdf`.

Romanowski:2008:NCOa

[Rom08a] Zbigniew Romanowski. Numerical calculation of overlap and kinetic integrals in prolate spheroidal coordinates. *International Journal of Quantum Chemistry*, 108(2):249–256, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Romanowski:2008:NCOb

[Rom08b] Zbigniew Romanowski. Numerical calculation of overlap and kinetic integrals in prolate spheroidal coordinates. II. *International Journal of Quantum Chemistry*, 108(3):487–492, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roy:2005:EAK

[Roy05a] Amlan K. Roy. Erratum: Amlan K. Roy, "Studies on some singular potentials in quantum mechanics," International Journal of Quantum Chemistry (2005) **104**(6) 861–870. *International Journal of Quantum Chemistry*, 105(1):99, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Roy05b].

Roy:2005:SSS

[Roy05b] Amlan K. Roy. Studies on some singular potentials in quantum mechanics. *International Journal of Quantum Chemistry*, 104(6):861–870, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Roy05a].

Roy:2008:GBD

[Roy08] Amlan K. Roy. Grid-based density functional calculations of many-electron systems. *International Journal of Quantum Chemistry*, 108(5):837–847, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rovira:2000:FPM

[RP00] Carme Rovira and Michele Parrinello. First-principles molecular dynamics simulations of models for the myoglobin active center. *International Journal of Quantum Chemistry*, 80(6):1172–1180, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/75502059/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75502059/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502059&PLACEBO=IE.pdf`.

Randic:2003:CMC

[RP03] Milan Randić and Dejan Plavšić. Characterization of molecular complexity. *International Journal of Quantum Chemistry*,

91(1):20–31, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Reinhardt:2009:NIB

[RP09] P. Reinhardt and J.-P. Piquemal. New intermolecular benchmark calculations on the water dimer: SAPT and supermolecular post-Hartree–Fock approaches. *International Journal of Quantum Chemistry*, 109(14):3259–3267, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Reis:2000:DCS

[RPB00] H. Reis, M. G. Papadopoulos, and I. Boustani. DFT calculations of static dipole polarizabilities and hyperpolarizabilities for the boron clusters B_n ($n = 3--8, 10$). *International Journal of Quantum Chemistry*, 78(2):131–135, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71005519/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71005519/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71005519&PLACEBO=IE.pdf`.

Ramseyer:2004:OOP

[RPHG04] C. Ramseyer, V. Pouthier, J. Humbert, and C. Girardet. Orientational ordering in physisorbed molecular layers induced by surface geometry and confinement. *International Journal of Quantum Chemistry*, 99(5):735–742, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Reining:2000:FPC

[RPPO00] Lucia Reining, Olivia Pulci, Maurizia Palummo, and Giovanni Onida. First-principles calculations of electronic excitations in clusters. *International Journal of Quantum Chemistry*, 77(6):951–960, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000977/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000977/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000977&PLACEBO=IE.pdf`.

Rastogi:2007:GPV

[RPS+07] V. K. Rastogi, M. A. Palafox, Surabhi Singhal, S. P. Ojha, and W. Kiefer. Geometrical parameters, vibrational wavenumbers, and relationships established with six difluorobenzonitriles. *International Journal of Quantum Chemistry*, 107(5):1099–1114, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ruhoff:2000:ACF

[RR00] Peder Thusgaard Ruhoff and Mark A. Ratner. Algorithms for computing Franck–Condon overlap integrals. *International Journal of Quantum Chemistry*, 77(1):383–392, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004281/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004281/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004281&PLACEBO=IE.pdf`.

Ritchie:2002:UFF

[RR02] Burke Ritchie and Merle E. Riley. Use of fast Fourier transform computational methods in electron scattering. *International Journal of Quantum Chemistry*, 90(2):792–798, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rissi:2003:ADF

[RRC03] Eduardo Rissi, Roberto Rivelino, and Sylvio Canuto. Applications of density functional theory methods in millimeter-wave spectroscopy. *International Journal of Quantum Chemistry*, 91(4):575–585, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rusu:2006:HBB

[RRD06] Victor H. Rusu, Mozart N. Ramos, and João Bosco P. Da Silva. Hydrogen bonds between hydrogen fluoride and aromatic azines: An ab initio study. *International Journal of Quantum Chemistry*, 106(13):2811–2817, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rignanese:2005:ETO

[RRGP05a] G.-M. Rignanese, X. Rocquefelte, X. Gonze, and Alfredo Pasquarello. Erratum: Titanium oxides and silicates as high-κ dielectrics: A first-principles investigation by G.-M. Rignanese, X. Rocquefelte, X. Gonze, Alfredo Pasquarello. *International Journal of Quantum Chemistry*, 103(3):354, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [RRGP05b].

Rignanese:2005:TOS

[RRGP05b] G.-M. Rignanese, X. Rocquefelte, X. Gonze, and Alfredo Pasquarello. Titanium oxides and silicates as high-κ dielectrics: A first-principles investigation. *International Journal of Quantum Chemistry*, 101(6):793–801, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [RRGP05a].

Ramirez-Ramirez:2005:TSF

[RRNG05] Víctor M. Ramírez-Ramírez and Ignacio Nebot-Gil. Theoretical study of the formation reaction of the methyl vinyl ketone: A conformational approach. *International Journal of Quantum Chemistry*, 105(5):518–526, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rasmussen:2007:FFM

[RRPJ07] Thomas D. Rasmussen, Pengyu Ren, Jay W. Ponder, and Frank Jensen. Force field modeling of conformational energies: Importance of multipole moments and intramolecular polarization. *International Journal of Quantum Chemistry*, 107(6):1390–1395, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Russo:2008:ITB

[RRUE08] Nino Russo, Maria J. Ramos, Jesus M. Ugalde, and Leif A. Eriksson. Introduction: Theoretical Biophysics Symposium, Cetraro, Italy, June 16–20, 2007. *International Journal of Quantum Chemistry*, 108(11):1873, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rosta:2000:ICB

[RS00] E. Rosta and P. R. Surján. Interaction of chemical bonds. V. Perturbative corrections to geminal-type wave functions.

International Journal of Quantum Chemistry, 80(2):96–104, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001286/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001286/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001286&PLACEBO=IE.pdf`.

Rao:2006:PAF

[RS06] J. Srinivasa Rao and G. Narahari Sastry. Proton affinity of five-membered heterocyclic amines: Assessment of computational procedures. *International Journal of Quantum Chemistry*, 106(5):1217–1224, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rozanska:2008:OCC

[RS08] Xavier Rozanska and Joachim Sauer. Oxidative conversion of C1–C3 alkanes by vanadium oxide catalysts. DFT results and their accuracy. *International Journal of Quantum Chemistry*, 108(12):2223–2229, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rolik:2009:MMP

[RS09] Zoltán Rolik and Ágnes Szabados. Multipartitioning Møller–Plesset perturbation theory: Size-extensivity at third order and symmetry conservation. *International Journal of Quantum Chemistry*, 109(11):2554–2563, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [RS11].

Rolik:2011:EMM

[RS11] Zoltán Rolik and Ágnes Szabados. Erratum: Multipartitioning Møller–Plesset perturbation theory: Size-extensivity at third order and symmetry conservation. *International Journal of Quantum Chemistry*, 111(14):3992, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [RS09].

Rivas-Silva:2000:TEQ

[RSDNSB00] J. F. Rivas-Silva, S. Durand-Niconoff, T. M. Schmidt, and M. Berrondo. Theoretical explanation of the quenching of luminescence in cerium-doped ytterbium oxyorthosilicate. *International Journal of Quantum Chemistry*, 79(3):198–203,

???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72508372/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72508372/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72508372&PLACEBO=IE.pdf`.

Rivas-Silva:2003:DSD

[RSFRB03] J. F. Rivas-Silva, A. Flores-Riveros, and M. Berrondo. DFT study of 1-D $Li_6Gd(BO_3)_3$. *International Journal of Quantum Chemistry*, 94(2):105–112, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rivas-Silva:2004:IAS

[RSFRDNA04] J. F. Rivas-Silva, A. Flores-Riveros, J. S. Durand-Niconoff, and N. Aquino. Ab initio analysis of some fluoride and oxide structures doped with Pr and Yb. *International Journal of Quantum Chemistry*, 97(3):815–825, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ringer:2008:LLS

[RSKC08] Ashley L. Ringer, C. David Sherrill, Rollin A. King, and T. Daniel Crawford. Low-lying singlet excited states of isocyanogen. *International Journal of Quantum Chemistry*, 108 (6):1137–1140, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Renugopalakrishnan:2003:RBD

[RSL+03] V. Renugopalakrishnan, A. Strzelczyk, Pingzou Li, A. A. Mokhnatyuk, Sachin H. Gursahani, Mahesh Nagaraju, M. Prabhakaran, H. Arjomandi, and Shoba L. Lakka. Retroengineering bacteriorhodopsins: Design of smart proteins by bionanotechnology. *International Journal of Quantum Chemistry*, 95(4–5):627–631, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ruette:2004:CPQ

[RSM+04a] F. Ruette, M. Sánchez, G. Martorell, C. González, R. Añez, A. Sierraalta, L. Rincón, and C. Mendoza. CATIVIC: Parametric quantum chemistry package for catalytic reactions: I. *International Journal of Quantum Chemistry*, 96(4):321–332, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ruette:2004:COC

[RSM+04b] F. Ruette, M. Sánchez, C. Mendoza, A. Sierraalta, G. Martorell, and C. González. Calculation of one-center integrals in parametric methods using simulated annealing and simplex methods. *International Journal of Quantum Chemistry*, 96 (4):303–311, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Razbirin:2007:OSC

[RSN+07] B. S. Razbirin, A. N. Starukhin, D. K. Nelson, E. F. Sheka, and M. Prato. Optical spectra and covalent chemistry of fulleropyrrolidines. *International Journal of Quantum Chemistry*, 107(14):2787–2802, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rivas-Silva:2000:ICA

[RSRMBFR00] J. F. Rivas-Silva, L. Rodríguez-Merino, M. Berrondo, and A. Flores-Riveros. Ab initio calculations for absorption and emission energies of alkali halide crystals doped with thallium. *International Journal of Quantum Chemistry*, 77(4):785–790, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70500242/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70500242/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70500242&PLACEBO=IE.pdf`.

Rennig:2008:IAA

[RST08] Amanda Rennig, Annette Slutter, and Lorena Tribe. Interactions of aminomethylphosphonic acid and sarcosine with montmorillonite interlayer surfaces. *International Journal of Quantum Chemistry*, 108(3):538–543, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Russo:2002:IBM

[RSTG02] Nino Russo, Emilia Sicilia, Marirosa Toscano, and Andrè Grand. On the interaction between manganese cation (Mn^{2+}) and the nucleic acid bases (T, U, C, A, G) in the gas phase. *International Journal of Quantum Chemistry*, 90(2):903–909, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ratkiewicz:2006:AMG

[RT06] Artur Ratkiewicz and Thanh N. Truong. Automated mechanism generation: From symbolic calculation to complex chemistry. *International Journal of Quantum Chemistry*, 106(1): 244–255, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rezania:2009:SMM

[RT09] Vahid Rezania and Jack A. Tuszynski. A stochastic model for microtubule dynamicity involving mixtures of tubulin isotypes. *International Journal of Quantum Chemistry*, 109(14): 3430–3440, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ruangpornvisuti:2009:DST

[Rua09] Vithaya Ruangpornvisuti. A DFT study of transformation of nitrosothiol isomers and their decomposition to nitric oxide in gas phase. *International Journal of Quantum Chemistry*, 109 (2):275–284, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ruiz:2005:HMMa

[Rui05a] María Belén Ruiz. Hylleraas method for many-electron atoms. I. The Hamiltonian. *International Journal of Quantum Chemistry*, 101(3):246–260, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ruiz:2005:HMMb

[Rui05b] María Belén Ruiz. Hylleraas method for many-electron atoms. II. Integrals over wave functions with one interelectronic coordinate. *International Journal of Quantum Chemistry*, 101 (3):261–273, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roeggen:2005:IPX

[RV05] I. Røeggen and L. Veseth. Interatomic potential for the $X\,^1\Sigma$ state of Be_2, revisited. *International Journal of Quantum Chemistry*, 101(2):201–210, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rosseto:2003:TMA

[RVD03] Renato Rosseto, Maria Domingues Vargas, and Jordan Del Nero. Theoretical modeling of alkynes. *International Journal of Quantum Chemistry*, 95(2):137–143, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Randic:2009:SLG

[RVNP09] Milan Randić, Marjan Vračko, Marjana Novič, and Dejan Plavšić. Spectrum-like graphical representation of RNA secondary structure. *International Journal of Quantum Chemistry*, 109(13):2982–2995, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rangelov:2006:QCM

[RVP06] Miroslav A. Rangelov, Georgi N. Vayssilov, and Dimiter D. Petkov. Quantum chemical model study of the acyl migration in 2′ (3′)-formylnucleosides. *International Journal of Quantum Chemistry*, 106(6):1346–1356, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ravichandran:2009:MDR

[RVP09] Lalitha Ravichandran, Nayana Vaval, and Sourav Pal. Magnetizability of doublet radicals using Fock space multi-reference coupled cluster method. *International Journal of Quantum Chemistry*, 109(10):2191–2198, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rak:2000:ESP

[RVR00] Janusz Rak, Alexander A. Voityuk, and Notker Rösch. Energetics of the splitting of pyrimidine photodimers induced by electron transfer to rhodium(III) complexes. A quantum chemical study. *International Journal of Quantum Chemistry*, 77(1):128–138, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004253/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004253/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004253&PLACEBO=IE.pdf`.

Ritchie:2000:NST

[RW00] Burke Ritchie and Charles A. Weatherford. Numerical solution of the time-dependent Schrödinger equation for continuum states. *International Journal of Quantum Chemistry*, 80(4–5):934–941, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505416/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505416/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505416&PLACEBO=IE.pdf`.

Red:2004:DGF

[RW04a] Eddie Red and Charles A. Weatherford. Derivation of a general formula for the Shibuya–Wulfman matrix. *International Journal of Quantum Chemistry*, 100(2):208–213, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ritchie:2004:RET

[RW04b] Burke Ritchie and Charles A. Weatherford. Relativistic electron theory: Is spin a property of the electron in vacuo or of the electromagnetic field interaction. *International Journal of Quantum Chemistry*, 100(6):1014–1018, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ritchie:2004:TDN

[RW04c] Burke Ritchie and Charles A. Weatherford. Time-dependent non-wavepacket theory of electron scattering. *International Journal of Quantum Chemistry*, 100(5):710–712, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ren:2001:TSC

[RWW+01] Yi Ren, Xin Wang, Ning-Bew Wong, An-Min Tian, Fu jiang Ding, and Liangfu Zhang. Theoretical study of the N_{10} clusters without double bonds. *International Journal of Quantum Chemistry*, 82(1):34–43, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76510764/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76510764/`

FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76510764&PLACEBO=IE.pdf.

Romeike:2006:CIM

[RWW+06] C. Romeike, M. R. Wegewijs, W. Wenzel, M. Ruben, and H. Schoeller. Charge-induced modulation of magnetic interactions in a $[2 \times 2]$ metal-organic grid complex. *International Journal of Quantum Chemistry*, 106(4):994–1000, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ren:2007:DHC

[RZ07] Haizhen Ren and Fuji Zhang. Double hexagonal chains with maximal energy. *International Journal of Quantum Chemistry*, 107(6):1437–1445, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sarkar:2009:RAF

[SA09] Biplab Sarkar and Satrajit Adhikari. A rigorous approach to the formulation of extended Born–Oppenheimer equation for a three-state system. *International Journal of Quantum Chemistry*, 109(4):650–667, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saalfrank:2000:QDL

[Saa00] Peter Saalfrank. Quantum dynamics of laser- and field-induced desorption of molecules from metal surfaces. *International Journal of Quantum Chemistry*, 80(2):210–219, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73001291/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001291/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001291&PLACEBO=IE.pdf.

Sadeghpour:2000:CIA

[Sad00] H. R. Sadeghpour. Channel interaction in alkali-halide photodissociation: Interferometric lineshapes and dynamic switching. *International Journal of Quantum Chemistry*, 80(4–5):958–965, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505421/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/

73505421/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505421&PLACEBO=IE.pdf.

Sadlej:2002:ISB

[Sad02] Joanna Sadlej. Ab initio study of bending modes in water cage clusters, $(H_2\ O)_n$, n 6–10. *International Journal of Quantum Chemistry*, 90(3):1191–1205, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sadlej:2006:IUZ

[Sad06] Andrzej J. Sadlej. Improving upon the ZORA Hamiltonian. *International Journal of Quantum Chemistry*, 106(12):2518–2524, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sierraalta:2008:IIS

[SAE08] Anibal Sierraalta, Paola Alejos, and Elena Ehrmann. Influence of isomorphous substitution on NO and N_2O thermochemistry on Au/ZSM-5 catalyst. *International Journal of Quantum Chemistry*, 108(10):1696–1704, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Safouhi:2004:HAN

[Saf04] Hassan Safouhi. Highly accurate numerical results for three-center nuclear attraction and two-electron Coulomb and exchange integrals over Slater-type functions. *International Journal of Quantum Chemistry*, 100(2):172–183, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2003:CEC

[Sah03] Bidhan C. Saha. Charge exchange in C^{6+} + H ($1s$) collisions at low energies. *International Journal of Quantum Chemistry*, 92(1):29–34, March 5, 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sahni:2004:ET

[Sah04] Viraht Sahni. On Ehrenfest's theorem. *International Journal of Quantum Chemistry*, 97(6):953–960, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sakai:2000:TAC

[Sak00] Shogo Sakai. Theoretical analysis of the Cope rearrangement of 1,5-hexadiene. *International Journal of Quantum Chemistry*, 80(4–5):1099–1106, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505417/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505417/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505417&PLACEBO=IE.pdf`.

Sakai:2002:TAC

[Sak02] Shogo Sakai. Theoretical analysis of cyclic reaction mechanisms of two ethylenes. *International Journal of Quantum Chemistry*, 90(2):549–554, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salam:2000:RII

[Sal00] A. Salam. Retarded intermolecular interactions involving diamagnetic molecules. *International Journal of Quantum Chemistry*, 78(6):437–442, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72502338/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72502338/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72502338&PLACEBO=IE.pdf`.

Salam:2005:GER

[Sal05] A. Salam. Generalized expressions for resonant excitation transfer and retarded dispersion energy shifts obtained using multipolar quantum electrodynamics. *International Journal of Quantum Chemistry*, 105(6):762–766, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salvador:2009:CAT

[Sal09] Pedro Salvador. Convergence acceleration techniques for non-Hermitian SCF problems. *International Journal of Quantum Chemistry*, 109(11):2564–2571, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sarma:2008:MIV

[SAM08] Manabendra Sarma, S. Adhikari, and Manoj K. Mishra. Mechanistic investigation of vibrational fine structure in e-H_2 scattering using local complex potential-based time dependent wave packet approach. *International Journal of Quantum Chemistry*, 108(6):1044–1051, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Serrano-Andres:2001:TSS

[SAMBS01] Luis Serrano-Andrés, Manuela Merchán, Antonio Carlos Borin, and Jonna Stålring. Theoretical studies on the spectroscopy of the 7-azaindole monomer and dimer. *International Journal of Quantum Chemistry*, 84(2):181–191, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502339/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502339/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502339&PLACEBO=IE.pdf`.

Sapirstein:2006:IRN

[Sap06] J. Sapirstein. Interplay of relativistic and nuclear effects in few-electron atoms and ions. *International Journal of Quantum Chemistry*, 106(15):3178–3185, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sang-Aroon:2008:DAA

[SAR08] Wichien Sang-Aroon and Vithaya Ruangpornvisuti. Determination of aqueous acid-dissociation constants of aspartic acid using PCM/DFT method. *International Journal of Quantum Chemistry*, 108(6):1181–1188, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sawicka:2003:DBA

[SASS03] Agnieszka Sawicka, Iwona Anusiewicz, Piotr Skurski, and Jack Simons. Dipole-bound anions supported by charge–transfer interaction: Anionic states of $H_nF_{3-n}N \rightarrow BH_3$ and $H_3N \rightarrow BH_nF_{3-n}$ ($n = 0, 1, 2, 3$). *International Journal of Quantum Chemistry*, 92(4):367–375, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Satkovskiene:2003:TJE

[Šat03] D. Šatkovskienė. Theoretical justification of empirical additivity schemes for conformational energies. *International Journal of Quantum Chemistry*, 91(1):5–12, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schreiber:2003:OBS

[SB03] Marko Schreiber and Volker Buss. Origin of the bathochromic shift in the early photointermediates of the rhodopsin visual cycle: A CASSCF/CASPT2 study. *International Journal of Quantum Chemistry*, 95(6):882–889, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szmytkowski:2004:VPB

[SB04] Radosław Szmytkowski and Sebastian Bielski. Variational principles for bound states of Schrödinger and Dirac equations allowing the use of discontinuous trial functions. *International Journal of Quantum Chemistry*, 97(6):966–976, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Safouhi:2006:EMI

[SB06a] Hassan Safouhi and Ahmed Bouferguene. Extrapolation methods for improving convergence of spherical Bessel integrals for the two-center Coulomb integrals. *International Journal of Quantum Chemistry*, 106(11):2318–2323, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Safouhi:2006:SPL

[SB06b] Hassan Safouhi and Ahmed Bouferguene. Symbolic programming language in molecular multicenter integral problem. *International Journal of Quantum Chemistry*, 106(1):65–78, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Swart:2006:OSW

[SB06c] Marcel Swart and F. Matthias Bickelhaupt. Optimization of strong and weak coordinates. *International Journal of Quantum Chemistry*, 106(12):2536–2544, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Ano07a].

Sen:2005:IQM

[SBB05] Kakali Sen, Samita Basu, and Dhananjay Bhattacharyya. Ab initio QM/MM study of excited state electron transfer between pyrene and 4,4′-bis(dimethylamino)-diphenylmethane with different solvent systems: Role of hydrogen bonding within solvent molecules. *International Journal of Quantum Chemistry*, 102(4):368–378, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sen:2006:ISE

[SBB06] Kakali Sen, Samita Basu, and Dhananjay Bhattacharyya. Ab initio studies on excited state intramolecular electron transfer in 4-amino-N-methylphthalimide and 3-amino-N-methylphthalimide. *International Journal of Quantum Chemistry*, 106(4):913–927, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szekeres:2005:GOC

[SBBL05] Zs. Szekeres, F. Bogár, F. Bartha, and J. Ladik. Geometry optimization of the cytosine molecules in a cytosine stack using the B3LYP crystal orbital method. *International Journal of Quantum Chemistry*, 105(1):74–78, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Seida:2003:IMS

[SBF03] Pamela R. Seida, Jeanne W. Bundens, and Michelle M. Francl. Ab initio MO study of the symmetrical and asymmetrical isomers of bridging alkynylaluminum and alkynylberyllium dimers. *International Journal of Quantum Chemistry*, 95(6): 806–809, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sokol:2004:HQM

[SBF+04] Alexey A. Sokol, Stefan T. Bromley, Samuel A. French, C. Richard A. Catlow, and Paul Sherwood. Hybrid QM/MM embedding approach for the treatment of localized surface states in ionic materials. *International Journal of Quantum Chemistry*, 99(5):695–712, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Silva:2005:DCS

[SBFV05] Gustavo R. Silva, Itamar Borges, Jr., and Jose D. Figueroa-Villar. DFT conformational studies of the HI-6 molecule. *International Journal of Quantum Chemistry*, 105(3):260–269, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Subbotina:2006:CDP

[SBHF06] Julia O. Subbotina, V. A. Bakulev, R. Herges, and W. M. F. Fabian. 1,7-cyclization of 1-diazo-2,4-pentadiene and its heteroanalogues: DFT study. *International Journal of Quantum Chemistry*, 106(10):2229–2235, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stirling:2009:PII

[SBK+09] András Stirling, Imre Bakó, László Kocsis, László Hajba, and János Mink. Pt(II)-ion hydration: Structural and vibrational characteristics from theory and experiment. *International Journal of Quantum Chemistry*, 109(11):2591–2598, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sawicka:2005:LEE

[SBKSS05] Agnieszka Sawicka, Joanna Berdys-Kochańska, Piotr Skurski, and Jack Simons. Low-energy (0.1 eV) electron attachment S — S bond cleavage assisted by Coulomb stabilization. *International Journal of Quantum Chemistry*, 102(5):838–846, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Song:2005:HBC

[SBL05a] Lianxiang Song, Yuxiang Bu, and Ping Li. Hydrogen bond character and proton transfer behavior in water–thiophenol clusters and their cation radicals: Insight into water number size dependence. *International Journal of Quantum Chemistry*, 105(2):186–198, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szekeres:2005:BBP

[SBL05b] Zs. Szekeres, F. Bogár, and J. Ladik. B3LYP, BLYP and PBE DFT band structures of the nucleotide base stacks. *International Journal of Quantum Chemistry*, 102(4):422–426, ????

2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Seijo:2000:IMP

[SBM00] Luis Seijo, Zoila Barandiarán, and Donald S. McClure. Ab initio model potential embedded cluster calculation of the absorption spectrum of Cs_2GeF_6:Mn^{4+}. Large discrepancies between theory and experiment. *International Journal of Quantum Chemistry*, 80(4–5):623–635, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505411/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505411/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505411&PLACEBO=IE.pdf`.

Sottile:2005:TMS

[SBM+05] Francesco Sottile, Fabien Bruneval, A. G. Marinopoulos, L. K. Dash, Silvana Botti, Valerio Olevano, Nathalie Vast, Angel Rubio, and Lucia Reining. TDDFT from molecules to solids: The role of long-range interactions. *International Journal of Quantum Chemistry*, 102(5):684–701, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sil:2007:ASU

[SBM07] A. N. Sil, S. Bhattacharyya, and P. K. Mukherjee. Atomic structure under external confinements: Effect of plasma. *International Journal of Quantum Chemistry*, 107(14):2708–2715, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2003:RAC

[SBMM03] B. Saha, S. Bhattacharyya, T. K. Mukherjee, and P. K. Mukherjee. Radial and angular correlation in heliumlike ions. *International Journal of Quantum Chemistry*, 92(5):413–418, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2003:DSS

[SBT+03] Rajendra Saha, S. P. Bhattacharyya, Christopher D. Taylor, Yong Zhao, and Thomas R. Cundari. Direct solution of the Schrödinger equation by a parallel genetic algorithm: Cases

of an exactly solvable 2-D interacting oscillator and the hydrogen atom. *International Journal of Quantum Chemistry*, 94(5):243–250, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shapley:2001:PPD

[SC01] Warwick A. Shapley and Delano P. Chong. PW86-PW91 density functional calculation of vertical ionization potentials: Some implications for present-day functionals. *International Journal of Quantum Chemistry*, 81(1):34–52, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/75502157/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75502157/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502157&PLACEBO=IE.pdf`.

Scofield:2002:QDM

[SC02a] D. F. Scofield and T. C. Collins. Quantum dynamical manifolds: Applications to excitonic coupled high temperature superconductivity. *International Journal of Quantum Chemistry*, 90(2):719–750, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Serrano:2002:EBL

[SC02b] Agostinho Serrano and Sylvio Canuto. Effect of bond-length alternation on the dipole hyperpolarizability of phenol blue. *International Journal of Quantum Chemistry*, 87(5):275–279, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90512104/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90512104/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90512104&PLACEBO=IE.pdf`.

Scofield:2004:QDM

[SC04] D. F. Scofield and T. C. Collins. Quantum dynamical manifolds: Pair states in high-temperature superconductivity. *International Journal of Quantum Chemistry*, 99(5):758–789, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Soscun:2006:BSD

[SCB+06] Humberto Soscún, Olga Castellano, Yaneth Bermúdez, Carlos Toro, Nestor Cubillán, Alan Hinchliffe, and Xuan Nguyen Phu. B3LYP study of the dipole moment and the static dipole (hyper)polarizabilities of para-nitroaniline in gas phase. *International Journal of Quantum Chemistry*, 106(5):1130–1137, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Scerri:2009:DST

[Sce09] Eric R. Scerri. The dual sense of the term "element," attempts to derive the Madelung rule, and the optimal form of the periodic table, if any. *International Journal of Quantum Chemistry*, 109(5):959–971, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Soriano-Correa:2003:PSP

[SCES03] Catalina Soriano-Correa, Rodolfo O. Esquivel, and Robin P. Sagar. Physicochemical and structural properties of bacteriostatic sulfonamides: Theoretical study. *International Journal of Quantum Chemistry*, 94(3):165–172, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Singh:2007:CAB

[SCG07] Ajeet Singh, Shampa Chakraborty, and Bishwajit Ganguly. Conformational analysis and the binding sites of nitrilotriacetamide: A computational study. *International Journal of Quantum Chemistry*, 107(6):1430–1436, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schulz:2000:ACC

[Sch00] L. P. Schulz. Algebraic criteria on chemical compound saturation and unsaturation. *International Journal of Quantum Chemistry*, 80(3):432–438, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501014/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501014/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501014&PLACEBO=IE.pdf`.

Schmidt:2002:HOB

[Sch02] P. P. Schmidt. Harmonic oscillator basis functions and Gaussian model potentials for the analysis of anharmonic vibrations. *International Journal of Quantum Chemistry*, 90(1): 202–226, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schiott:2004:PIC

[Sch04] Birgit Schiøtt. Possible involvement of collective domain movement in the catalytic reaction of soluble epoxide hydrolase. *International Journal of Quantum Chemistry*, 99(2):61–69, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schreckenbach:2005:DFC

[Sch05] Georg Schreckenbach. Density functional calculations of ^{19}F and ^{235}U NMR chemical shifts in uranium (VI) chloride fluorides $UF_{6-n}Cl_n$: Influence of the relativistic approximation and role of the exchange-correlation functional. *International Journal of Quantum Chemistry*, 101(4):372–380, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Soscun:2001:ABA

[SCHH01] Humberto Soscún, Olga Castellano, Javier Hernández, and Alan Hinchliffe. Acidity of the Brönsted acid sites of zeolites. *International Journal of Quantum Chemistry*, 82(3):143–150, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/77004285/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/77004285/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=77004285&PLACEBO=IE.pdf`.

Soscun:2002:TSS

[SCHH02] Humberto Soscún, Olga Castellano, Javier Hernández, and Alan Hinchliffe. Theoretical study of the structural, vibrational, and topologic properties of the charge distribution of the molecular complexes between thiophene and Brönsted acid sites of zeolites. *International Journal of Quantum Chemistry*, 87(4):240–253, ????

2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/88011402/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88011402/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88011402&PLACEBO=IE.pdf.

Sun:2007:TSS

[SCHW07] Lili Sun, Yingfei Chang, Bo Hong, and Rongshun Wang. Theoretical studies of structures and stabilities of endohedral fullerenes $X^{0/n+}$ @ $C_3 2$ (X = H, Li, Na, K, Be, Mg, Ca, B, Al, C, Si, N, P, n = 1–3). *International Journal of Quantum Chemistry*, 107(5):1241–1247, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sychrovsky:2000:BAA

[SČL00] Vladimír Sychrovský, Petr Čársky, and Hans Lischka. B_k approximation applied to the multireference configuration interaction method. *International Journal of Quantum Chemistry*, 76(2):185–196, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/69503171/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503171/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503171&PLACEBO=IE.pdf.

Su:2007:TCB

[SCLL07] Xinfang Su, Xinlu Cheng, Yonggang Liu, and Qinghuan Li. Theoretical calculation of bond dissociation energies and heats of formation for nitromethane and polynitromethanes with density functional theory. *International Journal of Quantum Chemistry*, 107(3):515–521, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sanz:2000:DVC

[SCM00] Javier Fdez. Sanz, Carmen J. Calzado, and Antonio Márquez. DFT *versus* CI determination of the electron-transfer matrix element in some case examples. *International Journal of Quantum Chemistry*, 76(3):458–463, January 20, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70000288/START; http:

//www3.interscience.wiley.com/cgi-bin/fulltext/70000288/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000288&PLACEBO=IE.pdf.

Szefczyk:2007:QCA

[SCMS07] Borys Szefczyk, Frederik Claeyssens, Adrian J. Mulholland, and W. Andrzej Sokalski. Quantum chemical analysis of reaction paths in chorismate mutase: Conformational effects and electrostatic stabilization. *International Journal of Quantum Chemistry*, 107(12):2274–2285, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Scofield:2000:QDM

[Sco00] D. F. Scofield. Quantum dynamical manifolds 5. Hydrogen mass-spacetime. *International Journal of Quantum Chemistry*, 80(3):369–393, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73501023/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501023/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501023&PLACEBO=IE.pdf.

Savin:2003:ACA

[SCP03] A. Savin, F. Colonna, and R. Pollet. Adiabatic connection approach to density functional theory of electronic systems. *International Journal of Quantum Chemistry*, 93(3):166–190, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shillady:2001:ECS

[SCR01] Donald D. Shillady, John Craig, and Sarah Rutan. Explicitly correlated SCF study of small hydrides. *International Journal of Quantum Chemistry*, 85(4–5):520–528, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Soriano-Correa:2008:CES

[SCRE08] Catalina Soriano-Correa, A. Raya, and Rodolfo O. Esquivel. Characterization of electronic structure and physicochemical properties of antiparasitic nifurtimox analogues: A theoretical study. *International Journal of Quantum Chemistry*, 108(8):1369–1379, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shillady:2002:ECS

[SCRR02] Donald D. Shillady, John Craig, Sarah Rutan, and Bijan Rao. Explicitly correlated SCF study of anharmonic vibrations in $(H_2O)_2$. *International Journal of Quantum Chemistry*, 90(4-5):1414–1420, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Soriano-Correa:2007:ESP

[SCRRE07] Catalina Soriano-Correa, Juan F. Sánchez Ruiz, A. Raya, and Rodolfo O. Esquivel. Electronic structure and physicochemical properties of selected penicillins. *International Journal of Quantum Chemistry*, 107(3):628–636, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Soriano-Correa:2005:EPP

[SCRSRE05] Catalina Soriano-Correa, Angélica Raya, Juan F. Sánchez-Ruiz, and Rodolfo O. Esquivel. Electronic and physicochemical properties of selected nitrofurans: A theoretical study. *International Journal of Quantum Chemistry*, 104(4):491–496, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [SCRSRE06].

Soriano-Correa:2006:EEP

[SCRSRE06] Catalina Soriano-Correa, Angélica Raya, Juan F. Sánchez-Ruiz, and Rodolfo O. Esquivel. Erratum: Electronic and physicochemical properties of selected nitrofurans: A theoretical study International Journal of Quantum Chemistry (2005) 104(4) 491–496. *International Journal of Quantum Chemistry*, 106(2):554, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [SCRSRE05].

Sukharev:2004:CPI

[SCSWF04] M. E. Sukharev, E. Charron, A. Suzor-Weiner, and M. V. Fedorov. Calculations of photodissociation in intense laser fields: Validity of the adiabatic elimination of the continuum. *International Journal of Quantum Chemistry*, 99(4):452–459, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stolterfoht:2009:SOC

[SCTK+09] N. Stolterfoht, R. Cabrera-Trujillo, P. S. Krstić, Y. Öhrn, E. Deumens, and J. R. Sabin. Stueckelberg oscillations in the

charge transfer into the n = 2 and n = 3 shells of He^2 on collision with H. *International Journal of Quantum Chemistry*, 109(13):3063–3074, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Si:2009:TSR

[SCW09] Yan-Ling Si, Wei-Lin Chen, and En-Bo Wang. Theoretical studies on redox properties, protonation sites, and electronic spectrum of a new type of polyoxometalate $[Ti_{12}Nb_6O_{44}]^{10-}$ by DFT. *International Journal of Quantum Chemistry*, 109 (7):1560–1565, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Staroverov:2000:CDS

[SD00a] Viktor N. Staroverov and Ernest R. Davidson. Charge densities for singlet and triplet electron pairs. *International Journal of Quantum Chemistry*, 77(3):651–660, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004060/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004060/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004060&PLACEBO=IE.pdf`.

Staroverov:2000:EDR

[SD00b] Viktor N. Staroverov and Ernest R. Davidson. Electron distributions in radicals. *International Journal of Quantum Chemistry*, 77(1):316–323, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004273/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004273/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004273&PLACEBO=IE.pdf`.

Smeyers:2003:PXB

[SD03] Yves G. Smeyers and Wagner B. De Almeida. Preface: XI Brazilian Symposium on Theoretical Chemistry, 18–21 November 2001, Hotel Glória, Caxambu, Minas Gerais, Brazil. *International Journal of Quantum Chemistry*, 95(2): 61–62, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Singh:2006:LOK

[SD06] C. Amuba Singh and O. Babynanda Devi. Ladder operators for the Kratzer oscillator and the Morse potential. *International Journal of Quantum Chemistry*, 106(2):415–425, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sarmah:2008:SER

[SD08] Pubalee Sarmah and Ramesh C. Deka. Solvent effect on the reactivity of CIS-platinum (II) complexes: A density functional approach. *International Journal of Quantum Chemistry*, 108 (8):1400–1409, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Springborg:2009:EC

[SD09] Michael Springborg and Yi Dong. Elemental chains. *International Journal of Quantum Chemistry*, 109(4):837–848, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Silva:2003:QCS

[SdACAG03] Washington B. Silva, Eberth de A. Corrêa, Paulo H. Acioli, and Ricardo Gargano. Quantum and classical study of vibrational states of H_2^+ and H_3^+ molecules. *International Journal of Quantum Chemistry*, 95(2):149–152, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sulston:2003:MBO

[SDB03] K. W. Sulston, S. G. Davison, and B. L. Burrows. Multisite bond and overlap treatment of polymer-chain band structure. *International Journal of Quantum Chemistry*, 94(6):341–346, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salva:2002:TST

[SDFM02] Antoni Salvà, Josefa Donoso, Juan Frau, and Francisco Muñoz. Theoretical studies on transimination of vitamin B6 analogs. *International Journal of Quantum Chemistry*, 89(1): 48–56, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schechner:2004:ELC

[SDS04] Martina Schechner, Annick P. Dejaegere, and Roland H. Stote. Effects of loop conformation on pKa and ligand binding in DNA gyrase B. *International Journal of Quantum Chemistry*, 98(4):378–387, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sinitsky:2002:ECF

[SDTM02] A. V. Sinitsky, M. B. Darhovskii, A. L. Tchougréeff, and I. A. Misurkin. Effective crystal field for trivalent first transition row ions. *International Journal of Quantum Chemistry*, 88(4): 370–379, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szczepanik:2007:COP

[SDW07] W. Szczepanik, M. Dulak, and T. A. Wesolowski. Comment on "On the original proof by reductio ad absurdum of the Hohenberg–Kohn theorem for many-electron Coulomb systems". *International Journal of Quantum Chemistry*, 107 (3):762–763, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Kry05].

Sterling:2007:CIE

[SDZ+07] Mark R. Sterling, O. Dolgounitcheva, V. G. Zakrzewski, Yu. Dahnovsky, and J. V. Ortiz. Correlated, ab initio electron propagators in the study of molecular wires: Application to a single molecular bridge placed between two model leads. *International Journal of Quantum Chemistry*, 107(15):3228–3235, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sorensen:2000:VSB

[SE00] Thomas E. Sorensen and Walter B. England. Valence states of BeO: Feynman's way. *International Journal of Quantum Chemistry*, 76(2):259–279, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503178/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503178/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503178&PLACEBO=IE.pdf`.

Scherlis:2002:SSS

[SE02a] Damián A. Scherlis and Darío A. Estrin. Structure and spin-state energetics of an iron porphyrin model: An assessment of theoretical methods. *International Journal of Quantum Chemistry*, 87(3):158–166, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89015697/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89015697/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89015697&PLACEBO=IE.pdf`.

Sorensen:2002:VSC

[SE02b] Thomas E. Sorensen and Walter B. England. Valence states of the cyano radical Feynman's way. *International Journal of Quantum Chemistry*, 90(2):516–533, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sonnino:2007:GTF

[SE07] Giorgio Sonnino and Jarah Evslin. Geometrical thermodynamic field theory. *International Journal of Quantum Chemistry*, 107(4):968–987, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sebastiani:2005:CDP

[Seb05] Daniel Sebastiani. Crystalline diamond polymorphs analyzed with first-principles ^{13}C NMR chemical shift calculations. *International Journal of Quantum Chemistry*, 101(6):849–853, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Seidl:2003:DFT

[Sei03] Michael Seidl. Density functional theory from the extreme limits of correlation. *International Journal of Quantum Chemistry*, 91(2):145–150, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szekeres:2005:FFS

[SEM05] Zsolt Szekeres, Thomas Exner, and Paul G. Mezey. Fuzzy fragment selection strategies, basis set dependence and HF–DFT comparisons in the applications of the ADMA method of macromolecular quantum chemistry. *International Journal*

of Quantum Chemistry, 104(6):847–860, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Smirnov:2002:WTA

[SEU02] V. P. Smirnov, R. A. Evarestov, and D. E. Usvyat. Wannier-type atomic functions and chemical bonding in crystals. *International Journal of Quantum Chemistry*, 88(5):642–651, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shilyaeva:2007:RRB

[SEY07] Ksenia Shilyaeva, Nils Elander, and Evgeny Yarevsky. Role of resonances in building cross sections: Comparison between the Mittag-Leffler and the T-matrix Green function expansion approaches. *International Journal of Quantum Chemistry*, 107(6):1301–1315, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Seybold:2008:APK

[Sey08] Paul G. Seybold. Analysis of the pK_a s of aliphatic amines using quantum chemical descriptors. *International Journal of Quantum Chemistry*, 108(15):2849–2855, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shilyaeva:2009:RRB

[SEY09] Ksenia Shilyaeva, Nils Elander, and Evgeny Yarevsky. The role of resonances in building cross sections: The Mittag-Leffler expansion in a two-channel scattering. *International Journal of Quantum Chemistry*, 109(3):414–424, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salvador:2009:QAE

[SFD09] Pedro Salvador, Xavier Fradera, and Miquel Duran. Quantitative assessment of the effect of basis set superposition error on the electron density of molecular complexes by means of quantum molecular similarity measures. *International Journal of Quantum Chemistry*, 109(11):2572–2580, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sawada:2009:SIA

[SFK09] Toshihiko Sawada, Dmitri G. Fedorov, and Kazuo Kitaura. Structural and interaction analysis of helical heparin oligosaccharides with the fragment molecular orbital method. *International Journal of Quantum Chemistry*, 109(9):2033–2045, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

San-Fabian:2003:DCC

[SFPA03] E. San-Fabián and L. Pastor-Abia. DFT calculations of correlation energies for excited electronic states using MCSCF wave functions. *International Journal of Quantum Chemistry*, 91 (3):451–460, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sousa:2008:MDA

[SFR08] Sérgio F. Sousa, Pedro A. Fernandes, and Maria João Ramos. Molecular dynamics analysis of farnesyltransferase: A closer look into the amino acid behavior. *International Journal of Quantum Chemistry*, 108(11):1939–1950, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Strajbl:2000:ILS

[ŠFW00] Marek Štrajbl, Jan Florián, and Arieh Warshel. Ab initio/LD studies of chemical reactions in solution: Reference free-energy surfaces for acylation reactions occurring in serine and cysteine proteases. *International Journal of Quantum Chemistry*, 77(1):44–53, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004294/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004294/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004294&PLACEBO=IE.pdf`.

Shigeta:2001:EPC

[SFZO01] Y. Shigeta, A. M. Ferreira, V. G. Zakrzewski, and J. V. Ortiz. Electron propagator calculations with Kohn–Sham reference states. *International Journal of Quantum Chemistry*, 85(4–5):411–420, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sala:2003:EEM

[SG03] Fabio Della Sala and Andreas Görling. Excitation energies of molecules by time-dependent density functional theory based on effective exact exchange Kohn–Sham potentials. *International Journal of Quantum Chemistry*, 91(2):131–138, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schmidt:2000:CF

[SGB00] Michael W. Schmidt, Mark S. Gordon, and Jerry A. Boatz. Cubic fuels? *International Journal of Quantum Chemistry*, 76(3):434–446, January 20, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000286/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000286/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000286&PLACEBO=IE.pdf`.

Seidel:2002:QMC

[SGGBB02] L. Seidel, C. González-Giralda, R. M. Benito, and F. Borondo. Quantum manifestations of classical trajectories in molecular systems. *International Journal of Quantum Chemistry*, 86(2):175–181, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85011803/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85011803/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85011803&PLACEBO=IE.pdf`.

Shishkin:2000:SNN

[SGHL00] Oleg V. Shishkin, Leonid Gorb, Pavel Hobza, and Jerzy Leszczynski. Structural nonrigidity of nucleic acid bases. Post-Hartree–Fock ab initio study. *International Journal of Quantum Chemistry*, 80(4–5):1116–1124, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505408/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505408/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505408&PLACEBO=IE.pdf`.

Schay:2001:PML

[SGLF01] Gusztav Schay, Rita Galantai, Monique Laberge, and Judit Fidy. Protein matrix local fluctuations and substrate binding in HRPC: A proposed dynamic electrostatic sampling method. *International Journal of Quantum Chemistry*, 84(2):290–301, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/84502326/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502326/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502326&PLACEBO=IE.pdf.

Schmiedekamp:2007:SCC

[SGP+07] Ann M. Schmiedekamp, Anthony Ginnetti, Brian Piccione, Kevin Cannon, and M. Dominic Ryan. Six-coordinate Co^{2+} with imidazole, NH_3, and H_2O ligands: Approaching spin crossover. *International Journal of Quantum Chemistry*, 107 (6):1415–1429, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Skurski:2000:HCO

[SGS00a] Piotr Skurski, Maciej Gutowski, and Jack Simons. How to choose a one-electron basis set to reliably describe a dipole-bound anion. *International Journal of Quantum Chemistry*, 80(4–5):1024–1038, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505397/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505397/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505397&PLACEBO=IE.pdf.

Skurski:2000:PBT

[SGS00b] Piotr Skurski, Maciej Gutowski, and Jack Simons. On the possibility of binding of two electrons to dipole potentials. *International Journal of Quantum Chemistry*, 76(2):197–204, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/69503172/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503172/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503172&PLACEBO=IE.pdf.

Safouhi:2000:NMR

[SH00] H. Safouhi and P. E. Hoggan. New method of rapid and accurate evaluation for multicenter bielectronic integrals over B functions. *International Journal of Quantum Chemistry*, 80(2):236–248, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001284/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001284/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001284&PLACEBO=IE.pdf`.

Safouhi:2001:RPA

[SH01] Hassan Safouhi and Philip Hoggan. Recent progress in the accurate and rapid evaluation of all Coulomb integrals over Slater-type orbitals. *International Journal of Quantum Chemistry*, 84(5):580–591, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85006929/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85006929/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85006929&PLACEBO=IE.pdf`.

Safouhi:2002:TCN

[SH02a] Hassan Safouhi and Philip Hoggan. Three-center nuclear attraction, three-center two-electron Coulomb and hybrid integrals over B functions evaluated using the nonlinear S transformation. *International Journal of Quantum Chemistry*, 90 (1):119–135, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sims:2002:HPH

[SH02b] James S. Sims and Stanley A. Hagstrom. High-precision Hy–CI variational calculations for the ground state of neutral helium and helium-like ions. *International Journal of Quantum Chemistry*, 90(6):1600–1609, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Springborg:2007:SCG

[SH07] Michael Springborg and Kaspar Hegetschweiler. Some continuous geometry transitions and the consequences for a

transition-metal atom. *International Journal of Quantum Chemistry*, 107(5):1073–1084, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shimazaki:2009:BZI

[SH09] Tomomi Shimazaki and So Hirata. On the Brillouin-zone integrations in second-order many-body perturbation calculations for extended systems of one-dimensional periodicity. *International Journal of Quantum Chemistry*, 109(13):2953–2959, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shavitt:2004:ETB

[Sha04] Isaiah Shavitt. Are exponential-type basis sets preferable to Gaussians? *International Journal of Quantum Chemistry*, 100 (2):105–108, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shahu:2006:CSM

[Sha06] Milena Shahu. CASSCF study into the mechanism for predissociation of the allyl radical. *International Journal of Quantum Chemistry*, 106(2):501–506, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shainyan:2007:CSF

[Sha07] Bagrat A. Shainyan. Computational study of 4-fluoro-4-chloro- and 4-fluoro-4-bromo-4-silathiacyclohexane S-oxides: Effect of halogen on the SO $\rightarrow$ Si intramolecular coordination in the boat and twist conformers. *International Journal of Quantum Chemistry*, 107(1):189–199, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Soscun:2000:IST

[SHC00] Humberto Soscun, Javier Hernández, and Olga Castellano. Ab initio study of the topology of the charge distribution of $H_3SiO(H)AlH_3$ conformers. *International Journal of Quantum Chemistry*, 76(1):1–9, January 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503201/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503201/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503201&PLACEBO=IE.pdf`.

Steinborn:2000:MCF

[SHE+00] E. O. Steinborn, H. H. H. Homeier, I. Ema, R. Lopez, and G. Ramírez. Molecular calculations with B functions. *International Journal of Quantum Chemistry*, 76(2):244–251, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503176/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503176/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503176&PLACEBO=IE.pdf`.

Soscun:2002:IDF

[SHE+02] Humberto Soscún, Javier Hernández, Ramón Escobar, Carlos Toro-Mendoza, Ysaías Alvarado, and Alan Hinchliffe. Ab initio and density functional theory calculations of the dipole polarizability and the second dipole hyperpolarizability of benzene. *International Journal of Quantum Chemistry*, 90(2): 497–506, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sheka:2004:IIC

[She04a] Elena F. Sheka. Intermolecular interaction in C_{60}-based electron donor–acceptor complexes. *International Journal of Quantum Chemistry*, 100(4):388–406, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sheka:2004:OEC

[She04b] Elena F. Sheka. Odd electrons and covalent bonding in fullerenes. *International Journal of Quantum Chemistry*, 100 (4):375–387, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shehadi:2007:TAF

[She07a] Ihsan A. Shehadi. THEMATICS analysis for functional ion channels. *International Journal of Quantum Chemistry*, 107 (11):2075–2081, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sheka:2007:OEM

[She07b] E. F. Sheka. Odd electrons in molecular chemistry, surface science, and solid state magnetism. *International Journal of*

Quantum Chemistry, 107(14):2935–2955, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sheka:2007:CSF

[She07c] Elena F. Sheka. Chemical susceptibility of fullerenes in view of Hartree–Fock approach. *International Journal of Quantum Chemistry*, 107(14):2803–2816, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sheka:2007:DAO

[She07d] Elena F. Sheka. Donor–acceptor origin of fullerene C_{60} dimerization. *International Journal of Quantum Chemistry*, 107 (13):2361–2371, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Small:2008:CMQ

[SHG08] David W. Small and Martin Head-Gordon. Central moments in quantum chemistry. *International Journal of Quantum Chemistry*, 108(7):1220–1231, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2006:TSM

[SHH+06] Hao Sun, Hong-Qing He, Bo Hong, Ying-Fei Chang, Zhe An, and Rong-Shun Wang. Theoretical study of the mechanism of CH_2CO + CN reaction. *International Journal of Quantum Chemistry*, 106(4):894–905, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shidlovskaya:2002:IEM

[Shi02] E. K. Shidlovskaya. Improved embedded molecular cluster model. *International Journal of Quantum Chemistry*, 89(4): 349–370, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shigeta:2004:HQM

[Shi04] Yasuteru Shigeta. Hybrid QM/MM studies on energetics of malonaldehyde in condensed phase. *International Journal of Quantum Chemistry*, 96(1):32–41, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shigeta:2005:OEP

[Shi05] Yasuteru Shigeta. Optimized effective potential method at finite temperature: An application to superconductivity. *In-*

ternational Journal of Quantum Chemistry, 101(6):774–782, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sakimoto:2009:TIT

[SHM09a] Yukiko Sakimoto, Kimihiko Hirao, and Djamaladdin G. Musaev. Theoretical insights into the thiol reductase activity of ebtellur. *International Journal of Quantum Chemistry*, 109(10):2297–2307, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sumpter:2009:TES

[SHM+09b] Bobby G. Sumpter, Jingsong Huang, Vincent Meunier, Jose M. Romo-Herrera, Eduardo Cruz-Silva, Humberto Terrones, and Mauricio Terrones. A theoretical and experimental study on manipulating the structure and properties of carbon nanotubes using substitutional dopants. *International Journal of Quantum Chemistry*, 109(1):97–118, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schulze-Halberg:2009:AOD

[SHZGP09] Axel Schulze-Halberg, E. Zamora-Gallardo, and J. J. Peña. Arbitrary-order Darboux transformations for position-dependent mass Schrödinger equations with noncentral potential. *International Journal of Quantum Chemistry*, 109(7): 1464–1471, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Santana:2009:ECS

[SI09] Juan A. Santana and Yasuyuki Ishikawa. Effective collision strengths for electron-impact excitation of transitions within the ground 1 s^2 2 s^2 2 p^4 manifold of O-like Fe^{18+}. *International Journal of Quantum Chemistry*, 109(9):1920–1927, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sinha:2000:SFC

[Sin00] Anjana Sinha. SWKB formalism for confined quantum systems. *International Journal of Quantum Chemistry*, 79 (5):267–273, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72512626/START;` `http://www3.interscience.wiley.com/cgi-bin/fulltext/`

72512626/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72512626&PLACEBO=IE.pdf.

Sugimori:2005:TSM

[SINN05] Kimikazu Sugimori, Tomoya Ito, Hidemi Nagao, and Kiyoshi Nishikawa. Theoretical study of multiphoton processes in diatomic molecules. *International Journal of Quantum Chemistry*, 105(6):596–604, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shoji:2008:TCBb

[SIS+08a] Mitsuo Shoji, Hiroshi Isobe, Toru Saito, Yasutaka Kitagawa, Shusuke Yamanaka, Takashi Kawakami, Mitsutaka Okumura, and Kizashi Yamaguchi. Theory of chemical bonds in metalloenzymes XI: Full geometry optimization and vibration analysis of porphyrin iron-oxo species. *International Journal of Quantum Chemistry*, 108(15):2950–2965, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shoji:2008:TCBa

[SIS+08b] Mitsuo Shoji, Hiroshi Isobe, Toru Saito, Hirotaka Yabushita, Kenichi Koizumi, Yasutaka Kitagawa, Shusuke Yamanaka, Takashi Kawakami, Mitsutaka Okumura, Masayuki Hagiwara, and Kizashi Yamaguchi. Theory of chemical bonds in metalloenzymes. VII. Hybrid-density functional theory studies on the electronic structures of P450. *International Journal of Quantum Chemistry*, 108(4):631–650, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sugimori:2006:TSD

[SIT+06] Kimikazu Sugimori, Tomoya Ito, Yusuke Takata, Kazuhiro Ichitani, Hidemi Nagao, and Kiyoshi Nishikawa. Theoretical study of the dissociation process by multiphoton absorption in the diatomic molecule. *International Journal of Quantum Chemistry*, 106(15):3079–3086, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shoji:2007:TCB

[SIT+07] Mitsuo Shoji, Hiroshi Isobe, Yu Takano, Yasutaka Kitagawa, Shusuke Yamanaka, Mitsutaka Okumura, and Kizashi Yamaguchi. Theory of chemical bonds in metalloenzymes. IX. Theoretical study on the active site of the ribonucleotide reductase

and the related species. *International Journal of Quantum Chemistry*, 107(15):3250–3265, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sandalov:2003:TSC

[SJE03] Igor Sandalov, Börje Johansson, and Olle Eriksson. Theory of strongly correlated electron systems: Hubbard–Anderson models from an exact Hamiltonian, and perturbation theory near the atomic limit within a nonorthogonal basis set. *International Journal of Quantum Chemistry*, 94(3):113–143, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stanchev:2008:SDS

[SJM08] Stancho Stanchev, Frank Jensen, and Ilia Manolov. Synthesis and DFT study of the spectral behavior of new 4-hydroxycoumarins. *International Journal of Quantum Chemistry*, 108(8):1340–1351, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sjoqvist:2000:DEN

[Sjö00] Erik Sjöqvist. Degree of electron-nuclear entanglement in molecular states. *International Journal of Quantum Chemistry*, 77(2):526–533, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70002212/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70002212/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70002212&PLACEBO=IE.pdf`.

Saha:2000:SCC

[SK00a] Bidhan C. Saha and Anil Kumar. State-changing collisions of low-Rydberg Na atoms with ground state He atoms: A low-energy study involving spherical and nonspherical initial target states. *International Journal of Quantum Chemistry*, 80(4–5):1011–1023, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505391/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505391/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505391&PLACEBO=IE.pdf`.

Shuford:2000:QCC

[SK00b] Kevin L. Shuford and Jeffrey L. Krause. Quantum control of charge carriers in quantum wells. *International Journal of Quantum Chemistry*, 77(1):393–402, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004282/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004282/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004282&PLACEBO=IE.pdf`.

Saha:2001:RIO

[SK01a] Bidhan C. Saha and Anil Kumar. Role of initial orbital alignment in $H^+ + K(4p)$ collisions at low energies. *International Journal of Quantum Chemistry*, 85(4–5):382–391, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2001:QCL

[SK01b] Qicun Shi and Sabre Kais. Quantum criticality at the large-dimensional limit: Three-body Coulomb systems. *International Journal of Quantum Chemistry*, 85(4–5):307–314, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stambuk:2001:NCA

[ŠK01c] Nikola Štambuk and Paško Konjevoda. New computational algorithm for the prediction of protein folding types. *International Journal of Quantum Chemistry*, 84(1):13–22, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84002437/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002437/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002437&PLACEBO=IE.pdf`.

Sirbu:2003:PAE

[SK03a] Ioana Sirbu and Harry F. King. Perturbational approach to the electron correlation cusp applied to helium-like atoms. *International Journal of Quantum Chemistry*, 92(5):433–450, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stambuk:2003:PSP

[ŠK03b] Nikola Štambuk and Paško Konjevoda. Prediction of secondary protein structure with binary coding patterns of amino acid and nucleotide physicochemical properties. *International Journal of Quantum Chemistry*, 92(2):123–134, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Selvarengan:2005:SMI

[SK05a] P. Selvarengan and P. Kolandaivel. Study of metal ions (Na^+, K^+) interaction with different conformations of glycine molecule. *International Journal of Quantum Chemistry*, 102 (4):427–434, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Site:2005:MMP

[SK05b] Luigi Delle Site and Kurt Kremer. Multiscale modeling of polymers on a surface: From ab initio density functional calculations of molecular adsorption to large-scale properties. *International Journal of Quantum Chemistry*, 101(6):733–739, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stanek:2005:WFR

[SK05c] Jerzy Stanek and Jerzy Konarski. Wigner function of the rotating Morse oscillator. *International Journal of Quantum Chemistry*, 103(1):10–18, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Selvarengan:2006:TSC

[SK06] P. Selvarengan and P. Kolandaivel. Theoretical study of CH. . . O hydrogen bond in proton transfer reaction of glycine. *International Journal of Quantum Chemistry*, 106(4):1001–1008, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Skala:2009:HUR

[SK09] L. Skála and V. Kapsa. Heisenberg uncertainty relations can be replaced by stronger ones. *International Journal of Quantum Chemistry*, 109(8):1626–1630, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shalabi:2005:TSL

[SKA05] A. S. Shalabi, M. A. Kamel, and H. Y. Ammar. Theoretical study of laser light generation and color image formation: F_{A1}:Cs^+ and F_{A2}:Li^+ centers at the low coordination (100) and (110) surfaces of AgCl and AgBr. *International Journal of Quantum Chemistry*, 103(4):432–448, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sode:2009:CCM

[SKHY09] Olaseni Sode, Murat Keçeli, So Hirata, and Kiyoshi Yagi. Coupled-cluster and many-body perturbation study of energies, structures, and phonon dispersions of solid hydrogen fluoride. *International Journal of Quantum Chemistry*, 109(9): 1928–1939, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shoji:2005:TCB

[SKK+05] M. Shoji, K. Koizumi, Y. Kitagawa, S. Yamanaka, T. Kawakami, M. Okumura, and K. Yamaguchi. Theory of chemical bonds in metalloenzymes II: Hybrid-DFT studies in iron–sulfur clusters. *International Journal of Quantum Chemistry*, 105(6): 628–644, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shoji:2006:TCB

[SKK+06] M. Shoji, K. Koizumi, Y. Kitagawa, S. Yamanaka, M. Okumura, K. Yamaguchi, Y. Ohki, Y. Sunada, M. Honda, and K. Tatsumi. Theory of chemical bonds in metalloenzymes V: Hybrid-DFT studies of the inorganic [8Fe–7S] core. *International Journal of Quantum Chemistry*, 106(15):3288–3302, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shoji:2007:TCBb

[SKK+07] Mitsuo Shoji, Kenichi Koizumi, Yasutaka Kitagawa, Shusuke Yamanaka, Mitsutaka Okumura, and Kizashi Yamaguchi. Theory of chemical bonds in metalloenzymes IV: Hybrid-DFT study of Rieske-type [2Fe — 2S] clusters. *International Journal of Quantum Chemistry*, 107(3):609–627, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sankararamakrishnan:2000:SSA

[SKMW00] R. Sankararamakrishnan, K. Konvicka, E. L. Mehler, and H. Weinstein. Solvation in simulated annealing and high-temperature molecular dynamics of proteins: A restrained water droplet model. *International Journal of Quantum Chemistry*, 77(1):174–186, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004257/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004257/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004257&PLACEBO=IE.pdf`.

Saito:2009:TSC

[SKN+09a] Toru Saito, Yusuke Kataoka, Yasuyuki Nakanishi, Toru Matsui, Yasutaka Kitagawa, Takashi Kawakami, Mitsutaka Okumura, and Kizashi Yamaguchi. Theoretical studies on chemical bonding between Cu(II) and oxygen molecule in type 3 copper proteins. *International Journal of Quantum Chemistry*, 109(15):3649–3658, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sakata:2009:LLE

[SKN09b] Tetsuya Sakata, Yukio Kawashima, and Haruyuki Nakano. Low-lying excited states of 7-aminocoumarin derivatives: A theoretical study. *International Journal of Quantum Chemistry*, 109(9):1940–1949, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sugimori:2008:DSI

[SKNN08] K. Sugimori, H. Kawabe, H. Nagao, and K. Nishikawa. A DFT study of infrared spectrum of sphingomyelin lipid molecule with calcium cation. *International Journal of Quantum Chemistry*, 108(15):2935–2942, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sugimori:2009:IDS

[SKNN09] K. Sugimori, H. Kawabe, H. Nagao, and K. Nishikawa. Ab initio and DFT study of ^{31}P-NMR chemical shifts of sphingomyelin and dihydrosphingomyelin lipid molecule. *International Journal of Quantum Chemistry*, 109(15):3685–3693, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Skorobogatov:2002:DKF

[Sko02] G. A. Skorobogatov. Deduction of the Klein–Fock–Gordon equation from a non-Markovian stochastic equation for real pure-jump process. *International Journal of Quantum Chemistry*, 88(5):614–623, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Samanta:2008:TDS

[SKSB08] Sudipta Samanta, Mukul Kabir, Biplab Sanyal, and Dhananjay Bhattacharyya. Twist-dependent stacking energy of base-pair steps in B-DNA geometry: A density functional theory approach. *International Journal of Quantum Chemistry*, 108 (6):1173–1180, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sahu:2009:DRI

[SKSS09a] V. K. Sahu, A. K. R. Khan, R. K. Singh, and P. P. Singh. Drug–receptor interaction-based quantitative structure–activity relationship of tetrahydroimidazodiazepinone. *International Journal of Quantum Chemistry*, 109(6):1243–1254, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Singh:2009:CQS

[SKSS09b] R. K. Singh, A. K. R. Khan, V. K. Sahu, and P. P. Singh. Comparative QSTR study of a series of alcohol derivatives against Tetrahymena pyriformis. *International Journal of Quantum Chemistry*, 109(2):185–195, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stepanov:2005:PMB

[SKT05] Nikolai F. Stepanov, Alexei A. Kubasov, and Yaroslav V. Tikhii. Properties of methanol bound to a defect of zeolitic structure. *International Journal of Quantum Chemistry*, 104 (2):214–222, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shoji:2007:TCBa

[SKT+07] Mitsuo Shoji, Kenichi Koizumi, Takeshi Taniguchi, Yasutaka Kitagawa, Shusuke Yamanaka, Mitsutaka Okumura, and Kizashi Yamaguchi. Theory of chemical bonds in metalloenzymes III: Full geometry optimization and vibration analysis

of ferredoxin-type [2Fe–2S] cluster. *International Journal of Quantum Chemistry*, 107(1):116–133, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shukla:2000:IES

[SL00] M. K. Shukla and J. Leszczynski. Investigations of the excited-state properties of isocytosine: An ab initio approach. *International Journal of Quantum Chemistry*, 77(1):240–254, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004264/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004264/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004264&PLACEBO=IE.pdf`.

Sahu:2005:MBI

[SL05a] Prabhat K. Sahu and Shyi-Long Lee. Many-body interactions of carbon monoxide cyclic oligomers: A computational study. *International Journal of Quantum Chemistry*, 103(3):314–321, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sen:2005:FOC

[SL05b] K. D. Sen and F. Javier Luque. First-order correlation-kinetic contribution to Kohn–Sham exchange charge density function in atoms, using quantal density functional theory approach. *International Journal of Quantum Chemistry*, 101(3):231–238, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shukla:2005:TDD

[SL05c] M. K. Shukla and Jerzy Leszczynski. Time-dependent density functional theory (TD-DFT) study of the excited state proton transfer in hypoxanthine. *International Journal of Quantum Chemistry*, 105(4):387–395, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sobrinho:2005:EAC

[SL05d] A. M. C. Sobrinho and M.-T. Lee. Elastic and absorption cross sections for electron–carbon monosulfide collisions. *International Journal of Quantum Chemistry*, 103(5):703–710, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sahu:2007:HBI

[SL07] Prabhat K. Sahu and Shyi-Long Lee. Hydrogen-bond interactions in THF–H_2O–HF: A theoretical study. *International Journal of Quantum Chemistry*, 107(10):2015–2023, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shainyan:2009:PSI

[SL09] Bagrat A. Shainyan and Natalia F. Lazareva. PO $\rightarrow$ Si intramolecular coordination in the derivatives of 1,4-phosphasilacyclohexane 1-oxides. *International Journal of Quantum Chemistry*, 109(2):301–307, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slanina:2005:CSE

[SLA+05] Zdeněk Slanina, Shyi-Long Lee, Ludwik Adamowicz, Filip Uhlík, and Shigeru Nagase. Computed structure and energetics of La@C_{60}. *International Journal of Quantum Chemistry*, 104(2):272–277, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Santos:2005:TII

[SLB+05] J. D. Santos, E. Longo, M. E. Banja, V. A. A. Espinoza, and C. A. Taft. A theoretical investigation of the interaction between H, Li, Na, K, and fullerenes. *International Journal of Quantum Chemistry*, 102(3):302–312, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2008:IHH

[SLB+08] Junyou Shi, Ping Li, Yuxiang Bu, Weihua Wang, Zhaoxia Mou, and Rui Song. Isomerization of HNO to HON in the singlet state assisted by amino acid residues and/or water molecules. *International Journal of Quantum Chemistry*, 108 (7):1246–1256, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Skouteris:2004:RAE

[SLCW04a] Dimitris Skouteris, Antonio Laganà, Gabriella Capecchi, and Hans-Joachim Werner. Rotational and alignment effects in a wave packet calculation for the Cl + H_2 reaction. *International Journal of Quantum Chemistry*, 99(5):577–584, ????

2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Skouteris:2004:WPC

[SLCW04b] Dimitris Skouteris, Antonio Laganà, Gabriella Capecchi, and Hans-Joachim Werner. Wave packet calculations for the Cl + H_2 reaction. *International Journal of Quantum Chemistry*, 96(6):562–567, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sandalov:2005:TSC

[SLE05] I. Sandalov, U. Lundin, and O. Eriksson. Theory of strongly correlated electron systems. I. Intersite Coulomb interaction and the approximation of renormalized fermions in total energy calculations. *International Journal of Quantum Chemistry*, 102(6):1019–1045, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2006:RMC

[SLL06] Shujuan Sun, Lan Li, and Zonghe Li. Radical-mediated cytosine and 5-methylcytosine hydrolytic deamination reactions. *International Journal of Quantum Chemistry*, 106(8):1878–1884, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schonherr:2002:SQC

[SLRS02] T. Schönherr, R. Linder, U. Rosellen, and V. Schmid. Spectroscopic and quantum chemical study on electronic and geometric properties of free and embedded dithizone molecules. *International Journal of Quantum Chemistry*, 86(1):90–99, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85008596/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85008596/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85008596&PLACEBO=IE.pdf`.

Silva:2005:CAD

[SLS+05] Carlos H. T. P. Silva, Andreia M. Leopoldino, Eloiza H. T. Silva, V. A. A. Espinoza, and C. A. Taft. Computer-aided design of a novel ligand for retinoic acid receptor in cancer chemotherapy. *International Journal of Quantum Chemistry*,

102(6):1131–1135, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slanina:2006:EES

[SLU+06] Zdeněk Slanina, Shyi-Long Lee, Filip Uhlík, Ludwik Adamowicz, and Shigeru Nagase. Excited electronic states and relative stabilities of C_{80} isomers. *International Journal of Quantum Chemistry*, 106(10):2222–2228, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2007:TSA

[SLW+07] Jiao Sun, Wen-Cai Lu, Hong Wang, Li-Zhen Zhao, Ze-Sheng Li, and Chia-Chung Sun. Theoretical study on Al_nO_2 ($n = 1--10$) clusters and O_2 adsorption on the Al(111) surface. *International Journal of Quantum Chemistry*, 107(9):1915–1924, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2007:ESC

[SLWS07] Xiao-Ying Sun, Zhi-Ru Li, Di Wu, and Chia-Chung Sun. Extraordinary superatom containing double shell nucleus: $Li(HF)_3Li$ connected mainly by intermolecular interactions. *International Journal of Quantum Chemistry*, 107(5):1215–1222, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Souza:2003:FCA

[SM03] Sarai S. Souza and Maria Matos. Finite-cluster approximation for deep-level impurities in silicon carbide. *International Journal of Quantum Chemistry*, 95(2):88–96, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Squire:2004:FSC

[SM04] Richard H. Squire and Norman H. March. Fulleride superconductivity compared and contrasted with RVB theory of high T_c cuprates. *International Journal of Quantum Chemistry*, 100(6):1092–1103, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sil:2005:EDPa

[SM05a] A. N. Sil and P. K. Mukherjee. Effect of Debye plasma on the doubly excited states of highly stripped ions. *International*

Journal of Quantum Chemistry, 102(6):1061–1068, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Singh:2005:MBP

[SM05b] A. K. Singh and P. C. Mishra. Mismatch base pairing of the mutagen 8-oxoguanine and its derivatives with adenine: A theoretical search for possible antimutagenic agents. *International Journal of Quantum Chemistry*, 102(3):343–351, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Squire:2005:QPT

[SM05c] Richard H. Squire and Norman H. March. Quantum phase transitions and superconductivity: Proposal for the phase diagram of alkali-doped fullerides and by universality HTSC including Wigner solids. *International Journal of Quantum Chemistry*, 105(6):883–897, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shepard:2006:ONW

[SM06a] Ron Shepard and Michael Minkoff. Optimization of nonlinear wave function parameters. *International Journal of Quantum Chemistry*, 106(15):3190–3207, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sil:2006:SPH

[SM06b] A. N. Sil and P. K. Mukherjee. Spectral properties of helium-like ions under strongly coupled plasma conditions. *International Journal of Quantum Chemistry*, 106(2):465–477, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Squire:2006:CIS

[SM06c] Richard H. Squire and Norman H. March. Changing an insulating state with Wigner-like correlations into a superconductor with applications to doped fullerides. *International Journal of Quantum Chemistry*, 106(15):3343–3363, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Singh:2007:ASC

[SM07a] A. K. Singh and P. C. Mishra. Off-atomic site charges in some anions, metal cations, and complexes: Significance for electrostatic properties and binding. *International Journal of Quantum Chemistry*, 107(3):597–608, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Squire:2007:ABB

[SM07b] Richard H. Squire and Norman H. March. Aspects of BCS to BEC "Crossover" as illustrated by fulleride superconductivity. *International Journal of Quantum Chemistry*, 107(15):3013–3027, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Squire:2008:PPI

[SM08] Richard H. Squire and Norman H. March. Preformed pair induced quantum phase transition in fulleride superconductivity. *International Journal of Quantum Chemistry*, 108(15): 2819–2836, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stashans:2009:QCI

[SM09] Arvids Stashans and Frank Maldonado. Quantum chemical investigation of lanthanum doping effects in tetragonal and rhombohedral PZT materials. *International Journal of Quantum Chemistry*, 109(7):1576–1583, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sambrano:2001:TAT

[SMAL01] J. R. Sambrano, J. B. L. Martins, J. Andres, and Elson Longo. Theoretical analysis on TiO_2 (110)/V surface. *International Journal of Quantum Chemistry*, 85(1):44–51, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85004197/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85004197/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85004197&PLACEBO=IE.pdf`.

Shepard:2007:NWF

[SMB07] Ron Shepard, Michael Minkoff, and Scott R. Brozell. Nonlinear wave function expansions: A progress report. *Inter-*

national Journal of Quantum Chemistry, 107(15):3203–3218, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Squire:2009:HCP

[SMB09] Richard H. Squire, Norman H. March, and Michael L. Booth. HTSC cuprate phase diagram using a modified Boson–Fermion–Gossamer model describing competing orders, a quantum critical point and possible resonance complex. *International Journal of Quantum Chemistry*, 109(15):3516–3532, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shimomura:2009:HRS

[SMDG09] Kenta Shimomura, Yasuji Muramatsu, Jonathan D. Denlinger, and Eric M. Gullikson. High-resolution soft X-ray spectral analysis in the C K region of titanium carbide using the DV-X_α molecular orbital method. *International Journal of Quantum Chemistry*, 109(12):2722–2727, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2003:ATS

[SMDM03] B. Saha, T. K. Mukherjee, A. K. Das, and P. K. Mukherjee. Allowed transitions in silicon isoelectronic ions. *International Journal of Quantum Chemistry*, 91(5):626–632, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Smentek:2002:TCE

[Sme02] Lidia Smentek. Two-center exchange interactions in rare earth doped materials. *International Journal of Quantum Chemistry*, 90(3):1206–1214, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sierraalta:2008:ISF

[SMEA08] Anibal Sierraalta, Guillermo Martorell, Elena Ehrmann, and Rafael Añez. Improvement of scale factors for harmonic vibrational frequency calculations using new polarization functions. *International Journal of Quantum Chemistry*, 108(6): 1036–1043, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szopa:2008:GSV

[SMK08] Katarzyna Szopa, Monika Musiał, and Stanisław A. Kucharski. Ground state and vertical excitation energies of the diazene isomers with the coupled cluster method. *International Journal of Quantum Chemistry*, 108(12):2108–2116, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Srikanth:2002:RES

[SMM02] K. Srikanth, V. R. Marathe, and Manoj K. Mishra. Role of electronic structure of ruthenium polypyridyl dyes in the photoconversion efficiency of dye-sensitized solar cells: Semiempirical investigation. *International Journal of Quantum Chemistry*, 89(6):535–549, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shinoda:2006:RRO

[SMM06] Hiroyuki Shinoda, Yoshihiro Mori, and Mineyuki Mizuguchi. Reinvestigation into the ring-opening process of monochloroethylene oxide by quantum chemical calculations. *International Journal of Quantum Chemistry*, 106(4):952–959, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Scherlis:2002:EEC

[SMOE02] Damián A. Scherlis, Marcelo A. Martí, Pablo Ordejón, and Darío A. Estrin. Environment effects on chemical reactivity of heme proteins. *International Journal of Quantum Chemistry*, 90(4-5):1505–1514, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sen:2002:SDQ

[SMS+02] K. D. Sen, B. Mayer, P. C. Schmidt, Jorge Garza, Rubicelia Vargas, and Alberto Vela. Static dipole and quadrupole polarizability of confined hydrogen atom with $Z = N/3(N = 1--5)$. *International Journal of Quantum Chemistry*, 90(2): 491–496, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shukla:2007:RGM

[SMS07] P. K. Shukla, P. C. Mishra, and S. Suhai. Reactions of guanine with methyl chloride and methyl bromide: O6-methylation

versus charge transfer complex formation. *International Journal of Quantum Chemistry*, 107(5):1270–1283, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Struniewicz:2002:TSH

[SMSM02] Cezary Struniewicz, Anne Milet, Joanna Sadlej, and Robert Moszynski. Theoretical study of the hydrogen chloride trihydrate. *International Journal of Quantum Chemistry*, 90(3): 1151–1162, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Solimannejad:2006:NSO

[SMT06] Mohammad Solimannejad, Seyed Kamran Moayedi, and Majid Tavakoli. Nonperturbative solutions for one-dimensional Schrödinger equation with position-dependent mass. *International Journal of Quantum Chemistry*, 106(5):1027–1031, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sumpter:2007:INS

[SMVMC07] Bobby G. Sumpter, Vincent Meunier, Álvaro Vázquez-Mayagoitia, and Ronald K. Castellano. Investigation of the nanoscale self-assembly of donor-σ-acceptor molecules. *International Journal of Quantum Chemistry*, 107(12):2233–2242, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2007:MOC

[SMY07] Rajiv Saha, Dongxia Ma, and Danny L. Yeager. Modification of optimal complete active space choices for the multiconfigurational spin-tensor electron propagator method for ionization potentials. *International Journal of Quantum Chemistry*, 107 (3):694–702, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sadygov:2002:DPC

[SN02] Rovshan G. Sadygov and Daniel Neuhauser. Dynamics of primary charge separation in bacterial photosynthesis using the multilevel Redfield-Davies secular approach. *International Journal of Quantum Chemistry*, 87(4):254–263, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/90511922/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90511922/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90511922&PLACEBO=IE.pdf.

Serr:2006:PHF

[SN06a] Andreas Serr and Roland R. Netz. Polarizabilities of hydrated and free ions derived from DFT calculations. *International Journal of Quantum Chemistry*, 106(14):2960–2974, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Srivastava:2006:NCO

[SN06b] Vipin Srivastava and A. Ramesh Naidu. New classes of orthogonal polynomials. *International Journal of Quantum Chemistry*, 106(5):1258–1266, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sobrinho:2008:MOE

[SNdAM08] A. M. C. Sobrinho, M. A. C. Nascimento, M. D. de Andrade, and L. A. C. Malbouisson. Molecular one-electron properties using the multireference Hartree–Fock CI method. *International Journal of Quantum Chemistry*, 108(13):2595–2602, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shalabi:2000:CVW

[SNH00] A. S. Shalabi, E. M. Nour, and W. S. Abdel Halim. Characterization of van der Waals interaction potentials D_{4h} and T_d configurations of He_4. *International Journal of Quantum Chemistry*, 76(1):10–22, January 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/69503192/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503192/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503192&PLACEBO=IE.pdf.

Shoji:2004:TCB

[SNM+04] M. Shoji, Y. Nishiyama, Y. Maruno, K. Koizumi, Y. Kitagawa, S. Yamanaka, T. Kawakami, M. Okumura, and K. Yamaguchi. Theory of chemical bonds in metalloenzymes I:

Analytical and hybrid-DFT studies on oxo and hydroxo diiron cores. *International Journal of Quantum Chemistry*, 100 (6):887–906, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Suzuki:2009:CES

[SNN+09] Chikashi Suzuki, Tsuyoshi Nishi, Masami Nakada, Mitsuo Akabori, Masaru Hirata, and Yoshiyuki Kaji. Calculation of the electronic structure of AmO_2 and Pr_6O_{11} for XANES analysis with redox property. *International Journal of Quantum Chemistry*, 109(12):2744–2752, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shigeta:2000:TSD

[SNT+00] Y. Shigeta, H. Nagao, J. Toyoda, Y. Morita, K. Nakasuji, Y. Yoshioka, and K. Yamaguchi. Theoretical study on dependency of conductivity on structure of the proton- and electron-coupled system. *International Journal of Quantum Chemistry*, 80(4–5):882–891, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505370/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505370/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505370&PLACEBO=IE.pdf`.

Shigeta:2001:ESC

[SNY01] Y. Shigeta, H. Nagao, and K. Yamaguchi. Electronic structure calculation by Monte Carlo diagonalization method. *International Journal of Quantum Chemistry*, 84(5):601–606, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/82003609/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/82003609/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=82003609&PLACEBO=IE.pdf`.

Sheka:2002:HSS

[SNZG02] Elena F. Sheka, Ekaterina A. Nikitina, Valentin A. Zayets, and Ilya Ya. Ginzburg. High-spin silicon fullerene Si_{60} and its oligomers. *International Journal of Quantum Chemistry*, 88(4):441–448, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saal:2004:VEC

[SO04a] Amar Saal and Ourida Ouamerali. Vibrational and electronic contributions to the polarizability and first hyperpolarizability of monosubstituted acetylene: Theoretical study. *International Journal of Quantum Chemistry*, 96(4):333–342, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sunel:2004:EBS

[SÖ04b] N. Sünel and O. Özsoy. Electronic band structure evolution as a carbon sheet rolls up to a SWCNT and a SWCNT closes to a torus, by using extended SSH model. *International Journal of Quantum Chemistry*, 100(2):231–235, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sabin:2009:ARS

[SO09a] John R. Sabin and Jens Oddershede. An analytical representation of shell corrections for stopping power. *International Journal of Quantum Chemistry*, 109(13):2933–2936, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sabin:2009:FHF

[SÖ09b] John R. Sabin and N. Yngve Öhrn. Frank E. Harris: The first 80 years. *International Journal of Quantum Chemistry*, 109(13):2801, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salter:2008:OIN

[SOEW08] E. A. Salter, Kerrie A. O'Brien, R. Wesley Edmunds, and A. Wierzbicki. ONIOM investigation of nucleotide selectivity in phosphodiesterases 3 and 4. *International Journal of Quantum Chemistry*, 108(6):1189–1199, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sokolov:2002:RAV

[Sok02] Alexey V. Sokolov. Radical addition to the vinyl C≡C bond: Quantum chemistry model of the reaction. *International Journal of Quantum Chemistry*, 88(4):358–369, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sokolov:2004:NAE

[Sok04] Alexey V. Sokolov. New aspects of electrophylic aromatic substitution mechanism: Computational model of nitration reaction. *International Journal of Quantum Chemistry*, 100(1): 1–12, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schiott:2004:TTB

[SOLI04] B. Schiøtt, J. Overgaard, F. K. Larsen, and B. B. Iversen. Testing theory beyond molecular structure: Electron density distributions of complex molecules. *International Journal of Quantum Chemistry*, 96(1):23–31, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sonnino:2004:TFT

[Son04] Giorgio Sonnino. Thermodynamic field theory with applications. *International Journal of Quantum Chemistry*, 98(2): 191–221, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stashans:2000:HPP

[SP00] Arvids Stashans and Henry Pinto. Hole polarons in pure $BaTiO_3$ studied by computer modeling. *International Journal of Quantum Chemistry*, 79(6):358–366, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72515276/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72515276/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72515276&PLACEBO=IE.pdf`.

Seo:2000:GPM

[SPH00] Dong-Kyun Seo, Garegin Papoian, and Roald Hoffmann. Generalized perturbational molecular orbital (PMO) theory. *International Journal of Quantum Chemistry*, 77(1):408–420, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004285/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004285/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004285&PLACEBO=IE.pdf`.

Salazar:2003:DFT

[SPH+03] Mary C. Salazar, José L. Paz, Antonio J. Hernández, Carlos Manzanares I, and Eduardo V. Ludeña. Density functional theory test study on the CO$\cdots$He dimer. *International Journal of Quantum Chemistry*, 95(2):177–183, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sasireka:2004:SLL

[SPI04] D. Sasireka, E. Palaniyandi, and K. Iyakutti. Study of local lattice relaxation of substitutional impurities in silicon and germanium. *International Journal of Quantum Chemistry*, 99 (3):142–152, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Serra:2003:BMD

[SPL03] Llorenç Serra, Antonio Puente, and Enrico Lipparini. Breathing modes of 2-D quantum dots with elliptical shape in magnetic fields. *International Journal of Quantum Chemistry*, 91 (3):483–489, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saarikoski:2003:ESC

[SPN03] H. Saarikoski, M. J. Puska, and R. M. Nieminen. Electronic structure calculations for 2-D quantum dots and laterally coupled quantum dot molecules in magnetic fields. *International Journal of Quantum Chemistry*, 91(3):490–497, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sulka:2008:EAM

[ŠPNU08] Martin Šulka, Michal Pitoňák, Pavel Neogrády, and Miroslav Urban. Electron affinity of the O_2 molecule: CCSD(T) calculations using the optimized virtual orbitals space approach. *International Journal of Quantum Chemistry*, 108(12):2159–2171, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Springborg:2000:ESP

[Spr00] Michael Springborg. Electronic and structural properties of extended-chain compounds and polymers. *International Journal of Quantum Chemistry*, 77(5):843–858,

???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/71000347/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000347/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000347&PLACEBO=IE.pdf.

SantAnna:2002:SST

[SPS02] Carlos Mauricio R. Sant'Anna, Vivian Passos De Souza, and Deogenes Santos De Andrade. Semiempirical simulation of a theta-class glutathione S-transferase-catalyzed glutathione attack to the allelochemical DIMBOA. *International Journal of Quantum Chemistry*, 87(5):311–321, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/91014545/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91014545/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91014545&PLACEBO=IE.pdf.

Srivastava:2005:ASB

[SPS05] H. K. Srivastava, F. A. Pasha, and P. P. Singh. Atomic softness-based QSAR study of testosterone. *International Journal of Quantum Chemistry*, 103(3):237–245, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shchavlev:2006:DCS

[SPS06] Andrew E. Shchavlev, Alexei N. Pankratov, and Alexei V. Shalabay. DFT computational studies on rotation barriers, tautomerism, intramolecular hydrogen bond, and solvent effects in 8-hydroxyquinoline. *International Journal of Quantum Chemistry*, 106(4):876–886, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Soujanya:2007:DSC

[SPSS07] Y. Soujanya, M. Punnagai, B. Sateesh, and G. Narahari Sastry. DFT study of core-modified porphyrin isomers. *International Journal of Quantum Chemistry*, 107(1):134–151, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Squire:2005:CFS

[Squ05] R. H. Squire. Can the Fulleride superconducting model (FSM) be extended? *International Journal of Quantum Chemistry*, 102(5):880–887, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Su:2002:QCS

[SQZ+02] Zhongmin Su, Yongqing Qiu, Hongmei Zhao, Rongshun Wang, Ruifeng Zhang, and Jiacong Shen. Quantum chemical study on ferromagnetic property on the N,N-dimethylaniline dimer radical cation. *International Journal of Quantum Chemistry*, 89(5):484–488, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sainudeen:2005:NOP

[SR05] Zuhail Sainudeen and Paresh Chandra Ray. Nonlinear optical properties of ionic NLO chromophores: An attempt to bridge the gap between computation and experiment. *International Journal of Quantum Chemistry*, 105(4):348–358, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stashans:2007:HDP

[SR07] Arvids Stashans and Richard Rivera. H-doped $PbTiO_3$: Structure and electronic properties. *International Journal of Quantum Chemistry*, 107(6):1508–1513, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2009:HMP

[SRA09] Soumen Saha, Ram Kinkar Roy, and Paul W. Ayers. Are the Hirshfeld and Mulliken population analysis schemes consistent with chemical intuition? *International Journal of Quantum Chemistry*, 109(9):1790–1806, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shapley:2002:IPG

[SRH02] Warwick A. Shapley, Jeffrey R. Reimers, and Noel S. Hush. INDO/S parameters for gold. *International Journal of Quantum Chemistry*, 90(1):424–438, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sunel:2006:ELM

[SRHÖ06] N. Sünel, E. Rizaoğlu, K. Harigaya, and O. Özsoy. Effects of Lagrangian multipliers on SWCNT in real space. *International Journal of Quantum Chemistry*, 106(9):2100–2106, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sulpizi:2005:OPM

[SRHR05] M. Sulpizi, U. F. Röhrig, J. Hutter, and U. Rothlisberger. Optical properties of molecules in solution via hybrid TDDFT/MM simulations. *International Journal of Quantum Chemistry*, 101(6):671–682, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Senthilkumar:2001:SCH

[SRK01] K. Senthilkumar, M. Ramaswamy, and P. Kolandaivel. Studies of chemical hardness and Fukui function using the exact solution of the density functional theory. *International Journal of Quantum Chemistry*, 81(1):4–10, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/75502155/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75502155/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502155&PLACEBO=IE.pdf`.

Seibert:2002:QMI

[SRO02] Eleanore Seibert, J. B. Alexander Ross, and Roman Osman. Quantum mechanical investigation of the electronic structure and spectral properties of 6,8-dimethylisoxanthopterin. *International Journal of Quantum Chemistry*, 88(1):28–33, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90010555/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90010555/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90010555&PLACEBO=IE.pdf`.

Smirnov:2004:CMC

[SRS+04] V. P. Smirnov, B. S. Razbirin, A. N. Starukhin, A. V. Chugreev, Yu. S. Grushko, S. Kolesnik, and B. P. Konstantinov. $C_{60}Cl_{24}$ molecule in crystalline toluene matrix. *Interna-*

tional Journal of Quantum Chemistry, 100(4):448–451, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2006:CMS

[SRW+06] Ying-Xin Sun, Yi Ren, Ning-Bew Wong, San-Yan Chu, and Ying Xue. Comprehensive mechanistic study of ion pair S_N 2 reactions of lithium isocyanate and methyl halides. *International Journal of Quantum Chemistry*, 106(7):1653–1663, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Scheurer:2000:CDS

[SS00a] P. Scheurer and W. H. E. Schwarz. Continuous degeneracy of sets of localized orbitals. *International Journal of Quantum Chemistry*, 76(3):428–433, January 20, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000285/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000285/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000285&PLACEBO=IE.pdf`.

Scheurer:2000:ELM

[SS00b] P. Scheurer and W. H. E. Schwarz. Externally localized molecular orbitals: A numerical investigation of localization degeneracy. *International Journal of Quantum Chemistry*, 76(3):420–427, January 20, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000284/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000284/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000284&PLACEBO=IE.pdf`.

Slamet:2001:QDF

[SS01] Marlina Slamet and Viraht Sahni. Quantal density functional theory of excited states: Application to an exactly solvable model. *International Journal of Quantum Chemistry*, 85(4–5):436–448, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Steen:2002:RST

[SS02a] Kay J. Steen and Lars Erik Smith. Reducing search time for optimal geometry of small molecular clusters. *International Journal of Quantum Chemistry*, 87(4):232–239, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90011777/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90011777/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90011777&PLACEBO=IE.pdf`.

Surjan:2002:CDP

[SS02b] Péter R. Surján and Ágnes Szabados. Constant denominator perturbative schemes and the partitioning technique. *International Journal of Quantum Chemistry*, 90(1):20–26, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2003:TDD

[SS03a] Aparna Saha and Pranab Sarkar. Tunneling dynamics of a double-well oscillator: Effects of barrier fluctuation and thermal modulation. *International Journal of Quantum Chemistry*, 93(4):280–285, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szabados:2003:OPP

[SS03b] Ágnes Szabados and Péter R. Surján. Optimized partitioning in PT: Application for the equation of motion describing ionization processes. *International Journal of Quantum Chemistry*, 92(2):160–167, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2004:TTF

[SS04a] Aparna Saha and Pranab Sarkar. Tunneling through a fluctuating barrier in the presence of a periodically driving field. *International Journal of Quantum Chemistry*, 97(5):914–921, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sahni:2004:SAN

[SS04b] Viraht Sahni and Marlina Slamet. State arbitrariness of the noninteracting fermion model in quantal density functional

theory. *International Journal of Quantum Chemistry*, 100 (6):858–866, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shen:2004:JME

[SS04c] Hujun Shen and Harris J. Silverstone. JWKB method as an exact technique. *International Journal of Quantum Chemistry*, 99(4):336–352, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2005:ETM

[SS05a] Aparna Saha and Pranab Sarkar. Effects of thermal modulation on tunneling through a fluctuating barrier in presence of bichromatic electromagnetic field. *International Journal of Quantum Chemistry*, 103(4):388–393, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szabados:2005:SDF

[SS05b] Ágnes Szabados and Péter R. Surján. Size dependence of Feenberg scaling. *International Journal of Quantum Chemistry*, 101(3):287–290, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sahni:2006:QDF

[SS06] Viraht Sahni and Marlina Slamet. Quantal density functional theory: Wave function arbitrariness of the noninteracting fermion model. *International Journal of Quantum Chemistry*, 106(15):3087–3096, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2008:EAD

[SS08a] Fu-Qiang Shi and Bao-An Song. Effect of AlH$\cdots$HO dihydrogen bond on the reaction between diphenylmethanol and pyrazolate-bridged dialuminum complex. An ONIOM DFT/AM1 study. *International Journal of Quantum Chemistry*, 108 (6):1107–1113, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szakacs:2008:SCC

[SS08b] Péter Szakács and Péter R. Surján. Stability conditions for the coupled cluster equations. *International Journal of Quantum Chemistry*, 108(12):2043–2052, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sadlej-Sosnowska:2009:TED

[SS09a] Nina Sadlej-Sosnowska. Transfer of electron density as a result of hydrogen bond formation. *International Journal of Quantum Chemistry*, 109(2):294–300, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slevinsky:2009:GTC

[SS09b] Richard Mikael Slevinsky and Hassan Safouhi. The S and G transformations for computing three-center nuclear attraction integrals. *International Journal of Quantum Chemistry*, 109 (8):1741–1747, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Smuczynska:2009:ELC

[SS09c] Sylwia Smuczyńska and Jack Simons. Effects of local Coulomb potentials on acid and base protonation–deprotonation rates and equilibria. *International Journal of Quantum Chemistry*, 109(13):3120–3130, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sygula:2009:SCC

[SS09d] Andrzej Sygula and Svein Saebø. π-π Stacking of curved carbon networks: The corannulene dimer. *International Journal of Quantum Chemistry*, 109(1):65–72, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2007:FGH

[SSA07] Aparna Saha, Pranab Sarkar, and S. Adhikari. Fourier grid Hamiltonian-based multidimensional Floquet propagator method for continuous, pulsed, and bichromatic laser field: Application to the multiphoton dissociation dynamics of HCN molecule. *International Journal of Quantum Chemistry*, 107 (6):1285–1294, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sendt:2000:QCS

[SSB00] Karina Sendt, Timothy W. Schmidt, and George B. Bacskay. Quantum chemical studies of the potential energy surfaces and vibrational frequencies of the $\tilde{X}(^1A')$, $\tilde{a}(^3A'')$ and $\tilde{A}(^1A'')$ states of CHCl and CFCl. *International Journal of Quantum Chemistry*, 76(3):297–305, January 20, 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000290/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000290/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000290&PLACEBO=IE.pdf`.

Subbotina:2007:DSC

[SSB+07] Julia O. Subbotina, Elena V. Sadchikova, Vasiliy A. Bakulev, Walter M. F. Fabian, and Rainer Herges. DFT study of cycloaddition reaction of isothiocyanates with diazoazoles to 4-imino-4H-pyrazolo[5,1-d] [1,2,3,5] thiatriazines. *International Journal of Quantum Chemistry*, 107(13):2479–2488, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shamsutdinov:2007:IMS

[SSC+07] A. F. Shamsutdinov, T. F. Shamsutdinov, D. V. Chachkov, A. G. Shamov, and G. M. Khrapkovskii. The influence of molecular structure on the change of the Arrhenius factor of gas-phase elimination of nitric acid from nitroalkanes. *International Journal of Quantum Chemistry*, 107(13):2343–2352, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stoyanova:2006:HME

[SSDB06] A. Stoyanova, C. Sousa, C. De Graaf, and R. Broer. Hopping matrix elements from first-principles studies of overlapping fragments: Double exchange parameters in manganites. *International Journal of Quantum Chemistry*, 106(12):2444–2457, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2005:ELT

[SSDM05] B. Saha, A. N. Sil, A. K. Das, and P. K. Mukherjee. Energy levels of two interacting particles in an anharmonic potential. *International Journal of Quantum Chemistry*, 102 (2):158–164, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Smith:2002:SPH

[SSF02] Garry T. Smith, Vedene H. Smith, Jr., and Alexei M. Frolov. Structures and properties of the hydrides of light elements.

International Journal of Quantum Chemistry, 90(4-5):1421–1427, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sharma:2009:QCS

[SSJ09] Smriti Sharma, Uddhavesh B. Sonavane, and Rajendra R. Joshi. Quantum chemical studies of peptide nucleic acid monomers and role of cyclohexyl modification on backbone flexibility. *International Journal of Quantum Chemistry*, 109 (4):890–896, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Suzuki:2005:CRD

[SSK+05] Ai Suzuki, Parasuraman Selvam, Tomonori Kusagaya, Seiichi Takami, Momoji Kubo, Akira Imamura, and Akira Miyamoto. Chemical reaction dynamics of PeCB and TCDD decomposition: A tight-binding quantum chemical molecular dynamics study with first-principles parameterization. *International Journal of Quantum Chemistry*, 102(3):318–327, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shankar:2009:CIP

[SSK09a] R. Shankar, K. Senthilkumar, and P. Kolandaivel. Calculation of ionization potential and chemical hardness: A comparative study of different methods. *International Journal of Quantum Chemistry*, 109(4):764–771, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sugihara:2009:HTP

[SSK09b] Sunao Sugihara, Chikashi Suzuki, and Ryohei Kameya. High thermoelectric performance of metal-substituted samples of α-Fe_2O_3 and computation of their electronic structures by the DV-X_α method. *International Journal of Quantum Chemistry*, 109(12):2788–2792, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sil:2005:EDPb

[SSM05] A. N. Sil, B. Saha, and P. K. Mukherjee. Effect of dense plasma on the spectral properties of hydrogenic ions. *International Journal of Quantum Chemistry*, 104(6):903–910, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salviano:2008:QRS

[SSMG08] Lucas R. Salviano, Geraldo M. E. Silva, João B. L. Martins, and Ricardo Gargano. Quantum reactive study of a potential energy surface obtained via genetic algorithm. *International Journal of Quantum Chemistry*, 108(13):2306–2311, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sivanesan:2001:SED

[SSN01] D. Sivanesan, V. Subramanian, and B. U. Nair. Solvent effect on DNA base stacked dimers: An isodensity polarizable continuum model approach. *International Journal of Quantum Chemistry*, 84(6):750–758, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502389/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502389/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502389&PLACEBO=IE.pdf`.

Schmiedekamp:2003:RBM

[SSN03] Ann Schmiedekamp, Mendel Schmiedekamp, and K. P. R. Nair. Rotational barriers of methyl fluorosulfonate and chlorosulfonate: Comparison between computational methods and experiment. *International Journal of Quantum Chemistry*, 95 (6):719–730, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sarma:2002:GSR

[SSR02] C. R. Sarma, N. Ravi Shankar, and S. Rettrup. A graphical scheme for representing many-electron spin-free configurations. *International Journal of Quantum Chemistry*, 86 (5):417–421, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86011222/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86011222/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86011222&PLACEBO=IE.pdf`.

Samsonowicz:2007:ETI

[SŚRL07] M. Samsonowicz, R. Świsłocka, E. Regulska, and W. Lewandowski. Experimental and theoretical IR, Raman, NMR spectra of 2-, 3-, and 4-nitrobenzoic acids. *International Journal of Quantum Chemistry*, 107(2):480–494, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Surjan:2002:NPT

[SSS02] Péter R. Surján, Ágnes Szabados, and Zsolt Szekeres. Non-symmetrical perturbation theory for improving coupled-cluster wave functions. *International Journal of Quantum Chemistry*, 90(4-5):1309–1320, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sugiyama:2005:ESA

[SSS+05] Ayumu Sugiyama, Kimikazu Sugimori, Tomofumi Shuku, Taichi Nakamura, Hiroaki Saito, Hidemi Nagao, Hiroyuki Kawabe, and Kiyoshi Nishikawa. Electronic structure of the active site with two configurations of azurin. *International Journal of Quantum Chemistry*, 105(6):588–595, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Seo:2007:SDE

[SSSK07] Hyun-Il Seo, Ju-Yong Sun, Chang-Ho Shin, and Seung-Joon Kim. Structure and dissociation energy of weakly bound $H_{2n+1}{}^{+}$ ($n = 5--8$) complexes. *International Journal of Quantum Chemistry*, 107(4):988–997, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sizova:2009:AOS

[SSSS09] Olga V. Sizova, Leonid V. Skripnikov, Alexander Yu Sokolov, and Vladimir V. Sizov. Atomic-orbital-symmetry based σ-, π-, and δ-decomposition analysis of bond orders. *International Journal of Quantum Chemistry*, 109(11):2581–2590, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sonawane:2000:CFS

[SST00] Kailas Dasharath Sonawane, Uddhavesh Bhaskar Sonavane, and Ravindra Tewari. Conformational flipping of the N(6) substituent in diprotonated N_6-(N-glycylcarbonyl)adenines:

The role of N(6)H in purine-ring-protonated ureido adenines. *International Journal of Quantum Chemistry*, 78(5):398–405, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72001896/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72001896/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72001896&PLACEBO=IE.pdf`.

Sawae:2002:QRW

[SST+02] Ryuichi Sawae, Toshio Sakata, Kenichi Takarabe, Minaru Tei, Youichi Mizuno, Yoshiyuki Mori, and Yoshinori Manmoto. Quantum random walks on the set of contingency tables. *International Journal of Quantum Chemistry*, 90(4-5):1321–1325, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sawae:2003:GCI

[SST+03] Ryuichi Sawae, Toshio Sakata, Minaru Tei, Kenichi Takarabe, and Yoshinori Manmoto. Gray code and the initialization problem of NMR quantum computers. *International Journal of Quantum Chemistry*, 95(4–5):558–560, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sindelka:2002:PES

[ŠŠU+02] Milan Šindelka, Vladimír Špirko, Jan Urban, Pavel Mach, and Jerzy Leszczynski. Potential energy surface and ro-vibrational energies of Ne in the ground electronic state. *International Journal of Quantum Chemistry*, 90(3):1232–1239, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2007:TIA

[SSZ+07] De-Heng Shi, Jin-Feng Sun, Zun-Lue Zhu, Heng Ma, Yu-Fang Liu, and Zheng-He Zhu. Theoretical investigations on analytical potential energy function and spectroscopic parameters for the state $b\,^3\Pi_u$ of dimer $^7Li_2$. *International Journal of Quantum Chemistry*, 107(9):1856–1863, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stefanov:2001:MPC

[ST01] V. E. Stefanov and A. A. Tulub. Migration of protons in a chain of tyrosine residues. *International Journal of*

Quantum Chemistry, 84(4):409–415, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/83002307/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/83002307/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=83002307&PLACEBO=IE.pdf.

Starikov:2000:NAO

[Sta00] E. B. Starikov. Nucleic acids as objects of material science: Importance of quantum chemical and quantum mechanical studies. *International Journal of Quantum Chemistry*, 77 (5):859–870, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/71000348/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000348/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000348&PLACEBO=IE.pdf.

Sabin:2000:MSC

[STAO00] John R. Sabin, S. B. Trickey, S. Peter Apell, and J. Oddershede. Molecular shape, capacitance, and chemical hardness. *International Journal of Quantum Chemistry*, 77(1):358–366, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70004278/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004278/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004278&PLACEBO=IE.pdf.

Stillinger:2006:PHP

[Sti06] Frank H. Stillinger. Perspective: An historical perspective. *International Journal of Quantum Chemistry*, 106(1):3, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2009:DFT

[STL+09] Haitao Sun, Ke Tang, Yanmin Li, Chunfang Su, Zhengyu Zhou, and Zhizhong Wang. Density functional theory study on the ionization potentials and electron affinities of thymine–formamide complexes. *International Journal of Quantum*

Chemistry, 109(6):1410–1417, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sugiyama:2006:DSE

[STN+06] Ayumu Sugiyama, Yuichiro Takamatsu, Keigo Nishikawa, Hidemi Nagao, and Kiyoshi Nishikawa. Docking stability and electronic structure of azurin–cytochrome c_{551} complex system. *International Journal of Quantum Chemistry*, 106(15): 3071–3078, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stone:2008:CSG

[Sto08] Anthony J. Stone. Comment: The symmetry group of nonrigid tetramethylsilane. *International Journal of Quantum Chemistry*, 108(8):1410, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Strasburger:2000:WHT

[Str00] K. Strasburger. Why Hylleraas-type functions failed to predict the existence of $PsLi^+$ and $^{2,3}PsHe^+$? *International Journal of Quantum Chemistry*, 79(4):243–252, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72512061/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72512061/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72512061&PLACEBO=IE.pdf`.

Svane:2000:SIC

[STS+00] A. Svane, W. M. Temmerman, Z. Szotek, J. Lægsgaard, and H. Winter. Self-interaction-corrected local-spin-density calculations for rare earth materials. *International Journal of Quantum Chemistry*, 77(5):799–813, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000343/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000343/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000343&PLACEBO=IE.pdf`.

Stuchebrukhov:2000:ICL

[Stu00] Alexei A. Stuchebrukhov. Ab initio calculations of long-distance electron tunneling in organometallic systems of bio-

logical origin. *International Journal of Quantum Chemistry*, 77(1):16–26, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004283/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004283/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004283&PLACEBO=IE.pdf`.

Sun:2005:DIM

[STW+05] Hao Sun, Yi-Zhen Tang, Zhan-Liang Wang, Xiu-Mei Pan, Ze-Sheng Li, and Rong-Shun Wang. DFT investigation of the mechanism of $CH_2CO + O(^3P)$ reaction. *International Journal of Quantum Chemistry*, 105(5):527–532, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slanina:2004:EES

[SUA+04] Zdeněk Slanina, Filip Uhlík, Ludwik Adamowicz, Kaoru Kobayashi, and Shigeru Nagase. Electronic excited states and stabilities of fullerenes: Isomers of C_{78} and $Mg@C_{72}$. *International Journal of Quantum Chemistry*, 100(4):610–616, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slanina:2004:CCE

[SUAL04] Zdeněk Slanina, Filip Uhlík, Ludwik Adamowicz, and Shyi-Long Lee. Computations of the catalytic effects in the Stone–Wales fullerene isomerizations: N and CN agents. *International Journal of Quantum Chemistry*, 99(5):634–639, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stavrev:2001:TSE

[SUH+01] K. K. Stavrev, S. Urahata, T. Herz, J. Han, and D. Coucouvanis. Theoretical study on the electronic structure and properties of synthetic $MoFe_3S_3$ compounds. *International Journal of Quantum Chemistry*, 85(4–5):469–474, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sedivcova-Uhlikova:2007:RTP

[ŠUKŽŠ07] Tereza Šedivcová-Uhlíková, Petra R. Kaprálová-Žďánská, and Vladimír Špirko. Radiative transition probabilities of CO^{2+}.

International Journal of Quantum Chemistry, 107(14):2654–2664, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sullivan:2000:BRa

[Sul00a] Neil S. Sullivan. Book review. *International Journal of Quantum Chemistry*, 78(1):65–66, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/71001660/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71001660/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71001660&PLACEBO=IE.pdf.

Sullivan:2000:BRb

[Sul00b] Neil S. Sullivan. Book review. *International Journal of Quantum Chemistry*, 78(1):67–68, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/71001651/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71001651/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71001651&PLACEBO=IE.pdf.

Slanina:2007:CSR

[SUL+07] Zdeněk Slanina, Filip Uhlík, Shyi-Long Lee, Ludwik Adamowicz, and Shigeru Nagase. Computed structures and relative stabilities of Be@C_{74}. *International Journal of Quantum Chemistry*, 107(13):2494–2498, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slanina:2008:CTI

[SUL+08] Zdeněk Slanina, Filip Uhlík, Shyi-Long Lee, Ludwik Adamowicz, and Shigeru Nagase. Computations on three isomers of La@C_{74}. *International Journal of Quantum Chemistry*, 108 (14):2636–2640, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2006:ESP

[Sun06] Mengtao Sun. Excited state properties of the chromophore of the asFP595 chromoprotein: 2D and 3D theoretical analyses. *International Journal of Quantum Chemistry*, 106(4):1020–

1026, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sutcliffe:2000:BR

[Sut00] Brian T. Sutcliffe. Book review. *International Journal of Quantum Chemistry*, 78(1):63–64, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71001659/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71001659/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71001659&PLACEBO=IE.pdf`.

Sutcliffe:2002:SOP

[Sut02] Brian Sutcliffe. Some observations on P.-O. Löwdin's definition of a molecule. *International Journal of Quantum Chemistry*, 90(1):66–79, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stashans:2008:QCS

[SV08] Arvids Stashans and Gabriela Vidal. A quantum-chemical study of phosphor impurity in $BaTiO_3$ crystal. *International Journal of Quantum Chemistry*, 108(5):992–995, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stevens:2005:IES

[SVC+05] F. Stevens, H. Vrielinck, F. Callens, E. Pauwels, V. Van Speybroeck, and M. Waroquier. Ab initio EPR study of S and Se defects in alkali halides. *International Journal of Quantum Chemistry*, 102(4):409–414, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Senent:2005:ISF

[SVDGFC05] M. L. Senent, M. Villa, R. Domínguez-Gómez, and A. Fernández-Clavero. Ab initio study of the far infrared spectrum of glycine. *International Journal of Quantum Chemistry*, 104 (4):551–561, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stashans:2006:EAS

[SVT06] Arvids Stashans, Ricardo Viteri, and Javier Torres. Ethanol adsorption on $SrTiO_3$ surfaces. *International Journal of*

Quantum Chemistry, 106(7):1715–1719, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salter:2002:TCP

[SW02] Edward A. Salter and A. Wierzbicki. Two charged particles in a two-dimensional well. *International Journal of Quantum Chemistry*, 89(3):121–128, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Safouhi:2009:I

[SW09] Hassan Safouhi and Ernst J. Weniger. Introduction. *International Journal of Quantum Chemistry*, 109(8):1617, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Swart:2003:ANL

[Swa03] Marcel Swart. AddRemove: A new link model for use in QM/MM studies. *International Journal of Quantum Chemistry*, 91 (2):177–183, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sharma:2003:IMD

[SWC03] Manu Sharma, Yudong Wu, and Roberto Car. Ab initio molecular dynamics with maximally localized Wannier functions. *International Journal of Quantum Chemistry*, 95(6): 821–829, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salter:2004:ISS

[SWL04] E. A. Salter, A. Wierzbicki, and T. Land. Ab initio studies of stepped 100 surfaces of KDP crystals. *International Journal of Quantum Chemistry*, 100(5):740–745, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Song:2009:ESP

[SWSH09] Jong-Won Song, Mark A. Watson, Hideo Sekino, and Kimihiko Hirao. The effect of silyl and phenyl functional group end caps on the nonlinear optical properties of polyynes: A long-range corrected density functional theory study. *International Journal of Quantum Chemistry*, 109(9):2012–2022, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salter:2004:HMC

[SWST04] E. A. Salter, A. Wierzbicki, G. Sperl, and W. J. Thompson. Homology models of the catalytic sites of phosphodiesterase 5A and 10A and molecular docking of selective apoptotic antineoplastic drugs (SAANDs). *International Journal of Quantum Chemistry*, 96(4):402–410, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Siegbahn:2001:TSM

[SWZ01] Per E. M. Siegbahn, Maria Wirstam, and Marc Zimmer. Theoretical study of the mechanism of peptide ring formation in green fluorescent protein. *International Journal of Quantum Chemistry*, 81(2):169–186, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76500935/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76500935/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76500935&PLACEBO=IE.pdf`.

Seminario:2005:IAE

[SY05] Jorge M. Seminario and Liuming Yan. Ab initio analysis of electron currents in thioalkanes. *International Journal of Quantum Chemistry*, 102(5):711–723, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shimazaki:2006:TSM

[SY06] Tomomi Shimazaki and Koichi Yamashita. Theoretical study of molecular conduction: I. Effective Green's function based on perturbation theory. *International Journal of Quantum Chemistry*, 106(4):803–813, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Seminario:2007:CCL

[SY07] Jorge M. Seminario and Liuming Yan. Cascade configuration of logical gates processing information encoded in molecular potentials. *International Journal of Quantum Chemistry*, 107 (3):754–761, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shimazaki:2009:TSM

[SY09] Tomomi Shimazaki and Koichi Yamashita. A theoretical study of molecular conduction. V. NEGF-based MP2 approach. *International Journal of Quantum Chemistry*, 109 (9):1834–1840, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Simeon:2005:IQC

[SYL05] Tomekia M. Simeon, Ilya Yanov, and Jerzy Leszczynski. Ab initio quantum chemical studies of fullerene molecules with substitutes $C_{59}X$ [X = Si, Ge, Sn], C_59X^- [X = B, Al, Ga, In], and C_59X [X = N, P, As, Sb]. *International Journal of Quantum Chemistry*, 105(4):429–436, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salci:2007:FEI

[SYLE07] Moses Salci, Evgeny Yarevsky, Sergey B. Levin, and Nils Elander. Finite element investigation of the ground states of the helium trimers $^4He_3$ and $^4He_2$ — ^3He. *International Journal of Quantum Chemistry*, 107(2):464–468, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2009:ISP

[SYZ+09] De-Heng Shi, Ben-Hai Yu, Jin-Ping Zhang, Yu-Fang Liu, and Zheng-He Zhu. Investigations on spectroscopic properties of $ND(X\,^3\Sigma^-)$ radical using coupled-cluster theory in combination with the correlation-consistent quintuple basis set augmented with diffuse functions. *International Journal of Quantum Chemistry*, 109(2):202–209, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Solkan:2008:MSD

[SZ08] V. N. Solkan and G. M. Zhidomirov. MP2 study on decomposition of nitrous oxide on the Ga-ZSM-5. *International Journal of Quantum Chemistry*, 108(14):2732–2743, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Soluyanov:2007:TEN

[SZA07] A. A. Soluyanov, S. N. Zagoulaev, and I. V. Abarenkov. Time evolution of the Neel state. *International Journal of Quantum*

Chemistry, 107(13):2320–2330, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Surong:2004:AEC

[SZJ+04] Qi-Mu Surong, Yongfang Zhao, Xiaogong Jing, Xinying Li, and Wenhui Su. Analysis of electron correlation in M_2Te (M = Cu, Ag, Au) systems. *International Journal of Quantum Chemistry*, 100(3):293–300, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Solkan:2007:DFT

[SZK07] V. N. Solkan, G. M. Zhidomirov, and V. B. Kazansky. Density functional theory studies of nitrous oxide adsorption and decomposition on Ga-ZSM-5. *International Journal of Quantum Chemistry*, 107(13):2417–2425, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2009:TIS

[SZL+09] De-Heng Shi, Jin-Ping Zhang, Yu-Fang Liu, Jin-Feng Sun, and Zun-Lue Zhu. Theoretical investigations on the SH^+ ($X\,^3\Sigma^-$) ion using coupled-cluster theory in combination with the correlation-consistent quintuple basis set augmented with diffuse functions. *International Journal of Quantum Chemistry*, 109(6):1159–1166, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2007:TSD

[SZML07] Hui Sun, Dongju Zhang, Chen Ma, and Chengbu Liu. Theoretical study on the Diels–Alder reaction of cyclopentadiene with methacrolein catalyzed by diethylimidazolium cation. *International Journal of Quantum Chemistry*, 107(9):1875–1885, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stashans:2002:SPP

[SZSP02] Arvids Stashans, Cesar Zambrano, Alfredo Sanchez, and Luis Miguel Procel. Structural properties of $PbTiO_3$ and $PbZr_xTi_{1-x}O_3$: A quantum-chemical study. *International Journal of Quantum Chemistry*, 87(3):145–151, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86513255/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86513255/`

FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86513255&PLACEBO=IE.pdf.

Szudy:2002:JSS

[Szu02] Józef Szudy. Józef Stanislaw ("Staszek") Kwiatkowski, (1936 to 2000). *International Journal of Quantum Chemistry*, 90 (3):991–994, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slanina:2004:CEE

[SZU+04] Z. Slanina, X. Zhao, F. Uhlík, S.-L. Lee, and L. Adamowicz. Computing enthalpy–entropy interplay for isomeric fullerenes. *International Journal of Quantum Chemistry*, 99(5):640–653, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shen:2001:QCS

[SZZ01] Ling-Ling Shen, Xiao-Dong Zhang, and Qi-Yuan Zhang. Quantum chemistry study of proteins in bacterial photosynthetic reaction center. *International Journal of Quantum Chemistry*, 83(1):30–40, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/79502657/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/79502657/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=79502657&PLACEBO=IE.pdf.

Tada:2002:AMO

[TA02] Tomofumi Tada and Yuriko Aoki. An analytical molecular orbital approach for modeling of low-dimensional conductors in molecular crystals. *International Journal of Quantum Chemistry*, 86(4):401–415, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/86011224/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86011224/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86011224&PLACEBO=IE.pdf.

Thompson:2006:TIB

[TA06] David C. Thompson and Paul W. Ayers. Thinking inside the box: Novel linear scaling algorithm for Coulomb potential

evaluation. *International Journal of Quantum Chemistry*, 106 (4):787–794, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tuzun:2007:MCD

[TA07] Nurcan Ş. Tüzün and Viktorya Aviyente. Modeling the cyclopolymerization of diallyl ether and methyl α-[(allyloxy)methyl]acrylate. *International Journal of Quantum Chemistry*, 107(4):894–906, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tachibana:2004:SSS

[Tac04] Akitomo Tachibana. Spindle structure of the stress tensor of chemical bond. *International Journal of Quantum Chemistry*, 100(6):981–993, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takahata:2008:IRE

[Tak08] Yuji Takahata. Inductive and resonance effects based on core-electron binding energy shift. *International Journal of Quantum Chemistry*, 108(13):2326–2333, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takatsuka:2009:TNB

[Tak09] Kazuo Takatsuka. Toward non-Born–Oppenheimer quantum chemistry. *International Journal of Quantum Chemistry*, 109 (10):2131–2142, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Talman:2003:NMM

[Tal03a] James D. Talman. Numerical methods for multicenter integrals for numerically defined basis functions applied in molecular calculations. *International Journal of Quantum Chemistry*, 93(2):72–90, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Talman:2003:ONO

[Tal03b] James D. Talman. Optimization of numerical orbitals in molecular MO-LCAO calculations. *International Journal of Quantum Chemistry*, 95(4–5):442–450, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Talman:2004:OID

[Tal04] James D. Talman. Overlap integrals for Dirac–Slater orbitals. *International Journal of Quantum Chemistry*, 100(2): 109–113, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Talman:2007:MEN

[Tal07] James D. Talman. Multipole expansions for numerical orbital products. *International Journal of Quantum Chemistry*, 107 (7):1578–1584, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tapia:2004:GED

[Tap04a] O. Tapia. Generalized electronic diabatic scheme: Diagonalizing the electronic Hamiltonian for artificial molecular systems. How do molecular meccanos move? *International Journal of Quantum Chemistry*, 97(1):637–650, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tapia:2004:MQT

[Tap04b] O. Tapia. Molecular quantum theory: Separable electronuclear wave functions and vibronic states—A generalized diabatic approach. *International Journal of Quantum Chemistry*, 99(4):373–384, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Taylor:2009:FHB

[Tay09] Howard S. Taylor. Frank Harris: The Berkeley years—A personal memoir. *International Journal of Quantum Chemistry*, 109(13):2817–2820, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Torres:2003:DFC

[TB03] M. B. Torres and L. C. Balbás. Density functional calculation of photoabsorption in metal clusters using an exchange-correlation potential with correct asymptotic behavior. *International Journal of Quantum Chemistry*, 91(2):263–269, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Taube:2006:NPU

[TB06] Andrew G. Taube and Rodney J. Bartlett. New perspectives on unitary coupled-cluster theory. *International Journal of Quantum Chemistry*, 106(15):3393–3401, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tasi:2009:EDB

[TB09] Gyula Tasi and Dóra Barna. Energy decomposition based on the extended virial theorem: Hartree–Fock and second-order Møller–Plesset results. *International Journal of Quantum Chemistry*, 109(11):2599–2605, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Torres:2009:RGA

[TBB09] Edmanuel Torres, P. Ulrich Biedermann, and Alexander T. Blumenau. The role of gold adatoms in self-assembled monolayers of thiol on Au(111). *International Journal of Quantum Chemistry*, 109(14):3466–3472, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Troche:2005:CCP

[TBCG05] Karla S. Troche, Scheila F. Braga, Vitor R. Coluci, and Douglas S. Galvão. Carcinogenic classification of polycyclic aromatic hydrocarbons through theoretical descriptors. *International Journal of Quantum Chemistry*, 103(5):718–730, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Telmini:2005:RMQ

[TBJ05] M. Telmini, S. Bezzaouia, and Ch. Jungen. R-matrix quantum defects of molecular hydrogen. *International Journal of Quantum Chemistry*, 104(4):530–537, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Talarico:2003:GCS

[TBJA03] Giovanni Talarico, Vincenzo Barone, Laurent Joubert, and Carlo Adamo. General computational strategy to study polymerization reactions at aluminum-based catalysts. *International Journal of Quantum Chemistry*, 91(3):474–482, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tergiman:2004:DEC

[TBM04] Y. S. Tergiman and M. C. Bacchus-Montabonel. Double-electron capture processes in charge transfer reactions. *International Journal of Quantum Chemistry*, 99(5):628–633, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Taveira:2006:MCC

[TBML06] A. M. A. Taveira, L. M. Brescansin, A. M. Machado, and M.-T. Lee. Multi-channel coupling effects for electronic excitations leading to the $b\,^3\Sigma$, $a\,^3\Sigma$, and $c\,^3\Pi_u$ states of H_2. *International Journal of Quantum Chemistry*, 106(9):2006–2013, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takahata:2005:EHS

[TC05] Yuji Takahata and Delano P. Chong. Estimation of Hammett sigma constants of substituted benzenes through accurate density-functional calculation of core-electron binding energy shifts. *International Journal of Quantum Chemistry*, 103 (5):509–515, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Torrens:2007:NCP

[TC07] F. Torrens and G. Castellano. Net charge and polarizability of zeolitic Brønsted acidic sites. *International Journal of Quantum Chemistry*, 107(13):2378–2383, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2002:I

[Tch02] Andrei L. Tchougréeff. Introduction. *International Journal of Quantum Chemistry*, 88(4):357, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2004:Ia

[Tch04a] Andrei L. Tchougréeff. Introduction. *International Journal of Quantum Chemistry*, 96(2):71–72, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2004:Ib

[Tch04b] Andrei L. Tchougreeff. Introduction. *International Journal of Quantum Chemistry*, 100(4):309–310, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2005:I

[Tch05] Andrei L. Tchougréeff. Introduction. *International Journal of Quantum Chemistry*, 104(2):101, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2006:I

[Tch06] Andrei L. Tchougréeff. Introduction. *International Journal of Quantum Chemistry*, 106(10):2171–2172, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2007:DMM

[Tch07a] A. L. Tchougréeff. Deriving a mechanistic model for potential energy surface of coordination compounds of nontransition elements. *International Journal of Quantum Chemistry*, 107 (13):2519–2538, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2007:I

[Tch07b] Andrei L. Tchougréeff. Introduction. *International Journal of Quantum Chemistry*, 107(13):2293, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2008:I

[Tch08] Andrei L. Tchougréeff. Introduction. *International Journal of Quantum Chemistry*, 108(14):2629, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tommasini:2001:EDM

[TCM01] M. Tommasini, V. Chernyak, and S. Mukamel. Electronic density-matrix algorithm for nonadiabatic couplings in molecular dynamics simulations. *International Journal of Quantum Chemistry*, 85(4–5):225–238, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Thonhauser:2009:NSP

[TCM09] T. Thonhauser, Davide Ceresoli, and Nicola Marzari. NMR shifts for polycyclic aromatic hydrocarbons from first-

principles. *International Journal of Quantum Chemistry*, 109 (14):3336–3342, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tang:2008:SEP

[TCS+08] Shu-Wei Tang, Ying-Fei Chang, Li-Li Sun, Hao Sun, Zhong-Min Su, and Rong-Shun Wang. Stabilities, electronic properties of exohedral fluorine and trifluoromethyl derivatives for T_dC_{28} fullerene $C_{28}F_{4-n}$ $(CF_3)_n$ $(n = 0, 1, 2, 3, 4)$. *International Journal of Quantum Chemistry*, 108(8):1391–1399, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2009:NER

[TD09] Andrei L. Tchougréeff and Richard Dronskowski. Nephelauxetic effect revisited. *International Journal of Quantum Chemistry*, 109(11):2606–2621, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Talman:2009:NOF

[TDF09] J. D. Talman, J. Delhalle, and J. G. Fripiat. Numerical orbital Fourier space approach to polymer band-structure calculations. *International Journal of Quantum Chemistry*, 109 (13):2968–2977, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Timoshkin:2002:RBE

[TDS+02] A. Y. Timoshkin, E. I. Davydova, T. N. Sevastianova, A. V. Suvorov, and H. F. Schaefer. Relationship between the energy of donor–acceptor bond and the reorganization energy in molecular complexes. *International Journal of Quantum Chemistry*, 88(4):436–440, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tyutyulkov:2007:NCN

[TDST07] N. Tyutyulkov, N. Drebov, A. Staykov, and A. Tadjer. New class of non-Kekulé radical polymethines: Theoretical study. *International Journal of Quantum Chemistry*, 107(6):1396–1404, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Temme:2000:CCE

[Tem00] F. P. Temme. Cayleyan s_n-encoded SU(2)×s_n ↓ } embeddings: Nuclear spin permutation symmetries via polyhedral lattice-point models, for modulo-i $\chi(\mathcal{C}_i(\mathcal{S}_n \downarrow \mathcal{G}))$ combinatorial invariance sets. *International Journal of Quantum Chemistry*, 78(2):71–82, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71005520/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71005520/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71005520&PLACEBO=IE.pdf`.

Temme:2002:UFD

[Tem02a] F. P. Temme. On uniform ($1 \leq I_i \leq 3$) n-fold $I^{\text{outer}}M(i_1 \cdots i_n)$ dual tensorial sets, spin irreps from $SU(3 \leq m) \times \mathcal{S}_n \supset \cdots \supset \mathcal{S}_n$ weight sets: a direct role for (n)-partitional catalogs of $\mathcal{S}_n$ combinatorics in spin physics. *International Journal of Quantum Chemistry*, 87(4):171–180, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85011505/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85011505/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85011505&PLACEBO=IE.pdf`.

Temme:2002:SSC

[Tem02b] F. P. Temme. Structural signs and carrier completeness of Liouvillian quasiparticle algebras: Dual group invariants for explicit $\mathcal{S}_n$-auxiliary tensor labels via projective mappings applicable to $[\mathrm{A}]_{n \leq 20}$ NMR spin ensembles. *International Journal of Quantum Chemistry*, 89(5):429–440, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Temme:2002:SAU

[Tem02c] F. P. Temme. SU(3)×$\mathcal{S}_{20}$ algebras for uniform spin-1 ensembles on $[^2\mathrm{H}^{12}\mathrm{C}]_{20}$, or $[^{14}\mathrm{N}]_{20}$, dodecahedrane-type lattices and analogous isotopomeric $[\mathrm{M}_{20}{}^1\mathrm{2C}_4\mathrm{0}]$ met - carb subensembles: M - based cardinalities and completeness of $\mathcal{S}_{20}$ spin irreps, via hierarchical $\mathcal{C}^{\lambda \vdash (n=20):(M)}$ designs of polyhedral combinatorics. *International Journal of Quantum Chemistry*, 90 (1):155–165, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Tem04].

Temme:2004:ESA

[Tem04] F. P. Temme. Erratum: SU(3)×$\mathcal{S}_{20}$ algebras for uniform spin-1 ensembles on $[^2H^{12}C]_{20}$, or $[^{14}N]_{20}$, dodecahedrane-type lattices and analogous isotopomeric $[M_{20}{}^12C_40]$ met - carb subensembles : M - based cardinalities and completeness of $\mathcal{S}_{20}$ spin irreps, via hierarchical $\mathcal{C}^{\lambda\vdash(n=20):(M)}$ designs of polyhedral combinatorics" International Journal of Quantum Chemistry Volume 87, Number 4, 2002, pages 171 - - 180. *International Journal of Quantum Chemistry*, 99(2):117, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Tem02c].

Temme:2009:LAF

[Tem09] Nico M. Temme. The leaky aquifer function revisited. *International Journal of Quantum Chemistry*, 109(13):2826–2830, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tergiman:2002:CTM

[TFBM02] Y. S. Tergiman, F. Fraija, and M. C. Bacchus-Montabonel. Charge transfer mechanism in N^{4+} + He and B^{3+} + He/H_2 ion–atom/molecule collisions. *International Journal of Quantum Chemistry*, 89(4):322–328, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tapia:2002:ECT

[TFS+02] O. Tapia, Henk Fidder, Vicent S. Safont, Mónica Oliva, and Juan Andrés. Enzyme catalysis: Transition structures and quantum dynamical aspects: Modeling Rubisco's oxygenation and carboxylation mechanisms. *International Journal of Quantum Chemistry*, 88(1):154–166, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89016141/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89016141/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89016141&PLACEBO=IE.pdf`.

Tielens:2001:HCP

[TG01] Frederik Tielens and Paul Geerlings. Henry constants predicted using multipole expansion for the interaction energies. *International Journal of Quantum Chemistry*, 84(1):

58–69, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/84502270/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502270/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502270&PLACEBO=IE.pdf.

Theophilou:2005:DEP

[TG05] Andreas K. Theophilou and Vitaly Glushkov. DFT with effective potential expressed as a mapping of the external potential: Applications to closed-shell molecules. *International Journal of Quantum Chemistry*, 104(4):538–550, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Trylska:2001:PAV

[TGG01] Joanna Trylska, Paweł Grochowski, and Maciej Geller. Parameterization of the approximate valence bond (AVB) method to describe potential energy surface in the reaction catalyzed by HIV-1 protease. *International Journal of Quantum Chemistry*, 82(2):86–103, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/77502747/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/77502747/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=77502747&PLACEBO=IE.pdf.

Toulouse:2006:SRV

[TGGS06] Julien Toulouse, Paola Gori-Giorgi, and Andreas Savin. Scaling relations, virial theorem, and energy densities for long-range and short-range density functionals. *International Journal of Quantum Chemistry*, 106(9):2026–2034, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Truhlar:2004:EAV

[TGGV+04] Donald G. Truhlar, Jiali Gao, Mireia Garcia-Viloca, Cristobal Alhambra, Jose Corchado, Maria Luz Sanchez, and Tina D. Poulsen. Ensemble-averaged variational transition state theory with optimized multidimensional tunneling for enzyme kinetics and other condensed-phase reactions. *International Journal of Quantum Chemistry*, 100(6):1136–1152, ???? 2004.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tsyshevsky:2009:MEP

[TGSK09] Roman V. Tsyshevsky, Guzel G. Garifzianova, Alexander G. Shamov, and Grigorii M. Khrapkovskii. Methane elimination from n-pentane. *International Journal of Quantum Chemistry*, 109(2):196–201, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tielens:2008:ERM

[THP08] Frederik Tielens, Vincent Humblot, and Claire-Marie Pradier. Exploring the reactivity of mixed ω-functionalized undecanethiol self-assembled monolayers—A DFT study. *International Journal of Quantum Chemistry*, 108(10):1792–1795, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Torsti:2003:MMB

[THPN03] T. Torsti, M. Heiskanen, M. J. Puska, and R. M. Nieminen. MIKA: Multigrid-based program package for electronic structure calculations. *International Journal of Quantum Chemistry*, 91(2):171–176, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tachikawa:2005:DDI

[TI05] Hiroto Tachikawa and Tetsuji Iyama. DFT and direct ab initio MD calculations of the gas hydrate: Hydrogen molecule trapped in water cluster $(H_2O)_{12}$. *International Journal of Quantum Chemistry*, 102(2):230–238, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Todorova:2009:CRC

[TIGD09] Tanya K. Todorova, Ivan Infante, Laura Gagliardi, and John M. Dyke. The chemiionization reactions Ce + O and Ce + O_2: Assignment of the observed chemielectron bands. *International Journal of Quantum Chemistry*, 109(10):2068–2079, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tadjer:2007:ESD

[TIV+07] A. Tadjer, A. Ivanova, Y. Velkov, S. Tzvetanov, M. Gotsev, and B. Radoev. Exploratory study of dielectric properties of

insoluble monolayers: Molecular models. *International Journal of Quantum Chemistry*, 107(8):1719–1735, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tovar:2008:ESM

[TJAS08] Roberto M. Tovar, Kyle P. Johnson, Keith Ashline, and Jorge M. Seminario. Effects of substituents on molecular devices. *International Journal of Quantum Chemistry*, 108(9): 1546–1554, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Trickey:2009:CKS

[TKJ09] S. B. Trickey, V. V. Karasiev, and R. S. Jones. Conditions on the Kohn–Sham kinetic energy and associated density. *International Journal of Quantum Chemistry*, 109(13):2943–2952, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Teng:2005:LCD

[TKS+05] Y. L. Teng, Y. H. Kan, Z. M. Su, Y. Liao, L. K. Yan, Y. J. Yang, and R. S. Wang. Luminescent compounds diphenylboron analogs of Alq_3 and its methyl substituents: A theoretical investigation of their electronic and spectroscopic properties. *International Journal of Quantum Chemistry*, 103(6): 775–780, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Teberekidis:2005:GSB

[TKT+05] Vasilios I. Teberekidis, Ioannis S. K. Kerkines, Constantinos A. Tsipis, Petr Čársky, and Aristides Mavridis. Ground states of BeC and MgC: A comparative multireference Brillouin–Wigner coupled cluster and configuration interaction study. *International Journal of Quantum Chemistry*, 102 (5):762–774, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takayanagi:2000:ICC

[TKY00] Toshiyuki Takayanagi, Yuzuru Kurosaki, and Keiichi Yokoyama. Ab initio calculations for the $N(^2D) + CH_4$ reaction: Does the $N(^2D)$ atom really insert into CH bonds of alkane molecules? *International Journal of Quantum Chemistry*, 79(3):190–197, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72508373/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72508373/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72508373&PLACEBO=IE.pdf.

Tu:2005:QCS

[TL05] Yaoquan Tu and Aatto Laaksonen. Quantum chemistry study of monomer electronic properties in water clusters and liquid water and methanol. *International Journal of Quantum Chemistry*, 102(5):888–896, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tacke:2006:RMC

[TLC06] Matthias Tacke, Rosaria Leyden, and Laurence P. Cuffe. Reactions of methyllithium with CO and CNMe: Theoretical study. *International Journal of Quantum Chemistry*, 106(3): 692–696, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tan:2006:TSG

[TLYW06] Xiaojun Tan, Ping Li, Xiuli Yang, and Dangsheng Wang. Theoretical studies of the geometries of H_2GeNaF an its insertion reaction with R — H (R = F, OH, NH_2, CH_3). *International Journal of Quantum Chemistry*, 106(8):1902–1906, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tzeli:2005:CXL

[TM05] Demeter Tzeli and Aristides Mavridis. $CH(X\,^2\Pi,\ a\,^4\Sigma^-)\ldots OH_2$ and CH_2 $(\tilde{X}\,^3B_1,\ \tilde{a}\,^1A_1)\ldots OH_2$ interactions. A first principles investigation. *International Journal of Quantum Chemistry*, 104(4):497–511, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Titov:2001:GMC

[TMAB01] A. V. Titov, N. S. Mosyagin, A. B. Alekseyev, and R. J. Buenker. GRECP/MRD-CI calculations of spin-orbit splitting in ground state of Tl and of spectroscopic properties of TlH. *International Journal of Quantum Chemistry*, 81 (6):409–421, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/76509319/START;

http://www3.interscience.wiley.com/cgi-bin/fulltext/76509319/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76509319&PLACEBO=IE.pdf.

Tei:2003:SDN

[TMM+03] Minaru Tei, Yoichi Mizuno, Yoshinori Manmoto, Ryuichi Sawae, and Kenichi Takarabe. Study of decoherence in a NMR quantum computer using tetrafluoropyridine. *International Journal of Quantum Chemistry*, 95(4–5):554–557, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Titov:2005:TSM

[TMPI05] A. V. Titov, N. S. Mosyagin, A. N. Petrov, and T. A. Isaev. Two-step method for precise calculation of core properties in molecules. *International Journal of Quantum Chemistry*, 104 (2):223–239, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tiwari:2008:SEA

[TMS08] Saumya Tiwari, P. C. Mishra, and S. Suhai. Solvent effect of aqueous media on properties of glycine: Significance of specific and bulk solvent effects, and geometry optimization in aqueous media. *International Journal of Quantum Chemistry*, 108 (5):1004–1016, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tasnadi:2003:SSD

[TN03] F. Tasnádi and Á. Nagy. Study of subspace density functional theory application of LSDA to excited states of atoms. *International Journal of Quantum Chemistry*, 92(2):234–238, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takano:2009:DFS

[TN09] Yu Takano and Haruki Nakamura. Density functional study of roles of porphyrin ring in electronic structures of heme. *International Journal of Quantum Chemistry*, 109(15):3583–3591, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tsumuraya:2003:OSS

[TNET03] Kazuo Tsumuraya, Takatoshi Nagano, Haruki Eguchi, and Hiroyuki Takenaka. Optimized structures of Si_{28} and $Ba@Si_{28}$ clusters: Ab initio study. *International Journal of Quantum Chemistry*, 91(3):328–332, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Toman:2005:OPS

[TNJL05] Petr Toman, Stanislav Nešpůrek, Jae Won Jang, and Cheol Eui Lee. Oligo[methyl(phenyl)silane] ion–radical conformations calculated by the B3LYP method. *International Journal of Quantum Chemistry*, 101(6):746–752, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takashima:2009:DSE

[TNO09] Akito Takashima, Toshiaki Nishii, and Jun Onoe. DV-X_α study on the electronic structure of C_{120} isomers derived from the general Stone–Wales rearrangement. *International Journal of Quantum Chemistry*, 109(12):2773–2779, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takahata:2003:OTE

[TNYY03] Masahiro Takahata, Masayoshi Nakano, Satoru Yamada, and Kizashi Yamaguchi. One- and two-exciton migration dynamics of a dendritic molecular aggregate. *International Journal of Quantum Chemistry*, 95(4–5):472–478, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Timokhina:2002:IQC

[TOB02] Helen N. Timokhina, Alexander A. Ovchinnikov, and Konstantin V. Bozhenko. Ab initio quantum chemical calculations of a cluster C_8H_{12}. *International Journal of Quantum Chemistry*, 88(4):433–435, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takahata:2006:DCC

[TOC06] Yuji Takahata, Andre K. Okamoto, and Delano P. Chong. DFT calculation of core-electron binding energies of pyrimidine and purine bases. *International Journal of Quantum*

Chemistry, 106(13):2581–2586, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tanaka:2000:ICH

[TOH+00] Kazuyoshi Tanaka, Mayumi Okada, Yuanhe Huang, Takao Yoshii, and Akihiro Ito. An instability condition for the Hartree–Fock solution of the infinite one-dimensional system with two-crossing bands. I. Singlet-instability check of metallic carbon nanotube. *International Journal of Quantum Chemistry*, 76(4):574–582, February 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000684/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000684/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000684&PLACEBO=IE.pdf`.

Takano:2000:DFP

[TOK+00] Y. Takano, T. Onishi, Y. Kitagawa, T. Soda, Y. Yoshioka, and K. Yamaguchi. Density functional and post-Hartree–Fock studies on effective exchange interaction of d-π-d conjugated systems involving m-phenylene-type bridge. *International Journal of Quantum Chemistry*, 80(4–5):681–691, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505428/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505428/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505428&PLACEBO=IE.pdf`.

Torrens:2002:CKS

[Tor02] F. Torrens. Computing the Kekulé structure count for alternant hydrocarbons. *International Journal of Quantum Chemistry*, 88(4):392–397, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Torrens:2004:ENC

[Tor04a] F. Torrens. Erratum: Nature of O_2, CO, and CN binding to hemoprotein models. *International Journal of Quantum Chemistry*, 99(6):981, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Tor04b].

Torrens:2004:NCC

[Tor04b] F. Torrens. Nature of O_2, CO, and CN binding to hemoprotein models. *International Journal of Quantum Chemistry*, 99 (6):963–971, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Tor04a].

Torrens:2006:COS

[Tor06] Francisco Torrens. Calculations of organic-solvent dispersions of single-wall carbon nanotubes. *International Journal of Quantum Chemistry*, 106(3):712–718, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Toutounji:2009:ZPL

[Tou09] Mohamad M. Toutounji. Zero-phonon line profiles in Markovian and non-Markovian schemes in high-temperature systems: Applications to glassy water and ethanol. *International Journal of Quantum Chemistry*, 109(14):3399–3409, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tsaune:2002:VPG

[TPGD02] A. Y. Tsaune, Y. A. Podolyak, V. N. Glushkov, and M. P. D'Yachenko. Variational problem for ground and excited rovibronic states on the basis of a molecular Hamiltonian in the principal central axes. *International Journal of Quantum Chemistry*, 89(4):260–267, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tel:2001:CHO

[TPRVC01] L. M. Tel, E. Pérez-Romero, C. Valdemoro, and F. J. Casquero. Cancellation of high-order electron correlation effects corresponding to eigenstates. *International Journal of Quantum Chemistry*, 82(3):131–137, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/77004289/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/77004289/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=77004289&PLACEBO=IE.pdf`.

Tan:2005:IHB

[TQC05] Hongwei Tan, Wenwen Qu, and Guangju Chen. Influence of hydrogen bonds between sidechains and cooperativity on self-assembly of the cyclopeptides. *International Journal of Quantum Chemistry*, 102(6):1106–1115, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tenorio:2000:SRC

[TR00] Francisco J. Tenorio and Juvencio Robles. On the stability and reactivity of C-Si heterofullerenes. *International Journal of Quantum Chemistry*, 80(2):220–226, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001275/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001275/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001275&PLACEBO=IE.pdf`.

Tokmachev:2009:EGH

[TR09] A. M. Tokmachev and M. A. Robb. Efficient generation of Heisenberg Hamiltonian matrices for VB calculations of potential energy surfaces. *International Journal of Quantum Chemistry*, 109(3):401–413, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tian:2000:TSS

[TRF+00] WeiQuan Tian, AiMin Ren, JiKang Feng, JingFu Guo, and ChiaChung Sun. Theoretical study on the structures and electronic spectra of $C_{120}O_n$ ($n = 1, 2$). *International Journal of Quantum Chemistry*, 79(5):291–307, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72512628/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72512628/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72512628&PLACEBO=IE.pdf`.

Trindle:2003:SPT

[Tri03] Carl Trindle. Spin preference in twenty-valence electron systems of form XCCY. *International Journal of Quantum Chemistry*, 93(4):286–293, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Trickey:2004:BR

[Tri04] Sam Trickey. Book review. *International Journal of Quantum Chemistry*, 100(1):60–61, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tieleman:2004:CSV

[TRMM04] D. Peter Tieleman, Kindal M. Robertson, Justin L. Maccallum, and Luca Monticelli. Computer simulations of voltage-gated potassium channel KvAP. *International Journal of Quantum Chemistry*, 100(6):1071–1078, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Thakkar:2001:FLC

[TS01a] Ajit J. Thakkar and Bhawani S. Sharma. A fresh look at the computation of spherically averaged electron momentum densities for wave functions built from Gaussian-type functions. *International Journal of Quantum Chemistry*, 85(4–5):258–262, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tieleman:2001:MDS

[TS01b] D. P. Tieleman and M. S. P. Sansom. Molecular dynamics simulations of antimicrobial peptides: From membrane binding to trans-membrane channels. *International Journal of Quantum Chemistry*, 83(3-4):166–179, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002583/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002583/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002583&PLACEBO=IE.pdf`.

Tang:2007:CAB

[TS07] Kai Tang and Fu Qiang Shi. Comparative analysis of blue-shifted hydrogen bond versus conventional hydrogen bond in methyl radical complexes. *International Journal of Quantum Chemistry*, 107(3):665–669, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Toulouse:2004:SRE

[TSF04] Julien Toulouse, Andreas Savin, and Heinz-Jürgen Flad. Short-range exchange-correlation energy of a uniform electron

gas with modified electron–electron interaction. *International Journal of Quantum Chemistry*, 100(6):1047–1056, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Trindle:2003:CMC

[TSH03] Carl Trindle, Gavin Sacks, and W. Dean Harman. Computational modeling of complexes of penta-ammine osmium (II) with aromatic ligands. *International Journal of Quantum Chemistry*, 92(5):457–456, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takahashi:2001:SEI

[TSK01] Masae Takahashi, Kenkichi Sakamoto, and Mitsuo Kira. Substituent effects on inversion motion of 4-silatriafulvene derivatives: An ab initio MO study. *International Journal of Quantum Chemistry*, 84(2):198–207, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502328/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502328/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502328&PLACEBO=IE.pdf`.

Takahata:2005:QDH

[TSN+05] Masahiro Takahata, Mitsuo Shoji, Hiroya Nitta, Ryo Takeda, Shusuke Yamanaka, Mitsutaka Okumura, Masayoshi Nakano, and Kizashi Yamaguchi. Quantum dynamics in high-spin molecules, spin dendrimers, and spin lattices. *International Journal of Quantum Chemistry*, 105(6):615–627, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tang:2007:DSMb

[TSP+07a] Yi-Zhen Tang, Hao Sun, Ya-Ru Pan, Xiu-Mei Pan, and Rong-Shun Wang. DFT studies on the mechanism of the reaction of C_2H_5S with NO_2. *International Journal of Quantum Chemistry*, 107(9):1907–1914, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tang:2007:DSMa

[TSP+07b] Yi-Zhen Tang, Hao Sun, Ya-Ru Pan, Xiu-Mei Pan, and Rong-Shun Wang. DFT studies on the multi-channel reaction of

CH_3 S+NO_2. *International Journal of Quantum Chemistry*, 107(6):1495–1501, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Trobec:2001:IEM

[TŠPJ01] R. Trobec, M. Šterk, M. Praprotnik, and D. Janežič. Implementation and evaluation of MPI-based parallel MD program. *International Journal of Quantum Chemistry*, 84(1): 23–31, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84002438/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002438/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002438&PLACEBO=IE.pdf`.

Trobec:2004:PPL

[TŠPJ04] R. Trobec, M. Šterk, M. Praprotnik, and D. Janežič. Parallel programming library for molecular dynamics simulations. *International Journal of Quantum Chemistry*, 96(6):530–536, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tawada:2009:LCP

[TSS+09] A. Tawada, K. Sugimori, M. Sano, S. Taniguchi, H. Nagao, and K. Nishikawa. Laser control of photodissociation process in diatomic molecule. *International Journal of Quantum Chemistry*, 109(14):3416–3422, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tang:2008:DFT

[TSZW08] Ke Tang, Haitao Sun, Zhengyu Zhou, and Zhizhong Wang. Density functional theory study on hydrogen-bonded complexes of adenine with polyformamide molecules. *International Journal of Quantum Chemistry*, 108(7):1287–1293, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tokmachev:2001:PES

[TT01] A. M. Tokmachev and A. L. Tchougréeff. Potential energy surfaces in hybrid quantum mechanical/molecular mechanical methods. *International Journal of Quantum Chemistry*,

84(1):39–47, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84002440/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002440/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002440&PLACEBO=IE.pdf`.

Tokmachev:2002:GMM

[TT02] A. M. Tokmachev and A. L. Tchougréeff. Generic molecular mechanics as based on local quantum description of molecular electronic structure. *International Journal of Quantum Chemistry*, 88(4):403–413, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2004:DMMa

[TT04a] A. L. Tchougréeff and A. M. Tokmachev. Deductive molecular mechanics of sp^3 carbon atom. *International Journal of Quantum Chemistry*, 96(2):175–184, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2004:DMMb

[TT04b] A. L. Tchougréeff and A. M. Tokmachev. Deductive molecular mechanics of sp^3 nitrogen atom and its application to analysis of a QM/MM interface. *International Journal of Quantum Chemistry*, 100(4):667–676, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takada:2005:HDS

[TT05] Tomoya Takada and Hiroto Tachikawa. Hybrid DFT study of the hyperfine coupling constants of methyl radicals in model matrix lattices. *International Journal of Quantum Chemistry*, 105(1):79–83, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tokmachev:2006:GFA

[TT06] A. M. Tokmachev and A. L. Tchougréeff. Group functions approach based on the combination of strictly local geminals and molecular orbitals. *International Journal of Quantum Chemistry*, 106(3):571–587, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tasaki:2004:CDD

[TTFP04] S. Tasaki, A. Tokuse, P. Facchi, and S. Pascazio. Control of decoherence: Dynamical decoupling versus quantum Zeno effect: A case study for trapped ions. *International Journal of Quantum Chemistry*, 98(2):160–172, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tamm:2002:TSE

[TTK02] Tarmo Tamm, Jüri Tamm, and Mati Karelson. Theoretical study of the effect of counterions on the structure of pyrrole oligomers. *International Journal of Quantum Chemistry*, 88 (2):296–301, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tokmachev:2001:EHA

[TTM01a] A. M. Tokmachev, A. L. Tchougréeff, and I. A. Misurkin. Effective Hamiltonian approach to catalytic activity of transition metal complexes. *International Journal of Quantum Chemistry*, 84(1):99–109, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84002445/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002445/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002445&PLACEBO=IE.pdf`.

Tokmachev:2001:IPW

[TTM01b] A. M. Tokmachev, A. L. Tchougréeff, and I. A. Misurkin. Ionization potentials within semiempirical antisymmetrized product of strictly localized geminals approach. *International Journal of Quantum Chemistry*, 85(3):109–117, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85011802/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85011802/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85011802&PLACEBO=IE.pdf`.

Tchougreeff:2007:TPI

[TTM07] A. L. Tchougréeff, A. M. Tokmachev, and I. Mayer. Towards a possible ab initio molecular mechanics. Transferability of density matrix elements. *International Journal of Quantum*

Chemistry, 107(13):2539–2555, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Topal:2006:CSS

[TUA06] Kevser Göçmen Topal, Canan Unaleroglu, and Viktorya Aviyente. Computational study of the synthesis of benzoin derivatives from benzil. *International Journal of Quantum Chemistry*, 106(7):1596–1610, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takahashi:2001:IFO

[TVK01] Masae Takahashi, Tamás Veszprémi, and Mitsuo Kira. Importance of frontier orbital interactions in addition reaction of water to disilene. *International Journal of Quantum Chemistry*, 84(2):192–197, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502333/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502333/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502333&PLACEBO=IE.pdf`.

Timofeeva:2002:RPD

[TVK+02] L. M. Timofeeva, Y. A. Vasilieva, N. A. Kleshcheva, G. L. Gromova, and D. A. Topchiev. Radical polymerization of diallylamine compounds: From quantum chemical modeling to controllable synthesis of high-molecular-weight polymers. *International Journal of Quantum Chemistry*, 88(5):531–541, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tran:2002:LBK

[TW02] Fabien Tran and Tomasz A. Wesołowski. Link between the kinetic- and exchange-energy functionals in the generalized gradient approximation. *International Journal of Quantum Chemistry*, 89(5):441–446, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Teng:2005:ESS

[TW05a] Qiwen Teng and Shi Wu. Electronic structures and spectra for triepoxides of fullerene $C_{78}O_3$. *International Journal of Quantum Chemistry*, 104(3):279–285, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tran:2005:TSN

[TW05b] Fabien Tran and Tomasz A. Wesołowski. Theoretical study of neutral and cationic complexes involving phenol. *International Journal of Quantum Chemistry*, 101(6):854–859, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tanaka:2008:DMD

[TW08] Genzo Tanaka and Charles Weatherford. Decomposition mechanisms of dinitrotoluene. *International Journal of Quantum Chemistry*, 108(15):2924–2934, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tsukamoto:2009:CCP

[TWSK09] Takayuki Tsukamoto, Hajime Wakabayashi, Yasuo Sengoku, and Noriyuki Kurita. Charge conducting properties of hydrated DNA duplex between Au electrodes obtained by molecular simulations and Green's function theory. *International Journal of Quantum Chemistry*, 109(10):2058–2067, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Teng:2003:TSS

[TWZ03] Qiwen Teng, Shi Wu, and Zheying Zhu. Theoretical studies on the structures and electronic spectra of $C_{75}B^-$. *International Journal of Quantum Chemistry*, 91(1):39–45, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tian:2009:DDS

[TWZW09] Wei Tian, Wenliang Wang, Yue Zhang, and Weina Wang. Direct dynamics study on the mechanism and the kinetics of the reaction of CH_3NH_2 with OH. *International Journal of Quantum Chemistry*, 109(7):1566–1575, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tian:2002:PTM

[TX02] Shan Xi Tian and Ke Zun Xu. Prototropic tautomers of 5-methylcytosine and enthalpy changes of their protonation, deprotonation, and deamination: Hybrid density functional B3LYP study. *International Journal of Quantum Chemistry*,

89(2):106–120, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takano:2007:HDF

[TY07] Yu Takano and Kizashi Yamaguchi. Hybrid density functional study of ligand coordination effects on the magnetic couplings and the dioxygen binding of the models of hemocyanin. *International Journal of Quantum Chemistry*, 107(15):3103–3119, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Taketsugu:2005:VAA

[TYG05] Tetsuya Taketsugu, Kiyoshi Yagi, and Mark S. Gordon. A vibrational analysis of the 7-azaindole-water complex: Anharmonicities using the quartic force field. *International Journal of Quantum Chemistry*, 104(5):758–772, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takeda:2007:ICD

[TYSY07] R. Takeda, S. Yamanaka, M. Shoji, and K. Yamaguchi. Ab initio calculation of the Dzyaloshinskii–Moriya parameters: Spin-orbit GSO-HF, DFT, and CI approaches. *International Journal of Quantum Chemistry*, 107(6):1328–1334, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takeda:2003:FON

[TYY03] R. Takeda, S. Yamanaka, and K. Yamaguchi. Fractional occupation numbers and spin density functional calculations of degenerate systems. *International Journal of Quantum Chemistry*, 93(5):317–323, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takeda:2004:ATP

[TYY04] R. Takeda, S. Yamanaka, and K. Yamaguchi. Approximate on-top pair density into one-body functions for CAS-DFT. *International Journal of Quantum Chemistry*, 96(5):463–473, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takeda:2005:SOC

[TYY05a] R. Takeda, S. Yamanaka, and K. Yamaguchi. Spin–orbit coupling of spin-frustrated systems. *International Journal*

of Quantum Chemistry, 102(1):80–89, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takeda:2005:FON

[TYY05b] Ryo Takeda, Shusuke Yamanaka, and Kizashi Yamaguchi. Fractional occupation number approaches for CAS (2,2) systems based on second-order density. *International Journal of Quantum Chemistry*, 101(6):658–665, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takeda:2006:RBS

[TYY06] R. Takeda, S. Yamanaka, and K. Yamaguchi. Resonating broken-symmetry approach to biradicals and polyradicals. *International Journal of Quantum Chemistry*, 106(15):3303–3311, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takeda:2007:SOR

[TYY07] Ryo Takeda, Shusuke Yamanaka, and Kizashi Yamaguchi. Spin-optimized resonating Hartree–Fock configuration interaction. *International Journal of Quantum Chemistry*, 107 (15):3219–3227, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ulander:2005:UEC

[UB05] Johan Ulander and Anders Broo. Use of empirical correction terms in calculating ionization constants. *International Journal of Quantum Chemistry*, 105(6):866–874, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Uddin:2004:EIS

[UBS04] M. Alfaz Uddin, A. K. Basak, and B. C. Saha. Electron-impact single ionization cross sections of helium isoelectronic systems. *International Journal of Quantum Chemistry*, 100 (2):184–198, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Urahata:2000:MCQ

[UC00] Sergio Urahata and Sylvio Canuto. Monte Carlo-quantum mechanics study of the UV-visible spectrum of benzophenone in water. *International Journal of Quantum Chemistry*, 80

(4–5):1062–1067, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505398/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505398/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505398&PLACEBO=IE.pdf`.

Umezawa:2006:ROB

[UC06] Naoto Umezawa and Toyohiro Chikyow. Role of the one-body Jastrow factor in the transcorrelated self-consistent field equation. *International Journal of Quantum Chemistry*, 106 (7):1477–1486, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ugalde:2004:I

[UE04] Jesus M. Ugalde and Leif A. Eriksson. Introduction. *International Journal of Quantum Chemistry*, 98(4):343, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Usvyat:2004:WFC

[UES04] D. E. Usvyat, R. A. Evarestov, and V. P. Smirnov. Wannier functions and chemical bonding in crystals with the perovskite-like structure: $SrTiO_3$, $BaTiO_3$, $PbTi_3$, and $LaMnO_3$. *International Journal of Quantum Chemistry*, 100 (4):352–359, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Urdaneta:2004:LAC

[UKAM04] I. Urdaneta, A. Keller, O. Atabek, and V. Mujica. Laser-assisted conductance of molecular wires: Two-photon contributions. *International Journal of Quantum Chemistry*, 99 (4):460–466, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ueno:2006:MSP

[UMDM06] Leonardo T. Ueno, L. R. Marim, A. Dal Pino, Jr., and Francisco B. C. Machado. MRCI study of the photoelectron spectrum of GeC and GeSi and their GeC^+ and $GeSi^+$ ions. *International Journal of Quantum Chemistry*, 106(13):2677–2688, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ujaque:2000:CSD

[UML00] Gregori Ujaque, Feliu Maseras, and Agustí Lledós. A comparative study of DFT and traditional ab initio methodologies on the OsO_4 molecule. *International Journal of Quantum Chemistry*, 77(2):544–551, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70002214/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70002214/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70002214&PLACEBO=IE.pdf`.

Urdaneta:2003:ADI

[UP03] I. Urdaneta and J. L. Paz. Algebraic derivation of the iterative-perturbative method as a global squeezing and displacement transformation. *International Journal of Quantum Chemistry*, 94(4):179–188, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Umari:2005:DFT

[UP05] P. Umari and Alfredo Pasquarello. Density functional theory with finite electric field. *International Journal of Quantum Chemistry*, 101(6):666–670, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Utzat:2004:CSB

[URBM04] Karissa Utzat, Albeiro A. Restrepo, Robert K. Bohn, and H. Harvey Michels. Conformational studies of benzyl alcohol and benzyl fluoride. *International Journal of Quantum Chemistry*, 100(6):964–972, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Upadhyay:2001:ISW

[USM01] D. M. Upadhyay, M. K. Shukla, and P. C. Mishra. An ab initio study of water clusters in gas phase and bulk aqueous media: $(H_2O)_n$, $n = 1--12$. *International Journal of Quantum Chemistry*, 81(1):90–104, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/75502171/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/75502171/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75502171&PLACEBO=IE.pdf`.

Umezawa:2003:TSC

[UT03] Naoto Umezawa and Shinji Tsuneyuki. Transcorrelated self-consistent calculation for electronic systems with variational Monte Carlo method. *International Journal of Quantum Chemistry*, 91(2):184–190, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

VanFaassen:2006:QDP

[Van06] M. Van Faassen. Quantum defect as a powerful tool for studying Rydberg transition energies with density functional theory. *International Journal of Quantum Chemistry*, 106(15): 3235–3241, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Varadwaj:2007:QCI

[Var07] Pradeep R. Varadwaj. Quantum chemical investigation of linear hydrogen bonding in ONCCN$\cdots$HX (X = F, Cl, Br) dimers. *International Journal of Quantum Chemistry*, 107 (5):1194–1204, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Varga:2008:LRA

[Var08] Štefan Varga. Long-range analysis of density fitting in extended systems. *International Journal of Quantum Chemistry*, 108(9):1518–1527, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vigo-Aguiar:2005:RMM

[VAS05] Jesús Vigo-Aguiar and T. E. Simos. Review of multistep methods for the numerical solution of the radial Schrödinger equation. *International Journal of Quantum Chemistry*, 103 (3):278–290, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vail:2006:SCE

[VAS06] Benjamin Vail, Damian Aris, and Mihai Scarlete. Symbolic computation engines and molecular modeling templates: Maple-assisted point group analysis of the vibrational activity of molecules. *International Journal of Quantum Chemistry*, 106(1):167–175, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valdemoro:2003:RDC

[VAT03] C. Valdemoro, D. R. Alcoba, and L. M. Tel. Recent developments in the contracted Schrödinger equation method: Controlling the N-representability of the second-order reduced density matrix. *International Journal of Quantum Chemistry*, 93(3):212–222, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valdemoro:2001:IBH

[VATPR01] C. Valdemoro, D. R. Alcoba, L. M. Tel, and E. Pérez-Romero. Imposing bounds on the high-order reduced density matrices elements. *International Journal of Quantum Chemistry*, 85 (4–5):214–224, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valdemoro:2009:TAP

[VATPR09] C. Valdemoro, D. R. Alcoba, L. M. Tel, and E. Pérez-Romero. Theoretical and applicative properties of the correlation and G-particle-hole matrices. *International Journal of Quantum Chemistry*, 109(11):2622–2638, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vysotsky:2004:CTP

[VB04] Y. B. Vysotsky and V. S. Bryantsev. Calculation of thermochemical properties of conjugated radicals. *International Journal of Quantum Chemistry*, 96(2):123–135, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Velasco:2001:RET

[VBML01] A. M. Velasco, E. Bustos, I. Martín, and C. Lavín. Rydberg electron transitions of the atmospherically important molecule N_2O. *International Journal of Quantum Chemistry*, 84(1): 70–77, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84002442/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002442/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002442&PLACEBO=IE.pdf`.

Velasco:2004:EMQ

[VBML04] A. M. Velasco, E. Bustos, I. Martín, and C. Lavín. Extension of the molecular quantum defect orbital methodology to the calculation of intensities and lifetimes for vibronic transitions within electronic Rydberg series of NO. *International Journal of Quantum Chemistry*, 99(4):511–521, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Villa:2004:ISS

[VBS+04] M. Villa, L. Bounaim, N. Smeyers, M. L. Senent, A. Ezamarty, and Y. G. Smeyers. Ab initio structural study of some substituted ibuprofen derivatives as possible anti-inflammatory agents. *International Journal of Quantum Chemistry*, 97(4): 883–888, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Velde:2007:ATT

[VBT+07] Christophe Vande Velde, Evi Bultinck, Karla Tersago, Christian Van Alsenoy, and Frank Blockhuys. From anisole to 1,2,4,5-tetramethoxybenzene: Theoretical study of the factors that determine the conformation of methoxy groups on a benzene ring. *International Journal of Quantum Chemistry*, 107 (3):670–679, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Varela:2000:SMP

[VCF+00] M. P. Béccar Varela, M. C. Caputo, M. B. Ferraro, P. Lazzeretti, M. C. Mariani, and D. Rial. Some mathematical properties of gauge transformations with respect to the Coulomb gauge: Variational analysis of an energy functional. *International Journal of Quantum Chemistry*, 77(3):599–606, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004063/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004063/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004063&PLACEBO=IE.pdf`.

VanSickle:2007:EDF

[VCHC07] Karina Van Sickle, Lori Marie Culberson, Jeremy Levin Holzmacher, and Mauricio Cafiero. Evaluation of density functional theory methods for the electronic interactions between

indole and substituted benzene: Applications to horseradish peroxidase. *International Journal of Quantum Chemistry*, 107 (6):1523–1531, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

VanMourik:2000:GBS

[VD00] Tanja Van Mourik and Thom H. Dunning, Jr. Gaussian basis sets for use in correlated molecular calculations. VIII. Standard and augmented sextuple zeta correlation consistent basis sets for aluminum through argon. *International Journal of Quantum Chemistry*, 76(2):205–221, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503173/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503173/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503173&PLACEBO=IE.pdf`.

Vikas:2004:GSE

[VD04] Vikas and B. M. Deb. Ground-state electronic energies and densities of atomic systems in strong magnetic fields through a time-dependent hydrodynamical equation. *International Journal of Quantum Chemistry*, 97(2):701–712, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Deb08].

Ventura:2006:EBT

[VDF+06] E. Ventura, S. A. Do Monte, W. Fragoso, C. F. Braga, and R. C. M. U. Araújo. Effects of π bond type, backbone size, and halogen on structural and spectroscopic properties of hydrogen-bonded complexes of the X H ... π type between alkenes or alkynes and haloacids (HF and HCl). *International Journal of Quantum Chemistry*, 106(4):1009–1019, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

vanderVaart:2000:CTB

[vdVM00] Arjan van der Vaart and Kenneth M. Merz, Jr. Charge transfer in biologically important molecules: comparison of high-level ab initio and semiempirical methods. *International Journal of Quantum Chemistry*, 77(1):27–43, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70004293/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004293/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004293&PLACEBO=IE.pdf`.

Visiers:2002:SMF

[VED+02] Irache Visiers, Barbara J. Ebersole, Stella Dracheva, Juan Ballesteros, Stuart C. Sealfon, and Harel Weinstein. Structural motifs as functional microdomains in G-protein-coupled receptors: Energetic considerations in the mechanism of activation of the serotonin 5-HT_{2A} receptor by disruption of the ionic lock of the arginine cage. *International Journal of Quantum Chemistry*, 88(1):65–75, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/89013452/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/89013452/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=89013452&PLACEBO=IE.pdf`.

Velarde:2004:SDS

[Vel04] Manuel G. Velarde. Solitons as dissipative structures. *International Journal of Quantum Chemistry*, 98(2):272–280, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Verwoerd:2005:NOC

[Ver05] W. S. Verwoerd. Nonlinear optical constants of polymers from molecular hyperpolarizabilities of donor–acceptor molecules. *International Journal of Quantum Chemistry*, 103(2):215–225, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vergenz:2009:RBA

[Ver09] Robert Vergenz. Remembering Bill Adams. *International Journal of Quantum Chemistry*, 109(15):3841–3843, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vasilescu:2002:QMM

[VG02] D. Vasilescu and R. Girma. Quantum molecular modeling of quercetin — Simulation of the interaction with the free radical

t-BuOO$^{\cdot}$. *International Journal of Quantum Chemistry*, 90 (2):888–902, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

VonOertzen:2006:DRT

[VG06] G. U. Von Oertzen and A. R. Gerson. O deficiency in the rutile TiO_2 (110) surface: Ab initio quantum chemical investigation of the electronic properties. *International Journal of Quantum Chemistry*, 106(9):2054–2064, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vilela:2005:QCD

[VGB05] Alessandra F. A. Vilela, Ricardo Gargano, and Patrícia R. P. Barreto. Quasi-classical dynamical properties and reaction rate of the Na + HF system on two different potential energy surfaces. *International Journal of Quantum Chemistry*, 103 (5):695–702, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vilela:2005:LMH

[VGM05] Alessandra F. Albernaz Vilela, Ricardo Gargano, and Geraldo Magela e Silva. Linking model Hamiltonians to ab initio and semiempirical methods in descriptions of impurities in conjugated polymers. *International Journal of Quantum Chemistry*, 103(5):537–542, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vilela:2003:QTC

[VGMN03] Alessandra F. A. Vilela, Ricardo Gargano, Kleber C. Mundim, and J. J. Soares Neto. Quasiclassical trajectory calculations of isotopic reactions $Na + XF \rightarrow NaF + X$ (X = D, T and Mμ) on two different potential energy surfaces. *International Journal of Quantum Chemistry*, 95(2):159–163, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valeyev:2000:ALR

[VH00] V. G. Valeyev and M. J. Hagmann. AC linear response of a resonant tunneling system. *International Journal of Quantum Chemistry*, 80(4–5):1007–1010, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505372/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505372/`

FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505372&PLACEBO=IE.pdf.

Vibok:2004:ANA

[VHM+04] Á. Vibók, G. Halász, A. M. Mebel, S. Hu, and M. Baer. Analytic–numerical approach to calculate electronic nonadiabatic coupling terms: Study of the C_2H molecule and the H_2 + H system. *International Journal of Quantum Chemistry*, 99(5):594–604, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

VanCauter:2005:CSK

[VHV+05] K. Van Cauter, K. Hemelsoet, V. Van Speybroeck, M. F. Reyniers, and M. Waroquier. Comparative study of kinetics and reactivity indices of free radical polymerization reactions. *International Journal of Quantum Chemistry*, 102 (4):454–460, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

VanSpeybroeck:2004:RAP

[VHWM04] V. Van Speybroeck, K. Hemelsoet, M. Waroquier, and G. B. Marin. Reactivity and aromaticity of polyaromatics in radical cyclization reactions. *International Journal of Quantum Chemistry*, 96(6):568–576, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vieito:2005:MIC

[VIGL+05] I. Vieito, M. Iglesias, J. M. García-Lastra, J. A. Aramburu, and M. Moreno. Molecular impurities in crystals: $(ReO_4)^{2-}$ Jahn–Teller ion in KCl. *International Journal of Quantum Chemistry*, 101(6):802–806, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vikas:2007:ACQ

[Vik07] Vikas. Associated and correlated quantum fluid dynamics in laser-induced ionization of helium. *International Journal of Quantum Chemistry*, 107(3):647–656, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Varga:2005:HBP

[VK05] Zoltán Varga and Attila Kovács. Hydrogen bonding in peptide secondary structures. *International Journal of Quantum*

Chemistry, 105(4):302–312, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vijayakumar:2007:ISC

[VK07] S. Vijayakumar and P. Kolandaivel. Isomerization study of C_5H_5NO molecules. *International Journal of Quantum Chemistry*, 107(4):769–781, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vijayakumar:2008:RMH

[VK08] S. Vijayakumar and P. Kolandaivel. Reaction mechanism of HSH and CH_3SH with $NH_2CH_2COCH_2X$ (X = F and Cl) molecules. *International Journal of Quantum Chemistry*, 108 (5):927–936, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vitnik:2006:MOI

[VKIJ06] Željko J. Vitnik, Vesna D. Kiricojević, Milovan D. Ivanović, and Ivan O. Juranić. Molecular orbital investigation of various reaction pathways in reaction of ketones with bromoform. *International Journal of Quantum Chemistry*, 106(6):1323–1329, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valone:2008:QBM

[VLJ08] Steven M. Valone, Jiabo Li, and Saryu Jindal. Quantum-based models of charge-dependent potential energy surfaces: Three-state models. *International Journal of Quantum Chemistry*, 108(9):1452–1464, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vitkovskaya:2008:TSM

[VLK+08] Nadezhda M. Vitkovskaya, Elena Yu. Larionova, Vladimir B. Kobychev, Natalia V. Kaempf, and Boris A. Trofimov. A theoretical study of methanol vinylation reaction mechanism. *International Journal of Quantum Chemistry*, 108(14):2630–2635, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

vanLenthe:2006:NCA

[vLvL06] J. H. van Lenthe and J. N. J. van Lingen. Note on the calculation of analytical Hessians in the zeroth-order regular approx-

imation (ZORA). *International Journal of Quantum Chemistry*, 106(12):2525–2528, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vadapalli:2006:ECC

[VM06a] Ravi K. Vadapalli and J. W. Mintmire. Endohedral carbon chains in chiral single-wall carbon nanotubes. *International Journal of Quantum Chemistry*, 106(11):2324–2330, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vayssilov:2006:P

[VM06b] Georgi Vayssilov and Tzonka Mineva. Preface. *International Journal of Quantum Chemistry*, 106(6):1285, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vila:2006:HBI

[VM06c] Antonio Vila and Ricardo A. Mosquera. Are the hydrogen bonds involving sulfur bases inverse or anomalous? *International Journal of Quantum Chemistry*, 106(4):928–934, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vayssilov:2007:PTH

[VM07a] Georgi Vayssilov and Tzonka Mineva. Preface: Third Humboldt Conference on Computational Chemistry. *International Journal of Quantum Chemistry*, 107(8):1651–1652, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Verberck:2007:NFC

[VM07b] B. Verberck and K. H. Michel. Nanotube field of C_{60} and C_{70} molecules in carbon nanotubes. *International Journal of Quantum Chemistry*, 107(13):2294–2319, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vetere:2003:DML

[VMA03] Valentina Vetere, Pascale Maldivi, and Carlo Adamo. Description of the metal–ligand bonding in f-element complexes: A DFT study including scalar relativistic effects. *International Journal of Quantum Chemistry*, 91(3):321–327, ????

2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Velasco:2005:MSP

[VML05] A. M. Velasco, I. Martín, and C. Lavín. MQDO study of photoionization cross-sections for carbon monoxide. *International Journal of Quantum Chemistry*, 104(4):517–521, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vorontsova:2004:WPM

[VMRA04] I. K. Vorontsova, I. D. Mikheikin, V. A. Rakitina, and I. A. Abronin. Words to a problem of multiplicity of carbenelike systems in the external electric fields. *International Journal of Quantum Chemistry*, 100(4):573–580, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Viterbo:2003:ISP

[VNB+03] V. C. Viterbo, J. L. Neves, J. P. Braga, R. P. G. Monteiro, and W. F. De Magalhães. Inversion of simulated positron annihilation lifetime spectra by moving boundary subspaces. *International Journal of Quantum Chemistry*, 95(2):97–102, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vracko:2000:CTE

[VNP00] Marjan Vračko, Marjana Novič, and Marko Perdih. Chemometrical treatment of electronic structures of 28 flavonoid derivatives. *International Journal of Quantum Chemistry*, 76(6):733–743, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70001599/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70001599/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70001599&PLACEBO=IE.pdf`.

VonSzentpaly:2000:MCD

[Von00] László Von Szentpály. Modeling the charge dependence of total energy and its relevance to electrophilicity. *International Journal of Quantum Chemistry*, 76(2):222–234, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503174/START; http:`

//www3.interscience.wiley.com/cgi-bin/fulltext/69503174/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503174&PLACEBO=IE.pdf.

Votyakov:2004:ISS

[VPS+04] S. L. Votyakov, A. V. Porotnikov, Yu. V. Shchapova, E. I. Yuryeva, and A. L. Ivanovskii. Ab initio simulation of the short-range order structure of Al ions and substitutional Fe, Cr impurities in S.S. Spinel ($MgAl_2O_4$). *International Journal of Quantum Chemistry*, 100(4):567–572, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

VanSpeybroeck:2005:SRD

[VPS+05] V. Van Speybroeck, E. Pauwels, F. Stevens, F. Callens, and M. Waroquier. Study of radical defects in crystalline lattices from first-principles molecular dynamics simulations. *International Journal of Quantum Chemistry*, 101(6):761–769, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vedernikova:2000:LAO

[VPSH00] I. Vedernikova, E. Proynov, D. Salahub, and A. Haemers. Local atomic and orbital reactivity indices from density functional calculations for hydrogen-bonded 1,2-dihydroxybenzene. *International Journal of Quantum Chemistry*, 77(1):161–173, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/70004256/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70004256/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70004256&PLACEBO=IE.pdf.

Varnai:2001:DFS

[VR01] Péter Várnai and W. Graham Richards. A density functional study of the interconversion of carbonyls and alcohols in solution: Comparison of reaction mechanisms involving NADPH, histidine, and tyrosine. *International Journal of Quantum Chemistry*, 84(2):276–281, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/84502336/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502336/

FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502336&PLACEBO=IE.pdf.

Valiente:2002:OSC

[VRA+02] R. Valiente, F. Rodríguez, J. A. Aramburu, M. Moreno, M. T. Barriuso, C. Sousa, and C. de Graaf. Optical spectroscopy of $(C_2H_5NH_3)_2CdCl_4$:Cu^{2+} under pressure: Study of Cu^{2+} local structure from theoretical calculations. *International Journal of Quantum Chemistry*, 86(2):239–244, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85006580/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85006580/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85006580&PLACEBO=IE.pdf.

Vrbik:2008:MCC

[Vrb08] Jan Vrbik. Monte Carlo computation of ground-state energy derivatives. *International Journal of Quantum Chemistry*, 108 (3):493–502, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Venkatraman:2004:SAS

[VRC04] Ramaiyer Venkatraman, Paresh Chandra Ray, and Chan Soo Choi. Self-assembly structure of the levulinic acid–melamine lattice. *International Journal of Quantum Chemistry*, 100 (5):758–763, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vrcek:2007:DSR

[Vrc07] Valerije Vrcek. DFT study of rearrangements in cyclopentylheptenyl carbocations. *International Journal of Quantum Chemistry*, 107(8):1772–1781, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Voloshina:2004:DAC

[VRE+04] Elena Voloshina, Gerhard Raabe, Michael Estermeier, Bert Steffan, and Jörg Fleischhauer. Determination of the absolute configuration of calliactine by quantum chemical calculations. *International Journal of Quantum Chemistry*, 100(6):1104–1113, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Venkatraman:2005:SNO

[VRFS05] Ramaiyer Venkatraman, Paresh Chandra Ray, Frank R. Fronczek, and Jagdish P. Singh. Structure and nonlinear optical properties of the HMT–CDA 1:1 adduct: Experimental and DFT approach. *International Journal of Quantum Chemistry*, 105(4):446–452, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valdes:2001:HLI

[VRS01] H. Valdés, V. M. Rayón, and J. A. Sordo. High-level ab initio predictions of CO_2 N_2 O structure. *International Journal of Quantum Chemistry*, 84(1):78–85, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84002443/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002443/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002443&PLACEBO=IE.pdf`.

V:2002:SEF

[VRSF02] J. C. López V., A. L. Rivera, Yu. F. Smirnov, and A. Frank. Simple evaluation of Franck–Condon factors and non-Condon effects in the Morse potential. *International Journal of Quantum Chemistry*, 88(2):280–295, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Virtuoso:2006:MPL

[VSBD06] Luciano S. Virtuoso, Rita C. O. Sebastião, João P. Braga, and Luis H. M. Da Silva. Macromolecular properties from light-scattering experimental data using linear inverse problem theory. *International Journal of Quantum Chemistry*, 106 (13):2731–2736, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vasyukov:2002:ISF

[VSD+02] V. N. Vasyukov, V. A. Shapovalov, V. P. Dyakonov, A. F. Dmitruk, E. I. Aksimentjeva, H. Szymczak, and S. Piechota. Investigation of structure of Fe^3+ magnetic center in polyparaphenylene. *International Journal of Quantum Chemistry*, 88(4):525–529, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Viskolcz:2007:TFC

[VSI+07] Béla Viskolcz, Milan Szori, Robert Izsak, Szilard N. Fejer, and Imre G. Csizmadia. Thermodynamic functions of conformational changes, part IV: Functional analysis of conformational entropy of substituted ethane and methanol. *International Journal of Quantum Chemistry*, 107(8):1826–1834, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vysotsky:2004:PES

[VSS04] Victor P. Vysotsky, George E. Salnikov, and Lyudmila N. Shchegoleva. Potential energy surfaces of fluorinated benzene radical cations. *International Journal of Quantum Chemistry*, 100(4):469–476, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valdemoro:2002:SBP

[VTA+02] C. Valdemoro, L. M. Tel, D. R. Alcoba, E. Pérez-Romero, and F. J. Casquero. Some basic properties of the correlation matrices. *International Journal of Quantum Chemistry*, 90 (6):1555–1561, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vongachariya:2009:ATP

[VTP09] Arthit Vongachariya, Sutheera Tantiwattanakul, and Vudhichai Parasuk. Accurate torsional potentials for monohalo and fluorohalo keto-enolate compounds. *International Journal of Quantum Chemistry*, 109(10):2199–2207, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valdemoro:2008:FNF

[VTPRA08] C. Valdemoro, L. M. Tel, E. Pérez-Romero, and D. R. Alcoba. Four new forms of the contracted Schrödinger equation and their connection with the second-order hypervirial condition. *International Journal of Quantum Chemistry*, 108(6):1090–1096, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Volkov:2004:IDF

[VTS04] Alexey N. Volkov, Alexey Y. Timoshkin, and Andrew V. Suvorov. On the importance of dimeric forms of Al and Ga

trichlorides in the electrophilic aromatic substitution reactions: An ab initio study. *International Journal of Quantum Chemistry*, 100(4):412–418, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Volkov:2005:PEA

[VTS05] Alexey N. Volkov, Alexey Y. Timoshkin, and Andrew V. Suvorov. Pathways of electrophilic aromatic substitution reactions catalyzed by group 13 trihalides: An ab initio study. *International Journal of Quantum Chemistry*, 104(2):256–260, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valderrama:2002:REE

[VU02] E. Valderrama and J. M. Ugalde. Role of electron-electron coalescence density in density functional theory. *International Journal of Quantum Chemistry*, 86(1):40–45, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85514353/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85514353/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85514353&PLACEBO=IE.pdf`.

Vidal:2005:DIA

[VV05] Luciano N. Vidal and Pedro A. M. Vazquez. Determination of ab initio absolute Raman excitation profiles using linear response theory. *International Journal of Quantum Chemistry*, 103(5):632–648, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Velkov:2007:FPS

[VVBT07] Zhivko Velkov, Yasen Velkov, Elena Balabanova, and Alia Tadjer. First principle study of the structure of conjugated amides and thioamides. *International Journal of Quantum Chemistry*, 107(8):1765–1771, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

VanSpeybroeck:2003:ISE

[VVW+03] V. Van Speybroeck, D. Van Neck, M. Waroquier, S. Wauters, M. Saeys, and G. B. Marin. Ab initio study on elementary radical reactions in coke formation. *International Journal*

of Quantum Chemistry, 91(3):384–388, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vadapalli:2003:TEF

[VWB+03] Ravi K. Vadapalli, Charles A. Weatherford, Ioana Banicescu, Ricolindo L. Cariño, and Jianping Zhu. Transient effect of a free particle wave packet in the hydrodynamic formulation of the time-dependent Schrödinger equation. *International Journal of Quantum Chemistry*, 94(1):1–6, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

VanSpeybroeck:2003:IES

[VWMS03] V. Van Speybroeck, M. Waroquier, Y. Martelé, and E. Schacht. Ab initio and experimental study on thermally degradable polycarbonates: Effect of structure on reactivity. *International Journal of Quantum Chemistry*, 91(3):363–368, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Veryazov:2004:DPQ

[VWSA+04] Valera Veryazov, Per-Olof Widmark, Luis Serrano-Andrés, Roland Lindh, and Björn O. Roos. 2MOLCAS as a development platform for quantum chemistry software. *International Journal of Quantum Chemistry*, 100(4):626–635, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Varandas:2004:GPE

[VX04] A. J. C. Varandas and Z. R. Xu. Geometric phase effect at N-fold electronic degeneracies in Jahn–Teller systems. *International Journal of Quantum Chemistry*, 99(4):385–392, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vyboishchikov:2008:PAE

[Vyb08] Sergei F. Vyboishchikov. Partitioning of atomization energy. *International Journal of Quantum Chemistry*, 108(4): 708–718, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2004:EMF

[WAJ04a] Y. Wang, R. Ahuja, and B. Johansson. Erratum: Mean-field potential approach to the quasiharmonic theory of solids. *In-*

ternational Journal of Quantum Chemistry, 97(1):700, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [WAJ04b].

Wang:2004:MFP

[WAJ04b] Y. Wang, R. Ahuja, and B. Johansson. Mean-field potential approach to the quasiharmonic theory of solids. *International Journal of Quantum Chemistry*, 96(5):501–506, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [WAJ04a].

Wang:2004:MPC

[WAJ04c] Y. Wang, R. Ahuja, and B. Johansson. Model for phase coexistence in phase transitions. *International Journal of Quantum Chemistry*, 97(6):961–965, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Walgraef:2004:RDA

[Wal04a] Daniel Walgraef. Reaction–diffusion approach to nanostructure formation and texture evolution in adsorbed monoatomic layers. *International Journal of Quantum Chemistry*, 98(2): 248–260, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wallace:2004:NMF

[Wal04b] Ron Wallace. Neural membrane field effects in a cytoskeleton corral: Microdomain regulation of impulse propagation. *International Journal of Quantum Chemistry*, 100(6):1038–1046, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2005:TSC

[WB05] Yixuan Wang and Perla B. Balbuena. Theoretical studies on cosolvation of Li ion and solvent reductive decomposition in binary mixtures of aliphatic carbonates. *International Journal of Quantum Chemistry*, 102(5):724–733, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wensheng:2000:EFS

[WBLQ00] Deng Wensheng, Gou Bingcong, Han Lihong, and Li Qianshu. Energies, fine structures, and transition rates of the

core-excited states in BeII. *International Journal of Quantum Chemistry*, 76(5):656–661, February 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000587/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000587/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000587&PLACEBO=IE.pdf`.

Wang:2009:P

[WBM09] Yan Alexander Wang, Erkki J. Brändas, and Jean Maruani. Preface. *International Journal of Quantum Chemistry*, 109 (14):3143–3144, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2004:USC

[WC04] Xiao-Gang Wang and Tucker Carrington, Jr. Using simply contracted basis functions with the Lanczos algorithm to calculate vibrational spectra. *International Journal of Quantum Chemistry*, 99(4):556–566, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2000:ISL

[WCP+00] Tao Wu, Xian-Yang Chen, Jian-Bo Peng, Chang-Sheng Shen, Guan-Zhi Ju, and Quan Ju. Isomers of $SiCl_3$ Li. *International Journal of Quantum Chemistry*, 79(1):17–24, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72504404/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72504404/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72504404&PLACEBO=IE.pdf`.

Winkler:2001:OPG

[WD01] Peter Winkler and Song-Tao Dai. The one-particle Green function — revisited. *International Journal of Quantum Chemistry*, 85(4–5):251–257, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2001:BSF

[WE01] Yan-Ni Wang and Leif A. Eriksson. B3LYP studies of the formation of neutral tyrosyl radical $Y_z^{\cdot}$ and regeneration of neutral tyrosine Y_z in PSII. *Interna-*

tional Journal of Quantum Chemistry, 83(3-4):220–229, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002584/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002584/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002584&PLACEBO=IE.pdf`.

Weiner:2003:NMG

[Wei03] B. Weiner. A novel method for generating approximate wavefunctions. *International Journal of Quantum Chemistry*, 95 (4–5):424–441, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weiner:2008:SSE

[Wei08] B. Weiner. Some simple explicit examples of correlated one-electron theory and density matrix functionals. *International Journal of Quantum Chemistry*, 108(15):2837–2848, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weniger:2000:ATT

[Wen00] Ernst Joachim Weniger. Addition theorems as three-dimensional Taylor expansions. *International Journal of Quantum Chemistry*, 76(2):280–295, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503179/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503179/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503179&PLACEBO=IE.pdf`.

Weniger:2002:ATT

[Wen02] Ernst Joachim Weniger. Addition theorems as three-dimensional Taylor expansions. II. B functions and other exponentially decaying functions. *International Journal of Quantum Chemistry*, 90(1):92–104, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weniger:2009:SHB

[Wen09] Ernst Joachim Weniger. The strange history of B functions or how theoretical chemists and mathematicians do (not) interact. *International Journal of Quantum Chemistry*, 109(8):

1706–1716, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Watts:2004:CCS

[WF04] John D. Watts and Joseph S. Francisco. Coupled-cluster studies of $HOONO^+$: Additional conformers of the $^2A'$ ON^+ OOH complex and a comparison of restricted and unrestricted open-shell Hartree–Fock coupled-cluster results. *International Journal of Quantum Chemistry*, 100(5):764–770, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2001:TSS

[WFS+01] Su-Fan Wang, Ji-Kang Feng, Chia-Chung Sun, Peng Liu, Zhen Gao, and Fan-Ao Kong. Theoretical study of silicon-sulfur clusters $(SiS_2)_n^-$ ($n = 1--6$). *International Journal of Quantum Chemistry*, 81(4):280–290, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76505742/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76505742/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76505742&PLACEBO=IE.pdf`.

Wade:2001:PIP

[WGD01] R. C. Wade, R. R. Gabdoulline, and F. De Rienzo. Protein interaction property similarity analysis. *International Journal of Quantum Chemistry*, 83(3-4):122–127, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/80002581/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/80002581/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=80002581&PLACEBO=IE.pdf`.

Wang:2002:IRM

[WGLX02] Zun Yao Wang, Xue Dong Gong, Jin Shan Li, and He Ming Xiao. An investigation on the reaction mechanism of the $F_2 + Cl_2 \rightarrow 2ClF$ using the B3LYP method. *International Journal of Quantum Chemistry*, 87(4):192–197, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90011778/START; http:`

//www3.interscience.wiley.com/cgi-bin/fulltext/90011778/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90011778&PLACEBO=IE.pdf.

Wang:2009:TID

[WGX09] Gui Xiang Wang, Xue Dong Gong, and He Ming Xiao. Theoretical investigation on density, detonation properties, and pyrolysis mechanism of nitro derivatives of benzene and aminobenzenes. *International Journal of Quantum Chemistry*, 109(7):1522–1530, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weber:2005:SQC

[WHD+05] K. C. Weber, K. M. Honório, S. L. Da Silva, R. Mercadante, and A. B. F. da Silva. Selection of quantum chemical descriptors by chemometric methods in the study of antioxidant activity of flavonoid compounds. *International Journal of Quantum Chemistry*, 103(5):731–737, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Whittaker:2002:MRM

[Whi02a] James W. Whittaker. Molecular relaxation and metalloenzyme active site modeling. *International Journal of Quantum Chemistry*, 90(4-5):1529–1535, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Whitten:2002:BEI

[Whi02b] J. L. Whitten. Bounds on electrostatic interactions. *International Journal of Quantum Chemistry*, 90(1):177–182, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Whitten:2003:LOI

[Whi03] J. L. Whitten. Localized orbital interactions: d-electron exchange and correlation. *International Journal of Quantum Chemistry*, 95(6):758–767, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wood:2004:VID

[WHKM04] D. M. Wood, P. Hochmann, L. Klasinc, and S. P. McGlynn. Vibronic intensities in diatomic molecules. *International Journal of Quantum Chemistry*, 99(4):522–532, ????

2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wilson:2004:AMM

[Wil04a] S. Wilson. Alternatives to multireference methods for the molecular electronic structure problem. *International Journal of Quantum Chemistry*, 99(6):925–935, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wilson:2004:BR

[Wil04b] S. Wilson. Book review. *International Journal of Quantum Chemistry*, 100(1):62–66, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wilson:2006:BR

[Wil06] S. Wilson. Book review. *International Journal of Quantum Chemistry*, 106(8):1970–1974, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Winkler:2004:EIW

[Win04] Peter Winkler. Electron interaction in weakly confining quantum dot potentials. *International Journal of Quantum Chemistry*, 100(6):1122–1130, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2009:CCP

[WJLL09] Dongling Wu, Dianzeng Jia, Lang Liu, and Anjie Liu. Conformation and coordination of 1-phenyl-3-methyl-4-benzal-5-pyrazolone thiosemicarbazone: A density functional study. *International Journal of Quantum Chemistry*, 109(6):1341–1347, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2003:MIT

[WK03] J. X. Wang and Sabre Kais. Metal–insulator transition in the Hubbard model on a triangular lattice with disorders: Renormalization group approach. *International Journal of Quantum Chemistry*, 93(5):360–374, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2006:USA

[WK06] Desheng Wang and Aron Kuppermann. Use of symbolic algebra in the calculation of hyperspherical harmonics. *Interna-*

tional Journal of Quantum Chemistry, 106(1):152–166, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Walewski:2006:SDE

[WKF+06] Ł. Walewski, D. Krachtus, S. Fischer, J. C. Smith, P. Bała, and B. Lesyng. SCC-DFTB energy barriers for single and double proton transfer processes in the model molecular systems malonaldehyde and porphycene. *International Journal of Quantum Chemistry*, 106(3):636–640, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2003:CSI

[WKS03] Jian Wu, D. J. Klein, and T. G. Schmalz. Computation on symmetry-invariant bases. *International Journal of Quantum Chemistry*, 94(1):7–22, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2000:ESP

[WL00] B. R. Wu and S.-L. Lee. Effect of spin polarization for hydrogen adsorbed on Si(111)(1×1) surface: First-principles calculations. *International Journal of Quantum Chemistry*, 79(1): 47–55, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72504315/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72504315/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72504315&PLACEBO=IE.pdf`.

Wang:2006:GMC

[WLWZ06] Weiping Wang, Bo Liao, Tianming Wang, and Wen Zhu. A graphical method to construct a phylogenetic tree. *International Journal of Quantum Chemistry*, 106(9):1998–2005, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2008:TIC

[WLZY08a] Yan-Hua Wang, Yun-Xiang Lu, Jian-Wei Zou, and Qing-Sen Yu. Theoretical investigation on charge-assisted halogen bonding interactions in the complexes of bromocarbons with some anions. *International Journal of Quantum Chemistry*, 108(1):90–99, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2008:UIC

[WLZY08b] Yan-Hua Wang, Yun-Xiang Lu, Jian-Wei Zou, and Qing-Sen Yu. Use of ab initio calculations to provide insights into the strength and nature of interfluorine interactions. *International Journal of Quantum Chemistry*, 108(6):1083–1089, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2008:DFC

[WML08] Fen Wang, Qingxi Meng, and Ming Li. Density functional computations of the cyclopropanation of ethene catalyzed by iron (II) carbene complexes Cp(CO)(L)FeCHR, L = CO, PMe_3, R = Me, OMe, ph, CO_2 Me. *International Journal of Quantum Chemistry*, 108(5):945–953, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2005:GES

[WNW05] J. P. Wang, C. J. Niu, and Z. J. Wu. Geometries and electronic structures of W_4 and W clusters. *International Journal of Quantum Chemistry*, 101(3):334–339, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weiner:2004:CUC

[WO04] B. Weiner and J. V. Ortiz. Construction of unique canonical coefficients for antisymmeterized geminal power states. *International Journal of Quantum Chemistry*, 97(5):896–907, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weiner:2005:COE

[WO05] B. Weiner and J. V. Ortiz. Correlated one-electron wave functions. *International Journal of Quantum Chemistry*, 104 (3):299–327, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wolff:2005:ASD

[Wol05] Stephen K. Wolff. Analytical second derivatives in the Amsterdam density functional package. *International Journal of Quantum Chemistry*, 104(5):645–659, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Woon:2002:IQC

[Woo02] David E. Woon. Ab initio quantum chemical studies of reactions in astrophysical ices. 4. Reactions in ices involving HCOOH, CH_2 NH, HCN, HNC, NH_3, and H_2O. *International Journal of Quantum Chemistry*, 88(1):226–235, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/88510649/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88510649/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88510649&PLACEBO=IE.pdf`.

Wathelet:2006:APE

[WPB+06] Valérie Wathelet, Julien Preat, Michaël Bouhy, Michèle Fontaine, Eric A. Perpète, Jean-Marie André, and Denis Jacquemin. Assessment of PBE0 for evaluating the absorption spectra of carbonyl molecules. *International Journal of Quantum Chemistry*, 106(8):1853–1859, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2000:PLM

[WQ00] Xuefeng Wang and Qi-Zong Qin. Peroxide linkage N_2 O_4 molecule: Prediction of new ONOONO isomers. *International Journal of Quantum Chemistry*, 76(1):77–82, January 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503197/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503197/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503197&PLACEBO=IE.pdf`.

Wadehra:2003:GES

[WRD03] Amita Wadehra, Amlan K. Roy, and B. M. Deb. Ground and excited states of one-dimensional self-interacting nonlinear oscillators through time-dependent quantum mechanics. *International Journal of Quantum Chemistry*, 91(5):597–606, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Worthington:2003:KIE

[WRK03] Sharon E. Worthington, Adrian E. Roitberg, and Morris Krauss. Kinetic isotope effects in the active site of *B. subtilis*

chorismate mutase. *International Journal of Quantum Chemistry*, 94(5):287–292, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2003:TDD

[WRRF03] Yuekui Wang, Gerhard Raabe, Charlotte Repges, and Jörg Fleischhauer. Time-dependent density functional theory calculations on the chiroptical properties of rubroflavin: Determination of its absolute configuration by comparison of measured and calculated CD spectra. *International Journal of Quantum Chemistry*, 93(4):265–270, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weatherford:2002:DPD

[WRW02] Charles A. Weatherford, Eddie Red, and Albert Wynn III. Designer polynomials, discrete variable representations, and the Schrödinger equation. *International Journal of Quantum Chemistry*, 90(4-5):1289–1294, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2000:DCE

[WS00] Jian Wang and Alexei A. Stuchebrukhov. DFT calculation of electron tunneling currents: Real-space (grid) molecular orbitals vs. Gaussian-type molecular orbitals. *International Journal of Quantum Chemistry*, 80(4–5):591–597, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505393/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505393/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505393&PLACEBO=IE.pdf`.

Wang:2005:ISD

[WSBV05] Haiyan Wang, Jan Szczepanski, Philip Brucat, and Martin Vala. Infrared spectra and dissociation pathways of the linear carbon–sulfur clusters C_nS and SC_nS (*nleq*29): Theoretical calculations. *International Journal of Quantum Chemistry*, 102(5):795–805, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2005:VAS

[WSC+05] Haiyan Wang, Jan Szczepanski, Andrew Cooke, Philip Brucat, and Martin Vala. Vibrational absorption spectra of C_nS

($n = 2, 6$) and C_nS_2 ($n = 7, 9, 11, 13, 15$) linear carbon–sulfur clusters. *International Journal of Quantum Chemistry*, 102 (5):806–819, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2003:SVB

[WSK03] Jian Wu, T. G. Schmalz, and D. J. Klein. Semiempirical valence-bond resonance energies for alternant conjugated hydrocarbons containing four-membered rings. *International Journal of Quantum Chemistry*, 95(4–5):455–460, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Willaime:2000:ESC

[WSNB00] F. Willaime, A. Satta, M. Nastar, and O. Le Bacq. Electronic structure calculations of vacancy parameters in transition metals: Impact on the bcc self-diffusion anomaly. *International Journal of Quantum Chemistry*, 77(6):927–939, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000984/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000984/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000984&PLACEBO=IE.pdf`.

Wu:2006:SEG

[WT06] Shi Wu and Qiwen Teng. Studies of equilibrium geometries and electronic spectra for $C_{78}O_4$. *International Journal of Quantum Chemistry*, 106(2):526–532, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weldon:2007:ICP

[WT07] Abby Jones Weldon and Gregory S. Tschumper. Intrinsic conformational preferences of and an anomeric-like effect in 1-substituted silacyclohexanes. *International Journal of Quantum Chemistry*, 107(12):2261–2265, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wasada-Tsutsui:2009:ESL

[WTWT09] Yuko Wasada-Tsutsui, Yoshihiro Watanabe, and Hiroshi Tatewaki. Electronic structures of lanthanide monofluorides in the ground state: Frozen-core Dirac–Fock–Roothaan calculations. *International Journal of Quantum Chemistry*, 109

(9):1874–1885, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weinstein:2002:P

[WV02] Harel Weinstein and Hugo O. Villar. Preface. *International Journal of Quantum Chemistry*, 88(1):3–4, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/91015230/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91015230/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91015230&PLACEBO=IE.pdf`.

Wang:2007:PMA

[WW07] Lei Wang and Haijun Wang. Planar mono-, di-aza- and phospha-naphthalene: Structure and aromaticity. *International Journal of Quantum Chemistry*, 107(9):1846–1855, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2008:ITC

[WW08] Yi-Lei Wang and Guo-Shi Wu. Improving the TDDFT calculation of low-lying excited states for polycyclic aromatic hydrocarbons using the Tamm–Dancoff approximation. *International Journal of Quantum Chemistry*, 108(3):430–439, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wasada:2009:TSA

[WWTHF09] Hiroaki Wasada, Yuko Wasada-Tsutsui, Tomohiro Hashimoto, and Shigenobu Funahashi. Theoretical study of acetonitrile-exchange reactions on hexasolvated divalent cations in the first transition series elements. *International Journal of Quantum Chemistry*, 109(10):2208–2226, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2007:TDD

[WWW+07] Hanlu Wang, Xueye Wang, Ling Wang, Hengliang Wang, and Aihong Liu. Time-dependent density functional theory study of electronic spectrum property for carbazolyl–pyridinyl alternating copolymers. *International Journal of Quantum Chemistry*, 107(4):937–945, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wybourne:2002:BFO

[Wyb02] Brian G. Wybourne. Bosons and fermions in a one-dimensional harmonic oscillator potential. *International Journal of Quantum Chemistry*, 90(3):1249–1252, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2006:UNE

[WZ06] Fan Wang and Tom Ziegler. Use of noncollinear exchange-correlation potentials in multiplet resolutions by time-dependent density functional theory. *International Journal of Quantum Chemistry*, 106(12):2545–2550, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wei:2004:REC

[WZJ04] Jichong Wei, Shuping Zhuo, and Guanzhi Ju. Rules of electron correlation energies of van der Waals' complexes RgX (Rg = Ar, Kr, X = F, Cl, Br). *International Journal of Quantum Chemistry*, 97(6):977–982, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2000:EMM

[WZL+00] Yue Wu, Hong Gang Zhao, Xiaoping Liu, Jiping Li, Kaihai Yang, and Hong Bin He. Evaluation of molecular moments by three methods. *International Journal of Quantum Chemistry*, 78(4):237–244, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72000077/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72000077/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72000077&PLACEBO=IE.pdf`.

Wang:2007:SEH

[WZL+07] Yan-Hua Wang, Jian-Wei Zou, Yun-Xiang Lu, Qing-Sen Yu, and Hui-Ying Xu. Single-electron halogen bond: Ab initio study. *International Journal of Quantum Chemistry*, 107(2): 501–506, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2009:ODM

[WZW+09] Fan Wang, Fei Zhao, Bing-Wu Wang, Ming-Wei Wang, Yuan-Zhu Zhang, Wei Wang, Song Gao, and Zhi-Da Chen. Orbital-dependent magnetic properties of molecular cluster containing high-spin Co(II) ions. *International Journal of Quantum Chemistry*, 109(14):3368–3378, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2006:FAD

[WZWC06] Yan-Qiu Wang, Jing-Yi Zhu, Li Wang, and Shu-Lin Cong. Field-assisted dissociative ionization of CH_2I_2 induced by femtosecond laser field. *International Journal of Quantum Chemistry*, 106(5):1138–1144, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2007:SNI

[WZWC07] Junyong Wu, Jingchang Zhang, Zhaoxu Wang, and Weiliang Cao. Study on the nature of interaction of BrCl with HF, H_2O, and NH_3. *International Journal of Quantum Chemistry*, 107 (9):1897–1906, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xiao:2004:SCD

[XBHL04] Chuanyun Xiao, Jessica Blundell, Frank Hagelberg, and William A. Lester, Jr. Silicon clusters doped with an yttrium metal atom impurity. *International Journal of Quantum Chemistry*, 96(4):416–425, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xie:2007:EAD

[XC07a] Hujun Xie and Zexing Cao. Electron attachment to the DNA bases adenine and guanine and dehydrogenation of their anionic derivatives: Density functional study. *International Journal of Quantum Chemistry*, 107(5):1261–1269, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xue:2007:TSE

[XC07b] Zhao-Ming Xue and Chun-Hua Chen. Theoretical study of electrical and electrochemical properties of cyclopentanepentaone and its dicyanomethylene derivatives. *International Journal of Quantum Chemistry*, 107(3):637–646, ???? 2007.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2008:ICN

[XCC+08] Xiang-Lan Xu, Wen-Kai Chen, Zhan-Hong Chen, Jun-Qian Li, and Yi Li. Interaction of CO and NO with the spinel $CuCr_2O_4$ (100) surface: A DFT study. *International Journal of Quantum Chemistry*, 108(9):1435–1443, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2003:API

[XCS+03] Xiao Ying Xu, Feng Cheng, Jian Hua Shen, Xiao Min Luo, Li Li Chen, Li Duo Yue, Yi Du, Fei Ye, Shan Hao Jiang, Da Yuan Zhu, Hua Liang Jiang, and Kai Xian Chen. Agonist–PPARγ interactions: Molecular modeling study with docking approach. *International Journal of Quantum Chemistry*, 93 (6):405–410, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2007:RMP

[XCW07] Dan Xu, Xian-Yang Chen, and Shu-Guang Wang. Reaction mechanism of platinum dimer cation with ammonia based on the relativistic density functional study. *International Journal of Quantum Chemistry*, 107(10):1985–1993, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xavier:2003:IMM

[XD03] Eder Severino Xavier and Hélio Anderson Duarte. Interaction of M — Sn (M = Ru, Rh, Pd) dimers with CH_2 and CF_2: A density functional study. *International Journal of Quantum Chemistry*, 95(2):164–176, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xiao:2006:TSI

[XFLX+06] Hua Xiao, Bei Feng-Li, Wang Xin, Yang Xu-Jie, and Lu Lu-De. Theoretical study of initiated reaction mechanism of polymerization of maleic anhydride catalyzed by OH^{-1} anion. *International Journal of Quantum Chemistry*, 106(5): 1145–1152, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2008:QCS

[XL08] Yu Xu and Qian Shu Li. A quantum chemistry study on boron nitrides $(BNN)_{2n}$ and $(BNN)_{2n}{}^{2+}$ $(n = 3{-}{-}8)$. *International Journal of Quantum Chemistry*, 108(2):296–306, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2009:HUD

[XLX+09a] Bing Xu, Qian-Shu Li, Yaoming Xie, R. Bruce King, and Henry F. Schaefer III. The highly unsaturated dimetal hexacarbonyls of manganese and rhenium: Alternatives to a formal metal–metal quintuple bond. *International Journal of Quantum Chemistry*, 109(13):3082–3092, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2009:IBM

[XLX+09b] Bing Xu, Qian-Shu Li, Yaoming Xie, R. Bruce King, and Henry F. Schaefer III. The interplay between metal–metal bonds, four-electron donor carbonyl groups, and five-electron donor nitrosyl groups in highly unsaturated binuclear rhenium carbonyl nitrosyls. *International Journal of Quantum Chemistry*, 109(10):2273–2285, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xue:2005:TPS

[XR05] Yongqiang Xue and Mark A. Ratner. Theoretical principles of single-molecule electronics: A chemical and mesoscopic view. *International Journal of Quantum Chemistry*, 102(5): 911–924, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2000:GPE

[XV00] Z. R. Xu and A. J. C. Varandas. Geometric phase effect in isotopomers of X_3 systems: Use of a split basis technique for the cone states of HD_2. *International Journal of Quantum Chemistry*, 80(3):454–460, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501025/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501025/`

FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501025&PLACEBO=IE.pdf.

Xu:2001:NDV

[XV01] Z. R. Xu and A. J. C. Varandas. Nuclear dynamics in the vicinity of a crossing seam: Vibrational spectrum of HD_2 revisited. *International Journal of Quantum Chemistry*, 83 (5):279–285, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/81002389/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/81002389/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=81002389&PLACEBO=IE.pdf.

Xiong:2005:AAW

[XVB05] Z. Xiong, M. I. Velgakis, and N. C. Bacalis. Analytic atomic wave functions of NMCSCF quality: Applications. *International Journal of Quantum Chemistry*, 104(4):418–429, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2004:ISD

[XVRL04] Hua Xu, J. S. J. Van Deventer, Szczepan Roszak, and Jerzy Leszczynski. Ab initio study of dissolution reactions of five-membered aluminosilicate framework rings. *International Journal of Quantum Chemistry*, 96(4):365–373, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xia:2008:DFS

[XXC08] Fei Xia, Hujun Xie, and Zexing Cao. Density functional study of protonation of deoxynucleosides: Electrophilic active sites and proton affinities. *International Journal of Quantum Chemistry*, 108(1):57–65, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xia:2003:DSC

[XXJG03] Qi Ying Xia, He Ming Xiao, Xue Hai Ju, and Xue Dong Gong. DFT study on cooperativity in the interactions of hydrazoic acid clusters. *International Journal of Quantum Chemistry*, 94(5):279–286, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xia:2004:SPH

[XXJG04] Qi Ying Xia, He Ming Xiao, Xue Hai Ju, and Xue Dong Gong. Structures and properties of $(H_2GaN_3)_n$ (n = 1–4) clusters: A DFT study. *International Journal of Quantum Chemistry*, 100(3):301–308, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2006:LHE

[XXMJ06] Xiao Juan Xu, He Ming Xiao, Xiu Fang Ma, and Xue Hai Ju. Looking for high-energy density compounds among hexaazaadamantane derivatives with CN, NC, and ONO_2 groups. *International Journal of Quantum Chemistry*, 106(7):1561–1568, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xue:2000:DFT

[XXY00] Ying Xue, Daiqian Xie, and Guosen Yan. Density functional theory studies on molecular structure and IR spectra of 9-methyladenine: A scaled quantum mechanical force field approach. *International Journal of Quantum Chemistry*, 76(6):686–699, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70001596/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70001596/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70001596&PLACEBO=IE.pdf`.

Xu:2005:TSS

[XXY+05] Xiufang Xu, Yumei Xing, Xia Yang, Guichang Wang, Zunsheng Cai, Zhenfeng Shang, Yinming Pan, and Xuezhuang Zhao. Theoretical study of structure and stability of fullerene derivative: $C_{50}O$. *International Journal of Quantum Chemistry*, 101(2):160–168, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xie:2003:TSR

[XYS+03] Xiao-Guang Xie, Song Ye, Nan-Hua Shi, Yong-Ming Zhou, and Huai Cao. Theoretical study of the reactions of the $^1\Sigma^+$ ground state of MS^+ (M = Sc, Y, and La) with oxygen-transfer reagent $MS^+ + CO \rightarrow ScO^+ + CS$ in the gas phase. *International Journal of Quantum Chemistry*, 92(6):478–483,

???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2007:HPA

[XZ07] Shoujun Xu and Heping Zhang. Hosoya polynomials of armchair open-ended nanotubes. *International Journal of Quantum Chemistry*, 107(3):586–596, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2006:FES

[XZGZ06] L. N. Xu, L. L. Zhang, Z. Guo, and L. X. Zhou. Full electronic structure calculation of the biological activity in P173L enzyme. *International Journal of Quantum Chemistry*, 106 (7):1544–1550, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yakushevich:2002:MIM

[Yak02] Ludmila V. Yakushevich. Modeling the internal mobility of the molecule of DNA. *International Journal of Quantum Chemistry*, 88(5):570–578, June 20, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yalcin:2004:BSC

[Yal04] Zeynel Yalçin. Bound state calculations for some three-body electronic and muonic atomic systems with Fues–Kratzer-type potential. *International Journal of Quantum Chemistry*, 98 (1):44–50, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamada:2004:TIC

[Yam04] Mitsuru Yamada. Trial introduction of a complex potential function for perturbation that causes quantum mechanical transition in a one-dimensional harmonic oscillator. *International Journal of Quantum Chemistry*, 99(3):127–141, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Yam05].

Yamada:2005:ETI

[Yam05] Mitsuru Yamada. Erratum: Trial introduction of a complex potential function for perturbation that causes quantum mechanical transition in a one-dimensional harmonic oscillator, Mitsuru Yamada, International Journal of Quantum Chemistry (2004) 99(3) 127–141. *International Journal of Quantum*

Chemistry, 102(6):1136–1138, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Yam04].

Yamaguchi:2009:TST

[Yam09] Yoichi Yamaguchi. Theoretical study of two-dimensionally fused zinc porphyrins: DFT calculations. *International Journal of Quantum Chemistry*, 109(7):1584–1597, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2006:SQT

[Yan06] Ciann-Dong Yang. Solving quantum trajectories in Coulomb potential by quantum Hamilton–Jacobi theory. *International Journal of Quantum Chemistry*, 106(7):1620–1639, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2009:TSSa

[Yan09] Yong Yang. Theoretical study of the SH$\cdots$O blue-shifted hydrogen bond. *International Journal of Quantum Chemistry*, 109(2):266–274, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yarzhemsky:2000:SGA

[Yar00] V. G. Yarzhemsky. Space-group approach to the nodal structure of superconducting order parameter in ferromagnetic and antiferromagnetic materials. *International Journal of Quantum Chemistry*, 80(2):133–140, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001281/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001281/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001281&PLACEBO=IE.pdf`.

Yalcin:2000:ESS

[YAŞ00] Zeynel Yalçın, Metın Aktaş, and Mehmet Şımşek. Exact solutions of the Schrödinger equation for ^{1,3} s states of the atom with Fues-Kratzer-type potential. *International Journal of Quantum Chemistry*, 76(5):618–625, February 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000583/START; http:`

//www3.interscience.wiley.com/cgi-bin/fulltext/70000583/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000583&PLACEBO=IE.pdf.

Yan:2005:TPC

[YBS05] Shihai Yan, Yuxiang Bu, and Lixiang Sun. Theoretical prediction of the contact distance dependence of the electron transfer reactivity of the ClO/ClO^- coupling system. *International Journal of Quantum Chemistry*, 101(3):305–319, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ye:2007:EPU

[YCN+07] J. F. Ye, H. Chen, R. Note, H. Mizuseki, and Y. Kawazoe. Excess polarizabilities upon excitation from the ground state to the first dipole-allowed excited state of diphenylpolyenes. *International Journal of Quantum Chemistry*, 107(10):2006–2014, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yuan:2009:ERA

[YCS09] Xiao-Li Yuan, Xin-Lu Cheng, and Xin-Fang Su. Effect of ring annelation on cations [M = H^+, Li^+, Na^+, K^+, Be^{2+}, Mg^{2+}, and Ca^{2+}]. . . benzene interaction: A density functional theory investigation. *International Journal of Quantum Chemistry*, 109(5):972–981, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ye:2001:TSD

[Ye01] Song Ye. Theoretical study of the dehydrogenate reaction of H_2S by Sc^+ (^1D). *International Journal of Quantum Chemistry*, 82(2):60–64, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/77502748/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/77502748/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=77502748&PLACEBO=IE.pdf.

Yu:2007:TST

[YF07] Yongming Yu and Shengyu Feng. Theoretical study of thermal rearrangements of α-silylalcohols: Effects of substituents attached to the silicon atom on the reactions. *International*

Journal of Quantum Chemistry, 107(1):105–115, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2005:EME

[YHC05] Xiaohua Yang, Haiquan Hu, and Zhida Chen. Effect of magnetic exchange, double exchange, vibronic coupling, and asymmetry on magnetic properties in $d^2 - d^3$ mixed-valence dimers. *International Journal of Quantum Chemistry*, 103 (2):190–197, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2000:DLA

[YHD00] Benhui Yang, Keli Han, and Shiliang Ding. Dynamical Lie algebraic approach to energy transfer of the scattering system A + BC. *International Journal of Quantum Chemistry*, 78(5):295–302, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72001897/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72001897/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72001897&PLACEBO=IE.pdf`.

Yu:2007:TSS

[YHD+07] Guang-Tao Yu, Xu-Ri Huang, Yi-Hong Ding, Wei Chen, and Chia-Chung Sun. Theoretical study of the Si_2NO potential energy surface. *International Journal of Quantum Chemistry*, 107(5):1181–1193, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2008:ESO

[YHF+08] Gang Yang, Wenhua Hou, Xiaomiao Feng, Xuefan Jiang, and Jin Guo. Electronic structure of oligoaniline doped by inorganic and organic acids. *International Journal of Quantum Chemistry*, 108(6):1155–1163, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yanai:2007:NIM

[YHN+07] Takeshi Yanai, Robert J. Harrison, Takahito Nakajima, Yasuyuki Ishikawa, and Kimihiko Hirao. New implementation of molecular double point-group symmetry in four-component relativistic Gaussian-type spinors. *International Journal of*

Quantum Chemistry, 107(6):1382–1389, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yuryeva:2004:IIB

[YI04] E. I. Yuryeva and A. L. Ivanovskii. Investigation of interatomic bonding in 3C-SiC:M by nonempirical quantum chemistry methods. *International Journal of Quantum Chemistry*, 96(2):136–141, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yildirim:2006:USN

[Yil06] Necmettin Yildirim. Use of symbolic and numeric computation techniques in analysis of biochemical reaction networks. *International Journal of Quantum Chemistry*, 106(1):256–265, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yanai:2000:NAE

[YINH00] Takeshi Yanai, Kazuhiro Ishida, Haruyuki Nakano, and Kimihiko Hirao. New algorithm for electron repulsion integrals oriented to the general contraction scheme. *International Journal of Quantum Chemistry*, 76(3):396–406, January 20, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000282/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000282/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000282&PLACEBO=IE.pdf`.

Ye:2000:ESL

[YJ00] Yuan-Jie Ye and Yan Jiang. Electronic structures and long-range electron transfer through DNA molecules. *International Journal of Quantum Chemistry*, 78(2):112–130, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71005518/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71005518/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71005518&PLACEBO=IE.pdf`.

Yanai:2009:ACI

[YKGC09] Takeshi Yanai, Yuki Kurashige, Debashree Ghosh, and Garnet Kin-Lic Chan. Accelerating convergence in iterative solution

for large-scale complete active space self-consistent-field calculations. *International Journal of Quantum Chemistry*, 109 (10):2178–2190, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamanaka:2005:CBL

[YKK+05] S. Yamanaka, K. Koizumi, Y. Kitagawa, T. Kawakami, M. Okumura, and K. Yamaguchi. Chemical bonding, less screening, and Hund's rule revisited. *International Journal of Quantum Chemistry*, 105(6):687–700, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yanov:2006:LMC

[YKS+06] Ilya Yanov, Yana Kholod, Tomekia Simeon, Anna Kaczmarek, and Jerzy Leszczynski. Local minima conformations of the Sc_3N @C_{80} endohedral complex: Ab initio quantum chemical study and suggestions for experimental verification. *International Journal of Quantum Chemistry*, 106(14):2975–2980, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaguchi:2002:AIS

[YKT+02] Kizashi Yamaguchi, Takashi Kawakami, Yu Takano, Yasutaka Kitagawa, Yoshifumi Yamashita, and Harunori Fujita. Analytical and ab initio studies of effective exchange interactions, polyradical character, unpaired electron density, and information entropy in radical clusters $(R)_N$: Allyl radical cluster ($N = 2--10$) and hydrogen radical cluster ($N = 50$). *International Journal of Quantum Chemistry*, 90(1):370–385, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yannouleas:2002:MFM

[YL02] Constantine Yannouleas and Uzi Landman. Magnetic-field manipulation of chemical bonding in artificial molecules. *International Journal of Quantum Chemistry*, 90(2):699–708, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yanov:2004:ETT

[YL04] Ilya Yanov and Jerzy Leszczynski. Electron transport throughout the DNA base pair. *International Journal of*

Quantum Chemistry, 96(4):436–442, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yanov:2004:MMS

[YLS+04] Ilya Yanov, Jerzy Leszczynski, E. Sulman, V. Matveeva, and N. Semagina. Modeling of the molecular structure and catalytic activity of the new fullerene-based catalyst (η^2-c_{60})pd(PPh_3)$_2$: An application in the reaction of selective hydrogenation of acetylenic alcohols. *International Journal of Quantum Chemistry*, 100(5):810–817, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yi:2003:TIC

[YLYD03] Hai-Bo Yi, Xiang-Yuan Li, Sheng-Yong Yang, and Xiao-Hui Duan. Theoretical investigation of charge transfer excitation and charge recombination in acenaphthylene–tetracyanoethylene complex. *International Journal of Quantum Chemistry*, 94(1):23–35, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2007:RPD

[YLZ07] Jing Yang, Qian Shu Li, and Shaowen Zhang. Reaction-path dynamics and theoretical rate constants for the reaction $CH_4 + O_3 \rightarrow HOOO + CH_3$. *International Journal of Quantum Chemistry*, 107(10):1999–2005, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yeager:2005:AMS

[YM05] Danny L. Yeager and Manoj K. Mishra. Algebraic modifications to second quantization for non-Hermitian complex scaled Hamiltonians with application to a quadratically convergent multiconfigurational self-consistent field method. *International Journal of Quantum Chemistry*, 104(6):871–879, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2004:TSF

[YMZH04] Guanghui Yang, Qingtian Meng, Xin Zhang, and Keli Han. Theoretical study on the formation mechanism of iso-CH_2I-Cl. *International Journal of Quantum Chemistry*, 97(2):719–724, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yarzhemsky:2004:GTD

[YN04] V. G. Yarzhemsky and V. I. Nefedov. Group theoretical description of two-electron wave functions in systems with subgroups of symmetry. *International Journal of Quantum Chemistry*, 100(4):519–527, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yavari:2006:IMO

[YNDJ06] Issa Yavari, Farough Nasiri, Hoorieh Djahaniani, and Arash Jabbari. Ab initio molecular orbital study of conformational properties of cyclohexyne, cycloheptyne, and cyclooctyne. *International Journal of Quantum Chemistry*, 106(3):697–703, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaguchi:2006:BHM

[YNN+06] K. Yamaguchi, M. Nakano, H. Nagao, M. Okumura, S. Yamanaka, T. Kawakami, S. Yamada, D. Yamaki, Y. Kitagawa, R. Takeda, and H. Nitta. N-band Hubbard models. III. Boson–fermion and interaction–boson models for high-T_c superconductivity. *International Journal of Quantum Chemistry*, 106(5):1052–1075, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamanaka:2009:RCC

[YNN+09] S. Yamanaka, S. Nishihara, K. Nakata, Y. Yonezawa, M. Okumura, T. Takada, H. Nakamura, and K. Yamaguchi. Resonating coupled-cluster CI approach to ion-radical systems: Comparison with the unrestricted coupled-cluster approach. *International Journal of Quantum Chemistry*, 109(15):3811–3818, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamanaka:2006:MDF

[YNU+06] Shusuke Yamanaka, Kazuto Nakata, Takeshi Ukai, Toshikazu Takada, and Kizashi Yamaguchi. Multireference density functional theory with orbital-dependent correlation corrections. *International Journal of Quantum Chemistry*, 106(15):3312–3324, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaki:2001:ADT

[YNY01] D. Yamaki, H. Nagao, and K. Yamaguchi. Analysis of difference two-electron density matrix between two states of magnetic molecules. *International Journal of Quantum Chemistry*, 85(4–5):204–213, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yuen:2009:IRQ

[YOGR09] Wai Kong Yuen, Daniel G. Oblinsky, Robert D. Giacometti, and Stuart M. Rothstein. Improving reptation quantum Monte Carlo. *International Journal of Quantum Chemistry*, 109(14):3229–3234, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yoshimoto:2001:NBO

[YOM+01] T. Yoshimoto, Y. Ohta, J. Maki, Y. Shigeta, H. Nagao, and K. Nishikawa. Non-Born–Oppenheimer density functional theory for excited states by using Green's function techniques. *International Journal of Quantum Chemistry*, 84(3):354–362, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/83002311/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/83002311/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=83002311&PLACEBO=IE.pdf`.

Yamaki:2004:FUR

[YONY04] Daisuke Yamaki, Tadafumi Ohsaku, Hidemi Nagao, and Kizashi Yamaguchi. Formulation of unrestricted and restricted Hartree–Fock–Bogoliubov equations. *International Journal of Quantum Chemistry*, 96(1):10–16, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamanaka:2003:GSD

[YOYY03] S. Yamanaka, T. Ohsaku, D. Yamaki, and K. Yamaguchi. Generalized spin density functional study of radical reactions. *International Journal of Quantum Chemistry*, 91(3):376–383, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yusha:2007:ESM

[YPD+07] Sergei N. Yusha, Alexander A. Projavkin, Ilia A. Dementyev, Andrei O. Kozin, and Dmitry V. Korolkov. The electronic structure of molybdenum (II) clusters with chelate ligands. *International Journal of Quantum Chemistry*, 107(13):2507–2518, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yuryeva:2005:ESC

[YPS05] E. I. Yuryeva, R. N. Pletney, and A. V. Skripov. Electronic structure, chemical binding, and elastic properties of M–H interactions as calculated by the X_α–DV method. *International Journal of Quantum Chemistry*, 104(2):143–147, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yalcin:2002:PHA

[YŞ02] Zeynel Yalçin and Mehmet Şimşek. Potential harmonic approximation in atomic three-body systems with Fues–Kratzer-type potential. *International Journal of Quantum Chemistry*, 88(6):735–741, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2005:SSA

[YS05] Y. J. Yang and Z. M. Su. Structure, stability, and aromaticity of M — SubPc (M = B, Al, and Ga): Computational study. *International Journal of Quantum Chemistry*, 103(1):54–59, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yan:2006:MMT

[YS06] Liuming Yan and Jorge M. Seminario. Moletronics modeling toward molecular potentials. *International Journal of Quantum Chemistry*, 106(8):1964–1969, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yan:2007:ETN

[YS07] Liuming Yan and Jorge M. Seminario. Electron transport in nano-Gold–Silicon interfaces. *International Journal of Quantum Chemistry*, 107(2):440–450, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2009:TSSb

[YS09] Guochun Yang and Zhongmin Su. Theoretical study on the second-order nonlinear optical properties of nonconjugated D-π-A chromophores. *International Journal of Quantum Chemistry*, 109(7):1553–1559, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamanaka:2001:GSO

[YSO+01] S. Yamanaka, Y. Shigeta, Y. Ohta, D. Yamaki, H. Nagao, and K. Yamaguchi. Generalized spin orbital GW theory for spin-frustrated and spin-degenerate systems. *International Journal of Quantum Chemistry*, 84(3):369–374, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/83002306/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/83002306/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=83002306&PLACEBO=IE.pdf`.

Yurenev:2006:ELH

[YSP06] P. V. Yurenev, A. V. Scherbinin, and V. I. Pupyshev. Energy levels of the hydrogen atom in a cylindrical cavity. *International Journal of Quantum Chemistry*, 106(10):2201–2207, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yurenev:2008:SHA

[YSP08] P. V. Yurenev, A. V. Scherbinin, and V. I. Pupyshev. Shifts of the hydrogen atom in a cylindrical cavity. *International Journal of Quantum Chemistry*, 108(14):2666–2677, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yurenev:2008:HIE

[YSS08] P. V. Yurenev, A. V. Scherbinin, and N. F. Stepanov. Hybrid Ab initio/EFP approach for calculating d-d absorption spectrum of hexaammineruthenium(II) ion in aqueous solutions. *International Journal of Quantum Chemistry*, 108(14):2711–2718, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yan:2005:EPS

[YST+05] Li-Kai Yan, Zhong-Min Su, Ke Tan, Min Zhang, Lun-Yu Qu, and Rong-Shun Wang. Electronic properties of Strandberg anions: A DFT study of $[X_2Mo_5O_{23}]^{n-}$, ($X = P^V$, S^{VI}, As^V, Se^{VI}), and $[(RP)_2Mo_5O_{21}]^{4-}$ ($R = H$, CH_3, C_2H_5). *International Journal of Quantum Chemistry*, 105(1):37–42, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2005:DSP

[YSV05] M. Yang, P. Senet, and C. Van Alsenoy. DFT study of polarizabilities and dipole moments of water clusters. *International Journal of Quantum Chemistry*, 101(5):535–542, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaki:2000:MTD

[YSY+00] D. Yamaki, Y. Shigeta, S. Yamanaka, H. Nagao, and K. Yamaguchi. MP2, Tamm–Dancoff, and RPA methods based on the generalized HF solution. *International Journal of Quantum Chemistry*, 80(4–5):701–707, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505412/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505412/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505412&PLACEBO=IE.pdf`.

Yamaki:2001:GSO

[YSY+01] D. Yamaki, Y. Shigeta, S. Yamanaka, H. Nagao, and K. Yamaguchi. Generalized spin orbital calculations of spin-frustrated molecules. *International Journal of Quantum Chemistry*, 84(5):546–551, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502939/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502939/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502939&PLACEBO=IE.pdf`.

Yoshimoto:2003:FPS

[YT03] Yoshihide Yoshimoto and Shinji Tsuneyuki. First-principles study of inter-nitrogen interaction energy of Cu(100)- c (2×2)N surface. *International Journal of Quantum Chemistry*, 91 (2):211–215, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamamoto:2005:CES

[YTD05] Shigeyoshi Yamamoto, Hiroshi Tatewaki, and Geerd H. F. Diercksen. Characterization of the excited states of ethylene by MRCI. *International Journal of Quantum Chemistry*, 103 (1):45–53, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamanaka:2003:SCF

[YTK+03] S. Yamanaka, R. Takeda, T. Kawakami, S. Nakano, D. Yamaki, S. Yamada, K. Nakata, T. Sakuma, T. Takada, and K. Yamaguchi. Spin correlation functions by generalized spin orbital density functional and multireference approaches. *International Journal of Quantum Chemistry*, 95(4–5):512–520, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamanaka:2005:QSC

[YTS+05] Shusuke Yamanaka, Ryo Takeda, Mitsuo Shoji, Yasutaka Kitagawa, Hiroaki Honda, and Kizashi Yamaguchi. Quantum spin correction scheme for ab initio spin-unrestricted solutions: Multiple bonds case. *International Journal of Quantum Chemistry*, 105(6):605–614, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamanaka:2007:DFS

[YUN+07] Shusuke Yamanaka, Takeshi Ukai, Kazuto Nakata, Ryo Takeda, Mitsuo Shoji, Takashi Kawakami, Toshikazu Takada, and Kizashi Yamaguchi. Density functional study of manganese dimer. *International Journal of Quantum Chemistry*, 107(15):3178–3190, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yuryeva:2006:DMO

[Yur06] Elmira I. Yuryeva. X_α-DVM modelling of oxygen transport in $YBa_2Cu_3O_{7-\delta}$ and $SrFeO_3$. *International Journal of*

Quantum Chemistry, 106(10):2290–2296, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yuryeva:2007:DSP

[Yur07] Elmira I. Yuryeva. X_α-DVM study of properties of active sites of hemoglobin upon substitution of Fe by other 3d-metal atoms. *International Journal of Quantum Chemistry*, 107(13): 2556–2563, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yuryeva:2008:DID

[Yur08] Elmira I. Yuryeva. X_α-DVM investigation of double water molecule interactions with active sites of α- and β-subunits of hemoglobin. *International Journal of Quantum Chemistry*, 108(14):2648–2656, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ye:2005:ISI

[YW05] Song Ye and Chaojie Wang. Ab initio study of the insertion reactions of Sc^+ (^1D) with HF, HCl, H_2O, H_2S, NH_3, PH_3, CH_4, and SiH_4. *International Journal of Quantum Chemistry*, 102(6):1080–1086, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yagi:2009:ISW

[YW09] Kiyoshi Yagi and Daichi Watanabe. Infrared spectra of water molecule encapsulated inside fullerene studied by instantaneous vibrational analysis. *International Journal of Quantum Chemistry*, 109(10):2080–2090, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yong:2007:TSA

[YWC07] Liu Yong, Shao Dan Wu, and Xian Xing Chi. Theoretical study of aromaticity in small hydrogen and metal cation clusters X^{3+} (X = H, Li, Na, K, and Cu). *International Journal of Quantum Chemistry*, 107(3):722–728, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2009:PTC

[YWZ+09] Gang Yang, Xiaomin Wu, Yuangang Zu, Chengbu Liu, Yujie Fu, and Lijun Zhou. Proton transfer at the carboxylic sites of amino acids: A single water molecule catalyzed process. *International Journal of Quantum Chemistry*, 109(2):320–327,

???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2004:WPS

[YY04] Bo-Yin Yang and Yeong-Nan Yeh. Wiener polynomials of some chemically interesting graphs. *International Journal of Quantum Chemistry*, 99(2):80–91, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2001:DLA

[YYHD01] Benhui Yang, Hongming Yin, Keli Han, and Shiliang Ding. Dynamical Lie algebraic treatment for the A+BC scattering. *International Journal of Quantum Chemistry*, 81(3):214–221, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76504661/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76504661/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76504661&PLACEBO=IE.pdf`.

Yamaguchi:2008:BHM

[YYI+08] K. Yamaguchi, S. Yamanaka, H. Isobe, M. Hagihara, D. Yamaki, M. Nishihara, Y. Kitagawa, T. Kawakami, and M. Okumura. N-bands Hubbard models. IV. Comparisons of electron- or hole-doped quaternary oxypictides LaOMPn superconductors with cuprates. *International Journal of Quantum Chemistry*, 108(15):3016–3041, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaguchi:2009:TCB

[YYI+09] Kizashi Yamaguchi, Syusuke Yamanaka, Hiroshi Isobe, Mitsuo Shoji, Toru Saito, Yasutaka Kitagawa, Mitsutaka Okumura, and Jiro Shimada. Theory of chemical bonds in metalloenzymes XIII: Singlet and triplet diradical mechanisms of hydroxylations with iron-oxo species and P450 are revisited. *International Journal of Quantum Chemistry*, 109(15):3723–3744, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaguchi:2003:BHM

[YYK+03] Kizashi Yamaguchi, Daisuke Yamaki, Yasutaka Kitagawa, Masahiro Takahata, Takashi Kawakami, Tadafumi Ohsaku,

and Hidemi Nagao. N-band Hubbard models II: Cooperative mechanisms of electron–phonon, electron correlation, and many-band effects toward high-T_c superconductors. *International Journal of Quantum Chemistry*, 92(1):47–70, March 5, 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamanaka:2001:GSD

[YYKY01] S. Yamanaka, D. Yamaki, S. Kiribayashi, and K. Yamaguchi. Generalized spin density functional theory for noncollinear molecular magnetism II — Influence of gradient correction and self-interaction correction. *International Journal of Quantum Chemistry*, 85(4–5):421–431, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yin:2006:DCR

[YYQ+06] Wenjuan Yin, Shihai Yan, Mei Qin, Zhiqiang Li, and Yuxiang Bu. Different catalysis role of in-loop and out-of-loop waters in assisting HNS/HSN proton transfer isomerizations: Bridging vs. surrounding effect. *International Journal of Quantum Chemistry*, 106(7):1528–1543, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamanaka:2000:GSD

[YYS+00] S. Yamanaka, D. Yamaki, Y. Shigeta, H. Nagao, Y. Yoshioka, N. Suzuki, and K. Yamaguchi. Generalized spin density functional theory for noncollinear molecular magnetism. *International Journal of Quantum Chemistry*, 80(4–5):664–671, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505394/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505394/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505394&PLACEBO=IE.pdf`.

Yamanaka:2001:NSD

[YYS+01] S. Yamanaka, D. Yamaki, Y. Shigeta, H. Nagao, and K. Yamaguchi. Noncollinear spin density functional theory for spin-frustrated and spin-degenerate systems. *International Journal of Quantum Chemistry*, 84(6):670–676, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502394/START; http:`

//www3.interscience.wiley.com/cgi-bin/fulltext/84502394/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502394&PLACEBO=IE.pdf.

Yamaguchi:2009:EHF

[YYS+09] Kizashi Yamaguchi, Syusuke Yamanaka, Jiro Shimada, Hiroshi Isobe, Toru Saito, Mitsuo Shoji, Yasutaka Kitagawa, and Mitsutaka Okumura. Extended Hartree–Fock theory of chemical reactions. IX. Diradical and perepoxide mechanisms for oxygenations of ethylene with molecular oxygen and iron-oxo species are revisited. *International Journal of Quantum Chemistry*, 109(15):3745–3766, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamanaka:2004:MMS

[YYT+04] Shusuke Yamanaka, Daisuke Yamaki, Ryo Takeda, Hidemi Nagao, and Kizashi Yamaguchi. *J*-model for magnetism and superconductivity of triangular, kagome, and related spin lattice systems. *International Journal of Quantum Chemistry*, 100(6):1179–1196, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yongjun:2001:ESF

[YYXC01] Liu Yongjun, Liu Ying, Zhao Xian, and Liu Chengbu. Electronic spectra and first-order hyperpolarizability of 4-(dicyanomethylene)-2,6-bis-(2′-thiophene-vinyl)-pyran derivatives. *International Journal of Quantum Chemistry*, 82(2): 65–72, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/77502749/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/77502749/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=77502749&PLACEBO=IE.pdf.

Yoshimoto:2000:NMC

[YYY+00] T. Yoshimoto, A. Yoshinaga, A. Yamada, Y. Ohta, and K. Nishikawa. Nonadiabatic Monte Carlo simulation of H and H_3. *International Journal of Quantum Chemistry*, 80 (4–5):907–915, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505402/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505402/FILE?TPL=ftx_start; http://www3.interscience.

wiley.com/cgi-bin/fulltext?ID=73505402&PLACEBO=IE.pdf.

Yamaki:2005:DHM

[YYY05] Daisuke Yamaki, Koji Yasuda, and Kizashi Yamaguchi. Determination of the Hubbard model parameters by using the unrestricted Hartree–Fock solutions, and improvement of their energies. *International Journal of Quantum Chemistry*, 103(1):73–81, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaguchi:2001:TDD

[YYYM01] Yoichi Yamaguchi, Yasunori Yokomichi, Shiyoshi Yokoyama, and Shinro Mashiko. Time-dependent density functional calculations of the Q-like bands of phenylene-linked free-base and zinc porphyrin dimers. *International Journal of Quantum Chemistry*, 84(3):338–347, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/84502346/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502346/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502346&PLACEBO=IE.pdf.

Yan:2005:MPG

[YYZ05a] Weigen Yan, Yeong-Nan Yeh, and Fuji Zhang. On the matching polynomials of graphs with small number of cycles of even length. *International Journal of Quantum Chemistry*, 105 (2):124–130, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yan:2005:OCT

[YYZ05b] Weigen Yan, Yeong-Nan Yeh, and Fuji Zhang. Ordering the complements of trees by the number of maximum matchings. *International Journal of Quantum Chemistry*, 105(2): 131–141, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2005:TSM

[YYZ+05c] Guanghui Yang, Li Yao, Xin Zhang, Qingtian Meng, and Ke-Li Han. Theoretical study of the mechanism for spin-forbidden quenching process $O(^1D) + CO_2\ (^1\Sigma) \rightarrow O(^3P) + CO_2\ (^1\Sigma)$. *International Journal of Quantum Chemistry*, 105

(2):154–159, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yuldasheva:2007:QCE

[YZ07] Gulnara Yuldasheva and Georgii M. Zhidomirov. Quantum-chemical examination of interaction of cytostatic-fluorouracil with deoxyribonucleic acids. *International Journal of Quantum Chemistry*, 107(13):2384–2388, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2008:KIL

[YZ08] Yujun Yang and Heping Zhang. Kirchhoff index of linear hexagonal chains. *International Journal of Quantum Chemistry*, 108(3):503–512, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yin:2009:CDH

[YZC09] Aixia Yin, Guiqiu Zhang, and Dezhan Chen. Chiral discrimination in hydrogen-bonded complexes of butan-2-ol (m-form) and hydrogen peroxide. *International Journal of Quantum Chemistry*, 109(7):1472–1480, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2006:BSR

[YZG06] Yong Yang, Weijun Zhang, and Xiaoming Gao. Blue-shifted and red-shifted hydrogen bonds: Theoretical study of the $CH_3CHO\cdots HNO$ complexes. *International Journal of Quantum Chemistry*, 106(5):1199–1207, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yao:2008:ESS

[YZW+08] Shujuan Yao, Chenggang Zhou, Jinping Wu, Jiaye Li, Bo Han, and Hansong Cheng. On the electronic structures and spectroscopic properties of polyyne and its derivatives. *International Journal of Quantum Chemistry*, 108(9):1565–1571, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2008:WPT

[YZX+08] Sheng-Yong Yang, Jun Zou, Ming-Li Xiang, Guo-Bin Xie, Bing Shi, and Yu-Quan Wei. Whether proton transition to the triphosphate tail of ATP occurs at protein kinase environment: A Car–Parrinello ab initio molecular dynamics study.

International Journal of Quantum Chemistry, 108(7):1239–1245, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yin:2001:PPT

[YZY+01] Hong-Ming Yin, Rui-Qin Zhang, Ben-Hui Yang, Ke-Li Han, and Guo-Zhong He. The properties and possible transformation path for $C_{12}B_{24}N_{24}$. *International Journal of Quantum Chemistry*, 84(3):363–368, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/84502350/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84502350/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84502350&PLACEBO=IE.pdf`.

Zurek:2009:NCC

[ZA09] Eva Zurek and Jochen Autschbach. NMR computations for carbon nanotubes from first principles: Present status and future directions. *International Journal of Quantum Chemistry*, 109(14):3343–3367, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zakharov:2004:ECS

[Zak04a] A. Yu Zakharov. Ensembles in classical statistical mechanics and their unification via nonlinear field theory. *International Journal of Quantum Chemistry*, 100(4):442–447, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zakharov:2004:IFR

[Zak04b] A. Yu. Zakharov. Intermolecular forces and random fields: Mutual renormalizations in classical statistical mechanics. *International Journal of Quantum Chemistry*, 96(3):234–238, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zalesny:2005:PRS

[ZB05] Robert Zaleśny and Wojciech Bartkowiak. Performance of the reduced-size polarized Z3PolX basis set in calculations of vibrational polarizabilities, infrared, and Raman intensities: Application to formaldehyde molecule. *International Journal*

of Quantum Chemistry, 104(5):660–666, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zechmann:2008:ISP

[ZB08] Gunther Zechmann and Mario Barbatti. Ab initio study of the photochemistry of aminopyrimidine. *International Journal of Quantum Chemistry*, 108(7):1266–1276, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zope:2008:CSU

[ZBPD08] Rajendra R. Zope, Tunna Baruah, Mark R. Pederson, and B. I. Dunlap. Comparative study of unscreened and screened molecular static linear polarizability in the Hartree–Fock, hybrid-density functional, and density functional models. *International Journal of Quantum Chemistry*, 108(2):307–317, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2002:TCA

[ZCFD02] Zhengyu Zhou, Xueli Cheng, Aiping Fu, and Dongmei Du. Theoretical calculation of activation energy barrier from vibrational frequencies for the reaction of $O(^3P)$ with CHFCl. *International Journal of Quantum Chemistry*, 87(5):280–287, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/90512110/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/90512110/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=90512110&PLACEBO=IE.pdf`.

Zhang:2004:LNF

[ZCWZ04] Congjie Zhang, Zexing Cao, Haishun Wu, and Qianer Zhang. Linear and nonlinear feature of electronic excitation energy in carbon chains $HC_{2n+1}H$ and $HC_{2n}H$. *International Journal of Quantum Chemistry*, 98(3):299–308, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2000:ISG

[ZCZ00] Q.-M. Zhang, Huimin Cai, and Zhenyu Zhang. Ab initio studies of Ge addimers on the Si(100) surface. *International Journal of Quantum Chemistry*, 80(4–5):708–712, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73505395/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505395/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505395&PLACEBO=IE.pdf.

Zhang:2007:TDD

[ZCZ+07] Yuexing Zhang, Xue Cai, Xianxi Zhang, Hui Xu, Zhongqiang Liu, and Jianzhuang Jiang. Time-dependent density functional theory studies of the electronic absorption spectra of metallophthalocyanines of group IVA. *International Journal of Quantum Chemistry*, 107(4):952–961, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2009:BGP

[ZCZC09] Hong Zhang, Frankie Cheung, Feng Zhao, and Xin-Lu Cheng. Band gaps and the possible effect on impact sensitivity for some nitro aromatic explosive materials. *International Journal of Quantum Chemistry*, 109(7):1547–1552, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2002:CSD

[ZCZF02] Zhengyu Zhou, Guang Chen, Xingmin Zhou, and Hui Fu. Computational studies on density function theory for the bimolecular metathesis reaction $CH_3 + HCl \leftrightarrow CH_4 + Cl$. *International Journal of Quantum Chemistry*, 87(1):49–57, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85515905/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85515905/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85515905&PLACEBO=IE.pdf.

Zhang:2006:IQC

[ZD06] Weichao Zhang and Benni Du. Ab initio quantum chemical studies of reaction mechanism for CN with CH_2CO. *International Journal of Quantum Chemistry*, 106(5):1076–1085, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2007:IQC

[ZD07a] Weichao Zhang and Benni Du. Ab initio quantum chemical studies of the reactions of CF_3CFHO_2 with HO_2. *International Journal of Quantum Chemistry*, 107(1):46–55, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zheng:2007:HEV

[ZD07b] Yujun Zheng and Shiliang Ding. Highly excited vibrational levels of triatomic molecule N_2O: U(4) algebraic model. *International Journal of Quantum Chemistry*, 107(4):1008–1014, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zheng:2008:PES

[ZD08] Yujun Zheng and Shiliang Ding. Potential energy surface and highly excited vibrational lines of NO_2 via algebraic approach. *International Journal of Quantum Chemistry*, 108(6):1059–1066, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2003:TII

[ZDAZ03] Zhengyu Zhou, Benni Du, Fu Aiping, and Weichao Zhang. Theoretical investigation of the isomers photolysis reaction for chlorine nitrate. *International Journal of Quantum Chemistry*, 94(1):44–50, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2008:MGP

[ZDMF08] Weichao Zhang, Benni Du, Lailong Mu, and Changjun Feng. Mechanism for the gas-phase reaction between OH and 3-methylfuran: A theoretical study. *International Journal of Quantum Chemistry*, 108(7):1232–1238, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zakrzewski:2000:EEP

[ZDO00] V. G. Zakrzewski, O. Dolgounitcheva, and J. V. Ortiz. Efficient electron propagator algorithms for shakeup final states: Anthracene and acridine. *International Journal of Quantum Chemistry*, 80(4–5):836–841, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.`

wiley.com/cgi-bin/abstract/73505404/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505404/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505404&PLACEBO=IE.pdf.

Zakrzewski:2009:SCE

[ZDO09] Viatcheslav G. Zakrzewski, Olga Dolgounitcheva, and J. V. Ortiz. Strong correlation effects in the electron binding energies of phthalocyanine. *International Journal of Quantum Chemistry*, 109(15):3619–3625, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2008:FPM

[ZDQF08] Jiang-Bo Zhu, Guo-Liang Dai, Ming-Hua Qiao, and Kang-Nian Fan. First principle MD study on the structural and electronic properties of liquid and amorphous $NI_{81}B_{19}$ and $NI_{80}P_{20}$ alloy. *International Journal of Quantum Chemistry*, 108(2):370–377, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zakjevskii:2007:EPS

[ZDZO07] V. V. Zakjevskii, O. Dolgounitcheva, V. G. Zakrzewski, and J. V. Ortiz. Electron propagator studies of vertical electron detachment energies and isomerism in purinic deoxyribonucleotides. *International Journal of Quantum Chemistry*, 107 (12):2266–2273, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zerner:2000:IKR

[Zer00] Michael C. Zerner. Introduction: Klaus Rüdenberg. *International Journal of Quantum Chemistry*, 76(2):115–130, January 15, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/69503165/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503165/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503165&PLACEBO=IE.pdf.

Zerner:2000:NOP

[ZFD+00a] Michael C. Zerner, Walter M. F. Fabian, Renate Dworczak, Dietmar W. Kieslinger, Gert Kroner, Hans Junek, and Max E. Lippitsch. Nonlinear optical properties of dicyanomethylene-derived heteroaromatic dyes: Semiempirical molecular or-

bital calculations and experimental investigations. *International Journal of Quantum Chemistry*, 79(4):253–266, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72512060/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72512060/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72512060&PLACEBO=IE.pdf`.

Zhou:2000:SDF

[ZFD00b] Zhengyu Zhou, Aiping Fu, and Dongmei Du. Studies on density functional theory for the electron-transfer reaction mechanism between M-C_6H_6 and M^+-C_6H_6 complexes in the gas phase. *International Journal of Quantum Chemistry*, 78(3):186–194, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71007687/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71007687/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71007687&PLACEBO=IE.pdf`.

Zanella:2005:ESP

[ZFD05] Ivana Zanella, A. Fazzio, and Antônio J. R. Da Silva. Electronic and structural properties of $C_{59}Si$ on the monohydride Si(100) surface. *International Journal of Quantum Chemistry*, 103(5):557–561, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2005:TSRb

[ZFFX05] Jie Zhang, Shengyu Feng, Dacheng Feng, and Ju Xie. Theoretical study of 1,2-rearrangement in silylmethanethiol. *International Journal of Quantum Chemistry*, 105(1):57–65, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zaider:2000:TSS

[ZFLL00] Marco Zaider, Albert Y. C. Fung, Jingdong Li, and J. Ladik. From track structure to stochastic chemistry and DNA damage: Microdosimetric perspective. *International Journal of Quantum Chemistry*, 80(3):327–340, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/73501013/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501013/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501013&PLACEBO=IE.pdf.

Zhang:2008:MKP

[ZFZ+08] Jianguo Zhang, Lina Feng, Shaowen Zhang, Hong Zheng, Tonglai Zhang, Li Yang, and Huihui Zheng. Mechanisms and kinetics for preparing carbohydrazide by reacting dimethyl carbonate with hydrazine: A theoretical study. *International Journal of Quantum Chemistry*, 108(9):1555–1564, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2003:DLA

[ZGY+03] Xian Zhao, Daren Guan, Xizhang Yi, Guibao Xu, and Minhua Jiang. Dynamic Lie algebraic formulation of second-order optical nonlinearity for substituted benzenes. *International Journal of Quantum Chemistry*, 93(5):335–343, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2005:APS

[ZH05] Jian-Ge Zhou and Frank Hagelberg. Adsorption of 1-propanol on the Si(100) surface. *International Journal of Quantum Chemistry*, 105(4):359–367, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2006:HOS

[ZH06] Xin Zhang and Ke-Li Han. High-order symplectic integration in quasi-classical trajectory simulation: Case study for $O(^1D) + H_2$. *International Journal of Quantum Chemistry*, 106(8): 1815–1819, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhanpeisov:2001:SCR

[ZHA01] Nurbosyn U. Zhanpeisov, Shinya Higashimoto, and Masakazu Anpo. Selective catalytic reduction of nitric oxide with ammonia: A theoretical ab initio study. *International Journal of Quantum Chemistry*, 84(6):677–685, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-

bin/abstract/84002452/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/84002452/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=84002452&PLACEBO=IE.pdf.

Zhou:2007:UBZ

[Zho07] Bo Zhou. Upper bounds for the Zagreb indices and the spectral radius of series-parallel graphs. *International Journal of Quantum Chemistry*, 107(4):875–878, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhechkov:2006:PGP

[ZHS06] Lyuben Zhechkov, Thomas Heine, and Gotthard Seifert. Physisorption of N_2 on graphene platelets: An Ab initio study. *International Journal of Quantum Chemistry*, 106(6):1375–1382, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ziesche:2002:CMH

[Zie02] P. Ziesche. Cumulant 2-matrix of the high-density electron gas and the density matrix functional theory. *International Journal of Quantum Chemistry*, 90(1):342–354, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zivkovic:2009:EMT

[Živ09] Tomislav P. Živković. Exact mathematical treatment of the modifications of finite-dimensional quantum systems. *International Journal of Quantum Chemistry*, 109(13):2831–2859, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2000:IPS

[ZJZ00] Yongfang Zhao, Xiaogong Jing, and Mingyu Zhang. Ab initio pseudopotential study of M_2 As^- and M_2 Br^+ (M = Cu, Ag, Au). *International Journal of Quantum Chemistry*, 80(1): 38–43, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72515497/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72515497/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72515497&PLACEBO=IE.pdf.

Zhang:2003:GTB

[ZKB03] X.-G. Zhang, P. S. Krstić, and W. H. Butler. Generalized tight-binding approach for molecular electronics modeling. *International Journal of Quantum Chemistry*, 95(4–5):394–403, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhukovskii:2007:PMQ

[ZKEE07] Yuri F. Zhukovskii, Eugene A. Kotomin, Robert A. Evarestov, and Donald E. Ellis. Periodic models in quantum chemical simulations of F centers in crystalline metal oxides. *International Journal of Quantum Chemistry*, 107(14):2956–2985, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zverev:2007:SRE

[ZKRS07] Vladislav V. Zverev, Valeriy I. Kovalenko, Irina P. Romanova, and Oleg G. Sinyashin. Structure and relative energies of regioisomers and valence isomers of C_{60} adducts. HF and DFT study. *International Journal of Quantum Chemistry*, 107(13): 2442–2453, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhanpeisov:2004:IBG

[ZKYA04] Nurbosyn U. Zhanpeisov, Yukiya Kanazawa, Hiromi Yamashita, and Masakazu Anpo. Intrinsic band gap shift in Ti silicalites modified by V ion implantation: Ab initio and density functional theory study. *International Journal of Quantum Chemistry*, 96(4):349–354, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2000:ISI

[ZL00] Yu-Fang Zhou and Cheng-Bu Liu. Ab initio study of ice catalyzation of HOCl + HCl reaction. *International Journal of Quantum Chemistry*, 78(4):281–284, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72000072/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72000072/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72000072&PLACEBO=IE.pdf`.

Zhao:2004:KSS

[ZL04] Jun Fang Zhao and Qian Shu Li. A kinetic stability study of MN_5^+ (M = Be, Mg, Ca, Sr, and Ba). *International Journal of Quantum Chemistry*, 98(6):485–494, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2006:TSM

[ZL06] Yi-Quan Zhang and Cheng-Lin Luo. Theoretical study of the magnetic exchange coupling behavior substituting Cr(III) with Mo(III) in cyano-bridged transition metal complexes. *International Journal of Quantum Chemistry*, 106(7):1551–1560, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zaporotskova:2004:SRH

[ZLC04] I. V. Zaporotskova, N. G. Lebedev, and L. A. Chernozatonskii. Single and regular hydrogenation and oxidation of carbon nanotubes: MNDO calculations. *International Journal of Quantum Chemistry*, 96(2):149–154, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2007:TSS

[ZLF+07] Feng Zhu, Rui Li, Dacheng Feng, Maoxia He, and Zhengting Cai. Theoretical studies of sulbactam: Reactions after acylation. *International Journal of Quantum Chemistry*, 107(9): 1925–1934, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zuo:2008:BFA

[ZLH+08] Ming-Hui Zuo, Hui-Ling Liu, Xu-Ri Huang, Jin-Hui Zhan, and Chia-Chung Sun. A barrier-free atomic radical-molecule reaction: N (^{2}D NO_2 ($^2A_1$)) mechanistic study. *International Journal of Quantum Chemistry*, 108(8):1309–1315, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2002:ISR

[ZLHL02] Dongju Zhang, Yongjun Liu, Haiquan Hu, and Chengbu Liu. Inner-sphere reorganization for redox pairs $M(NH_3)_6^{2+/3+}$ (M = Mn, Fe, and Co): Models and calculations. *International Journal of Quantum Chemistry*, 86(5):468–477, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print),

1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/86011221/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/86011221/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=86011221&PLACEBO=IE.pdf`.

Zheng:2009:IBT

[ZLJ+09] Guishan Zheng, Marcus Lundberg, Jacek Jakowski, Thom Vreven, Michael J. Frisch, and Keiji Morokuma. Implementation and benchmark tests of the DFTB method and its application in the ONIOM method. *International Journal of Quantum Chemistry*, 109(9):1841–1854, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2005:TSRa

[ZLL+05] Aihua Zhang, Kun Liu, Lan Li, Siyu Ma, and Zonghe Li. Theoretical study of the ring-closing reaction of 5′-AMP to cAMP and H_2O in the gas phase. *International Journal of Quantum Chemistry*, 104(3):373–378, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2009:TSSa

[ZLL+09a] Jinglai Zhang, Yonghong Li, Junfeng Li, Xing Chen, and Zexing Cao. Theoretical studies on structures and electronic spectra of linear carbon chains $C_{2n}H^+$ ($n = 1--5$). *International Journal of Quantum Chemistry*, 109(5):1116–1126, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2009:TSSb

[ZLL+09b] Min Zhang, Ze-Sheng Li, Yan Li, Jia Liu, and Jia-Zhong Sun. Theoretical study on the spectroscopic properties and electronic structures of heteroleptic phosphorescent Ir(III) complexes. *International Journal of Quantum Chemistry*, 109(6): 1167–1176, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2005:TSS

[ZLML05] Hongmei Zhao, Kun Liu, Siyu Ma, and Zonghe Li. Theoretical study of stabling function of the NO to the $(CH_3)_3$ CO · radical. *International Journal of Quantum Chemistry*, 101 (1):113–117, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zheng:2007:PES

[ZLS07] Xuehe Zheng, Ngan M. Ly, and Alexei A. Stuchebrukhov. Photoactivated excited states of DNA repair photolyase: Dynamical and semiempircal identification. *International Journal of Quantum Chemistry*, 107(15):3126–3131, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2006:TSH

[ZLSL06] Aihua Zhang, Lan Li, Shujuan Sun, and Zonghe Li. Theoretical studies of the hydrolysis reaction of 5′-AMP. *International Journal of Quantum Chemistry*, 106(8):1870–1877, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2007:TSR

[ZLX+07] Hongyu Zhang, Qimin Liang, Yueyuan Xia, Mingwen Zhao, Yanju Ji, Chen Song, Xiangdong Liu, and Bingyun Zhang. Theoretical study of the ·H reaction with cytosine. *International Journal of Quantum Chemistry*, 107(1):240–246, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2007:SSC

[ZLXL07] Yi Zhao, Nan Li, Wen Guo Xu, and Qian Shu Li. Structure and stability of Be_6, Be, and Be clusters. *International Journal of Quantum Chemistry*, 107(1):81–91, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2005:MEI

[ZLY05] Yi-Quan Zhang, Cheng-Lin Luo, and Zhi Yu. Magnetic exchange interactions in cyano-bridged Mo^{III} binuclear complexes: Broken-symmetry and density functional theory calculations. *International Journal of Quantum Chemistry*, 102 (2):165–173, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2009:BCA

[ZLY+09] Zhong-Jun Zhou, Hui-Ling Liu, Jian-Kang Yu, Guang-Tao Yu, and Xu-Ri Huang. Bonding and correlation analysis of various Si_2CO isomers on the potential energy surface. *International Journal of Quantum Chemistry*, 109(5):907–919,

???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2005:TPE

[ZLZ05] Jian-Guo Zhang, Qian Shu Li, and Shao-Wen Zhang. Triplet potential energy surface for BH_2N: A DFT study. *International Journal of Quantum Chemistry*, 103(4):422–431, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhanpeisov:2004:CCB

[ZMAL04] Nurbosyn U. Zhanpeisov, Kazuhiko Mizuno, Masakazu Anpo, and Jerzy Leszczynski. C_1 C_2 bond cleavage in vinylidenecyclopropanes: Theoretical density functional theory study. *International Journal of Quantum Chemistry*, 96(4):343–348, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zamora:2003:CES

[ZMB+03] Miguel A. Zamora, Marcelo F. Masman, José A. Bombasaro, Mónica L. Freile, Valdir Cechinel Filho, Silvia N. López, Susana A. Zacchino, and Ricardo D. Enriz. Conformational and electronic study of N-phenylalkyl-3,4-dichloromaleimides: Ab initio and DFT study. *International Journal of Quantum Chemistry*, 93(1):32–46, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zeng:2009:CNM

[ZMMK09] Tao Zeng, Hirotoshi Mori, Eisaku Miyoshi, and Mariusz Klobukowski. Calibration of new model core potentials for main group elements. *International Journal of Quantum Chemistry*, 109(14):3235–3245, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zaragoza:2000:DSI

[ZMMS+00] I. P. Zaragoza, J. M. Martínez-Magadán, R. Santamaria, D. Dixon, and M. Castro. DFT study of the interaction of the HZSM-5 zeolite with the benzene molecule. *International Journal of Quantum Chemistry*, 80(2):125–132, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73001287/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73001287/`

FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73001287&PLACEBO=IE.pdf.

Zheng:2005:DIW

[ZMS05] Xuehe Zheng, Dmitry M. Medvedev, and Alexei A. Stuchebrukhov. Does internal water influence electron tunneling in proteins? Example of cytochrome c oxidase. *International Journal of Quantum Chemistry*, 102(5):473–479, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2005:NPD

[ZMX+05] Mei-Yu Zhao, Qing-Tian Meng, Ting-Xian Xie, Ke-Li Han, and Guo-Zhong He. Nonadiabatic photodissociation dynamics. *International Journal of Quantum Chemistry*, 101(2):153–159, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2000:TPS

[ZMZ+00] Lixin Zhou, Chaoyong Mang, Yongfan Zhang, Shengchang Xiang, and Zunxing Huang. Theoretical predictions of the structure, gas-phase acidity, and aromaticity of tetrathiosquaric acid. *International Journal of Quantum Chemistry*, 78 (6):443–449, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/72502339/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72502339/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72502339&PLACEBO=IE.pdf.

Zhang:2009:PES

[ZMZ+09] Y. H. Zhang, J. Meng, X. Q. Zhang, Hui Li, and C. A. Taft. Pressure effects on the structural, electronic, and optical properties of Si_n @SWCNTs. *International Journal of Quantum Chemistry*, 109(6):1385–1395, May 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhanpeisov:2005:DFTa

[ZNF05] N. U. Zhanpeisov, S. Nishio, and H. Fukumura. Density functional theory study of vibrational properties of the 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) molecule: IR,

Raman, and UV-vis spectra. *International Journal of Quantum Chemistry*, 105(4):368–375, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Znojil:2000:NPM

[Zno00] Miloslav Znojil. New perturbation method with the matching of wave functions. *International Journal of Quantum Chemistry*, 79(4):235–242, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72512063/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/72512063/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72512063&PLACEBO=IE.pdf`.

Zulicke:2000:IDC

[ZNZS00] L. Zülicke, R. Neumann, Ch. Zuhrt, and J. Schretter. Intramolecular dynamics of cationic van der Waals complexes: Case study of $ArHCl^+$. *International Journal of Quantum Chemistry*, 80(3):486–498, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73501026/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73501026/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73501026&PLACEBO=IE.pdf`.

Zhanpeisov:2005:DFTb

[ZOK+05] N. U. Zhanpeisov, K. Ohta, S. Kajimoto, J. Hobley, K. Hatanaka, and H. Fukumura. Density functional theory study of the origin of IR and Raman band shifts in H-bond complexes of triethylamine with water. *International Journal of Quantum Chemistry*, 105(4):376–386, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zotev:2006:CNM

[Zot06] V. S. Zotev. Comment on "New methods for old Coulomb few-body problems". *International Journal of Quantum Chemistry*, 106(2):550–551, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2004:DFT

[ZPW+04] Ziyan Zhou, Xiumei Pan, Xue Wu, Zhongmin Su, Yuhe Kan, and Yuzhong Xie. Density functional theory study on isomerization reactions of pyridazine derivatives bearing N,N-dialkylaminoethyl group. *International Journal of Quantum Chemistry*, 98(6):515–521, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2002:DFC

[ZQF+02] Zhengyu Zhou, Yuhui Qu, Aiping Fu, Benni Du, Faxin He, and Hongwei Gao. Density functional complete study of hydrogen bonding between the water molecule and the hydroxyl radical ($H_2O\cdots HO$). *International Journal of Quantum Chemistry*, 89(6):550–558, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2003:AOC

[ZR03] Wusheng Zhu and Herschel Rabitz. Attaining optimal controls for manipulating quantum systems. *International Journal of Quantum Chemistry*, 93(2):50–58, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zeng:2007:DFT

[ZR07] Yi Zeng and Yi Ren. Density functional theory study of tautomerization of 2-aminothiazole in the gas phase and in solution. *International Journal of Quantum Chemistry*, 107 (1):247–258, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zou:2009:SEO

[ZRF+09] Lu-Yi Zou, Ai-Min Ren, Ji-Kang Feng, Xue-Qin Ran, Yan-Ling Liu, and Chia-Chung Sun. Structural, electronic, and optical properties of phenol-pyridyl boron complexes for light-emitting diodes. *International Journal of Quantum Chemistry*, 109(7):1419–1429, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2005:TII

[ZRRC05] Hua-Jie Zhu, Yi Ren, Jie Ren, and San-Yan Chu. Theoretical investigation of ion pair S_N 2 reactions of alkali isothiocyanates with alkyl halides. Part 1. Reaction of lithium isothiocyanate and methyl fluoride with inversion mechanism. *In-*

ternational Journal of Quantum Chemistry, 101(1):104–112, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zayets:2004:TSC

[ZS04a] Valentin A. Zayets and Elena F. Sheka. TUNCUR: Sequential codes for semiempirical quantum chemical calculations of tunneling current. *International Journal of Quantum Chemistry*, 100(4):695–708, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zielinski:2004:SSD

[ZS04b] Ryszard Zieliński and Henryk Szymusiak. Structure of stable double-ionic model water clusters of quaternary alkylammonium surfactants with some monovalent counterions as derived by the DFT method. *International Journal of Quantum Chemistry*, 99(5):724–734, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zahradnik:2005:FPC

[ZŠ05] Rudolf Zahradník and Libuše Šroubková. Formation and physical characteristics of van der Waals molecules, cations, and anions: Estimates of complete basis set values. *International Journal of Quantum Chemistry*, 104(1):52–63, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhidomirov:2004:PMS

[ZSKV04] G. M. Zhidomirov, A. A. Shubin, V. B. Kazansky, and R. A. Van Santen. Possible molecular structure of promoted Lewis acidity sites in ZnZSM-5. *International Journal of Quantum Chemistry*, 100(4):489–494, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2009:DSR

[ZSL+09] Jinsheng Zhang, Wei Shen, Ruiqiu Liu, Youqing Yu, Hailing Wu, and Ming Li. DFT study on Ru^{II}-catalyzed cyclization of terminal alkynals to cycloalkenes. *International Journal of Quantum Chemistry*, 109(4):679–687, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zheng:2001:TSR

[ZSM+01] Neng Wu Zheng, Yujie Sun, Dongxia Ma, Ruyi Yang, Tao Zhou, and Tao Wang. Theoretical study on regularity of changes in quantum defects in Rydberg state series of many-valence electron atoms within WBEPM theory. *International Journal of Quantum Chemistry*, 81(3):232–237, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76504671/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76504671/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=76504671&PLACEBO=IE.pdf`.

Zambrano:2003:SEP

[ZSPS03] Cesar Zambrano, Alfredo Sanchez, Luis Miguel Procel, and Arvids Stashans. Structural and electronic properties of $PbZr_xTi_{1-x}O_3$ ($x = 0.5, 0.375$): A quantum chemical study. *International Journal of Quantum Chemistry*, 95(1):37–43, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zheng:2000:TPL

[ZSW+00] Neng-Wu Zheng, Yu-Jie Sun, Tao Wang, Dong-Xia Ma, Yi Zhang, and Wei Su. Transition probability of lithium atom and lithiumlike ions with weakest bound electron wave functions and coupled equations. *International Journal of Quantum Chemistry*, 76(1):51–61, January 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/69503195/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/69503195/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=69503195&PLACEBO=IE.pdf`.

Zhang:2007:NMM

[ZSWL07] Dongju Zhang, Hui Sun, Fang Wang, and Chengbu Liu. NO migration from N-methyl-N-nitrosobenzene-sulfonamide to 3,6-dibromocarbazole: Concerted or stepwise reaction path? *International Journal of Quantum Chemistry*, 107(7): 1585–1589, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zaitsevskii:2002:IQC

[ZT02] Andréi Zaitsevskii and Christian Teichteil. Ab initio quasirelativistic calculations on electronic transitions in ICl by the multireference many-body perturbation theory. *International Journal of Quantum Chemistry*, 88(4):426–432, June 15, 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2004:TPD

[ZT04a] Wuming Zhu and S. B. Trickey. Tests of perturbative DFT total energy estimates implemented in a Gaussian basis. *International Journal of Quantum Chemistry*, 100(3):245–253, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ziesche:2004:MES

[ZT04b] P. Ziesche and F. Tasnádi. Methods for electronic-structure calculations: Overview from a reduced-density-matrix point of view. *International Journal of Quantum Chemistry*, 100 (4):495–508, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2008:MER

[ZT08] Bo Zhou and Nenad Trinajstić. Maximum eigenvalues of the reciprocal distance matrix and the reverse Wiener matrix. *International Journal of Quantum Chemistry*, 108(5):858–864, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2009:KIM

[ZT09] Bo Zhou and Nenad Trinajstić. The Kirchhoff index and the matching number. *International Journal of Quantum Chemistry*, 109(13):2978–2981, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhekova:2007:TSS

[ZTI+07] H. Zhekova, A. Tadjer, A. Ivanova, J. Petrova, and N. Gospodinova. Theoretical study of the structure and electronic spectra of fully protonated emeraldine oligomers. *International Journal of Quantum Chemistry*, 107(8):1688–1706, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ziesche:2000:HCS

[ZTSP00] Paul Ziesche, Jianmin Tao, Michael Seidl, and John P. Perdew. How correlation suppresses density fluctuations in the uniform electron gas of one, two, or three dimensions. *International Journal of Quantum Chemistry*, 77(5):819–830, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71000345/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71000345/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71000345&PLACEBO=IE.pdf`.

Zhu:2007:QCS

[ZTSZ07] Yanyan Zhu, Mingsheng Tang, Xiaoyu Shi, and Yufen Zhao. Quantum chemical study of cyclic dipeptides. *International Journal of Quantum Chemistry*, 107(3):745–753, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2009:GPP

[ZTW+09] Jing Zhao, Ming-Sheng Tang, Dong-Hui Wei, Chu-Feng Zhao, Wen-Jing Zhang, and Hong-Ming Wang. Gas-phase pyrolysis mechanisms of 3-anilino-1-propanol: Density functional theory study. *International Journal of Quantum Chemistry*, 109 (5):1036–1044, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zagidullina:2007:QCI

[ZVVT07] Aygul E. Zagidullina, Ivan V. Vakulin, Olga S. Vostrikova, and Rifkat F. Talipov. Quantum chemical investigation of donor–acceptor complexes of trimethylaluminum with Lewis bases of group 15 elements. *International Journal of Quantum Chemistry*, 107(13):2372–2377, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zheng:2003:IPE

[ZW03] Neng Wu Zheng and Tao Wang. Ionization potential of excited states of Be-like sequence in the concept of iso-spectrum-level series. *International Journal of Quantum Chemistry*, 93 (5):344–350, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zheng:2004:CES

[ZW04] Neng Wu Zheng and Tao Wang. Calculation of excited-state ionization potential for boron-like sequence. *International Journal of Quantum Chemistry*, 98(6):495–501, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2007:ATE

[ZW07] Baojing Zhou and Yan Alexander Wang. An accurate total energy density functional. *International Journal of Quantum Chemistry*, 107(15):2995–3000, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2009:PWA

[ZW09a] Yu Zhang and J. L. Whitten. Photoemission into water adsorbed on metals: Probing dissociative electron transfer using theory. *International Journal of Quantum Chemistry*, 109 (15):3541–3551, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2009:UDV

[ZW09b] Yu Adam Zhang and Yan Alexander Wang. Are the unconventional density variations really unconventional? *International Journal of Quantum Chemistry*, 109(14):3199–3216, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2002:ISE

[ZWJ02a] Weihua Zhu, Guo-Shi Wu, and Yuansheng Jiang. Incorporation of solvent effects into density functional predictions of molecular polarizabilities and hyperpolarizabilities. *International Journal of Quantum Chemistry*, 86(4):347–355, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/88010695/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/88010695/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=88010695&PLACEBO=IE.pdf`.

Zhu:2002:SEM

[ZWJ02b] Weihua Zhu, Guo-Shi Wu, and Yuansheng Jiang. Substitution effects on the molecular structures and the lon-

gitudinal molecular polarizabilities of all-trans polyacetylene oligomers of increasing size. *International Journal of Quantum Chemistry*, 86(4):390–400, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/85515906/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85515906/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85515906&PLACEBO=IE.pdf`.

Zheng:2004:WBE

[ZWM+04] Neng-Wu Zheng, Tao Wang, Dong-Xia Ma, Tao Zhou, and Jing Fan. Weakest bound electron potential model theory. *International Journal of Quantum Chemistry*, 98(3):281–290, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zheng:2002:SMP

[ZWMZ02] Nengwu Zheng, Tao Wang, Dongxia Ma, and Tao Zhou. Simple method for the precise calculation of atomic energy levels of IB elements in the periodic table. *International Journal of Quantum Chemistry*, 87(5):293–302, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/91012969/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91012969/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91012969&PLACEBO=IE.pdf`.

Zhang:2004:AGM

[ZWMZ04] Liling Zhang, Wei Wu, Yirong Mo, and Qianer Zhang. Applications of graphic method to C_{20}, C_{60}, and achiral single-wall nanotubes. *International Journal of Quantum Chemistry*, 98 (1):51–58, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhuo:2001:RPE

[ZWSJ01] Shuping Zhuo, Jichong Wei, Changsheng Shen, and Guanzhi Ju. Rules on pair electron correlation in MOH (M = H, Li, Na). *International Journal of Quantum Chemistry*, 83(6):311–317, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/81502111/START; http:`

//www3.interscience.wiley.com/cgi-bin/fulltext/81502111/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=81502111&PLACEBO=IE.pdf.

Zhang:2002:TSH

[ZXX02] Ji Zhang, Jijun Xiao, and Heming Xiao. Theoretical studies on heats of formation for cubylnitrates using density functional theory B3LYP method and semiempirical MO methods. *International Journal of Quantum Chemistry*, 86(3):305–312, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/85004525/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/85004525/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=85004525&PLACEBO=IE.pdf.

Zhang:2009:FPS

[ZXZ+09] Hong Zhang, Lian-Jun Xu, Fu-Chun Zhang, Xin-Lu Cheng, and Guang-Wen An. First principles study on the structure and electronic properties of 2-nitrimino-1-nitroimidazolidine. *International Journal of Quantum Chemistry*, 109(4):720–725, March 15, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zheng:2004:FEC

[ZY04] Weiying Zheng and Lung-An Ying. Finite-element calculations for the helium atom. *International Journal of Quantum Chemistry*, 97(1):659–669, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2006:TMH

[ZY06] Yi-Liang Zhang and Zhong-Zhi Yang. Tautomerism and the maximum hardness principle. *International Journal of Quantum Chemistry*, 106(8):1723–1735, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2007:RDK

[ZY07] Heping Zhang and Yujun Yang. Resistance distance and Kirchhoff index in circulant graphs. *International Journal of Quantum Chemistry*, 107(2):330–339, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2009:CDH

[ZYC09] Guiqiu Zhang, Aixia Yin, and Dezhan Chen. Chiral discrimination in hydrogen-bonded complexes of 2-methylol oxirane with hydrogen peroxide. *International Journal of Quantum Chemistry*, 109(5):920–930, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zheng:2000:RIM

[ZYG00] Yujun Zheng, Xizhang Yi, and Daren Guan. Rotationally inelastic molecule-surface scattering: dynamical lie algebraic method. *International Journal of Quantum Chemistry*, 76(4):500–510, February 5, 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/70000681/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/70000681/FTSTART; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=70000681&PLACEBO=IE.pdf`.

Zhang:2005:FQM

[ZZ05] Da W. Zhang and John Z. H. Zhang. Full quantum mechanical study of binding of HIV-1 protease drugs. *International Journal of Quantum Chemistry*, 103(3):246–257, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2009:TSR

[ZZC09] Hongwei Zhou, Zhiqiang Zhang, and Hon-Yeung Cheung. Theoretical study on the reactive sites and intramolecular interactions in taxol and its four analogues. *International Journal of Quantum Chemistry*, 109(2):362–372, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2006:TSR

[ZZDY06] Liqun Zhang, Zhengyu Zhou, Dongmei Du, and Pei Yuan. Theoretical study of the reaction mechanism of proton transfer in glycinamide. *International Journal of Quantum Chemistry*, 106(9):2082–2089, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2000:TSS

[ZZFL00] Dongju Zhang, Bingyou Zhuang, Dacheng Feng, and Chengbu Liu. Theoretical study of self-exchange electron-transfer reactions for the $M(H_2O)$ (M = V, Cr, Mn, and Fe) systems. *International Journal of Quantum Chemistry*, 78(1):32–41, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/71001656/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/71001656/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=71001656&PLACEBO=IE.pdf`.

Zhang:2008:BAN

[ZZHL08] Ping Xia Zhang, Yong Fang Zhao, Feng You Hao, and Xin Ying Li. Bonding analysis for NgAuOH (Ng = Kr, Xe). *International Journal of Quantum Chemistry*, 108(5): 937–944, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2007:ESS

[ZZKS07] Yulan Zhu, Shuyu Zhou, Yuhe Kan, and Zhongmin Su. Electronic structures and spectra of porphyrin with fused benzoheterocycles: DFT and TDDFT-PCM investigations. *International Journal of Quantum Chemistry*, 107(7):1614–1623, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zakharov:2004:CBG

[ZZL04] A. Yu. Zakharov, M. A. Zakharov, and O. V. Loginova. Connection between generalized lattice model of multicomponent systems and Ginzburg–Landau theory. *International Journal of Quantum Chemistry*, 100(4):435–441, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zakharov:2005:GLM

[ZZL05] A. Yu Zakharov, M. A. Zakharov, and V. V. Lebedev. Generalized lattice model of multicomponent equilibrium and nonequilibrium systems. *International Journal of Quantum Chemistry*, 104(2):126–132, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2009:TCT

[ZZM09] Tian-Yi Zhang, Neng-Wu Zheng, and Dong-Xia Ma. Theoretical calculations of transition probabilities and oscillator strengths for Ti III and Ti IV. *International Journal of Quantum Chemistry*, 109(2):145–159, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zakharov:2005:STB

[ZZUO05] A. Yu. Zakharov, M. A. Zakharov, A. L. Udovsky, and H. A. J. Oonk. Statistical thermodynamics of binary systems with variable valent states of one of the components. *International Journal of Quantum Chemistry*, 104(2):133–142, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2006:RCI

[ZZW+06] Xin-Ming Zhou, Zheng-Yu Zhou, Qun-Yan Wu, Abraham F. Jalbout, and Nan Zhang. Reaction of CH_3O_2 and HO_2: Ab initio characterization of dimer structure and vibrational mode analysis for reaction mechanisms. *International Journal of Quantum Chemistry*, 106(2):514–525, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2007:SCO

[ZZWM07] Shulei Zhao, Zhengyu Zhou, Wenjuan Wang, and Hongkun Ma. Study of conformational and optical rotation for the alaninamide. *International Journal of Quantum Chemistry*, 107 (4):1015–1026, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2008:IFM

[ZZZ+08] An-Guo Zhang, Hui Zhang, Zheng-Yu Zhou, Zhao-Kun Jia, and Rui-Yan Hou. The influence of formamide (model of protein unit) on the intramolecular proton transfer in the DNA simple base guanine: A density functional theory study. *International Journal of Quantum Chemistry*, 108(9):1589–1600, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).