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Title word cross-reference

($N-1$) [ACD+13a, ACD+13b]. ($n=2,3,4$) [VSP19]. (σ^3,λ^3) [TR12]. (σ^3,λ^5) [TR12]. + [CXW14, GTK10, NMLD13]. 0 [UD12]. 1 [MG15, TS15b, YZLZ18]. $1-n$ [CYG+15]. 10 [AC11b, TS15b]. 13 [WYGW12, SIT18]. 15 [AC11b]. 17 [GZZ12]. 18 [LW16]. 2 [CWT+12, CBDS19, GSS13, MSBF16, MH10, SJD14, WvRSM14, YDL+10, YZLZ18]. 20 [AC11b, LYL16, YVEI+17]. 24 [TS15b]. 3 [AARP17, CM16, DVVP14, GMMH+16, GSS13, GPK12, GBG+19, HSW+19, LTT16, MG15, MA16, MYT+14, MP19b, MSSP17, PSS14, Pop18, RVCFF13, TS15b, VVMY18, YLL11, YZLZ18, dLvNC18b]. 4 [AFSW16, GWJJ12, ZTH+15]. 4*d* [Hil13]. 4*f* [Hua16]. 4×1 [LGKS17]. 4×4 [SH14]. 5 [APY+16, LZH16, WFL+19, YLL11]. 5^{12} [MKH15]. 6 [MCAY15, Rab12, TSZQ12]. 6^2 [MKH15]. 6^3 [MKH15]. 6^4 [MKH15]. 7×7 [UGK18]. 8 [CSC+18, TN12]. 8×2 [LGKS17]. $[2+2]$ [LXFC17]. $[5+1]$

[YZL+15]. [5 + 2] [LXFC17]. [n] [uLhY11]. + [DDM+15, FD16, FHG+19, GMBM18, HDM+19, LCL+10, LdSRR16, LTR18, LCWW10, NH19, RLA+11, RRF11, SS19, SFBT17, UT14, YCGA10, YZ15b, ZCK+16, ZWY+10a]. +/0/− [TG12b]. + · · · π [CCCLCGRO14]. − [ATP18, CXW14, HBL12, JLH+14, LCWW10, RDT14, TDT19, YCGA10, Yu12a, ZWY+10b]. $\bar{}_{18}$ [YLT+19]. 0/+ [GTT10]. 0/+ [TN12]. 1
[Ben17, KSK11, LGW12, LX11, LWD13, PTK11, Pie14]. 11 [HJ13]. 129 [SKMS13]. 13 [Ben17, GMSV14, HJ13, OPR16, PTK11, Pie14, VAMS14]. 15 [RDT14]. $^{15}_{2}$ [RDT14]. 19 [DKE+17]. $^{1}\Delta_g$ [WLF19]. $^{1}\Sigma$ [LWD13]. $^{1}\Sigma^{+}$ [Kop15b]. $^{1}\Sigma^{+}_{g}$ [ZZZ+19]. 2 [GTK10, LGW12, LWD13, OZLSBH12]. 2+ [BHB+17, BHB19, BMFG16, DAdGR15, LBC+19, LPE+10, LWXC16, MG11, PGY15, RRF11, RHT+15, TLY+12, WRG+17, vSGP10]. $^{2}_{18}$− [YLT+19]. 29 [HAI+16]. 2•− [LGW12]. $^{2}\Pi$ [GTK10, LWD13]. 3
[GTK10, HZ11, HCD+10, TCPPC14, dCRN18]. 3+ [DAdGR15]. 3− [RDT14]. 31 [HAI+16]. 35 [Tsi19]. 4+ [YW12]. 43 [HBI+17]. 51 [MG11]. 77 [RK15]. ^{I} [WJX+10]. ^{II} [CM16]. ^{IV} [LLSW14, MG11]. ^{LHM} [BS10c]. ^{p} [vSGP10]. $'$ [KPL15]. $_{(ads)}$ [LLTC12]. $_1$ [ILKR11, II10, KIOY19]. $_1 + x$ [SMiN+19]. $_{1,2}$ [WHL+10]. $_{10}$ [GSS13, LdSRR16, TFQ+11, WWKS16]. $_1 2$ [BHP19, CC18c, DM15, LLLM11, LLB+12, LLD17, LCWW10, VIT+15]. $_{13}$ [JCG+11, LAHS16, SC17]. $^{+}_{13}$ [OPR16]. $^{+}_{15}$ [OPR16]. $_{16}$ [WZH+18]. $_{18}$ [DM15, TFQ+10, VIT+15]. $_{19}$ [DM15, VIT+15]. $\bar{}_{19}$ [YLZ+19]. $_2$ [AS15a, AR10, BE14, BPE16, BŁF14, BCNH+11, BPLL12, BLG10, BWKW10a, BWKW10b, BS10b, BS16b, CK10, CCJ+11, CCM15, CKL+11, CXS10, CSNCS+18, DSB+19, DOM+11, DLSD13, DT19, DLW12, DHE+12, DSHLM18, EVR18, EP15, EBPK17b, EB18, FMNC11, GLZ17, GK10, GWJR18, GNI18, GY12, GWJJ12, HSJ18, HYL+11, HZ11, HSY+11, HFSO12, HBL12, HYD10, HRL11, HVS16, Ibr17, JCG+10, JLS+10, JLH+14, KBC12, KIOY19, KMS+19, KKR+13, Kop16, Kop18, Kop19b, KCL+14, LZTV10, LWW12, LYC+13, LAHS16, LBTV12, LLSW14, LWXC16, LLLW19, LPLB16, LCWW10, LWD13, LJG+11, LLL+12, MLQ+12, MLGB16, MP19a, MG15, MKH15, MCUJ15, MLCD11, MS15, MCAY15, NGAS17, NC14, NMLD13, NKD18, OKY18, PVL+13, PLFS18, PBE16, RHNN10, RAGLL11, RDT14, RRC+15, RVdMB16, RHT+15, RSKG14, RSK+15, SSC+19, ŠBD+17, SC17, STS+10]. $_2$ [SSX+14, SLY+19, TLdG+12, TNY18, Tak11, TSJ+10, TSZQ12, Tsi17, UvSvdWK19, VP19, VT14, VV14, WKC10a, WHL+10, WGL+11, WMW11, WLHZ12, WC13, WWKS16, WLF19, WRM+12, WGN+16, WGLG+16, WYGW12, XFX+16, XCLZ19, YR13, YHX19, YLL11, Yu12a, YZ15b, YXZZ17, ZRCC11, ZRCC12, ZZ10, ZZL+10b, ZSWL12, ZLLL12, ZYG+14, ZLY+16, ZZZ+19, ZZL19, dSDdAR10]. $_{20}$ [GBGR16, JCG+11, LdSRR16, MCK17b]. $\bar{}_{20}$ [YLZ+19]. $_{24}$ [GBGR16, YW12]. $_{26}$ [LAHS16]. $_{28}$ [MCK17a]. $^{+}_{2}$ [CG12, EVR18, MH11]. $^{-}_{2}$ [MN19, Sak18]. $_{2h}$ [ZLY+16]. $_3$ [Alg17, AR10, ATP18, ASS+17, ABB+12, ABB+13, BE12, CK10, CCJ+11, CXW14, EB12, EBK13, FD16, FHG+19, GSMZ19, HSJ18, HDM+19, Ibr17, JCG+10, KT19, KKR+13, LLBO12, LLLM11, LLB+12,

LZL+15b, LGW12, LLX+19, LLTC12, LBTV11, LBTV12, LJG+11, MLQ+12, MLGB16, MP19b, MCUJ15, MCAY15, NMLD13, OKIS17, ONTTL16, RGVC+19, Sak18, ŠBD+17, SLY+19, TLdG+12, TCPPC14, UT14, UT15, VVY17, VVMY18, VV14, VDVR14, VED10, WKLC12, WGL+11, WLHZ12, WRM+12, XCLZ19, YR13, YKH15, YXZZ17, ZZ10, ZZL+10b, ZZL+10a, ZYLL12, ZLLL12, ZLX+19, dSDdAR10, dCRN18]. $_{3-x}$ [CWT+12]. $_{30}$ [TFQ+10]. $_{36}$ [GNI18]. $\bar{}_{39}$ [YLZ+19]. $^{+}_{3}$ [PMG+16]. $_{3d}$ [RSKG14, TFQ+10]. $_{3h}$ [RSKG14]. $_{3v}$ [TFQ+10]. $_{4}$ [BS16b, DOM+11, GY12, HVS16, KD10, KBC12, KMS+19, LLLM11, LLB+12, LL10c, LCL+18, MLQ+12, OZLSBH12, Sch13, SZBM13, SMiN+19, Sie18, SSX+14, TLdG+12, TSJ+10, UvSvdWK19, WKC10a, YKH15, ZXS+10, ZLY+16, ZBB16, ZZZ+19]. $_{48}$ [YW12]. $_{5}$ [Bac12, CG12, Ibr17, JLS+10, PBE16, RDT14, SJD11, STS+10, SSX+14, VP19, XFX+16]. $_{56}$ [TFQ+11]. $_{57}$ [SNKS10]. $_{58}$ [GWT+17]. $_{6}$ [BTMS12, BS16b, Cas14, CG12, GBGR16, KV14, LLL+12, OPR16, SWMW10, SSX+14, TNY18, Tak11, WMW11, WRG+17, YKH15, YOPB16, YHW17, ZZZ+19]. $_{6}0$ [LTR18, KP10, LLC17, MSV16, NKD18, RLA+11, SKMS13, SBW12, TFQ+10, WLW+10, WCY+11, WL14, YDGZ15, ZZL19]. $_{62}$ [GWT+17]. $_{7}$ [GBGR16, OPR16]. $_{70}$ [ZSL+11]. $_{71}$ [VL17b]. $_{76}$ [ZYG+14]. $_{8}$ [GNI18, WWKS16, WCL+11, YW12, YOPB16]. $_{80}$ [ZLX+19]. $_{84}$ [FL15]. $_{89}$ [SNKS10]. $_{9}$ [Cas14]. $_{980}$ [WTH+16]. $_{9k}$ [TJR19]. $_{A}$ [GK15a, SK15a, WGN+16, PG18, SK12, SK17, Zha12b, Zha12a]. $_{ax}$ [SNDK16]. $_{CARBO}$ [PLH16]. $_{d}$ [Sch13]. $_{glyc}$ [PFVL14]. $_{h}$ [GM17]. $_{HH}$ [HCD+10]. $_{m}$ [GTT10, JM11, SIT18, TS15b]. $^{q}_{m}$ [XhD15]. $_{N}$ [ATP18, HOM+16, LGW12, RWR+13, YZGS14b, Yu12b, Yu12a, ZYR+15, ASS10, AC11b, CKL+11, GTT10, GNI18, GWPJ11, GWJJ12, JM11, JLH+14, LLX+19, MCAY15, NC14, OKY18, PZBA13, Rab12, RVCFF13, SN16a, TN12, Tak10, Tak11, TSZQ12, TS15b, TDT19, WYGW12, XhD15, YVEI+17, vSGP10]. $_{n-m}$ [SIT18]. $_{n=1--10}$ [HDM+19]. $_{n} = 1 - 4$ [AM19a]. $^{+}_{n}$ [ABB+12, ABB+13]. $^{-}_{n}$ [GZZ12, GWJJ12]. $^{-/0}_{n}$ [YLL11]. $^{-/0}_{n}$ [TT18]. $_{nv}$ [PZBA13]. $_{sp2}$ [TKCN19]. $_{x}$ [CWT+12, LZTV10, SB11]. $_{ZF}$ [YZWC11]. a [TN10]. α [CCOH14, DBG11, DB12, FFA14, HPT16a, HHT+13a, HHT+13b, KKK+19, LJW+11b, LDH+14, NDG14, RWR+13, SWM10, SH14, SKY+11, WXL+12, WCAH10, XLYZ10, YR13, YZL+15, ZYR+15, ZKH+10, LFB14]. B [GWX+12]. $\bar{1}$ [HSH15]. β [AKMT11, BŁS10, CYY+17, CCOH14, DBG11, HPT16a, IO13b, LLvG10, LJW+11b, LvG13a, LvG13c, LJL+11, NGAS17, yOaCG10, Pop18, SZB19, SKY+11, WS10, WXL+12, XWSW13, YZ17, ZX11, ZBP11, ZP13, ZKH+10]. β_2 [CV12, VKC10, LLHM16]. c [TN10]. $\cdot$ [ATP18, BH13, LZL+15b, RAGLL11, TNY18, YKH15, ATP18, BZH14]. $\cdots$ [CROB16, TDT19, VVJ15, WvRSM14]. $\cdots\pi$ [BSF18, CCCLCGRO14]. $\cdots\pi\cdots$ [YZZ+17]. χ [DPSL16]. χ_1 [SZBM13]. χ_2 [SZBM13]. d [CAT+13, JXSW15, KTK17, MCK17a, SM17, TDKT10]. d^6 [BF19a, TS15a]. d_4 [Kow11]. e^- [HBL12]. e_2 [WCY+11]. η^2 [RHPWS13]. η^6 [ZCK+16]. f

[CAT+13, JXSW15, MCK17a, TDKT10]. f^n [BBG+18b]. γ [BTB+11, DBG11, YLCX10]. J [KNP+12, LZH+11]. k [Hug14, YS15]. κ [YSRSS10]. λ [BH15]. λ^3 [SLT14]. λN [XHLH16]. $\leftrightarrow$ [RSK+15]. M [ATIP18, AM19a, LLX+19, MP19b, YLT+19, NMH19]. $m = 1, 2$ [SIT18]. $m = 2$ [TS15b]. $m = 2, 3$ [TS15b]. M_5^- [ATIP18]. μ [RHPWS13]. N [AARP17, HPT17, JSW10, KYCL11, KYKR15, KSK11, LHL+10, LXZ+10, MB16, PHT17, PM18b, QZM11, RF15, YLZ+10, ZWY+10a, ZBP11, dSdLBNB17, BŁBG+13, BS10b, HCB11, JLH+14, LLX+19, LXFC17, OKY18, RRF11, SLY+19, TCGNT18, TT18]. $n + m = 4$ [XhD15]. $n + m \leq 3$ [GTT10]. $n = 0$ [MCAY15]. $n = 1$ [GWJJ12, Rab12, RVCFF13, TN12, TSZQ12, YLL11, TS15b]. $n = 1, 2$ [ABB+12, ABB+13]. $n = 10$ [TS15b]. $n = 12$ [YVEI+17]. $n = 2$ [WYGW12, TS15b]. $n = 3$ [SIT18]. $n = 4$ [GZZ12, TS15b]. $n = 5$ [AC11b]. $n \leq 20$ [ASS10]. $n \leq 25$ [Tak11]. $n \leq 55$ [Tak10]. $N \log N$ [AO10]. $O(N)$ [BSL11]. $O(N \log N)$ [FGM11]. p [HNN+17, MCK17b]. π [AH10, BŁBG+13, BSF18, CLFRO18, CKL+11, DLMH12, GNC+18, GZZM16, HSZ+11, KV14, KDS17, MUN+19, MVKS10, MIS+15, OOK11, PM18a, RF15, SSGS15, SDF12, SWW+19, YJN+11, Zha11, ZZMW19]. $\pi \cdots$ [YZZ+17]. $\pi \cdots \pi$ [CCCLCGRO14]. pK_a [BA11, CPK19]. Ψ [Lüc14]. $q = 0, \pm 1, -2$ [XhD15]. r_m^2 [RCM+13b]. $\rightarrow$ [CK10, Chu10, GTK10, HZ11, HBL12, LWD13, NMLD13]. S_1 [KKL+13]. σ [DPSL16, GZZM16, LZL+15b, PM18a]. $\sigma\pi$ [CZY11, YWZ14]. $\tilde{\mathrm{A}}^1\mathrm{A}'$ [MCLD10]. $\times$ [SRS14]. $\rightarrow$ [CSNCS+18, SB19, XCLZ19]. $v = 0$ [LWD13]. X [AM19a, Sak18, UT15]. $x = 1$ [CWT+12, LZTV10]. Y [UT15].

-1 [dLvNC18a]. **-5** [LL10c]. **-A** [YJN+11]. **-acceptor** [MIS+15]. **-Ace** [LHL+10]. **-acetals** [YZL+15]. **-Acetate** [BHP19]. **-Aceto-** [SJD14]. **-acetyl-** [ZBP11]. **-acetylation** [LHL+10]. **-adrenergic** [LLHM16, VKC10]. **-Al** [YR13]. **-alkenoyl** [YZL+15]. **-alumina** [SH14]. **-amination** [YZ17]. **-amino** [ZKH+10]. **-aminopolycarboxylate** [ĆMD13]. **-arene** [ZCK+16]. **-atomic** [JXSW15]. **-ATPase** [II10]. **-azacrown-5** [ZWY+10a]. **-barrel** [yOaCG10, WXL+12]. **-based** [BPE16, EBK13, EP15, EB18, LFB14, MP19a, PBE16]. **-benzaldehyde** [Lu11]. **-bipyridinyl** [KPL15]. **-block** [CAT+13, MCK17b, TDKT10]. **-bond** [CKL+11]. **-bound** [XWSW13]. **-butane** [TCGNT18]. **-butanol** [BS10b]. **-butene** [MSBF16, WvRSM14]. **-butyl-** [MG15]. **-butylbenzene** [HCB11]. **-carboxylates** [AARP17]. **-carrabiose** [YSRSS10]. **-catalyst** [SSD19]. **-catalyzed** [YXZZ17]. **-cation** [MUN+19]. **-chloridophenylacetohydroxamate** [CBDS19]. **-conjugated** [BŁBG+13]. **-coumaric** [HNN+17]. **-couplings** [LZH+11]. **-Cu** [NGAS17]. **-curcumin** [AMK11]. **-cyclodextrin** [DBG11]. **-dimensional** [MB16]. **-dimethylaminophenyl** [YLZ+10]. **-effect** [RWR+13]. **-electron** [KTK17, LW16, LYL16, HPT17, PHT17]. **-erythrose** [SM17]. **-expanded** [MLQ+12]. **-F12a** [MLCD11]. **-form** [GWX+12]. **-glucosamine**

[FWS+18]. **7-tetraene** [ABDGN12]. **7.0** [GLW19].

8 [AAC+16]. **8-formyl-7-hydroxycoumarin** [LZHH11]. **8-naphthoquinone** [HWB19]. **8R** [BG13].

9 [Sch10, Spr10, SOvG12, ZQ14]. **9-dimethylacridine** [FWS+18]. **978** [Sch10]. **978-0-19-530573-9** [Sch10]. **9H** [ZQ14]. **9H-9-borafluorenes** [ZQ14].

= [ATP18, ATIP18, ASS+17, AM19a, AM19b, CXS10, EPH+15, GPK+16, GNI18, JLH+14, JJAB16, JJJ16, LDJ+10, LLL+11, LZJ+11, Li14a, Li14b, LGW12, LLX+19, LZSM19, LCWW10, LWD13, MP19b, MCK17a, MCK17b, OKY18, PGS+15, PMG+16, Rab12, RDT14, SPS+12, Sak18, SLIB12, TLdG+12, TFQ+11, TT18, TG12b, UT15, WWKS16, XhD15, YW12, YLT+19, YS13, YHCS11, ZYLL12, ZLLL12, ZLX+19].

A-B [LLLM11]. **A-band** [KT19]. **A-site-ordered** [LLB+12]. **Ab-Initio** [PAK15, XYZ18]. **ABC** [SM16a]. **ABEEM** [LWZ+19, CZY11, YWZ14]. **ability** [LLL+10, PGS+15, RTS+13]. **above** [MK17]. **Absolute** [Gri13, HLW+17, KB11b, KYB13, VED10]. **absorbing** [NPG+18]. **Absorption** [RS17a, ZLL+10, DMD+18, FD13, HNN+17, KB16, LLBO12, LX11, LXZ+10, MKK+19, PMC+17, PDMT10, PDG+16, SGDT10, TYN15, TZ12, Tsi14, WWD14, ZTH+15, ZDX11, QCR12]. **abstraction** [AAMD+11, BS10b, CSXZ17, GY12, JCG+10, LJW+11b, PNE18, WLHZ12, dCRN18]. **Ac** [SNKS10]. **ACCDB** [MP19c]. **Accelerated** [MFEM15, MFEM16, SH19a, YKNN19, AGB13, BDTP11, CVT+11, CF18, DWC17, GBL+11, HEMCZE+14, HAP+12, KV13, LL11, MLN+18, REV+17, YLGX14, YSG12, ZC14, ZLL+13]. **accelerates** [HS17b]. **Accelerating** [HASR+12, HB19, LZ12, YWJ+16, HP10a]. **Acceleration** [BKŠ+11, ON14, SOM+13, UTM11, WSGN11, OOT15]. **accelerator** [SBV10]. **accelerators** [KK17a]. **acceptance** [BB11b, KB11c, NDW15, dRBO13]. **acceptor** [EHT19, Gil11, Lu11, MSV16, MIS+15, SB19, ZSTRS+18, ZZL19]. **acceptor-bridge-donor** [ZSTRS+18]. **acceptors** [KKK+19, uLhY11, TZ12]. **accessibility** [HPL+18, LHL+10]. **accessible** [FZY+12, WXL+12, WBF17]. **Accessing** [JZZM14]. **accompanying** [HSN14]. **according** [GM17, LPE+10, YZZ16]. **account** [EPH+13, Tsi18]. **Accounting** [XML+15, HH11, MBC11]. **Accuracy** [ASW19, DBM+15, FCE15, KFY+13, LLH17, BPB11, GRARO+14, HWLW11, KSR+16, LZ12, LDZW17, MLG18, NTNY15, yOaCG10, RS13, RVCFF13, Rob13, TO10, VVW+18, ZYS+10, AIM+18, Gil11, SDIP18]. **Accurate** [BS16b, BS18, CX10, CSXZ17, EFOD13, FLM11, IN13, KG15, LYC+13, LLH11, LWL+10, MK13b, MFR+11, NWW17, Pol13, PVJ10, Sch12, SRR16, SY11, ŚSB+16, SYZ+17, TH13, VSP19, WL14, YB16, ZWLX11,

ZWX19, AF14, ABS+19, BS10a, BPM15, Ben17, CCLP12, CSGOA17, CRZ+18, DKE+17, GAI13, GBW+14, GWZX12, HRC13, KKH18, LC17b, LZZ14, MAK+14, ME10, MFR+17, NHN16, yOTn16, dlRL11, RB13a, RCR+16, RDDS10, RR14, SH15, SS16b, VAMS14, VDVR14, VRKT19, WXS+12, WJG+13, WX12, XSZL11, YOMT14, dVZ17, dSAdSL13].
Accurately [Bow16, LFB14, MA16, Zha12b]. **ACE** [WCDM11, LHL+10].
acetaldehyde [AS11, AAMD+11]. **acetals** [YZL+15]. **acetamides** [JSW10].
Acetate [BHP19]. **acetic** [KSNT19]. **Aceto** [SJD14]. **acetohydroxyacid** [XLYZ10]. **acetonitrile** [KT18, RS14]. **acetyl** [ZBP11, ZP13].
acetylacetone [SJWE10]. **acetylation** [FHK+12, IMK+16, LHL+10].
acetylcholine [SRA17]. **acetylene** [GRCL12, HSY+11, LT13, Tak10].
achieve [PH17, RAR+11]. **Achieving** [SLY+19, NNK+16]. **Achim** [Spr10].
acid [BLG11, CYY+17, CC18b, CFC15, CM16, CB11d, FD14, FZL+15, Fel10, FP17b, FCE15, GRL+11, GRL+12, HPT16a, HNN+17, HGY15, HCP15, KSNT19, KLS10, KMLS10, LBC+12, LXL+11, LFM12, LP11b, LPMT17, MSLS10, MRO17, NHF+10, OXBW16, PHDH13, PG18, SISK10, SZBM13, SGY+18, SBW12, SV11, TKCN19, TL16, VMPS17, WC14, WG12, XVN17, ZSB+11, ZWP11, ZHHX11, dSH19]. **acid-arsenic** [KSNT19].
acid-catalyzed [CYY+17]. **acid-phosphoric** [KSNT19]. **acid-water** [TL16]. **acid/base** [VMPS17]. **acidic** [APY+16, TTC+18, YDX16].
acidities [ALK+15]. **acidity** [CRZ+18, CPK12]. **Acids** [WBKS19, BSG+18b, CCCLCGRO14, DKE+17, EHSPT16, FCE15, GREA11, RSL16, SCF+19, SST+18, XLYZ10, ZKH+10]. **ACP** [STM+15, SJ16]. **across** [AAC+16, GMPB12, MGS+16]. **acrylate** [LZL+16]. **act** [LC10]. **acting** [BT18]. **Actinide** [SvLK18, RTS+13]. **action** [XLY12]. **activated** [CV12, FWS+18, KSR17, ZGZ19]. **Activation** [Niz13, AALCM11, DR11, DSM+11, FB12, KMT+19, LSL+19, MRR11, MBFG15, PG18, SH19b, TM18, TS15a, WC11, XLYZ10, YXZZ17].
activation-strain [FB12]. **activator** [BM12]. **active** [AIGP15, BHF+18, Cas13, DAP+18, DPB+12, EB18, LZTV10, NH19, PDG+16, SCSW13, SC18b, XTn18]. **active-site** [DAP+18]. **active-space** [NH19, PDG+16, XTn18]. **actives** [EOO+16]. **activities** [AHK+19].
activity [BPC13, DXL+10, GAI13, GHL17, GFPSD17, MJLV14a, RCM+13b, SLY+10, TD10, TTB+11, YB13, ZsA10, ZDW18]. **acute** [TTL+12]. **acyclic** [NMH19, ZKH+10]. **acyl** [PS10]. **adamantane** [EHSPT16].
adamantane-based [EHSPT16]. **Adapted** [ELKE19, FF11, SSSM15, TH13, YKH15]. **Adaptive** [ISK14, KEMP17, LZS+17, AOW11, BGR13, DSK17, FHMB15, HDM+15, LL19a, MJC14, MBFP15, MJG+15, OZ14, PN13, SNS13, WTD+19, WMW+10].
Adaptive-numerical-bias [KEMP17]. **adaptively** [ER18, SR18].
adcluster [IN13]. **Adding** [PFAS+19, XHLH16, Zha12b]. **addition** [FWB14, KSO+19, KS13b, NDG14]. **Additive** [XVA+16, DPNM11, HM13, TSR+16, VHA+10, VMPS17]. **additivity** [VRKT19, ZRL+15]. **address** [LG14]. **Addressing** [MMH19, cCVG+14].

[RHJ11, SHMO11, SHL+11, ZC14, LMZ11a]. **annihilation** [BL12]. **annulated** [RS17a]. **anode** [GNI18, YZLZ19]. **Anomerization** [SM17]. **anomers** [HH11]. **ansa** [OSA19]. **ansa-zirconocene** [OSA19]. **ansa-zirconocene/borate** [OSA19]. **ansatz** [Bou14, WGA18]. **answer** [SJWE10, Tan19]. **ant** [ZsA10]. **antagonists** [LLL+10]. **anthrax** [JAH+17]. **Anti** [WFZ+18, ZsA10]. **Anti-Electrostatic** [WFZ+18]. **anti-HIV-1** [ZsA10]. **antiaromatic** [TDKT10]. **antibiotics** [PG15]. **antibody** [UNT16]. **anticancer** [AJA+19, SZZ+18]. **Anticooperativity** [TDT19]. **antiferromagnetic** [ZB18]. **Antiferromagnetically** [SZL19]. **antigen** [JAH+17]. **antimicrobials** [PPUBGD10]. **antioxidant** [GAI13, ZDW18]. **antiparasitic** [PPUBGD10]. **antisense** [ICS+12, ICS+13]. **antitrypanosomal** [PSdPE+10]. **antitubercular** [TD10]. **AO** [YOPB16]. **AOFORCE** [vW11]. **APBS** [UHH+11]. **API** [LAS+14, ZW18]. **AppA** [XBSS19]. **Applicability** [MAK+14, DI11, GHL17, GKR13, HH15, JZZM14, KMS+19, Ray13, RKG11, VHS+19]. **applicable** [CL16, WGL+11]. **Application** [AFBR17, BAMR13, BPE16, DAG19, GCCM15, HTS15, LDG+15, MBA11, MTS+19, MH10, OL13, PAK15, RVP+11, SMP17a, SRS14, SC17, SDL14, SMM+18, Tak18, VKTRJ15, WH11, WFS19, ZsA10, vSGP10, CSAdOM17, CJPTC18, DGPM14, Elk16, GLB16, GFG11, GCW16, HYSF19, IUK+11, KT19, KFY+13, KS18, KSK11, LLHM16, LP11a, LLL+10, LLLC11, LvG13c, MDTD13, MdOdQ18, PHC13, RZG+13, RCM+13b, SMDP18, SN16a, SLX+15, SYH12, VV14, VKC10, WCDM11, You10, AFPI13, BD11, CZNA11, Fer13b, Fer13a, FCOGM12, GAI13, HYUS11, KUDG12, MCC11, Pet11, PW12, SPZP19, TSZQ12]. **Applications** [KGHC15, LCPS13, LCA17, Spr18, APK14, CGPP11, EVR18, Fel10, GBFD12, HZY+10, HCD+10, IO13b, KKO+16, uLhY11, LJR+12, MG11, NS18, SSSM15, SGM+13, ISP+10]. **applied** [BLG11, CTP13, GKR13, KKR+13, LTT16, PM18b, Ray13, RKG11, SZTSM10]. **Applying** [KB11a, ZSLL17, CC11]. **Approach** [Coo19, NNT+19, VSP19, ACD+13b, BPE16, BBG+18a, BVHI17, BGR13, CCLP12, CRZ+18, CHC+13, CXS10, DK11, DGPM14, DVVP14, DFF+15, DHE+12, FRSA14, Fer17, FNSF+11, FCCP17, FD16, FSD+18, dCGCRN19, GPE13, GZ14, GH16a, HRC13, HDH12, HNN+17, HHBY10, HZSS17, ITY+19, JCX10, KV12, KV13, KHLM19, KT19, Kid19, KSK11, KT10, KSHP+19, KKK+19, KKH18, LLTC12, LH14a, LG14, MZZ11, Man19b, MGWR12, ME10, Mor15, NSK18, NB19, NLL19, NO16, OT12, PRP15, PMC+17, PSdPE+10, PH10b, PBE16, PPUBGD10, PLP+16, RKGN10, RB12, RVP+11, SLT14, SZdB19, SEF+16, SH11b, SY16a, Sti15, SLLL13, SGH+16, SM17, TO19, TAG16, TSR+16, VVLG17, WFS19, XZ11, YKO+11, ZSLL17, ZLW10, AIM+18, GFG11, ACD+13a]. **approaches** [BP18, BH13, CME11, DBM+17, ECZWD17, HBI+17, IT19, LSH+11, RLDJ17, RŠRR15, VLB+10, YJ11, ZDT18]. **Appropriate** [LZLC13]. **Approximate** [Gav12, KV12, KV13, RP15, RZ16, SM14a, HH16a]. **approximation** [AO10, Boz18, Cas13, HH17, Kid19, Sch12, WHM10, WDKT19, YD17, YN15].

[KRSC12, HLH+12, Hug12, LH11, LJR+12, SKKS13]. **beta-barrel** [LJR+12]. **beta-complex** [SKKS13]. **Beta-decomposition** [KRSC12]. **beta-peptides** [HLH+12]. **Bethe** [KK17b]. **better** [AF14, BM12, JT18, KDS17, yOaCG10, XHLH16]. **Between** [ELKE19, ALW+10, ASL+11, AR10, ACS12, AHK+19, BSF18, BSD18, CCCLRO14, CC18b, CZH12, CQFC10, CCOH14, CB11a, dRCFGRB18, DHF+11, Den12, FD14, FC16, GYX+10, GO13, Gav12, GKSS14, HSJ18, HTY19, HvM16, HvM17, HHWL17, Jab18a, Jia19, KTT16, KHWB17, KPH+19, LDJ+10, LLL+11, LW11, LYL16, LWL+16, LvG13b, Lüc14, MS17, MUGNVJ+18, MSSP17, MvBD18, OHNK11, OCL11, PRJ+17, PL14, RŠRR15, SBW12, TTR+12, TSN16, WCT+11, WFZ+18, WDS+19, Wei12b, YHG+11, YKH15, YFH+19, YDGZ15, ZY14, ZB18, ZBMZH15]. **Beyond** [PNW+16, JND+19, RLA18, SCOJ13]. **BH** [LBTV11, LBTV12, Kop15b]. **Bi** [ATIP18, RDT14, DM15, VIT+15, HSJ18]. **bias** [KEMP17, KS12]. **biased** [BG17, ZGZC19]. **biasing** [MJC14, OZ14]. **bibliography** [Pyy13]. **bicarbonate** [VPR10]. **BiCu** [LLLM11]. **bicyclically** [Alg17]. **bifunctional** [BEM14, BEPM14, WFL+19]. **Big** [WDKT19, MPA12]. **big-bang** [MPA12]. **BiH** [HSJ18]. **Bilayer** [vRWGS17, II18, KLN16, RBOH11, SLX+15, WHAS+10, WHAS+16]. **Bilayers** [BPPS19, BPPS17, GBL+11, PVM10, PS10, RI10, TG12a]. **Bimetallic** [GEP+14, DAdGR15, GTT10, KKPT11, SIT18]. **bimolecular** [CSAdOM17]. **binary** [Hua16, LAS+14]. **Binding** [AIM+18, ELKE19, FPB12, GRS15, HVS16, KJDB12, NN19, SSP+13, SMD18, YKNN19, ZP13, AALCM11, ALW+10, ABD11, AS10, AC11a, ACS12, BHNS14, BTMS12, BVHI17, BEL+11, CBP+15, ĆMD13, CLA16, CIKT13, CZY11, CS17, CZAF17, CHR+12b, CHR+12a, CPK12, CXD+19, DHF+11, DS12b, DVVP14, DAB16, DPOS16, ETLS17, GHK12, GDV17, GWZ15, GEP+14, GPdC+16, GAJ+17, HDK+12, HYYZ13, HDM+19, HPL13, HNWF07, HNWF12, HG13, HHWL17, ISP+10, JCP14, JZ12, KZZ+16, KTO11, KTO13, KDT+12, Lar12, LL10b, LJW11a, LW11, LCA17, LBS10, MSY19, MLZZ12, MLN+18, MGWR12, MSÅK12, MAP18, MFR+17, MNNK10a, NST14, NHN16, NWW17, NZM18, NFG+13, NF17, NN18, NO16, NNK+16, OBW12, Oht16, OHNK11, OSR16, OCLM14, OOT15, PGCT+12, PBLdS12, PGS+15, Pla11, RLDJ17, RCR+16, RDDS10, RAR+11, RO14b, RZ16, RF15, Rez19]. **binding** [SPS+12, SRA17, SOD+11, STM+15, TYZ+16, TJR19, TS15a, UNT16, VVG13, Vor10, VM11, VHS+19, WS10, WNP+16, WLLH18, WWW19, WL14, XHLH16, YZ15a, YZZ16, YJXZ13, YHH+13, ZZ14, ZJZM13, ZYvIZ14, ZLX+13, dRBO13]. **binding-based** [MAP18]. **binding-site** [ISP+10]. **binds** [XHLH16]. **BINOL** [HPT16a]. **BINOL-phosphoric** [HPT16a]. **Binor** [WJX+10]. **Binor-S** [WJX+10]. **binuclear** [KMS+19, LZTV10]. **bio** [MSvG12, RZ16]. **biochemical** [DGSVGVM19, RB12]. **biofuels** [LGC19]. **bioisosterism** [EdOdS18]. **BioLayer** [JAH+17]. **biological** [BHB12, Ben17, CLK11, DLL+10, DMN15, GREA11, GFPSD17, GLM+17,

ASS+17, ASW19, BLG11, BS15, CK10, CvM19, CXS10, DDP+18, GNC+18, GTT10, GPK+16, GLW19, HDB15, HvM16, HvM19, Ibr11, JCGVPHT17, JSF19, JXSW15, JT18, LYL16, LCC18, LBTV11, LBTV12, LTP11, LYSS11, LZSM19, MDTD13, MDTD16, MCK17a, Niz13, PKK17, PD11, PZM15, RDT14, Rez19, RLA18, RSKG14, SFM+18, SLY+19, SKGB13, TY10, TS10b, TG12b, TS15b, TZ11, TL16, VVY17, WHL+10, WCT+11, WGL12, WHX+10, Wei12a, Wei12b, WvRSM14, WZK+13, YLZ+10, YZL+15, ZY14, ZYW+16, vSGP10, EHSPT16]. **bonding-induced** [YLZ+10]. **bonding/back** [PKK17]. **bonding/back-bonding** [PKK17]. **Bonds** [ELKE19, JLLW19, WFZ+18, BT18, CXD+19, DGB+13, ED15, FPRS14, Gra18, HH15, Jab14, JJJ16, LZH+11, LZL+15b, LZY12b, LDG+15, OOK11, PGI19, Rob13, SM16a, SK13, SJ16, TDT19, WS19, XMA+19, YLT+19, YLL11, YKH15, YJ17, ZLY+16, Jab18b, YLZ+19]. **BonnMag** [BBG+18b]. **Book** [CD19, Sch10, Spr10]. **Boolean** [CDC19]. **boost** [KV15a]. **BOP** [SH19a]. **borafluorenes** [ZQ14]. **borane** [BEPM14, Kop15b, LC10, SJZ+15]. **borane-cyclic** [LC10]. **borate** [OSA19]. **borates** [GWJJ12]. **border** [SK12, SK17]. **borides** [ZWMW10]. **born** [AB16b, BLZ+13, DSF17, FCE15, HWLW11, KCPMG12, LL10a, LCH10, MT19b, PS13, RSB+13, SZTSM10, SSBW14, VMPS17, WWKS11]. **boron** [BEPM14, Gra18, GAMAC+14, LT14, Oht16, PGC12, VS14]. **boron-** [BEPM14]. **boron-doped** [VS14]. **boron-nitride** [LT14]. **boronate** [HLI+19]. **boryl** [LC10]. **BOSS** [VKTRJ15]. **BOSS-Gaussian** [VKTRJ15]. **Bosutinib** [GMASBF16]. **both** [AST+16, FNSF+11, LX11, TH13, WZ19, WS19]. **bottleneck** [SRR16]. **bound** [FLM11, GPK+16, LFM12, MAK+14, PMG+16, PZA15, XWSW13]. **Boundary** [Coo19, KB14a, Lun12, MTvG12, NO16, PL14, PS13, SSP19a, Sie15, VECT12, YAO18]. **Boundary-Integral** [Coo19]. **bounded** [LL19b, Pol13, SL10]. **bowls** [WL14]. **box** [Pla11, WS13]. **boxB** [XHLH16]. **Boys** [WO15]. **bptz** [CWT+12]. **bpy** [LWXC16]. **Br** [ATP18, ASS+17, EPH+15, GPK+16, LDJ+10, LLL+11, LZJ+11, PMG+16, YS13, ZLLL12, LZL+15b, MKH15, MSPC19, XhD15, ZWY+10b]. **Branch** [Ish10]. **branching** [BEL+11, OZLSBH12, STM17]. **BrBr** [LGW12]. **Breaking** [HRID16, SRR16, WWWW18, Man19b]. **bridge** [CVG14, PH15, ZSTRS+18, dLvNC18a]. **bridged** [HLI+19, KGR+16, ZLZ14, ZLY+16, ZB18, ZZWX11]. **bridges** [MLY+13, PH15]. **Bridging** [YLL11, dCDP15, LJL+11, MIS+15, BPC13]. **Brillouin** [QS19]. **Bringing** [RR11]. **broad** [MP19c, TZ12]. **broken** [XKW18]. **broken-symmetry** [XKW18]. **bromide** [MG15, OC19]. **bromination** [SGS+16]. **Bromine** [LWL+16]. **BROMOC** [DMN15]. **Bromosuccinimide** [QQY+18]. **Brooker** [TYN15, TKYN17]. **Brooks** [HIS17]. **Brownian** [DMN15, DZT11, LJR+12]. **brushes** [DQ16]. **BSSE** [OLPB19]. **BSSE-correction** [OLPB19]. **btmgp** [RHT+15]. **BtuF** [WWW19]. **buck** [KPF+15, KPF+19]. **Buckybowls** [HVS16, CCCLRO14]. **buffered** [MJG+15, MEH18]. **build** [APK14]. **builder**

EBK13, EB18, FAA15, FRC18, FA18, FE14, GRARO+14, GA18, GMO16, HASR+12, HYL+11, HS14a, HB14, HSH15, Hel13, HG10, HG13, HBL12, HYUS11, HGW18, Ibr17, IMSR18, ISM18, JCG+11, KK17a, KB10, KKNN11, KGHK12, KMS+19, KKR+13, KERY+16, KFT18, KCPMG12, KKL+13, KSH+17, KKH18, LEdOLdlV17, LRVM18, LOB18, LMZ11a, LCH10, LYC+13, LCA17, LvG13b, LCK+18, LCM+14, Lun12, MK17, MK19, MUGNVJ+18, MLN+18, MCLD10, MEH18, MCK17a, MCK17b, NWW17, NZM18, NLL19, NCT18, NN18, OHNK11, OLPB19]. **calculations** [OLA15, OOT15, OZLSBH12, PBLdS12, PTK11, PHK14, POB13, PBBP11, PDG+16, PN13, PGW+17, RAR+11, RLZ+18, RHT+15, RLD12, RR11, REV+17, RI10, RK15, SH15, SRSLO15, SP13, SPHF+18, SS16b, SCW11, SWPR11, SRS14, SMP17b, SDMS13, SHB17, SKTT11, SPZP18b, SPZP19, TLdG+12, TNY18, TS10a, TNI19b, UHH+11, VLB+10, VKAM12, VKNT16, VHR16, VFRAR16, VMPS17, VI17, WC13, WSZW15, WHK+12, WTH+16, WGA18, WXY14, XYW+14, YWJ+16, YD17, YN15, YJ19, ZRCC11, ZLT13, ZLZ14, ZWMW10, ZH12, MSPC19, NQB19]. **calculator** [dCLFGL13]. **calibrate** [VVLG17]. **Calibration** [CBP14, DDM+15]. **calix** [GMASBF16, PRRT+10, YCGA10, ZWY+10a, ZWS+10, GMASBF16]. **Call** [ZPF14]. **CAMERRA** [JLS18]. **Can** [ASMS10, IMSR18, KV15b, LZW+11, NH19, PŁAG11, SHL+13, SPZP18a, CIKT13, LCB10, TCPPC14, Zha12b]. **CANADA** [Fel10]. **cancer** [NS10, WC11]. **Canepa** [LHMM11]. **cannabinoid** [ILKR11]. **Canonical** [CPN+17, RHNN10, BW11a, HRK+10, HHNK19, KCK+17, PHH+12]. **Canterakis** [UCRL18]. **CaO** [BL12]. **CAP** [EFS16]. **CAP/SAC** [EFS16]. **CAP/SAC-CI** [EFS16]. **capabilities** [AAC+16]. **capability** [LC10]. **capacity** [KOP+14, PGC12, WKC10a, WKLC12]. **capillary** [NFPD13]. **caps** [WDS+19]. **capture** [GLZ17, SMD18]. **Car** [DL19, KCK+15]. **CARB1/TIP3P** [SA10]. **carbazole** [JYS+12, SLC+17, YJN+11]. **carbazole-based** [SLC+17]. **carbazole-fluorene** [YJN+11]. **CarbBuilder** [KSW16]. **carbene** [CWT+12, LXZ+10, TCPPC14, WS11, WS12, YJ19, dSdLBNB17]. **carbenes** [BAD+19, BSDP16, KYKR15, RF15]. **carbocation** [ONTTL16]. **carbocations** [OPR16]. **carbocyclic** [BAD+19]. **Carbohydrate** [ZYvIZ14, NMF+14]. **Carbohydrate-binding** [ZYvIZ14]. **carbohydrates** [CP15, HH11, JSD+11, PLH16]. **Carbon** [JLLW19, SC17, AJA+19, AS15a, AAMR18, ASL+11, BPE16, CME11, DI11, Den12, DC13, Fom13, FTR15, GSMM15, GPK+16, GBS+17, GZZ12, JWO15, KGHK12, KV14, KPH+19, KHE+19, KGJZ19, LPLS16, LL10c, LT14, LK16b, MSY19, OCW+15, RHNN10, RRK16, Sie18, TSR+16, VS14, WYL+15, WDZN16, YZN13, YZZ+17, ZYW+16, ZLY+16, ZWF15, OSI+19]. **carbon-beryllium** [CME11]. **carbon-carbon** [KGJZ19]. **carbon-germanium** [GSMM15]. **carbonate** [ZSWL12]. **Carbondioxide** [Sea10]. **carbonic** [SSP+13]. **carbons** [MKB+13, RVB+12]. **carbonyl** [BH19, CZH12, CROB16, TS10b, ZBMZH15]. **carbonylation** [MRC+18].

[Sán17, ZBMZH15]. **Chloroammonium** [VVMY18]. **chloroform** [GC11, WG12]. **chloroform-to-water** [WG12]. **CHOC** [LHHW14]. **choice** [LvG13b, Mor15, NCV10, SPZP18b, TLA10, WGA18]. **Cholesky** [GCW16, PS17]. **Cholesterol** [BPPS19, BPPS17, RBOH11]. **choline** [PP19]. **choline-O-sulfate** [PP19]. **chondroitin** [CHKR10]. **chondroitin-6-sulfate** [CHKR10]. **Chou** [FZL+15, GRL+11, GRL+12, ZHHX11]. **chromophore** [GA18, PGW+17, SGWA17]. **chromophores** [SGDT10, UD12]. **CI** [CME11, EFAC13, EFS16, FE14, IN13, KMS+19, KSHP+19, MN19, PH10b, SRF+17, SCF+19]. **circuits** [RVB+12]. **circular** [HNHR13, SEJ+18, ŠB13, ŠB15]. **circularly** [SEJ+18]. **Cis** [CSM16, MSBF16, WvRSM14, WS19, ZLHH14]. **Cis-** [CSM16, MSBF16, WvRSM14]. **CISD** [dALdS+15]. **cisplatin** [dRCFGRB18, CK17, PML+12]. **Cl** [ATP18, ASS+17, CXS10, EPH+15, GPK+16, KKR+13, LDJ+10, LLL+11, LZJ+11, LGW12, PMG+16, Rab12, RVdMB16, Sak18, TFQ+10, TFQ+11, Tsi19, TDT19, WGN+16, WGLG+16, YS13, ZCK+16, ZLLL12, CSNCS+18, JCG+10, JLS+10, JLH+14, LZL+15b, MSPC19, WLHZ12, WLF19, ZWY+10b]. **Clar** [KDS17]. **Clarifying** [RML+15]. **class** [DWL11, HHWL17, LD18, ZLW10]. **classical** [Aki16, BEM14, DHF+11, GA19, HS14a, HLvdV13, LRvdSM15, LM18a, LPE+10, LM18b, MS15, PVAM16, Ras17, RTS+13, RO14b, SM14b, SKA19, WKC+10b, WG14, Yu12a, ZM10]. **classification** [EP15, UT15]. **classifier** [YHH+13]. **classifying** [TO19]. **Clay** [BHB19, BHB+17]. **ClC** [KJ10]. **ClCH** [RVdMB16]. **ClCHO** [SS19]. **ClCl** [LGW12]. **clean** [CCJ+11]. **cleaning** [YR13]. **cleavage** [HEM+17, MS11]. **click** [TKXT13]. **CLL** [dACP12]. **ClNH** [VVMY18]. **close** [BLZ+13, MK17, RS13]. **Closed** [CYI+10, MA16, MS12, WWD14]. **closed-shell** [MA16, WWD14]. **Closo** [HJ13]. **Closo-carboranes** [HJ13]. **closure** [ABDGN12, NR11]. **cloud** [TF15]. **cluspro** [XML+15]. **Cluster** [AST+16, Hes19, MPNS13, SL17, ACD+13a, ACD+13b, AC11b, Avd18, BBG+18a, BYE+16, Cas14, CC18c, DI11, DM15, FF11, GNGCA10, GMG+10, GA18, GS11, HAGK10, HSB+19, HSH15, Höf14, HGCCGR+16, HBI+17, Les19, MC12, MG14, NLL19, Oht16, PGS+15, PB14, PMT16, RS14, RLZ+18, SB11, SLLL13, SM17, TLdG+12, TNY18, TTn19, VIT+15, VV14, WC13, XTn18]. **Cluster-based** [MPNS13]. **cluster-continuum** [WC13]. **cluster-expansion** [HAGK10]. **cluster-in-molecule** [NLL19]. **cluster/configuration** [FF11]. **cluster/Kohn** [VV14]. **clustering** [BSZ+12, LZS+17, PL19, YZ15a, ZSS+13]. **Clusters** [NSN19, SC17, TT18, AFPI13, ATIP18, AF14, Ano11, ASS10, AC12, BPM15, BACSCJ+10, CJL+13, CZZL19, DAG19, DH11, FCW+14, GTT10, GC18, GRD+10, GAMAC+14, GZZ12, GBGR16, GBG+19, HS14a, HS16b, HDM+19, Hsu14, JM11, JCP14, JHMB+09, JHMB+11, JCG+11, KD10, KKPT11, KOP+14, KSNT19, KDB13, LZTV10, LK13, LZZ+11, LCH+15, LCWW10, MCS11, Man19b, MPA10, MPA12, MP13, MBFG15, MBRC16, MCAY15, NC13, NC14, OKY18, PM18b, QZ10b, Rab12, RGVC+19, RSB+13,

SN16a, SBGP18, SB11, SIT18, SMP17a, TN12, TNI+19a, Tak10, Tak11, Tak18, TSZQ12, TNI19b, TS11, Tsu19, TDT19, US11, WHL+10, WYGW12, WZH+18, YVEI+17]. **CM1** [VSA11]. **CM3** [VSA11]. **CN** [TS15b, YKH15, KIOY19, STS+10, TCPPC14, WHDL11]. **CNH** [DBGO+17]. **CNO** [OKIS17]. **cNOR** [BS16a]. **CO** [Bac12, BPLL12, FD16, FHG+19, OKY18, SC17, SSX+14, YXZZ17, ZBB16, Spr10, WWKS16, BPLL12, CCJC10, DHE+12, DSHLM18, GLZ17, GWJR18, HFSO12, HVS16, KD10, LLC17, LPLB16, MG15, MBFG15, SSC+19, SKTT11, WC13, AAMR18, CMM18, HYL+11, JCG+11, SCSM19, WJX+10, YMY+19]. **coadsorbed** [LLTC12]. **coal** [WZC+19]. **Coarse** [CPK19, KZP+18a, MSLS10, MT20, NST14, BJP15, BLKP12, CAD16, GMPB12, HYSF19, HHWL17, JC16, KCK+17, KVQC+11, KLS10, KMLS10, LZ12, LZX16, LZZ14, LZLMP16, MT19a, MBC11, MBC13, ML14, RSG+10, SLX+15, SDZ17, SOM+13, SJ17, SGY+18, SM15, SAvG15, WBF17]. **Coarse-Grain** [CPK19]. **Coarse-Grained** [MT20, KZP+18a, MSLS10, NST14, BLKP12, CAD16, HYSF19, HHWL17, JC16, KCK+17, KVQC+11, KLS10, KMLS10, LZ12, LZX16, LZZ14, LZLMP16, MT19a, MBC11, MBC13, RSG+10, SLX+15, SDZ17, SJ17, SGY+18, SM15, SAvG15]. **coarse-graining** [BJP15, GMPB12]. **cobalamin** [AALCM11]. **cobalamin-dependent** [AALCM11]. **cobalt** [DSHLM18]. **Code** [HB19, REL+14, BTT10, CPRS18, GHK12, GP12, LLH14, LCPS13, RJR14, RRFV+18, WKC+10b, vW11]. **codes** [KSH+17, RKGN10]. **coding** [QLQ11, YS10]. **Codoped** [RLZ+18]. **coefficient** [FSD+18, WH11, WF16, WZWW18]. **coefficients** [AR10, JIS13, KCL+14, LRVM18, NMLD13, PN13, WG12, YAS13]. **cofactor** [ZX11]. **cofactors** [AKMYB18, GLM+17, ZSYH12]. **cogs** [DL16]. **coherent** [EVR18, LCH10]. **coinage** [Rab12]. **cold** [VL17b]. **collapse** [SCMA+17]. **collection** [BRGN12, MP19c]. **collective** [CF18]. **colliding** [YHX19]. **Collision** [FBvdB18, ZHS+18, dCLFGL13]. **Collision-free** [FBvdB18]. **collisions** [KCL+14, LPLB16]. **colony** [ZsA10]. **color** [DBM+17, GK15b, LWL+11, PE11]. **Combination** [JIS13, Jia19, NO16, Pon10, ST11, EP12, IM17, KHLM19, Tak14]. **combinations** [PD11]. **combinatorial** [GD10, SR10]. **Combined** [CMM18, PGW+17, ZZY+16, ASL+11, DWL11, DHF+11, GGM+12, IN13, KSSH13, KOP+14, LFN+10, Man19b, MCRL17, NC12, NF17, PMC+17, SGS+16, SNDK16, SH19a, SDL14, SPZP19, Tak10, VVJ15, WLF19, XDL+10, YKH15]. **combines** [WX12]. **Combining** [ALRM18, MBC11, PVAM16, SDF+17, ZGZC19, AS15b, AKN16, BKŠ+11, CQFC10, FBEM11, LWZ+19, MOS12, NHK+13, Vor10, Gon12]. **combustion** [IT19, MB14]. **Coming** [Ano16-75, Ano16-80, Ano16-81, Ano16-82, Ano16-83, Ano16-84, Ano16-85, Ano16-86, Ano16-87, Ano16-88, Ano16-76, Ano16-77, Ano16-78, Ano16-79, Yan16]. **commemorate** [HIS17]. **Comment** [Ihl12, JW12, Kne11b, LHMM11, Man13, NSN19, Ray13, RSR+12, RSLML12, dSdS12b, Can11, GKR13, GPGSM12, LAT11, QB10, QB11, SFLG+17, WM12, vLBBR12, VVB13]. **Commentaries** [CDM10]. **Commentary**

[RSR+12]. **commercial** [TF15]. **Common** [HTS17, RNP13, PH15]. **commonly** [PGY15, Pie14, PŁAG11, SPR+13]. **Communication** [PH15, KP10, LAT11]. **Communications** [CDB10, CDBM11]. **CoMnO** [LLL+12]. **Comp** [ABB+13, CHR+12b, HNWF12, ICS+13, Kne11b, MSK+12]. **compact** [RLD12]. **compactness** [PTB+15]. **comparable** [Gil11]. **Comparative** [GZZM16, GVP+10, LAM19, LAW+16, MJC14, MS13, SPR+13, WYGW12, BT18, BPC13, BS10c, JJAB16, RSSG18, VMRSH+17, ZYG+15, CJZS10, PS10]. **compared** [SGWA17]. **Comparing** [FBEM11, GMPB12, Hug14, MS16, SRF+17, VMPS17, SJC11]. **Comparison** [BBG+18a, BK13, BK17b, BVC13, GPM17, MHO18, MVKS10, NFPD13, NTNY15, OCL11, PGY15, Sch18, SLP+12, SIT18, STM+15, TLY+12, YAS13, dRBO13, AGR11a, BAMR13, BB11b, CDM+15, DLL+10, FED17, GR11, HCB11, HBI+17, HM13, KDT+12, KMLS10, LLSW14, MJLV14a, MvBD18, PXXW10, PKK17, PD11, RKGN10, Rob13, RŠRR15, TG12a, UD12, VVBL17, WTH+16, WG12, YLGX14, Kar17, Mat10, SA10, YJ11]. **comparisons** [BMR11]. **compatibility** [EOO+16]. **compatible** [KYB13, MPBJ11, RO14a, SOYC12, VHA+10]. **competing** [SLT14]. **Competition** [HvM16, LZL+15b, HvM17]. **Competitive** [ZSL+11, GMBX+16, RLDJ17]. **compilation** [NKJ16]. **complementarity** [GPS10, OAN15b]. **Complementary** [EVR18]. **Complete** [SN16b, CSKH15, LYC+13, OAN15a, SPS+12, SCSW13, TCB16]. **completeness** [Leh15]. **completeness-optimization** [Leh15]. **Complex** [DLT17, HBL12, KKGW19, ANH+11, BŁF14, BH19, DK19, DAdGR15, Dry14, FFA14, GCWS15, HBJ+17, Ish10, KBC12, KMS+19, KGHC15, KPG18, KZP+18b, KSW16, LLL+11, LZJ+11, LL11, LWXC16, MLGB16, MTS+19, MY17a, MY17b, NH19, NCV10, ODB18, OME16, OC14, PPUBGD10, QLYL10, SLT+15, SKKS13, SL17, SYN+12, SPM+19, TDP+12, TNI19b, WKLC12, WCWW11, WHX+10, WSWD19, ZT14]. **complexation** [CBP+15, SNS16]. **Complexes** [BF19a, BGS+19, EHSPT16, GPdC+16, SvLK18, SKGB13, AvKSP16, AMK11, ASMS10, AK10, AM19a, BCSCJ+13, BŁFZ13, BLDK+13, BSG+18b, CSGOA17, CPRS18, CWT+12, ĆMD13, CZH12, CGPP11, CAT+13, CBDS19, CMS13, CM16, CB11d, DS12b, DLP11, EPH+13, ED15, FHW+11, FCE15, FPB12, FB14b, GK15a, GHL17, GPK+16, Gil11, dCGCRN19, Gra18, HDK+12, HSY+11, HKR12, HLB15, HRJ+14, HGHP14, HRJ+15, HDPM14, HG10, HQSZ19, ITY+19, JRSHP14, KT12, KPL13, KTK17, LS11a, LLC+10, LWL+11, LHHW14, LZL+15b, LDZW17, LXZ+10, LYSS11, LJL+11, MUN+19, MLG18, MC10, MFR+11, MKK+19, OSHG17, OOT15, PGCT+12, PHK14, PM13, PZBA13, ŘRH12, RHPWS13, RLD12, SB10, SZdB19, SLIB12, SPR+13, SCSM19, SDL14, SGH+16, TLY+12, TS15a, Tru18, TKCN19, TS10b, Tsi19, VLB+10, VVP12, VVY17, WL14, XMSZ16, YMY+19, YKH15]. **complexes** [ZCK+16, ZRCC12, ZZL+12, ZLZ14, ZDX11, ZWY+10b, ZWY+10a, ZZL19, ZBMZH15, vSGP10]. **complexity** [GP12, NSP15].

GP11a, KSK11, KNP+12, KKA+18, Kos16, KKH18, LLB+12, LSH+11, LWD13, MG11, MCP18, PLFS18, PS17, Rui11, RRK16, SPHF+18, SH18a, SACdG14, Wu10, YB11, ZTH+15, ZLZ14, ZYvIZ14, GA19]. **couplings** [CSEMB+16, LK11, LZH+11, YFH+19, ZB18, dVAG16]. **covalency** [HS14a]. **Covalent** [WBT10, FCCP17, HAI+16, KAR12, MŘ17, OZS+13, RS13, SFA17]. **CovalentDock** [OZS+13]. **covalently** [CZNA11]. **Cover** [Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g, Ano12h, Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n, Ano12o, Ano12p, Ano12q, Ano12r, Ano12s, Ano12t, Ano13a, Ano13l, Ano13t, Ano13u, Ano13v, Ano13x, Ano13y, Ano13w, Ano13z, Ano13-27, Ano13-28, Ano13-29, Ano13-30, Ano13-31, Ano13b, Ano13c, Ano13d, Ano13e, Ano13f, Ano13g, Ano13h, Ano13i, Ano13j, Ano13k, Ano13m, Ano13n, Ano13o, Ano13p, Ano13q, Ano13r, Ano13s, Ano13-32, Ano13-43, Ano13-51, Ano13-52, Ano13-53, Ano13-55, Ano13-56, Ano13-57, Ano13-58, Ano13-54, Ano13-59, Ano13-60, Ano13-61, Ano13-62, Ano13-63, Ano13-64, Ano13-33, Ano13-34, Ano13-35, Ano13-36, Ano13-37, Ano13-38, Ano13-39, Ano13-40, Ano13-41, Ano13-42, Ano13-44, Ano13-45, Ano13-46, Ano13-47, Ano13-48, Ano13-49]. **Cover** [Ano13-50, Ano14a, Ano14b, Ano14c, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14n, Ano14o, Ano14p, Ano14q, Ano14r, Ano14s, Ano14t, Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14-28, Ano14-29, Ano14-30, Ano14-31, Ano14-32, Ano14-33, Ano14-34, Ano14z, Ano14-35, Ano14-36, Ano14-37, Ano14-38, Ano14-39, Ano14-40, Ano14-41, Ano14-42, Ano14-43, Ano14-44, Ano14-45, Ano14-46, Ano14-47, Ano14-50, Ano14-51, Ano14-52, Ano14-53, Ano14-54, Ano14-55, Ano14-27, Ano14-48, Ano14-49, Ano14-56, Ano14-57, Ano14-58, Ano14-59, Ano14-60, Ano14-61, Ano14-62, Ano14-63, Ano14-64, Ano14-65, Ano14-66, Ano14-67, Ano14-68, Ano14-69, Ano14-70, Ano14-71, Ano14-72, Ano14d, Ano14e, Ano14f, Ano15a, Ano15b, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n, Ano15o]. **Cover** [Ano15p, Ano15q, Ano15r, Ano15s, Ano15t, Ano15u, Ano15y, Ano15z, Ano15-27, Ano15-28, Ano15-29, Ano15-30, Ano15-31, Ano15-32, Ano15-33, Ano15-34, Ano15-35, Ano15-36, Ano15-39, Ano15v, Ano15-40, Ano15-41, Ano15-42, Ano15-43, Ano15-44, Ano15w, Ano15x, Ano15-37, Ano15-38, Ano15-45, Ano15-46, Ano15-47, Ano15-48, Ano15-49, Ano15-50, Ano15-51, Ano15-52, Ano15-53, Ano15-54, Ano15-55, Ano15-56, Ano15-57, Ano15c, Ano15d, Ano15e, Ano15f, Ano15g, Ano15h, Ano16a, Ano16b, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m, Ano16n, Ano16o, Ano16p, Ano16q, Ano16r, Ano16u, Ano16v, Ano16w, Ano16x, Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16-29, Ano16-30, Ano16-31, Ano16-32, Ano16-33, Ano16-34, Ano16-35, Ano16-36, Ano16c, Ano16-39, Ano16-40, Ano16-41, Ano16s, Ano16t]. **Cover** [Ano16-37, Ano16-38, Ano16-42, Ano16-43, Ano16-44, Ano16-45, Ano16-46, Ano16-47, Ano16-48, Ano16-49, Ano16-50, Ano16-51, Ano16-52, Ano16-53, Ano16-54, Ano16-55, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h, Ano17a, Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x, Ano17z, Ano17-27,

AAB+19, BMBJ11, FFA14, GS14, GCW16, dCGCRN19, ISN13, KNE11a, KRSC12, Les19, NJX+10, ODB18, PS17, RSLML12, Sak18, SSGS15, SEJ+18, STM17, SKGB13, WWU12, WES13, dSdS12a, dSdS12b, dLC17, dLvNC18b].

SFG+17, SHL+18, Sea10, SCW11, SDM+16, SEF+16, SE14, SH14, ST13, SHL+13, SPR+13, SZX13a, SZX13b, SMM15a, SMM15b, SMM+18, SKTT11, SZZS16, STS15, SK11, TLdG+12, TN10, VGV+11]. **density** [VAR12, VECT12, VV14, Vik11, VL17a, VI17, VED10, VHS+19, Vyb16, WKC10a, WHL+10, WGL+11, WCWW11, WWU12, WWCL15, WHX+10, WL14, WTH+16, XYW+14, YLZ+10, YS13, Yu12b, ZTH+15, ZXS+10, ZSWL12, ZKE+17, ZDX11, ZLHH14, ZCWX18, ZGS+10, dSdS12b, dSdLBNB17, dLC17, dLvNC18a, CDM10, FAS+18, VV19]. **density-based** [LZS+17]. **density-density** [DSAS19, SS16a]. **density-fitting** [Boz18, Hil13]. **Density-Functional** [YKNN19, Oht16, CHG+16, HNWF07, HNWF12, IM17, JCP14, KZZ+16, MFR+17, NF17, NN18, NO16, NNK+16, Rez19, RHPWS13, SPS+12, VED10]. **density-peaks** [LZS+17]. **deoxy** [VM11]. **deoxyribonucleoside** [XVN17]. **deoxyribonucleosides** [RJWW12]. **dependant** [PNG10]. **Dependence** [CFM+19, BRLS08, BRLS12, ELP19, FE14, GZZ12, KKO+16, KGM12, Lar12, LPE+10, LLTC12, MP17b, PZA15, PBE16, PS10, SGPJS+17, SY16b, AD10, MGWR12]. **Dependences** [NNT+19, SMM+18]. **dependency** [DKT13, PHDH13]. **Dependent** [YKNN19, AALCM11, BS16a, CHG+16, CP15, CKP10, DP15, EPD+10, GTK10, HNWF07, HNWF12, HG10, HYUS11, JYS+12, KS18, KCPMG12, LPLS16, LZ12, LZGS11, Mat10, NS10, PAK17, PPJ14, PVJ10, RHPWS13, REL17, SY16a, SFBT17, Vik11, WHL+10, WHX+10, YLZ+10, ZXS+10, ZDX11]. **depending** [Lin18]. **depolarized** [KKK+19]. **deposition** [SE14]. **depth** [DDP+18]. **derivates** [UGK18]. **derivation** [SCMA+17, VVV+15b]. **derivative** [MY17b, TPL+10]. **Derivatives** [KTSW11, CWHH11, CZH12, CBTZ16, CROB16, GRN19, HSZ+11, JS17a, JYS+12, KG11, KPL15, LWGZ15, LWWG12, MFR+11, MIS+15, NS10, NF18, PC14, RVB+12, RFN15, REH13, SBR13, SZX13a, SZX13b, VVJ15, VVY18, VSD10, WGL+11, WRG+17, WDP+12, ZsA10, ZWZ11, ZZ12, ZZWX11]. **derive** [RVP+11]. **derived** [CIKT13, GMMH+16, KSR+16, LRVM18, LZGS11, MUGNVJ+18, MCLD10, OSS10, PLZ17, REL17, SOYC12, SE14, TBSM12]. **Deriving** [CCYL11]. **descent** [MS16]. **describe** [LCK+18, RHRCH16, RS13]. **described** [BM12, CCB15, KDS17]. **Describing** [MKGA10, CGA19, DAP+18, JCP14, JBSQG11, MY17b, VBD11]. **Description** [FD16, MŘ17, Rez19, SWW+19, BBG+18a, BD12, BE16, Cam15, CRZ+18, LAM19, LZLC13, MFR+11, PM13, PLH16, PVAM16, RVM19, SRF+17, SSA+17, TKNN10, WvRSM14, WL14]. **descriptor** [DFF+15, MA16, PRYI+17, TMJ15, WMW+10, Yap11]. **descriptor-based** [DFF+15]. **Descriptors** [ELKE19, STF+19, CBDS19, FCL+10, FZL+15, GJMPAM+14, MdOdQ18, MCF+18, MH10, NKJ16, PKIC11, RB13b, SIT18, TTB+10, Wei12b, YLCX10, Yap11, YDX16, ZWX16]. **Design** [LI19, LLX+19, LCM16, Spr18, SCSM19, Tak14, TZ12, VBD11, AM10, AFBR17, BAMR13, BEPM14, BPC13, CBP14, DPB+12, DPOS16, DGL+13,

GS14, GMZ12, HSW+19, HHBY10, ISP+10, KSD+12, LABSG17, LBS10, MS16, NPG+18, PC11, SYDS11, SGM+13, Sti15, TKXT13, TRA+16, VVY17, VVMY18, VMV19, VMPS17, XHLH16, ZSB+11, ZWP11, ZYW+16, ZWS+10].
designed [BŁŁ13]. **Designing** [PSdPE+10, CSC+18, ZA15, Fel10].
desolvation [BK17a]. **Desorption** [UGK18]. **destabilization** [XMA+19].
detailed [ABB+12, ABB+13, GPdC+16, KGJZ19, MP13, MO15, MC10].
details [MBA14, RSG+10]. **Detect** [RMRBH+19]. **detected** [TCPPC14].
Detecting [DVVP14, HW19]. **Detection**
[CBP+15, BV14, CLX+10, Man19a, ZLM+15]. **detectors** [SK13].
determinant [PM18b]. **Determination**
[BP18, Cam19, KLS10, KMLS10, AFPI13, BŁS10, FSC+14, KR12, Kne11b, LPS12, LK11, LAT10, LAT11, MS13, NHN16, PG14, PBG17, SS16b, SPR+13, WAM17, WOH18, XLYZ10, YKO+11]. **determine** [VDVR14].
determined [CHP11, IM17, YK13]. **Determines** [PK19]. **Determining**
[DSD+11, SGPJS+17, CSNCS+18, SDB+16, WOH16]. **deterministic**
[ITY+19]. **detonation** [LWWG12]. **Deuterated** [NQB19]. **developers**
[GKV+13]. **Developing** [CK17, DSK17, LPS+13]. **Development**
[BSD18, FPH+19, GLB16, GMMH+16, HYSF19, LLJ12, MMB+17, MMZW14, MCP18, NB19, ND19, RZG+13, RLD12, SC17, TNYN16, WPM+15, ZA15, CYG+15, GMASBF16, GCP+13, LPLA13, PZA15, PPM15, WDHZ13, YWZ14, ZsA10, ZSYH12, CRC13, VKC10, WCDM11].
Developments [LJC+19, YWJ+16]. **Deviation** [CSAdOM17]. **deviations**
[HDL+14, KG15]. **devices** [DJX+11b, DJX+11a]. **Dewar** [Bac12]. **DF**
[Chu10]. **DFT**
[BRLS12, CLFRO18, CPR18, SIG+15, YJ17, ZZY+16, AALCM11, AR10, AF14, ASMS10, BTMS12, BRLS08, BIL10, BTB+11, CLFRO18, CMM18, CCB15, CH10, cCVG+14, CBDS19, CXS10, DSB+19, DJD12, EFAC13, FVP14, FPRS14, GMASBF16, GRN19, dCGCRN19, HDM+19, HSH15, HRJ+14, HRJ+15, HBI+17, HL19, JRSHP14, KG15, Kar17, KT12, KKL+13, KM13, KP10, LEdOLdlV17, LBC+19, LRBB12, LZL+10, LZHH11, LXZ+10, LSH+11, LYSS11, LZLC13, LH14a, LLSW14, LCM+14, MUN+19, MMS16, MPJ+19, MDTD16, MG15, Mat10, MS11, MVKS10, Mor15, MCK17a, MCK17b, NKJ16, NC12, NMLD13, PTK11, PHK14, QLYL10, RS17a, RDF+11, RS14, RRC+15, RLZ+18, RN17, REL17, RKB+14, RK15, SRF+17, SWM10, SCF+19, SRL+15, SCSM19, SWW+19, SDL14, SZZ+18, SPZP18b, TNI+19a, TSNC+17, TG12b, Tsi14, TS15b, Tsi17, VVJ15]. **DFT**
[VECT12, VL19, VAMS14, WKLC12, WYGW12, XKW18, YZGS14a, YZLZ19, YSRSS10, YZ15b, YXZZ17, ZCK+16, ZWGO16, ZZWT12, dSDdAR10, vS18].
DFT-based [NKJ16, NC12]. **DFT-D** [SWW+19]. **DFT-derived** [REL17].
DFT-MD [GMASBF16]. **DFT-predicted** [WKLC12]. **DFT/MM** [RN17].
DFT/TD [LXZ+10]. **DFT/TD-DFT** [LXZ+10]. **DFT/TDDFT** [MS11].
DFTB [SA10, FHT+15, MŘ17, MAP18]. **DFTB/MM** [RN17]. **DFTB3**
[IY18, KWG15, VHS+19]. **DGeCl** [MCLD10]. **DH** [SGPJS+17]. **DH2**
[SBW12]. **di-mannose** [VM11]. **di-tetrazine-tetroxide** [MCAG+16].

[CSXZ17, SZX13a, SZX13b, ZWLX11, ZWX19]. **Douglas** [YS13]. **DOX** [RCR+16]. **DPO** [WGL+11]. **DPPC** [LBDP12, vRWGS17]. **DPT** [BH13, BZH14]. **Dramatic** [MLY+13]. **dramatically** [CSC+18]. **Draw** [LBB+15]. **drawback** [BRGN12]. **Drew** [IPAA11]. **driven** [BSL11, BG17, DSM+11, GA19, HXM+16, KC13b, LZL+13, LLL+12, REL17]. **Driving** [YZLZ18, RN17, YZ17]. **Droplet** [SJSS19]. **Drude** [ALRM18, LRvdSM15, LM18a, Ric16, SM14b, ZM10, HLEM18]. **Drug** [GSHM10, MBA14, AJA+19, FLM11, GMASBF16, HSW+19, Ibr11, ISP+10, PC11, PVJ10, SZZ+18, VHA+10, Won18]. **drug-like** [VHA+10]. **druggability** [LG14]. **drugs** [PPUBGD10]. **DSCs** [YJN+11]. **DSiCl** [LX11]. **DSPMP** [FZL+15]. **DsRed.M1** [SGDT10]. **DSS** [GZM11]. **DSSCs** [ZSTRS+18]. **DTTO** [MCAG+16]. **dual** [JCG+10, MA16, TMJ15]. **Duncanson** [Bac12]. **duplex** [HDK+12]. **Durandal** [BSZ+12]. **during** [GBPCC19, GNDA+12, LBC+12, MJLV14a, MJLV14b, OSA19, PNG10, RSKG14, dCDP15]. **dyad** [KP10]. **dyads** [KCK+15]. **Dye** [MP19a, ACS12, JYS+12, LZL+15a, SLP+12, YJN+11]. **dye-aggregates** [SLP+12]. **dye-sensitized** [ACS12, JYS+12, LZL+15a, MP19a, YJN+11]. **dye-sensitizer** [YJN+11]. **Dyes** [FAS+18, DBM+17, NPG+18, VÅA14, WJG+13, YJN+11, ZSTRS+18]. **dyes*** [FA18]. **Dynamic** [LKL10, SFA17, SZB19, VSP19, TNYN16, AKK+16, BS10a, BMB13, CVT+11, ESM+12, GBL+11, Hel13, MB14, NYN17, OPR16, Vor12, WFS19, PBDW11]. **dynamical** [ALH+10, EFOD13, Ham11, VVMY18, VPR10]. **dynamically** [HS17a]. **Dynamics** [AIM+18, BHF+18, BHB19, CPV+12, LK13, MFEM16, NNT+19, NN19, AASP18, AJA+19, AALCM11, AG11, AS15a, Aki16, ASL+11, ABD11, APK14, AB16a, ALH+10, BHB12, BSL11, BDTP11, BJSI12, BW15, BF17, BMBJ11, Bow16, BEL+11, CTR13, CS14, CH16, CCOH14, CCW+10, CHKR10, DASA15, DGH+11, DMN15, DSD+11, DZT11, DJS+18, DLZ15, DDM+15, DL19, EP10, EK15, EPH+13, ETLS17, EFOD13, EvRC+18, Fom13, FBEM11, FPH+19, GBL+11, GDV17, GR11, GKB+19, GWZ15, GCW14, GGM+12, GPdC+16, GP11b, GC11, HZ11, HS17b, HKNH18, HHNK19, HCD+10, HP10b, HPT17, HPSK12, HJ10, HHWL17, HLEM18, HRID16, HC14, IUK+11, ISK14, IN19, IM17, II10, IPAA11, JIS13, JA10, JBSQG11, JCG+10, JAH+17, JLS18, JWST10, JMS14, JS17b, JND+19, KT19, KCK+17, KCK+15, KVQC+11, KUDG12, KSNT19]. **dynamics** [KGHC15, KCC+18, KDB13, KB14a, KNE11a, KERY+16, KLOS10, KJM+17, Kop19b, KSR+16, KG13, KZP+18a, KNR+18, KV15a, KVR10, LL15, Lar12, LWK+14, LH11, LJR+12, LL13a, LRvdSM15, LCH10, LYC+13, LMI+14, LPE+10, LLTC12, LZS+17, LPLB16, LLT12, LBDP12, MBT14, MMH19, MSY19, Man19b, MKS+12, MSC+10, MJC14, MN15, MCRL17, MLN+18, MFEM15, MADWB11, MKM+17, MB16, MHRR11, MO17, MIOM13, NPTS16, NST14, NFPD13, NFG+13, NNK+16, NHK+13, NTNY15, Oht16, ON14, OGL10, OCL11, OLY17, OT12, OCW+15, PMC+17, PSS14, PAK15, PH17, PP19, PL14, PM13, PD12, PHT17, PVZ13, PS10,

PVAM16, RD18, RS12, Ras17, RO14a, RO14b, RFN15, RR14, RdA12, RVdMB16, RC18, RLG14, REL+14, RŠRR15, RSB+13, SHMO11, SF18, SLT+15, SKA19, SWM10, SSWX14, SS19, SSNT19, SOM+13, SCK18].
dynamics
[SJ17, SR18, SYN+12, SM16b, SK13, SKMS13, SFLG+17, SLLL13, SJ16, SZZ+18, SV11, SPZP19, SBvG14, SAvG15, Tac19, Tac17, TNYN16, TFYO19, TJR19, TTC+18, US11, UGK18, Vor10, VM11, WKLC12, WBN+13, WAM17, WC11, WHL+10, WH11, WWKS11, WLC12, WLF19, WES13, WG14, Won18, Wu10, WBVE16, XCLZ19, YPvD13, YO19, YHX19, YJXZ13, Yon16, Yu12a, YFH+19, ZZY+16, ZX11, ZDKM12, ZBP11, ZP13, dCLFGL13, dSVdM+16].
Dynamics-Based [AIM+18, Vor10]. **DynamO** [BSL11]. **dysprosium** [BP18].

E-field [XMA+19]. **E-I** [GM17]. **EA** [MLCD11]. **EADock** [GZM11]. **Early** [Tsi18, CBP+15]. **earth** [Ano11, JHMB+09, JHMB+11, WD10]. **Easy** [SJL18, QS19, TKT11, VVV+15b, Yes12]. **easy-to-use** [QS19]. **Ebola** [OLY17]. **echo** [OC19]. **economic** [PN13]. **Ecoupling** [dVAG16]. **edge** [DWZ+17, DJX+11b, KHE+19, PDG+16]. **edge-modified** [DJX+11b].
editing [You10]. **Editor**
[GKR13, GPGSM12, JW12, Ray13, RSLML12, WM12, dSdS12b, vLBBR12, Ihl12, BCJC+14, Cor17, KR14, Man13, SFLG+17, VVB13]. **Editorial** [Ano16-56, Ano16-103, Ano16-104, Ano16-105, Ano16-106, Ano16-107, MWC19, Yan16, Ano16-129, Ano16-108, Ano16-109, Ano16-110, Ano16-130, Ano16-111, Ano16-112, Ano16-113, Ano16-114]. **Editorials** [BEFS13]. **Effect** [ABD11, CBG17, CS17, DSHLM18, GEG11, HYL+11, JZ12, KMT+19, OBW12, RRF11, SJSS19, TJR19, VS14, WZ19, dALdS+15, AB10, CSKH16, CR19, CD11, CXS10, DKT13, DJX+11b, DLW12, FCOGM12, FHK+12, GFGS18, GA19, HLBLCCG15, JWO15, JYS+12, KTT16, KCL+14, KLN16, LLvG10, MTvG12, ONTTL16, RWR+13, SLT14, SBC+11, SY16a, Tsi19, UT15, VLGK+17, WDLG12, ZJZM13, ZLL+10, BLG10, CC11, IYK11].
Effective [GKV+13, IM17, YZ16, AASP18, CVG14, DR11, DMN14, DMN15, GA12, HKNH18, KS13a, KS15, LCM+14, PHC13, PRYI+17, PS13, RLD12, ŚSB+16, UCFR16, WXS+12, YZZ16, YZ15b, ZKH+10]. **Effects**
[CS14, GBG+19, HTY19, JAH+17, JLLW19, LGOM+15, LCH+15, Mor15, NNT+19, SEM12, Tac17, WWTL19, YCK16, dCRN18, AS15a, ATIP18, AS18, AK10, ASK18, BBI+11, DMD+18, EPH+13, FAA15, FD16, GNC+18, GMG+10, HS16b, HDM+19, HLBLCCG15, INT18, IN19, JMX+16, KIOY19, KG11, KYCL11, KHE+19, KKA+18, LGVA14, LHT15, LWD13, LKZM18, MUN+19, MKGA10, MBC11, MRK11, MLY+13, MCUJ15, MGS+16, MKK+19, NASH15, ORZ11, OSHG17, OCW+15, PLFS18, PDMT10, PP19, PC14, RMGB11, RRK16, SSWX14, SMP17a, SFLG+17, TM16, TYN15, TY10, UT14, VP19, VKAM12, WXY14, YNH+17, YJ11, ZPP+16, Zha11, ALW+10, THP+15]. **Efficacy** [LC17a]. **efficiencies** [RO14a]. **Efficiency** [AC11b, BB11b, BB11c, FE14, GBSE11, XFG+16, AC12, FSSW19, GSHM10,

LY10, LWL+11, LZL+15a, MKGA10, RO14a, XFG+15, vLBBR12]. **Efficient** [AB16a, BC13, BAS14, Cas13, DSV+19, DMAH15, DSAS19, DBF14, EP10, GCWS15, GRN19, GWW19, GPK12, Ham11, HNS16, Hes19, HDL+14, HHWL17, JMS13, KNR+18, LZ11, Les19, LGKS17, MKS+12, NYN17, PSS14, PAK15, Ran12, RJS17, SS16b, SSP19a, TJB12, UCRL18, WHAS+16, WM12, ZZ14, ZKE+17, AM10, BW11a, Boz18, CBP14, CHG+16, CY09, CY13, CZZL19, CMS13, DS15, DGL+13, GREA11, GWZX12, HDL+17, ISK14, JZ17, Kid19, KB11a, KKH18, KV15b, LFB14, LPK16, LLZA12, LZL+15a, LZS+17, LAS+14, MP19a, NPTS16, NF18, NN18, OK16, PW12, PBG17, Ran13, RR14, Rod13, RSL16, SCOJ13, SA13, SSMW09, SCSW13, SWB+12, Sun15, TO10, WJG+13, WOH18, WLQ19, ZWP11, Zha12b, Zha12a, vLBBR12, WHAS+10]. **Efficiently** [WES13, ASMS10, DDK14]. **EFP** [CBG17]. **egg** [Pla11, ZP13]. **egg-box** [Pla11]. **EGRAD** [vW11]. **Ehrenfest** [Dil15, FED17]. **eigensolver** [KZZ+16, KCC+18]. **eigensolvers** [ZVY+15]. **eigenvalue** [Coh18, HLXH17, HLXH18]. **eight** [HDK+12]. **either** [TCPPC14]. **elastic** [ECZWD17, LBTV11, QB10, QB11, SH11a, XTY+14]. **Electric** [GH16b, LL13b, BŁFZ13, BŁBG+13, BS10a, CXS10, GH16a, KMT+19, KZK+12, MRB14, PdSC18, SH15, SLX+15, Yan11, YJ11, YCK16, ZSLL17, ZX19]. **electrical** [LLLM11]. **electro** [TMJ15]. **electro/nucleophilicity** [TMJ15]. **electrochemical** [SKGP19, SIG+11, SGH+16, YJ11]. **electrochemistry** [DSK17]. **Electrode** [IN19, MKO+13]. **electrodynamics** [Tac19]. **electrolyte** [KS18]. **electrolytes** [HAL14]. **electrolytic** [SV11]. **electromagnetic** [SEM12]. **Electron** [BK11, Bar14, BLG11, BWKW10a, BWKW10b, CEBO15, HS16a, HRMAL+13, HGCCGR+16, KGR+16, KKGW19, LLX+19, Pil17, VSP19, VV19, WWU12, ACD+13a, ACD+13b, ABDGN12, BHB12, BT18, CDB10, CAA10, CWHH11, CC18c, CJPTC18, CTP13, CXD+19, DAdGR15, ED15, EP12, ESM+12, EP15, FRSA14, FWS+18, FED17, FCPJM14, GNDA+12, HSH15, HPT17, HEMCZE+14, HAP+12, HBL12, IYK11, Jan16, JBSQG11, JSF19, KPL13, KTK17, KKA+18, KYG+15, LW16, uLhY11, LRVM18, LHO17, LYL16, LLJ12, LP11c, MRC+18, MKGA10, MRB14, MT19b, Mat14, MBFP15, MKH+13, MCK17a, NYH+17, NLL19, NS17, PAK17, PGdO+16, PSC11, PS17, PN13, PTB+15, PHT17, PC16, Ras17, Rod13, REL17, RSKG14, SFM+18, SZB19, SB14, SHB17, SGHL13, SK11, SSA+17, UCRL18, VGV+11, VECT12, VL17a, VCL18]. **electron** [VI17, Vyb16, WLW+10, WMW11, XBSS19, YKH+10, YLL11, ZPP+16, ZCWX18, ZGS+10, dLC18a, dLvNC18a, GMBM18, SDIP18]. **electron-correlation** [NYH+17]. **electron-deficient** [YLL11]. **electron-hole** [PTB+15]. **Electron-pair** [WWU12]. **electron-sharing** [JSF19]. **electron-vibrational** [CJPTC18]. **electron-withdrawing** [CWHH11]. **Electronegativity** [FCPJM14, vS18]. **Electronic** [AMQ+14, AM19a, AM19b, ASS10, BAD+19, DSB+19, DAdGR15, DGSVGVM19, GNDA+12, GNI18, HLWD15, Ibr17, JLLW19, KYCL11, KKL+13, KKGW19, LLBO12, LS11b, LKZM18, MT19b, MP19b, MAPB10,

NSN19, ND19, NIIT15, PMC+17, RLA+11, SZL19, TN12, TNI+19a, TN10, TFQ+10, TS15b, VI17, WRM+12, YW12, ZRCC11, ZLX+19, AR15, AK10, AC12, BLZ+13, CPRS18, DKE+17, DHOG13, DMD+18, EVR18, EH13, EWK+13, EBPK17b, FB10, GTT10, GRARO+14, GWX+12, GZZ12, HASR+12, HS14a, HSB+11, Hua16, IIF+10, KKH19, KKPT11, KSM17, KG11, KKA+18, Kop15b, Kos16, KP10, LGOM+15, LX11, LBTV11, LBTV12, LXZ+10, LSH+11, LLSW14, MC10, MA16, MCF10, MCF+18, Mat10, NC14, NS18, NCT18, NFI+16, OLA15, PdSC18, PHK14, PTB+15, PVAM16, Pyy13, RCM+13a, RML+15, RR12, RR11, SFA17, SLP+12].
electronic
[SIT18, SB19, SRS14, ŠB15, SKGB13, Tac19, TFQ+11, TD10, TS15a, TNG+10, TS11, TG12b, Tsu19, TEDT18, VVP12, VHR16, VAR12, VBMA13, VLGK+17, VGTL16, WHL+10, WGL12, WJG+13, WO15, WSGN11, WZK+13, YK13, YFH+19, ZJZM13, wZbZ11, ZBB16, ZZZ+19, dCDP15, dVAG16, vSGP10].
Electronically [SCSM19, BSL+16, LSH+11, LYSS11, RIJ+11, SFCCK+14, SFCCK+15, YB11]. **electronics** [RN17]. **Electrons**
[Sah18, EKH14, FHZA+18, WCY+11, WRG+17, XhD15, YCGA10, SGP18].
electrophilic [MA16, WDS+19]. **electrophilicity** [YB16]. **Electrostatic**
[CLA16, LP11b, MLZZ12, Sch18, VSP19, WFZ+18, ALRM18, AS18, BT18, BCNH+11, BSF18, BK13, CCC+11, CS14, CPK12, CB11c, DLSA14, ER18, GBL+11, HOK17, IO13a, KTNN10, KYG+15, Lar11, LCA17, LCM16, Mat14, NF18, OHPR18, PVJ10, RB13b, TY10, VMRSH+17, VVY18, YKO+11, YWJ+16, YAO18, YMP14, YZL+15, ZDZM13, ZBP11, KGM12].
Electrostatics [BSG18a, CZY11, FGM11, FP17a, KFY+13, LPLA13, MBA11, MBC13, NLP+16, SDZ17, SWPR11, UHH+11, XYX17, YMP14].
element [BCCO10, GPK+16, RMGB11, TG12b, TCX+13, XYX17].
elementary [LPLB16, Zim13]. **Elements** [TKN13, BV14, CWZB10, Hil13, JJJ16, LFB14, SK15a, TDKT10, Tsi14, WS12, XhD15, MSPC19]. **elevation** [HH10]. **ELF** [RSKG14]. **ELI** [BWKW10a, BWKW10b]. **ELIA**
[BWKW10a, BWKW10b]. **Eliminating** [vS18]. **elimination**
[SL10, dCDP15]. **Elisabeth** [Ihl12]. **ellipsoidal** [DGB+13, LDG+15].
Elongation [OLA15, MKGA10, MKGA10]. **Elongation-MP2** [MKGA10].
Elucidating [HNHR13, TDP+12]. **Elucidation** [CPLL11, TNYN16].
embedded [DSF17, GMG+10, HSH15, KMT+19, ZFS18]. **embedding**
[CCB15, ESD18, ESM+12, HH16a, HH17, Höf14, HOK17, KSR17, NF18, NOKJ16, RR12, SDF+17, SS16b]. **Embelin** [CPR18]. **emerges** [MNNK10a].
emission [CSC+18, LX11, MCLD10, PLP+16, SGWA17, WDP+12, ZLL+10].
emitted [PE11]. **emitters** [FWS+18, ZGZ19]. **emitting** [FWS+18, ZGZ19].
Emphasis [RCM+13b, PD11]. **Empirical**
[BA11, DLMH12, KLN12, CK17, DAG19, KB10, LL11, MPBJ11, PTK11, RJPB12, SZBM13, SBvG14, TM16, ZRL+15, ZM10]. **empirically** [VCL18].
employing [GP11b, MLCD11, TG12b]. **empowered** [BPLL12, RLLHL12].
enabled [Aou16, BK17c, KYG+15, LL10a, SR11]. **enables**
[KK17a, RC18, XHLH16]. **Enabling** [PHH+12]. **enamine** [AS11].

Enantioselective [ORZ11]. **enantioselectivity** [OAN15b]. **encapsulated** [EOO$^+$16, STS15]. **encapsulating** [WZH$^+$18]. **encapsulation** [YDGZ15]. **encoded** [RSL16]. **encoder** [LDH$^+$14]. **end** [HDL$^+$17, SL10]. **ended** [RJR14, Zim15]. **endo** [FB14a]. **Endohedral** [NKD18, FL15, GLF16, MCK17a, MCK17b, ZSL$^+$11, ZYG$^+$14]. **endohedrally** [DM15, VIT$^+$15]. **endothelial** [JAH$^+$17]. **endpoint** [BB11a]. **ene** [GRCL12, FB12]. **enediyne** [DCHL12]. **Energetic** [JCHT18, JW12, CG15, MCAG$^+$16, MvBD18, PBG17, SB18, SLHW09, TPL$^+$10, YSRSS10, ZZWX11, ZYL$^+$12]. **Energetics** [JL19, SFM14, TT18, BK17a, BMFG16, DT19, DSF17, GAJ$^+$17, HEM$^+$17, JJH$^+$13, KB13, MP13, MBRC16, OCW$^+$15, SJD11, SNS16, SL17, SDB$^+$16, ST13, SFBT17]. **Energies** [ELKE19, AF14, AS14, AG12, ABS$^+$19, BW11a, BŁF14, BVHI17, BS16b, BE16, BS18, CHG$^+$16, ĆMD13, CR19, CH10, CTP13, CXD$^+$19, CBG16, DHOG13, DMJ17, DHF$^+$11, DPOS16, FGM11, GRN19, Gil11, GP11a, Gri13, HAGK10, HH10, HH11, HLW$^+$17, HDM$^+$19, HHWL17, IKN13, KSH13, Kar17, KSM17, KJDB12, KB11b, KYB13, LJW11a, LW11, LHHW14, LH14a, MCS11, MS13, Min18, MSÅK12, MBE16, MMJ10, NWW17, NMF$^+$14, OBW12, yOTn16, OAN15a, OSR16, PGCT$^+$12, PPJ14, RLDJ17, Ran19, RDDS10, RAR$^+$11, RO14b, RZ16, RR14, Rob13, RJS17, SRR16, SK12, SHL$^+$13, SOD$^+$11, STM$^+$15, SGWA17, TS14, TSN16, UD12, VVG13, VECT12, VM11, WBT10, WS10, WJG$^+$13, WFS19, WGA18, WG12, WX12, YAS13, YMP14, ZZ14, dALdS$^+$15, dRBO13, NQB19]. **Energy** [DK11, ELKE19, GS16, IIHY15, JCGVPHT17, Jia19, Kop19a, LFN$^+$10, LPLB16, MYKO18, NK19, OSI$^+$19, PK19, SN16b, SSGS15, Spr18, SKGB13, VL19, VSP19, WM12, ZQH19, AMGB10, AAB$^+$19, AC11a, Ano10a, AK10, AKN16, BCSCJ$^+$13, BPM15, BRE16, BH15, BS16a, BRLS08, BRLS12, BACSCJ$^+$10, BG17, Bou14, Boz18, BD11, BWMSM10, BB11b, BB11c, BG12, CM13a, CK10, CDM$^+$15, CLA16, CY09, CX10, CZY11, CY13, CH16, CSXZ17, Che17, CF18, CS17, CHR$^+$12b, CHR$^+$12a, COHI19, CKP10, CMvG10, CPK12, CWZB10, DGH$^+$11, DWR17, DBG11, DS12b, DH14, DWC17, EV14, FMNC11, Fer17, FED17, FCOGM12, FSSW17, FCCP17, FLM11, GS14, GS15, GHK12, GO13, dCGCRN19, GMO16, HNyH19, HDL$^+$17, HHNK19, Hel13, HDM$^+$15, HH15, HG13, HYMZ16, HYUS11, HJKJ13, HGW18, HYD10, HDHL15a, HDHL15b]. **energy** [HDHL15c, IMK$^+$16, ISN13, IT19, JCPC11, JMLL13, JZ12, JZZM14, JCX10, KCB$^+$12, KTT16, KB10, KIOY19, KNHN16, KN17, KHWB17, KDR$^+$18, Kid19, KB11a, Kop15a, Kop16, Kop17a, Kop17b, Kop18, KLS10, KMLS10, KCL$^+$14, LRVM18, LMZ11a, LZ12, LYC$^+$13, LZZ14, LGL11, LP11b, LX11, LHG11, LSH$^+$11, LZY12b, LLSW14, LAW$^+$16, MCvdV13, MCC11, MK13b, MPA10, MPA12, MSC$^+$10, MJLV14a, MSBF16, MHO18, MK19, MUGNVJ$^+$18, MLN$^+$18, MSÅK12, MAP18, MB14, MB16, MLCD11, MIOM13, NZM18, NCT18, NFI$^+$16, OKIS17, OSR16, OK16, OOT15, OZS$^+$13, PBLdS12, PG18, PBLS19, PZCL16, PBBP11, PM18b, PBE16, PJ13, RS17a, RLDJ17, RAR$^+$11, RDT14, RS13, RCM$^+$13a, RML$^+$15, RF15, RVVK13, RLA18,

RDRC16, SM14a, SM16a, SRF$^+$17, SRSLO15, SFR$^+$11, SYDS11, SISK10, SWPR11, SY11, SC15, SOJ14, SH11b, SSMW09, SC18b, SBN13a, SBN13b]. **energy** [SOvG12, SLG15, SNS13, SN10, SHB17, SMM15a, SMM15b, SMM$^+$18, TM18, TSN16, UCFR16, UGK18, VLB$^+$10, VT14, VGV$^+$11, VL17a, Vyb16, WKC$^+$10b, WLF11, WSH10, WGL$^+$11, WWWW18, WZ19, WHM10, XHLH16, XYW$^+$14, XFX$^+$16, XVN17, XCLZ19, YOMT14, Yan14, YHX19, Yu12b, ZPF14, ZLT13, ZGZC19, ZH12, ZSB$^+$16, vLBBR12, SGP18]. **energy-adjusted** [HH15]. **enforced** [BW11b]. **engine** [BEFS13, DBDP16, HC14]. **engineering** [KLZ$^+$18]. **enhance** [EPH$^+$15, LZL$^+$15b, MIS$^+$15]. **Enhanced** [CFC15, HTS15, IMK$^+$16, KvdV14, SSO19, Bou14, CF18, KKO$^+$16, KJM$^+$17, LC16, MBFG15, SLLL13, ZLM$^+$15]. **enhancement** [LLL$^+$11, MA17]. **enhancements** [Abr11]. **enhances** [HYNS19]. **Enhancing** [MP19a]. **enol** [FD14]. **enones** [KSO$^+$19]. **enoyl** [STM$^+$15, SJ16]. **enoyl-ACP** [STM$^+$15, SJ16]. **Ensemble** [PKIC11, MKM$^+$17, YHH$^+$13, ZWP11]. **ensembles** [CDM$^+$15, GO13, Gri13, PBDW11, PKIC11, RLDJ17, RO14a]. **entatic** [HBR17]. **enterprise** [WDY13]. **enthalpies** [cCVG$^+$14, HDK$^+$12, LLH11, LWL$^+$10, MRR11, SHL$^+$18, WKC11, WDW12, ZWLX11, MSPC19]. **enthalpy** [UCFR16, vADC$^+$14]. **entropic** [CHR$^+$12b, CHR$^+$12a, Pro16]. **entropy** [BMPML$^+$13, Hug14, KCPMG12, LMZ$^+$11b, OBW12, STM$^+$15, SDMS13, XSZL11]. **entropy-based** [BMPML$^+$13]. **enveloping** [HDK$^+$12]. **environment** [CCW$^+$10, CB11a, JWST10, KKR$^+$13, KSR17, Lar12, LvG13b, LLT12, RVM19, SK18, TLY$^+$12, UvSvdWK19]. **environmental** [GMG$^+$10, GCC14, HS16b, LGVA14, SIG$^+$11]. **environments** [JBSQG11, PAT$^+$10]. **enzymatic** [GH10, LT13, RIJ$^+$11]. **enzyme** [BHNS14, BG13, Can10, Can11, DGH$^+$11, JDW$^+$19, LHMM11, RN17, SSP$^+$13, SC18b]. **Enzymes** [HRHI17, CQFC10]. **EOM** [KK17a, KKL$^+$13]. **EOM-CCSD** [KK17a, KKL$^+$13]. **EPIC** [TNG$^+$10]. **epidermal** [BHF$^+$18, WC11]. **epimers** [HH11]. **epitope** [CGBK13]. **epitopes** [GRP$^+$12]. **epoxidation** [MUN$^+$19, WCDM11]. **epoxide** [DSHLM18]. **epoxides** [BCP$^+$10]. **epoxy** [HTY19, LPMT17, PPH$^+$14]. **epoxy-carboxylic** [LPMT17]. **epoxy-phenol** [PPH$^+$14]. **equality** [ABS$^+$19]. **equalization** [vS18]. **Equation** [Coo19, NNT$^+$19, AA18, BCCO10, CD16, CLA16, Fer13b, Fer13a, FCE15, Fra15, Fra16, FC18, KS18, KK17b, RSLS13, SK15a, SM16a, SG10a, WBVE16, XYX17, YS18]. **equations** [BYE$^+$16, ZR10]. **equilibrated** [WHAS$^+$10, WHAS$^+$16]. **equilibrating** [OPR16]. **equilibration** [LBDP12, SMP17a]. **equilibria** [GWJR18, LC17b, PLH16]. **equilibrium** [DSD$^+$11, FD14, LLvG10, LvG13a, MCLD10, NHN16, SJWE10, WXY14]. **Ergodicity** [KCK$^+$17]. **Eric** [Sch10]. **ERKALE** [LHSH12]. **Ermod** [SM14a]. **Errata** [CHR$^+$12b, HRJ$^+$15]. **Erratum** [ACD$^+$13a, Ano15-59, Ano15-58, Ano17-35, ABB$^+$13, BRLS12, CY13, Fra16, GLW13a, HNWF12, HvM17, HDHL15a, HDHL15b, HLXH18, ICS$^+$13, JHMB$^+$11, Li14a, MT20, MSK$^+$12, RK16a, SFCCK$^+$15, SBN13b, SZX13b, SMM15a, WHAS$^+$16]. **error** [HAGK10, Hua16, KFT18, PHK14, PD11, WNP$^+$16, ZH12]. **errors**

[LEdOLdlV17, vS18]. **erythrose** [SM17]. **ESCAPE** [WFS19]. **ESCF** [vW11]. **esculetin** [LYSS11]. **ESES** [LWZ+17]. **eSHAFTS** [HSW+19]. **Essential** [DASA15, SKMS13, XTY+14]. **Establishing** [ZKH+10]. **Esters** [AGM+13, HLI+19]. **Estimates** [GS16, GS15, NFG+13]. **Estimating** [DWR17, RF15, KB11b, TTB+11]. **Estimation** [RLDJ17, ABS+19, BPE16, CZY11, Fer17, GLM+17, HHWL17, Hug14, JKS+16, MSV16, MRR11, OZS+13, PHK14, SY11, TM18, WFS19, YOMT14, ZH12]. **Estimations** [RLA18]. **estimator** [FCPJM14, WBF17]. **etching** [KHE+19]. **ethane** [Tak11, ZLT13]. **Ethanedithial** [SMB18]. **ethenol** [AAMD+11]. **ether** [HLB15, TFYO19, WLC12]. **ethers** [GKR13, Ray13, RKG11]. **ethylene** [KCB+12, KT12, LL13a, MCC11, SFM14, TLA10, XZ11, YMY+19, SMB18]. **Etomica** [SK15b]. **ETS** [CSM16, DBGO+17]. **ETS-NOCV** [CSM16, DBGO+17]. **Eulerian** [LWZ+17]. **eV** [KKH19]. **evaluate** [BY11, KPL13]. **evaluated** [VECT12]. **Evaluating** [DKE+17, Sch18, SJ16, WG12, HLS12, JLS18, VL17a, XSZL11]. **Evaluation** [AYYO17, CHR+12b, CHR+12a, EP12, HG10, LLC+10, MBE16, MCK17a, ŘRH12, RB13b, WNM17, YD17, BMR11, BŁFZ13, BŁF14, DLT17, DS12b, GS11, HBI+17, ISO+13, Kid19, KLOS10, Kos16, KT18, KSC16, LJW11a, LW11, LHHW14, LZY12b, NN18, PW12, SF18, UM13, VBDS+11, VM11, WO15, PŁAG11]. **evaluations** [HP10a]. **evaporation** [RSB+13]. **event** [BSL11, HNS16]. **event-driven** [BSL11]. **events** [LRvE17, Lun12, ONTTL16]. **evidence** [RS17b]. **Evolution** [RSKG14, WCY+11, CJL+13, GAMAC+14, MGCC19, NGAS17, Niz13, YHH+13, Yes15]. **evolutionary** [BDdS13, CDS16]. **evolving** [SL17]. **Ewald** [AG11, NO16, YWJ+16]. **EX** [PMG+16]. **EX3** [GPK+16]. **Exact** [BKLA13, GREA11, RP15, dLC18a, BSZ+12, BTB+11, KTSW11, LLZA12, Vyb15]. **exacting** [BS10b]. **Examination** [DT19]. **example** [BBG+18a, GREA11, MS15, RRK16]. **Examples** [HJG09, LK16b]. **EXAT** [JCGM18]. **ExcelAutomat** [LSL+19]. **Excess** [LLX+19, WLW+10, Fra15, Fra16, WCY+11, YCGA10]. **Exchange** [CKH19, DAB16, GS16, Rui11, VL19, XFG+16, ZLZ14, BTB+11, CSKH15, CSKH16, CKH17, CGPP11, CH16, CCOH14, CAT+13, ENKK+17, GS15, GWX+12, HG10, IYK11, IIHY15, IO13a, KCK+17, KTO11, KTO13, KCL+14, LPAS11, LC17a, LL11, LMI+14, MC10, MS16, OGL10, OL13, OLY17, OZ14, PW12, RFHG10, SH18a, SPH11, SH19a, SBN13a, SBN13b, SH18b, SSA+17, TKT11, VL17a, Vyb15, Vyb16, WYT17, XFG+15, ZC14]. **exchange-correlation** [HG10, SH18a, Vyb16]. **exchange-coupled** [CAT+13]. **exchange-repulsion** [CGPP11, ENKK+17]. **exchanged** [DAP+18, LZTV10]. **Excitation** [KDR+18, CHG+16, EFAC13, Les19, MEH18, PTB+15, SHB17, TG12b, TSN16, UD12, WJG+13, WZ19, WGA18]. **excitations** [ACD+13a, ACD+13b, CMF+17, FE14, IIF+10, PVAM16, WWD14, XTn18]. **Excited** [CH10, FHG+19, GBPCC19, SGWA17, YKNN19, ZXS+10, BSL+16, BH19, DSV+19, EK17, ESM+12, FD14, FAA15, FD16, GA18, HNWF07,

HNWF12, HH17, HZSS17, HDHL15a, HDHL15b, HDHL15c, JCGVPHT17, KT19, KPG18, KB14b, LLBO12, LLW12, LWW12, LWGZ15, LGC19, LX11, LSH+11, LYSS11, MPSG11, MGCC19, MEH18, NYN17, PH10b, RHRCH16, RR14, SFCCK+14, SFCCK+15, SRF+17, SZZS16, TSN17, WHL+10, WHX+10, YD17, YHX19, YLZ+10, YB11, YYT12, LZL+10, PGW+17].
Excited-State
[FHG+19, YKNN19, SGWA17, FD14, GA18, HH17, HZSS17, KT19, LWGZ15, MPSG11, NYN17, PH10b, WHL+10, WHX+10, YD17, YYT12, LZL+10].
excited-states [LLBO12]. **exciton**
[HRH+17, LSH+11, SEJ+18, WZ19, ZZL19]. **exciton-phonon** [WZ19].
EXcitonic [JCGM18, NNT+19, LCK+18, ZMMM12]. **excluded**
[LWZ+17, Yan14]. **exclusive** [dLC18a]. **Exhaustive** [DKV18]. **exhibited**
[RWR+13]. **Existence** [BMB13, WD10, NKD18]. **existing** [KT18].
Exothermic [LWL+16]. **expand** [BK17c, Car14]. **expanded**
[MLQ+12, TSNC+17, YSSB12]. **Expanding** [GMZ12, UCRL18]. **Expansion**
[Hes19, HAGK10, HSN14, LYC+13, LRER13, NF17, SS16a, SNS13].
expansions [LZGS11]. **Expected** [Clo15, AF14]. **Expedited** [DJD12].
expensive [LDZW17]. **experiment** [GNC+18, JAH+17, SA10].
Experimental [Cam19, MRC+18, NHF+10, AvKSP16, BRGN12, DCOD13, EOO+16, GPdC+16, HJ13, KP10, Pog10, RO14a, SB10, SGS+16, SKMS13, VZ14, CYI+10]. **experiments** [CBP14, HCB11]. **explained** [FL15].
Explicit [WG14, BEM14, CCOH14, CBG16, EK15, ENKK+17, GLB16, HDL+17, KJDB12, LH11, RdA12, SYH12, SKMS13, Zha12b]. **Explicitly**
[yOTn16, SM17]. **Exploiting** [HB14, BYE+16]. **Exploration**
[FHG+19, OSI+19, ZGS+10, BGL+18, CF18, LWW12, LAW+16, NJR18, OKIS17, OKY18, RDRC16, Sti15, SSP+19b]. **explore**
[JCPC11, MSC+10, MCC12]. **explored** [WLF19]. **explorer** [SYN+12].
Exploring
[BHB12, BPPS17, BPPS19, BCG10, DSHLM18, ELKE19, FDH19, MTM14, PJ13, Tsi17, VHS+19, ZSTRS+18, ZT14, dSdLBNB17, RDRC16, NOKJ16].
explosion [GC18]. **explosive** [YPC+10]. **Exponential** [BBOB16, BB11b].
expressions [Gav12]. **extended**
[GWZX12, IN19, KUDG12, LRvdSM15, SSWX14, TSN17, YB16, Pon11].
Extending [LMZ11a, Man13, TTn19, VBV13a, VVB13, PHH+12].
extensible [GCW14, JYC+16, LAS+14]. **Extension** [AlQ19, HSN14, PFVL14, SDZ17, VVW+18, YHVM12, Cam15, LL11, RLLHL12, Ras17].
extensions [NYH+17]. **Extensive** [JW12, SLHW09, YB11, CF14, KM13].
Extent [OSA19, GFGS18]. **exterior** [HL19]. **exterior/interior** [HL19].
external
[GKSS14, KMT+19, PdSC18, SEM12, XTn18, XMA+19, ZSLL17, ZX19].
extra [PFAS+19]. **extract** [MDTD16]. **extracted** [HNTS15]. **Extracting**
[WSWD19]. **Extraction** [CVG14, UvSvdWK19, VVG13]. **extrapolation**
[CC11, LYC+13, OAN15a, SRR16]. **Extreme**
[HRHI17, Cam15, DS12a, JBSQG11, CCR18]. **eXtreme-Pressure** [CCR18].

ZL11, ZP13, ZM10, ZCGM11]. **force-constant** [WOH18]. **Force-field** [COHI19, DMAH15, LLvG10, MBC11, WTH+16, ZL11]. **force-fields** [CCLP12]. **force-matched** [KSR+16]. **forcefield** [LDB+17, MMZW14]. **forcefields** [CBP14]. **ForceFit** [WKC+10b]. **forces** [EPD+10, Elk16, Has14, HNWF07, HNWF12, IO13a, RN17, SDB+16]. **ForConX** [LDB+17]. **forest** [WZ17]. **Foreword** [Mor19]. **form** [GKB+19, GWX+12, LZSM19, YZ15b]. **formaldehyde** [CYY+17, GNGCA10, OKY18, YPvD13]. **formaldehydes** [TKCN19]. **Formalism** [MKGA10, SFCCK+14, SFCCK+15, SMP17a]. **formamides** [JSW10]. **format** [LAS+14]. **formate** [CJZS10]. **formate-lyase** [CJZS10]. **Formation** [BPPS19, DWZ+17, BPPS17, CD11, ED15, GRCL12, KSM16, KAR12, KK19, LLH11, LWL+10, MCK17b, NMH19, Oht16, RVP+11, SHL+18, TDP+12, UCFR16, WNM17, WKC11, WDW12, YPC+10, ZSWL12, ZWX19, ZWX16, ZYL+12, MSPC19]. **formations** [HTS17]. **formats** [REL+14]. **formed** [RVB+12]. **formic** [TKCN19, TL16]. **forming** [Car14, ONTTL16]. **FORMS** [RMPAM15, FD14, KG11, PS14]. **formula** [BB11b, Ish12, MA16]. **formulas** [KTSW11]. **Formulation** [BD12, SSSM15, CSKH16, DLMH12, KCL+14, MBA11, SMM15a, SMM15b, WRHF10, ZKE+17]. **formyl** [LZHH11]. **förster** [RCM+13a, Kos16, RML+15]. **forsterite** [DOM+11, DBM+15]. **forth** [PNW+16]. **forward** [KZP+18a]. **Four** [PRJ+17, RK15, BHI19, EB12, HKR+14, JKS+16, LLC+10, LWGZ15, WS11, WS12, ZWZ11, OSI+19]. **Four-component** [RK15, HKR+14, JKS+16]. **four-membered** [WS11, WS12, OSI+19]. **Fourier** [IY18, NZM18, YWJ+16, Ish12, LL13a, SZTSM10]. **fpmb** [CWT+12]. **fraction** [Gil11]. **fractionations** [NASH15]. **fracture** [FPH+19]. **Fragment** [GK15b, IIF+10, LSL+19, WLLH18, CIKT13, DR11, FMG12, GWF11, GKV+13, HB14, ISM18, KS13a, KS15, LMZ11a, LFN+10, MFR+17, NF18, NMH19, NF17, OOT15, OOK11, RKGN10, SZdB19, VBV13b, WCT+11, dLC17]. **Fragment-based** [GK15b, WLLH18, FMG12, HB14, LMZ11a, SZdB19]. **fragment-separation** [NMH19]. **fragmentation** [EFB16, SS19]. **fragmented** [JSXH16]. **fragments** [CM16, Kos16, KSR17, ODB18, Sax12]. **fragments-rooted** [CM16]. **Frame** [AlQ19]. **framework** [BFH+13, EH13, GRN19, GP11a, HPT17, JBB+11, KTNN10, MKGA10, OM12, PHT17, RCM+13a, RML+15, Řez16, SK15b, SWB+12, WDY13]. **frameworks** [LSD+10, PLZ17, RNS19, VVV+15b, VVW+18]. **francium** [TH13]. **Franck** [CHC+13, MCLD10, MLCD11]. **Free** [Bou14, CBG16, GS16, GO13, GMO16, Jia19, MCvdV13, MUGNVJ+18, MYKO18, OCW+15, PK19, PZCL16, SISK10, SC18b, ZQH19, AC11a, Ano10a, AK10, ABS+19, AKN16, BKŠ+11, BSL11, BH15, BS16a, BD11, BB11b, BB11c, BG12, CY09, CX10, CZY11, CY13, Che17, CF18, CZZL19, CS17, CHR+12b, CHR+12a, CMvG10, DSB+19, DMJ17, DGH+11, DHF+11, DPOS16, Fer17, FHZA+18, FBvdB18, GS15, GHK12, GJMPAM+14, Gri13,

HLS12, HH10, HH11, HDK+12, HLW+17, HDL+17, HHNK19, HDM+15, HG13, HYUS11, HKR+14, HGW18, HHWL17, IMK+16, JMLL13, JCX10, KHWB17, Kid19, KB11a, KB11b, KYB13, LRVM18, LMZ11a, LGL11, LP11b, LAW+16, MSC+10, MS13, MHO18, Mau14, MLN+18, MSÅK12, MAP18, MBE16, MIOM13, NZM18, OSR16, OK16, PGCT+12, PBLdS12, PBBP11, PPJ14, RLDJ17, RDDS10, RAR+11, RO14b, RZ16, RR14, RR19]. **free** [SM14a, SFR+11, SWPR11, SY11, SH11b, SOD+11, SOvG12, SN10, SMM15a, SMM15b, SMM+18, TS11, VLB+10, VVG13, VM11, WSH10, WCT+11, WWWW18, WG12, XTG+11, XVN17, YOMT14, YAS13, Yan14, YHH+13, ZZ14, ZPF14, ZGZC19, ZWY+10b, ZH12, ZVY+15, dRBO13, WLF11, XYW+14]. **Free-Energy** [MYKO18, GO13, GMO16, BH15, CY09, HHNK19, HDM+15, HYUS11, IMK+16, JCX10, Kid19, MHO18, MIOM13, OSR16, PBBP11]. **free-software** [GJMPAM+14]. **free-standing** [TS11]. **freely** [CH16]. **Frenkel** [SEJ+18]. **Frenkel-exciton** [SEJ+18]. **frequencies** [DT19, LBH+11, LLH17, SST+18, TKCN19, WX12]. **frequency** [BMPML+13, CK10, KKA+18, LCW12, LS11b, yOTn16]. **frequency-independent** [yOTn16]. **FRET** [RO14a]. **Friedel** [CYY+17]. **friendly** [DBF14, SFR+11, SPM+19]. **frontier** [MGS+16, TZ12]. **frozen** [BVC13, Fer13b, Fer13a, HH16a, HH17, Höf14, SDF+17]. **frozen-density** [HH16a, HH17, Höf14, SDF+17]. **fructose** [RAR+11]. **fructose-1** [RAR+11]. **fuel** [SV11]. **Fukui** [BVC13, PRYI+17, SBR13, YVEI+17]. **Full** [STM17, ACD+13a, ACD+13b, BPLL12, PS17, TSC+13, XCLZ19, YBS19, dSDdAR10]. **full-dimensional** [XCLZ19]. **full-pivoting** [PS17]. **Fullerene** [Avd18, NKD18, GKSS14, KCK+15, KP10, LTR18, Oht16, TPL+10, TFQ+11, TTB+10, XFTW15, YDGZ15, ZSL+11, ZZ12, SWA13]. **fullerene-based** [TTB+10]. **fullerenes** [GZH10, GLF16, MCK17a, MCK17b, SWA13, STS15, WTH+16]. **Fullrmc** [Aou16]. **Fully** [AG12, NLL19, SR19, ZSTI14, FBY+17, GBL+11, KG13, LZL+13, Pop18]. **fulvenes** [AS18]. **Function** [GMBM18, Kop19a, ABDGN12, AB16b, BLG11, CKP10, DSAS19, GS14, GNDA+12, GEG11, HH16a, HBL12, HYMZ16, IY18, JLCA17, JMS13, KSHP+19, Kop15a, LL13a, LHG11, LCB10, LIRL+16, LL19b, MLG18, MB16, yOTn16, ON14, Pil17, PRYI+17, RZG+13, RvL11, SS16a, SFG+17, SK18, TCB16, TO10, UM13, UCFR16, WO15, WDHZ13, YVEI+17, ZLT13, ZCWX18, vSGP10]. **function-based** [WDHZ13]. **function-guided** [YVEI+17]. **Functional** [BHB19, CKH19, FAS+18, FPV13, LLX+19, MP19b, NN19, YKNN19, AMK11, ALK+15, Ali18, ASW19, Ano15-59, AG12, ASS10, BY11, BŁBG+13, BS19, BK17b, BZB+13, BG13, CHG+16, CRZ+18, CR14, CWHH11, CSKH15, CSKH16, CKH17, CSXZ17, CC11, CNK97, CPLL11, CB11d, DAP+18, FD16, GAI14, GHL17, GZL+12, GNGCA10, GSS13, GEG11, GAJ+17, GWPJ11, Han11, HDL+17, HNWF07, HNWF12, HPT17, HG10, HZSS17, INT18, IKN13, IM17, JCP14, JLH+14, JW16, JYS+12, KD10, KKPT11, KOP+14, KGHK12, KB13, KZZ+16,

KLN12, LCW12, ŁBGS16, LGW12, LBTV11, LBTV12, LHKS12, LH14b, LLH17, LPMT17, MMH19, MSY19, MAK+14, MWJ+11, MAP18, MFR+17, Mor15, MMJ10, NS18, NF17, NN18, NO16, NNK+16, Oht16, ORZ11, OM12, PAK17, PPH+14, Pie14, PD11, QZ10b, RJPB12, RS13, Rez19, RB12]. **functional** [RSLML12, RHPWS13, RHT+15, RNS19, RR19, Rui11, SPS+12, SH15, SFG+17, SHL+18, SCW11, SBT17, SEF+16, SE14, SH14, ST13, SHL+13, SPH11, SH19a, SMM15a, SMM15b, SMM+18, SKTT11, SZZS16, STS15, TLdG+12, TG12a, TS10b, UvSvdWK19, VV14, Vik11, VL17a, VI17, VLGK+17, VED10, VHS+19, WKC10a, WHL+10, WCWW11, WDLG12, WYT17, WHX+10, WL14, WTH+16, WGN+16, WZC+19, XYW+14, YJ11, YLZ+10, YS13, ZXS+10, ZWLX11, ZSWL12, ZLZ14, ZDX11, ZYG+14, ZWY+10b, ZWY+10a, ZLHH14, ZGZ19, ZGS+10, dSdS12a, dSdS12b, CKH19]. **functional/basis** [PD11]. **Functionalities** [LJC+19, KAG+12]. **functionalization** [WWTL19]. **functionalized** [KYKR15, LdSRR16, LTR18, MSY19]. **functionals** [Ben17, CCB15, CGR16, CXD+19, DH17, DOM+11, DWC17, ELP19, FPRS14, GWJR18, HG10, HBI+17, KB10, KSH13, KSSH13, Kar17, KM13, LBH+11, LAM19, LH14a, LK16a, PW12, RSG14, Rui11, SGPJS+17, Sea10, SDM+16, SH18a, SPR+13, SZX13a, SZX13b, VCL18, WYT17, Yu12b, ZTH+15, ZWX19, dSdLBNB17]. **functions** [BP18, BLZ+13, CD13, COHI19, CC11, CVG14, Fer13b, Fer13a, FFA14, Fra15, Fra16, GSHM10, GZ14, KK17a, KS18, LRER13, MY17b, Mit13, MLCD11, PHT17, Pro16, RHRCH16, RVM19, SFM14, SYDS11, SM18, Sun15, TNYN16, UCRL18, WZ17, TKN13]. **fundamental** [CD16, VCL18, XLYZ10]. **furan** [LGC19]. **furanosides** [KRTB10]. **Further** [RTS+13, FVB10, PZA15]. **fused** [CZY11]. **fusion** [OLY17]. **Fuzzy** [FPV13, SK12, SK17]. **fuzzy-border** [SK12, SK17]. **FXeOXeF** [ARLP13].

G [Ano15-59, BZH14, LWD13, PHK14, ILKR11]. **g-tensors** [PHK14]. **G2R3** [Gil11]. **g_membed** [WHAS+16, WHAS+10]. **Ga** [UT15, Mit13]. **Gabedit** [All11]. **GAFF** [MPBJ11]. **galactosidase** [AKMT11]. **GALAMOST** [ZLL+13]. **GalaxyDock2** [SKKS13]. **GalaxyDock3** [YBS19]. **GalaxyTongDock** [PBLS19]. **gallium** [GKB+19, YR13]. **gallium-supertetrahedral** [GKB+19]. **gamepad** [HH16b]. **GAMESS** [LRBB12, WSGN11]. **GAMESS-UK** [WSGN11]. **GAMPMS** [LMA15]. **gap** [NPG+18, QZ10b, RS17a, THP+15, VLGK+17, WZH+18]. **gaps** [TSN16, VCL18]. **GARLEEK** [PFAS+19]. **Garriga** [Ihl12]. **Garriga-Sust** [Ihl12]. **Gas** [ATM18, ABB+12, BGS+19, PLZ17, ARLP13, CC18c, DHE+12, GYX+10, GC18, JKS+16, KD10, LPK16, LJW11a, LPLB16, MP13, MFM+12, NIIT15, PGS+15, PMG+16, PSC11, RWR+13, Sea10, SYZ+17, STS15, YHG+11, ZSZ+14, ZYR+15, ZLHH14, ABB+13]. **Gas-Phase** [ATM18, ABB+12, GYX+10, LPLB16, PSC11, RWR+13, YHG+11, ZYR+15, ABB+13]. **gaseous** [HCB11, YHW17]. **gases** [LZ14, DHE+12, SMD18]. **gateway** [RK15]. **Gating** [SFBT17]. **GaudiMM** [PSG+17]. **Gauss** [MY17a]. **Gauss-type** [MY17a]. **GAUSSIAN**

VKTRJ15, VL17b, WPM+15, ZWL13]. **interfaces** [BBG+18a, PGCT+12, RRF11, SSAS10]. **interfacial** [HTY19, IN19, NFPD13, SHFJ18]. **Interfacing** [MSvG12]. **interference** [KIOY19]. **Interferometry** [JAH+17]. **interior** [HL19]. **intermediate** [TDP+12]. **intermediates** [BIL10, MRC+18, RB12]. **Intermolecular** [FMNC11, VECT12, Ano10a, BŁF14, BLDK+13, CCLP12, KSNT19, KCL+14, LZY12b, LZLC13, ŘRH12, SN10, TY10, TNG+10, VVP12, VMV19, WGD+16, ZZL+12, ZLT13]. **Internal** [AlQ19, LL15, REH13, LWK+14, NCV10, PH10a, TNG+10, VLGK+17, VBV13b, WBN+13]. **Internal-to-Cartesian** [REH13]. **internally** [SMP17b]. **Internucleotide** [LZH+11]. **interoperability** [REL+14]. **interphase** [BVY+12]. **Interplay** [FC16, LLL+11, YKH15, BSF18, CCCLCGRO14]. **interpolated** [MK19]. **interpolation** [Min18]. **Interpretation** [STF+19, ZDW18, DCOD13, TLA10, WXL17, XFX+16]. **Interpreting** [AVHB18, CLA16]. **interprotein** [JZ12]. **intersection** [Mat18]. **intersite** [LLLM11]. **interstitial** [GM17]. **intersystem** [AMQ+14, QCR12]. **intervalence** [DAdGR15]. **intervals** [LL11]. **intra** [LZY12b]. **intra-** [LZY12b]. **intraminimum** [ABD11]. **Intramolecular** [DBG11, GWF11, KP10, MH17, Spr18, CROB16, HB15, KFY+13, KV14, LWGZ15, LTP11, MTM14, MPSG11, SSB11, SSB13, VVJ15, YK13, YLZ+10, dALdS+15, dLC17]. **intraphase** [BVY+12]. **intrinsic** [AMGB10, OVPK15]. **intrinsically** [LC16]. **Introducing** [DJD12]. **Introduction** [HIS17, LL19b, Sie15, SJ17]. **intuitive** [EFAC13]. **invariant** [CWZB10, MK19]. **Inverse** [KTT16, GD10, JMS13, SKGP19, WHK+12]. **inversion** [HLI+19, Hei18, SP13, SM18, GG10]. **invert** [KZZ+16]. **inverted** [UT15, YJ17]. **investigate** [dSAdSL13]. **investigated** [SLY+10, SCW11, YS13]. **Investigating** [KGJZ19]. **Investigation** [ALW+10, CAP17, GY10, PH10b, WS10, YZLZ19, ZY14, AvKSP16, AMK11, ABB+12, ABB+13, BAD+19, CWT+12, CYY+17, CR19, CZH12, CH10, GDV17, HXM+16, KCB+12, KV15b, LLLM11, LLB+12, LZY+12a, LLD17, LXZ+10, MLQ+12, MP13, OAN15b, PZA15, PVS12, QCR12, RDT14, RRC+15, SBGP18, SH14, Tak11, TPL+10, TS10b, TR12, VVP12, VM19, YS18, YJN+11, Yu12a, ZZ10, ZSWL12, ZBMZH15]. **Investigations** [DL19, NSN19, GZL+12, HDM+19, KSO+19, KAR12, LWWG12, TSJ+10, Tsu19, WS12, YPvD13]. **Invisible** [SDM+16]. **involving** [ARLP13, CC18c, GNDA+12, LEdOLdlV17, LRER13, MEH18, NFG+13, OSHG17, SLT14, SLT+15, SWW+19, YZZ+17]. **iodanes** [SLT14]. **iodate** [SC18a]. **iodine** [ACS12, SLT14, SLT+15, KLN12]. **iodothyronine** [CFM+19]. **Ion** [Fra15, Fra16, LZTV10, BP18, DMN14, DMN15, EK15, JAH+17, JLCA17, KTK17, KJ10, LEdOLdlV17, LJR+12, LPE+10, MMB+17, MH11, NSK18, NC13, PGY15, PL14, RTS+13, SSGS15, SC18a, SMiN+19, SV11, TO19, TNY18, TJR19, Tru18, TCX+13, VPR10, Vik11, WC14, YZLZ19, ZZ10]. **ion-associated** [ZZ10]. **Ion-exchanged** [LZTV10]. **ion-pair** [TNY18].

Ano14-42, Ano14-43, Ano14-44, Ano14-45, Ano14-46, Ano14-47, Ano14-50, Ano14-51, Ano14-52, Ano14-53, Ano14-54, Ano14-55, Ano14-27, Ano14-48, Ano14-49, Ano14-56, Ano14-57, Ano14-58, Ano14-59, Ano14-60, Ano14-61, Ano14-62, Ano14-63, Ano14-64, Ano14-65, Ano14-66, Ano14-67, Ano14-68, Ano14-69, Ano14-70, Ano14-71, Ano14-72, Ano14d, Ano14e, Ano14f, Ano15a, Ano15b, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n, Ano15o]. **Issue** [Ano15p, Ano15q, Ano15r, Ano15s, Ano15t, Ano15u, Ano15y, Ano15z, Ano15-27, Ano15-28, Ano15-29, Ano15-30, Ano15-31, Ano15-32, Ano15-33, Ano15-34, Ano15-35, Ano15-36, Ano15-39, Ano15v, Ano15-40, Ano15-41, Ano15-42, Ano15-43, Ano15-44, Ano15w, Ano15x, Ano15-37, Ano15-38, Ano15-45, Ano15-46, Ano15-47, Ano15-48, Ano15-49, Ano15-50, Ano15-51, Ano15-52, Ano15-53, Ano15-54, Ano15-55, Ano15-56, Ano15-57, Ano15c, Ano15d, Ano15e, Ano15f, Ano15g, Ano15h, Ano16a, Ano16b, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m, Ano16n, Ano16o, Ano16p, Ano16q, Ano16r, Ano16u, Ano16v, Ano16w, Ano16x, Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16-29, Ano16-30, Ano16-31, Ano16-32, Ano16-33, Ano16-34, Ano16-35, Ano16-36, Ano16c, Ano16-39, Ano16-40, Ano16-41, Ano16s, Ano16t]. **Issue** [Ano16-37, Ano16-38, Ano16-42, Ano16-43, Ano16-44, Ano16-45, Ano16-46, Ano16-47, Ano16-48, Ano16-49, Ano16-50, Ano16-51, Ano16-52, Ano16-53, Ano16-54, Ano16-55, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h, Ano16-75, Ano16-89, Ano16-80, Ano16-94, Ano16-81, Ano16-95, Ano16-82, Ano16-96, Ano16-83, Ano16-97, Ano16-84, Ano16-98, Ano16-85, Ano16-99, Ano16-86, Ano16-100, Ano16-87, Ano16-101, Ano16-88, Ano16-102, Ano16-76, Ano16-90, Ano16-77, Ano16-91, Ano16-78, Ano16-92, Ano16-79, Ano16-93, Ano16-129, Ano16-108, Ano16-109, Ano16-110, Ano16-130, Ano16-111, Ano16-112, Ano16-113, Ano16-114, Ano16-103, Ano16-104, Ano16-105, Ano16-106, Ano16-107, Ano16-115, Ano16-121, Ano16-122, Ano16-123, Ano16-124, Ano16-125, Ano16-126, Ano16-127, Ano16-128, Ano16-116, Ano16-117, Ano16-118, Ano16-119, Ano16-120, Ano16-57, Ano16-58, Ano16-59, Ano16-60, Ano16-61, Ano16-62, Ano16-63]. **Issue** [Ano16-64, Ano16-65, Ano16-66, Ano16-67, Ano16-68, Ano16-69, Ano16-70, Ano16-71, Ano16-72, Ano16-73, Ano16-74, Ano17a, Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x, Ano17z, Ano17-27, Ano17-28, Ano17y, Ano17-29, Ano17-30, Ano17-31, Ano17-32, Ano17-33, Ano17-34, Ano17b, Ano17c, Ano17d, Ano17e, Ano17f, Ano17g, Ano17h, Ano17i, Ano17j, Ano17k, Ano17l, Ano17m, Ano17o, Ano17p, Ano17q, Ano17r, Ano17s, Ano17-36, Ano17-37, Ano17-62, Ano17-63, Ano17-64, Ano17-65, Ano17-66, Ano17-67, Ano17-38, Ano17-39, Ano17-40, Ano17-41, Ano17-42, Ano17-43, Ano17-44, Ano17-45, Ano17-46, Ano17-47, Ano17-48, Ano17-49, Ano17-50, Ano17-51, Ano17-52, Ano17-53, Ano17-54, Ano17-55, Ano17-56, Ano17-57, Ano17-58, Ano17-59, Ano17-60, Ano17-61, Ano18a, Ano18b, Ano18t, Ano18u, Ano18v, Ano18w, Ano18x, Ano18y]. **Issue** [Ano18z, Ano18-27, Ano18-28, Ano18-30, Ano18-31, Ano18-32, Ano18n, Ano18-29, Ano18-33, Ano18-34, Ano18-35, Ano18-36, Ano18-37, Ano18-38, Ano18c, Ano18d, Ano18e, Ano18f, Ano18g, Ano18h, Ano18i, Ano18j, Ano18k,

ABB+13, GNDA+12, NDG14, WLHZ12, WHDL11, YZGS14b].
mechanochemical [QB16]. **mediated**
[MRR11, QQY+18, RVP+11, XYW+14]. **medium**
[FE14, IPAA11, LRvE17, RK15, SC18b, WWD14]. **medium-size** [FE14].
medium-sized [LRvE17, RK15, WWD14]. **meets** [PNE18]. **melanin**
[LLL+10]. **melanin-concentrating** [LLL+10]. **mellitus** [PC11]. **Melting**
[FCW+14]. **membered** [HCD+10, OSI+19, TDKT10, WS11, WS12].
Membrane [OLY17, WCJ+14, YL13, BHI19, DSF17, HPL13, II18, JIS13,
KYT+17, MOS12, yOaCG10, PRP15, RBOH11, RI10, SSBW14, TO19,
WNM17, WHAS+10, WHAS+16, YS18]. **membrane-embedded** [DSF17].
membrane-water [JIS13]. **Membranes**
[LLH+19, BHI19, DLSA14, HBJ+17, SDZ17, WLO+17]. **MembrFactory**
[LLH+19]. **memory** [Gon12, Gra15, KNR+18, UIW+10, vW11]. **MEMPOT**
[DLSA14]. **merocyanine** [TYN15, TKYN17]. **mesh** [AG11, NO16].
MesoBioNano [SYN+12]. **mesogenic** [CRC13]. **mesoionic** [AR15].
Message [ZWL13, CSSB11]. **Mestres** [Ihl12]. **meta**
[BG13, LBH+11, WHK+12]. **meta-program** [WHK+12]. **Metabolic**
[TDP+12]. **Metabolic-intermediate** [TDP+12]. **metadiiodobenzene**
[PH12]. **Metadynamics**
[GS16, AKN16, GS15, KEMP17, Nav18, PZCL16, PPJ14, SH11b].
metadynamics-based [PPJ14]. **metaheuristic** [DS15]. **Metal**
[BF19a, MP19b, ND19, WWTL19, AJA+19, Ano11, AM19a, AM19b,
BBG+18a, BSF18, CGPP11, CMS13, DAP+18, DDM+15, FZL+19, GK15a,
GRD+10, GBG+19, HG10, JSF19, JAH+17, JHMB+09, JHMB+11, KLZ+18,
LYL16, LDZW17, LKZM18, LLL+12, MC10, MKK+19, PGS+15, PHK14,
PDG+16, Rab12, RNS19, ŠBD+17, SSGS15, SNS16, SFLG+17, SSX+14,
SSAS10, THP+15, UvSvdWK19, VVV+15b, VVW+18, VLGK+17, VHS+19,
WWKS16, WZH+18, YWZ14, YHCS11, ZYW+16, ZWY+10a, ZWS+10].
metal-atom [LKZM18]. **Metal-catalyzed** [WWTL19]. **metal-exchanged**
[DAP+18]. **metal-organic** [BBG+18a, RNS19, VVV+15b, VVW+18].
metallaborane [LK16b]. **Metallic**
[VVBL17, DAP+18, LZZ+11, MMS16, SPL+18, SWMW10, TG12a].
metallization [ASK18]. **metallo** [ED15, KTK17, MLQ+12]. **metallo-bis**
[KTK17]. **metallo-organic** [ED15]. **metalloenzyme** [GPdC+16].
metalloenzymes [DSM+11, Sti15]. **metallofullerene** [ZYG+14].
metallofullerenes [FL15]. **metalloid** [MMS16]. **metalloproteinase**
[VKNT15, VKNT16]. **metalloproteinase-2** [VKNT15, VKNT16].
metalloproteins [WC14, YWZ14]. **Metalophilic** [Li14a, Li14b].
Metamitron [BHB19]. **metamodels** [CBP14]. **metastable** [GKB+19].
metathesis [MJLV14a, MJLV14b, RS17b]. **meteorite** [SSNT19]. **methane**
[ARRC15, DR11, DAP+18, GYX+10, KMT+19, LZLC13, NH19, Niz13,
TLY+12, YHG+11, ZWZ11]. **methane-to-methanol** [DAP+18]. **methanol**
[AAMD+11, DAP+18, GYX+10, GNGCA10, HLH+12, MHRR11, NJX+10,
TKYN17, ZLL+10, NQB19]. **methionine** [AALCM11]. **Method**

[FBKD19, LI19, VSP19, WNP+16, ZQH19, AIGP15, AOW11, BBG+11, BMR11, BAMR13, BF15, BS19, BCCO10, BMBJ11, BRP+12, BMFG16, BD11, BB11b, BK17c, CIKT13, CZY11, CL16, CH16, DK11, DCŠ15, EFS16, EVR18, EPD+11, FGM11, Fer17, FRN15, FHZA+18, GLB16, GKJ+19, GBVA11, GKV+13, GA12, dCGCRN19, GWZX12, HLS12, HH10, HTS15, HNTS15, HNS16, HYNS19, HSN14, HNWF07, HNWF12, HAI+16, HBL12, HYUS11, HGW18, HHWL17, HLXH17, HLXH18, HL19, ITIN15, ISK14, ISO+13, ISM18, IO13a, IO13b, JZ17, JLH+14, JMS14, JS17b, KV12, KS13a, KS15, Kan15, KSSH13, KG15, KKNN11, KTO13, KB19, KB11c, KTNN10, KLS10, KZP+18b, KB14b, KWG15, LLHM16, LFB14, ŁBGS16, LPK16, LCH10, LL11, LLZA12, LWZ+19, LN15, LLSW14, LL19a, MK13a, MTM14, MHT+18, MC12, MKGA10, MPA12, MN15, Mat10, MDT10]. **method** [MRK11, MA17, MJG+15, MFR+17, MS15, MNNK10b, MH10, NF18, NR11, NFPD13, NF17, NO16, OLA15, OK16, OOT15, PSS14, Pet11, PSC11, PKIC11, PPJ14, PŁV+11, PM18b, Pon10, QLQ11, QB10, QB11, RHRCH16, RKGN10, RSLS13, RGVC+19, Rod13, RKB+14, RFHG10, SSO19, SF18, SS13a, SCM+15, SBB10, SSWX14, SBN13a, SBN13b, ŠB15, STM17, SG13, SSAS10, Tak14, TKNN10, Tak10, Tak18, TSZQ12, TSNC+17, US11, UIW+10, VLB+10, VDVR14, Vor10, WXS+12, WJG+13, WLQ19, WHM10, WTH+16, YO19, YWJ+16, Yon16, YAO18, YN15, YHH+13, ZDZM13, ZMMM12, Zha12b, Zha12a, ZLM+15, ZGZC19, ZZMW19, ZW17, ZFS18, ZH12, ZA15, ZZZ+19, Zim15, CKH19, JCHT18]. **method-based** [GKJ+19]. **Methodological** [VKNT16]. **methodologies** [Rob13]. **Methodology** [CPK19, Aki16, FF11, GAI13, GMASBF16, HPT17, OHPR17, OHPR18, RJWW12, HCD+10]. **Methods** [SGP18, Ano12u, Ano15-59, ASMS10, BG13, CLFRO18, CSGOA17, CXS10, CNK97, DKE+17, DCOD13, DBM+15, EWK+13, ESM+12, EV14, Fer13b, Fer13a, FB10, FSSW17, FSSW19, GAI14, GFPSD17, GD10, GSS13, GMO16, HCB11, HSB+11, Höf14, HWLW11, JJH+13, KSM17, KB13, KHWB17, LEdOLdlV17, LZLC13, LLSW14, MS13, MY17b, MHO18, MŘ17, MVKS10, MOS12, NYH+17, NASH15, NC13, NC14, NTNY15, OSHG17, PN13, PVAM16, RZG+13, ŘRH12, Rez19, SRF+17, ŚSB+16, SACdG14, STM+15, SWW+19, SGWA17, TG12b, TS15b, Tsi17, WBT10, WX12, YLCX10, YAS13, YJ17, ZGS+10, dSdLBNB17]. **methoxy** [PNE18]. **methoxybenzyl** [YZLZ18]. **methyl** [AARP17, BIL10, CPLL11, GZL+12, GMG+10, LK11, LZL+16, MG15, MSBF16, VKTRJ15, YYT12]. **methyl-methyl** [LK11]. **methylacetamide** [HLH+12, KSK11]. **methylacetylene** [WCWW11]. **methylated** [LRVM18]. **Methylation** [SCW11, KYCL11, QZM11, dALdS+15]. **methylbenzyl** [NDG14]. **methylcobalamin** [KKL+13]. **methylformamides** [JSW10]. **methyllysine** [GHK12]. **methyltransferase** [CPLL11, GH10, PBLdS12]. **Methyluracil** [HvM17, HvM16]. **MetREx** [Sti15]. **metric** [CXS10, LLFH16, PKIC11, SOJ14, ZT14]. **metrics** [Hug14, PBBP11, RCM+13b]. **Metropolis** [MO15, Pon10]. **Mezey** [HJJ13]. **MF** [YKH15]. **Mg** [HDM+19, LDJ+10, LLX+19, BMFG16, DOM+11,

[LLLW19]. **MNX** [AM19b]. **MO** [BRP+12, UIW+10, ZY14]. **moanalyzer** [DJD12]. **mobilities** [SFDE16]. **Mode** [AIM+18, BHR15, GVP+10, IY18, SRA17, SBB10, YHCS11, YXZZ17]. **Mode-tracking** [BHR15]. **Model** [Ale19, BŁS10, HM16, Jia19, MT20, Pog10, AASP18, AOW11, AS10, ALRM18, ATP18, AS15b, APA+14, AB16b, Bac12, BK17a, BH19, BEEL14, BS10b, BBG+18b, Cam15, Can10, Can11, CGP12, CGA19, CBTZ16, CFC15, CAD16, CG12, CMS13, CJZS10, DLL+10, DSF17, FCE15, FNSF+11, GRN19, GRS15, GM17, Gil11, GKR13, HLS12, HAL14, HLH+12, HOK17, HZSS17, Hug12, HRH+17, ISO+13, IN13, II18, JSXH16, Jor17, KFY+13, KCK+17, KMS+19, KR12, KOY+12, KD18, KCPMG12, KB14b, KDS17, LSL+19, LTT16, LY10, LRvdSM15, LFN+10, LPS+13, LHHW14, LZL+15a, LDG+15, LCK+18, LHMM11, MSLS10, MT19a, MPJ+19, MBC11, MBC13, MMB+17, MHO18, NJX+10, NTNY15, OPBR17, PB14, PCLL11, Pla11, Pon11, Ray13, RTS+13, Ric16, RMRBH+19, REL+14, RKG11, SM14b, SDF+17, SHF11, SSBW14, SK12]. **model** [SK17, SLX+15, SDZ17, SZBM13, SB11, TYN15, TCC+13, Tia12, TLA10, TTn19, UIW+10, VV14, VHS+19, WWKS11, WXL+12, WC13, WWW19, WNM17, WRHF10, WKC11, WCAH10, XZ11, XTY+14, XP13, YS18, YOMT14, YB13, YSG12, ZSTI14, ZKH+10, ZM10, dSDdAR10, dSH19, CCR18, FAS+18, MJBM12]. **model-tuned** [HZSS17]. **modeled** [MPA12]. **modeler** [BHI19, KLJ+17]. **Modeling** [ASW19, CB11a, DLSA14, FD13, FTW12, GMG+10, GBS+17, HPL13, JW16, KDR+18, Mat14, NS10, NDLW13, PLP+16, SZdB19, SK11, Tia12, Vyb15, AKMT11, Aou16, BEM14, BPC13, Bow16, BS10c, ĆMD13, CLA16, CZNA11, DAG19, DWR17, DSX+11, DLMH12, EBPK17a, FXC+13, GH10, GP12, GMZ12, GWJR18, GR10b, GWZX12, HLvdV13, HBJ+17, JC16, JCL+17, KSD+12, LABSG17, LLH14, LZGS11, LT13, LN15, MBA11, MJLV14b, MA17, MBA14, MPBJ11, NSO+14, NW17, PHC13, PSS14, PSG+17, PMT16, QLKI19, RJS17, SN16a, SKGP19, TTR+12, VKNT15, VÅA14, VCM15, WXL17, WPM+15, WLO+17, XDL+10, XLY12, YMY+19, YJ11, ZX11, DHE+12]. **modelling** [DBM+15]. **Models** [Hes19, NNT+19, ND19, BEM14, BLKP12, BPB11, CD11, Cor17, CBG16, CK17, DDP16, DSM+11, DI11, DGC14, DLC18b, EK15, EPD+10, GMPB12, GMMH+16, GMG+10, GKR13, GCP+13, GCC14, GAJ+17, HS16b, HGY15, JCP14, JGS+17, KJDB12, KKO+16, KB11b, KSR+16, KSW16, LTT16, LKL10, LZ12, LLSW14, LM18b, MPSA17, MSÅK12, MCUJ15, MKB+13, NNS15, OL13, PHC13, PGY15, PL18, Ray13, RTP+13, RKG11, SPHF+18, SCMA+17, SFLG+17, SAvG15, TH13, TTB+11, TTL+12, VKC10, VMPS17, VZ14, WS10, WXY14, WSWD19, XTn18, YJ11, YL13, ZsA10, ZDW18, dSdLBNB17]. **modern** [AB16a, AB16b, DH17, Fom11, LMR14, SF18, SDM+16]. **modes** [CBP+15, EB18, GMPB12, KKH18, LLTC12, MS17, dSH19, dSAdSL13]. **modification** [Ano12u, MIS+15]. **modified** [BD12, CH16, DPSL16, DJX+11b, GSD10, MRO17, Mit13, SMM15a, SMM15b, SMM+18, XYX17, XVA+16, ZZ12]. **modify** [ZX19]. **Modifying**

[CYG+15, LBS10]. **modular**
[HPT+16b, JP15, LWK+14, MBR+15, PSG+17]. **modulate** [WC13].
Modulating [LTR18]. **modulation** [PE11, RS17a]. **modulator** [ILKR11].
modulators [SRA17]. **module** [PHH+12, VBV13b]. **MOFs** [LPK16].
moieties [SPL+18]. **MOLCAS** [ADF+10, VBV13b, AAC+16]. **Moldyn**
[HPSK12]. **Molecular**
[AASP18, AJA+19, Ale19, BDTP11, BSF18, BHB19, CRZ+18, ĆMD13, CF18, Cor17, DGH+11, DHF+11, DSX+11, EvRC+18, Fom13, GKB+19, HKNH18, HTY19, HLEM18, Ibr11, JA10, KUDG12, KB14a, LWZK13, LBDP12, MM19, MFEM16, NN19, PP19, PL14, Pla11, RKGN10, RO14a, RRK14, Sch18, SBT17, SFLG+17, SV11, TFYO19, VSD10, WC11, WWKS11, XFG+16, XLY12, Yan16, YJXZ13, ZWS+10, AALCM11, AG11, AST+16, AFPI13, AS15a, ASL+11, AS10, APK14, AS18, AGB13, AS15b, AGR11b, AJR16, AB16a, ASK18, ALH+10, BMR11, BAMR13, BEM14, BSL11, BF15, BBOB16, BS19, BJSI12, BV14, BW15, BF17, BJP15, BGL+18, BMBJ11, BE16, BS18, BVC13, BEL+11, CBP14, CMM18, CCR18, CM13a, CDBM11, CD13, Car14, CTR13, CAF+13, CEBO15, CGA19, CIKT13, CGPP11, CS14, CXW14, CBTZ16].
molecular
[CH16, CCOH14, CBDS19, CVG14, CCW+10, CHKR10, CJPTC18, CB11b, CB11c, CM16, DMJ17, DSD+11, DJX+11b, DJX+11a, DJS+18, DLZ15, DDM+15, DN19, DL19, DL16, EP10, EK15, EJ13, EPH+13, EPH+15, ENKK+17, EPD+11, Fer13b, Fer13a, FBvdB18, FBEM11, FDH19, FSC+14, FPH+19, GBL+11, GDV17, Gar12, GJMPAM+14, GSHM10, GR11, GMZ12, GPM17, GMMH+16, GFGS18, GY10, GWZ15, GCW14, GGM+12, GBW+14, GEP+14, GPdC+16, GP11b, GR10b, GPK12, HS17b, HHNK19, HSW+19, HB14, HS12, HCD+10, HDM+15, HPSK12, HH16b, HWLW11, HJ10, HXM+16, HHWL17, HRID16, HC14, IUK+11, IIF+10, IN19, ISM18, IM17, II10, JIS13, JBSQG11, JAH+17, JSXH16, JWST10, JGS+17, Jor17, JMS14, JS17b, JND+19, JP15, KT19, KCK+17, KCK+15, KVQC+11, KGHK12, KSNT19, KGHC15, KCC+18, KLN12, KJDB12, KDB13, KERY+16].
molecular [KTSW11, KLOS10, KJM+17, KC14, KKK+19, Kos16, KSR+16, KG13, Kow11, KTNN10, KZP+18a, KV15a, KVR10, KSW16, LPAS11, LL15, LRVM18, Lar12, LWK+14, LBGS16, LH11, LL13a, LZ12, LFN+10, LLC+10, LL11, LZY+12a, LMI+14, LAHS16, LPE+10, LLTC12, LCB10, LZW+11, LTP11, LZL+13, LWXC16, LZS+17, LJL+11, LP11c, LAS+14, MSY19, MRB14, Man19b, MKS+12, MSC+10, MJC14, MCRL17, Mat10, Mat14, MSvG12, MLN+18, MWJ+11, MFEM15, MADWB11, Min18, MPNS13, MKM+17, MBA14, MHRR11, MCC12, MFR+17, MO17, MS12, NPTS16, NF18, NSO+14, NPG+18, NLP+16, NST14, NPG17, NFPD13, NFG+13, NF17, NNK+16, NHK+13, NS17, NTNY15, ODB18, Oht16, OHNK11, ON14, OGL10, OHPR17, OHPR18, OCL11, OLY17, OT12, OME16, OVPK15, OOT15, OCW+15, OZS+13, OOK11, PMC+17, PSS14, PAK15, PAK17, PH17, PSG+17, PL19]. **molecular**
[PM13, PGW+17, PVZ13, PJ13, PBG17, PS10, PVAM16, PLP+16, Pro16,

PH15, PVJ10, RJBH18, RD18, RMPAM15, RLLHL12, RNSF+16, RNP13, RNVP13, RS12, Ras17, RHJ11, RO14b, RR14, RdA12, RC18, RLG14, RŠRR15, REH13, SHMO11, SSO19, SF18, SLT+15, Sax12, SWM10, SK15b, SA13, SZTSM10, Sch12, SFR+11, SHFJ18, SHF11, SMRM+17, SS19, SSNT19, SOM+13, SJ17, SR18, SYN+12, SK13, SWB+12, SLLL13, SJ16, SDMS13, SKY+11, SZZ+18, SPZP18a, SPZP19, SBvG14, SAvG15, TNYN16, TKNN10, TZ12, TJR19, TTC+18, US11, UGK18, VYM15, Vik11, Vor10, Vor12, VM11, WKLC12, WBN+13, WAM17, WLW+10, WH11, WCY+11, WLC12, WOH16, WXL17, WOH18, WES13, WBF17, WCDM11, WO15, WCWV15, WL14, WG14, Won18, WDKT19, XDL+10, XFG+15, YKO+11, YPvD13, YNH+17, YO19, YLGX14, YLCX10, Yap11]. **molecular** [YPKB12, Yes12, Yes15, Yon16, ZSTI14, ZWL13, ZZY+16, ZX11, ZDKM12, ZSS+13, ZLY+16, ZP13, ZWX16, ZLL+13, ZA15, ZBMZH15, dSdLBNB17, dCLFGL13, dLvNC18a, AIM+18, IPAA11, KSD+12, MJLV14b, ZBP11, ZKH+10]. **molecular-mechanical** [ZSTI14]. **molecular-orbital** [US11]. **MoleculaRnetworks** [MCC12]. **Molecule** [KR12, vRWGS17, BT18, DHOG13, DGL+13, ETLS17, FAA15, GAI14, GCWS15, GBVA11, HLvdV13, HHWL17, ISO+13, IIHY15, KB11b, KKA+18, LIRL+16, MCUJ15, NLL19, PCLL11, RLL+10, SG10b, VGV+11, WF16, XYW+14, XMSZ16]. **molecule-mediated** [XYW+14]. **Molecule-specific** [KR12]. **molecule-transcription** [XMSZ16]. **Molecules** [ATM18, Cam19, ELKE19, PdSC18, AIGP15, Ali18, AWF+18, ARAG17, AGR11a, BŁBG+13, BS10a, BTMS12, BSF18, BPC19, Ben17, BS16b, BL12, CPZ19, CHG+16, CC18c, CQFC10, CYG+15, CCOH14, CXS10, CZNA11, FDH19, FE14, GWF11, GKJ+19, GP12, GPGSM11, GPGSM12, GAJ+17, HRB+17, HSB+11, Hug12, Ihl12, Kan15, KLJ+17, KGJZ19, KYG+15, LPS12, LHSH12, LvG13b, LH14b, LJL+11, LG14, MA16, MS13, Mat10, MSS+13, MH17, MBE16, MPBJ11, NIIT15, OGL10, OT12, PZBA13, Pyy13, RSSG18, RSG14, RK15, SFCCK+14, SFCCK+15, Sch13, SG10b, SFLG+17, SY16b, SM17, TZCK18, TSR+16, UNT16, VVV+15a, VHA+10, VVY18, VDVR14, WC13, WSZW15, WFS19, WWD14, WX12, You10, YKH15, YHW17, ZPP+16, Zha12b, ZLX+13, ZBB16, ZCGM11, MSPC19, SMB18]. **Møller** [FSSW17, FSSW19, Hil13, KKNN11, KN17, MCC11, YKH15]. **MOLSIM** [JP15]. **molSimplify** [IGK16]. **molten** [LCL+18]. **MolTPC** [WHJH13]. **molUP** [FRC18]. **Molybdatricarbaboranes** [LK16b]. **molybdocene** [PM13, SDL14]. **Moment** [Cam19, SS16a, JCG+11, KCB+12, Yan11]. **Moments** [GH16b, Ali18, BLDK+13, CP15, CTP13, DHOG13, GH16a, Lar11, NOKJ16, Tru18]. **momentum** [EP12, GWF11, NCT18, PH17]. **monazite** [RKB+14]. **monazite-type** [RKB+14]. **mono** [HvM19]. **mono-** [HvM19]. **monoanion** [YZGS14a]. **monoboronyl** [VVBL17]. **monododecyl** [TFYO19]. **Monohydride** [Kop19a]. **monohydroxide** [Kop17a]. **Monolayer** [SJSS19]. **monolayered** [RSKG14]. **monolayers** [LBDP12, RSK+15]. **Monomer** [SC17]. **Monomeric** [LLT12, CAT+13]. **mononuclear** [BCSCJ+13, OSS10]. **monosaccharide** [MSÅK12].

[SvLK18, Aou16, BBG+11, BCSCJ+13, BCJC+14, BACSCJ+10, CCC+11, CJPTC18, DDK14, Dra19, GBW+14, HSN+18, KR14, KVQC+11, KCC+18, KWG15, KYG+15, LWK+14, LHSH12, MLN+18, SKA19, SWA13, SHFJ18, SMRM+17, SJ17, SJ16, UU12, VBV13b, WSGN11, ZCS+15]. **packages** [MSvG12, MJG+15]. **packet** [LWD13]. **packing** [MCAG+16, MP17b, NS11]. **PaDEL** [HLS+13, Yap11]. **PaDEL-DDPredictor** [HLS+13]. **PaDEL-descriptor** [Yap11]. **PAEM** [ZY14]. **PAEM-MO** [ZY14]. **paint** [BEFS13]. **pair** [BSF18, BH13, CYG+15, CVG14, Hei18, KS18, MPA12, OM12, Sch12, SSGS15, SB14, TNY18, WCY+11, WWU12]. **Paired** [ZR10, WAB17]. **pairing** [KTK17, ZLL+10, ZM11]. **pairs** [BSG18a, DKT13, ENKK+17, LEdOLdlV17, LZH+11, MPSG11, Mau14, PL19, GMBM18]. **Pairwise** [GS14, Gon12, RVM19, VMPS17, XTY+14]. **pairwise-additive** [VMPS17]. **palladium** [MRC+18, WCWW11, YHG+11, dCDP15]. **palladium-catalyzed** [dCDP15]. **palladium-phenanthroline** [MRC+18]. **paper** [GPGSM12, Ihl12, JW12, WM12, HP10a]. **para** [KYCL11]. **para-substituted** [KYCL11]. **paracyclophane** [KGR+16]. **paracyclophane-bridged** [KGR+16]. **Paradoxical** [UT14]. **Parallel** [BTB+11, FBKD19, KDB13, NN18, UIW+10, WWKS16, BW11a, BTT10, CEBO15, CSSB11, GJMPAM+14, GRARO+14, GC18, HP10a, HS17b, HPSK12, KS13a, KNHN16, KN17, KZZ+16, KCC+18, KJM+17, KDT+12, LL10a, LPLA13, MBR+15, MCRL17, MYT+14, MJM+15, NNK+16, OPB+12, RFN15, SHMO11, TCX+13, TJB12, WHK+12, Yes15, ZWL13, ZSS+13, CJL+13, KDT+12, LMR14]. **parallel-generalized** [LL10a]. **Parallel-ProBiS** [KDT+12]. **parallelism** [FRN15, Gon12]. **Parallelization** [AB16b, RC18, VDL+13, BWMSM10, IUK+11, JMS14, KS15, KKNN11, LLZA12, RŠRR15, SHL19, vW11, ZDKM12]. **parallelize** [vW11]. **Parallelized** [AlQ19, DBDP16]. **parallelizing** [BMBJ11]. **parameter** [NB19, PFVL14, SH19a, VCL18, VVLG17, WDHZ13, LL11]. **Parameterization** [HK18, HJLV16, ILKR11, IHJ+13, MPSA17, PRRT+10, TCC+13, BAS14, CCLP12, DLMH12, KYB13, LTP11, LCL+18, MSS+13, VLB+10, VBD11, VHS+19]. **parameterizations** [SH15]. **parameterized** [OZS+13]. **Parameters** [CTR13, AG11, AKMYB18, BCSCJ+13, BCJC+14, BSD18, BW15, BC13, CYG+15, DPSL16, DMAH15, FHT+15, GSD10, HLS12, HM16, HBI+17, HLH+12, KvdV14, KGHK12, KGJZ19, LvDH13, LPS+13, LLvG10, LSH+11, MRO17, MP11, PBLS19, Pog10, RKB+14, SOYC12, SZBM13, SPR+13, SPZP18b, VYM15, VLGK+17, WAM17, WOH16, WOH18, WC14, YWZ14, ZRL+15]. **Parametric** [LM18b]. **Parametrization** [PG15, COHI19, DGPM14, GCWS15, SPS+12]. **Paramfit** [BW15]. **parasite** [FZL+15]. **paratropic** [CPN+17]. **Parrinello** [DL19, KCK+15]. **Part** [HRJ+15, CDBM11, CD13, HRJ+14, Fer13b, SK13]. **Partial** [HTS17, JMLL13, SMP17b, WOH16, GVP+10, MPBJ11, PL14]. **Partially** [XTn18, UT14]. **participating** [GSMZ19]. **particle** [AG11, BSD18, BK13, Cas13, ER18, Hei18, NO16, PH17, RJBH18, SCK18, ZDKM12]. **particle-field** [ZDKM12]. **particle-mesh** [AG11]. **Partition**

CPK19, DMN15, DJD12, DVVP14, DBDP16, DDK14, DWC17, DSK17, ESB13, EWK+13, FN12, FSC+14, GMSdG15, Gar12, GJMPAM+14, GLW13b, GS12, GCP+13, GCC14, GBW+14, GH16b, HLS+13, HRB+17, HDH12, HPT+16b, HPSK12, HHT+13b, HH16b, HG13, HYMZ16, HKR+14, HBJ+17, HL14, HC14, IGK16, JHH+13, JJW+14, JLCA17, JP15, JCGM18, KS13a, KS15, KK17a, Kan15, KR14, KB16, KKR+13, KDR+18, KLJ+17, KJM+17, KDT+12, Kos16, KG13, KWL+16, KK17b, KWG15, KSD+12, KYG+15, KAG+12, KSW16, KPF+15, LPS12, LJR+12, LHSH12, Leh15, LRvdSM15, LRvE17, LDB+17, LLZA12, LBB+15, LWZ+17, LC12, LAS+14, MHT+18, MDTD16, MBR+15, MYT18, MSSP17, MB14, MB16, NKJ16, OV14].

Software
[OPB+12, OZS+13, OC14, PSS14, PGL+15, PSG+17, PW12, PPM15, PHH+12, PVZ13, PG14, RLLHL12, RNSF+16, Ras17, Řez16, RR14, RdA12, RSR+12, RCM+13b, SM14a, SFG+17, SK15b, SWA13, SMRM+17, She12, SC15, Sie15, SJ17, SvLK18, SJL18, SWB+12, SDMS13, TNYN16, TSC+13, TTR+12, TTL+12, UU12, VMRSH+17, VVV+15b, VAR12, VBV13b, WdVN12, WDY13, WPM+15, WF16, Wei12b, WHK+12, WHJH13, WG14, WCJ+14, XML+15, XYX17, YWJ+16, YZZ16, Yes12, Yes15, YHH+13, ZFOS19, ZDKM12, ZLL+13, dVAG16, CCC+11, DBF14, EdOdS18, FRC18, HSW+19, MSvG12, MJG+15, SF18, SBV10, SGM+13, Yap11, ZCS+15, She12].

softwares [All11]. **solar** [ACS12, DGL+13, JYS+12, LZL+15a, MP19a, SLC+17, TZ12, VÅA14, YJN+11]. **Solid** [MP19b, RSK+15, ASS10, ASK18, CL16, HLS12, HBI+17, KLN12, KKH18, LOB18, OLPB19, POB13].

Solid-state [RSK+15, HBI+17, KLN12, KKH18, LOB18, OLPB19, POB13].

solids [BK11, BPC19, HAI+16, MDTD13, MS15, dlRL11, Pon11, SN16a].

Solubility [MSY19, KKO+16, WZWW18]. **solubilization** [TFYO19].

solute [BRLS08, BRLS12, EOA+11, RVM19, TKT11, YKO+11, Yan11].

solute/solvent [RVM19]. **solutes** [GC11, PAK15]. **Solution** [Cam19, PK19, AvKSP16, AK10, DR11, DBM+17, DP15, EOA+11, GAI13, GAI14, HDK+12, HAL14, HNN+17, KS18, KTNN10, KVR10, LLvG10, MMB+17, MFM+12, PMC+17, PGW+17, SJWE10, TKNN10, UCFR16, WHL+10, WC13, WLF19, XTG+11, ZLL+10, ZZ10, vADC+14]. **solutions** [Ber17, CFC15, EK15, Kri10, OC19, OCW+15, SM14a]. **Solvation** [Jia19, RNSF+16, ZBP11, ALRM18, CBG17, CBG16, FGM11, GMMH+16, GPK12, HRC13, JMLL13, JGS+17, Jor17, KSK11, LP11b, MS13, MPSA17, MBE16, NW17, OBW12, PL14, RK16a, RK16b, SM14a, SK12, SY11, SMM15a, SMM15b, SMM+18, TKYN17, TCC+13, WXL17, WWWW18, YOMT14, YAS13, Yan14, ZCS+15]. **solvation-free-energy** [SMM15a, SMM15b]. **solvational** [FCL+10]. **Solvatochromic** [MKH15]. **Solvatochromism** [TKYN17]. **solve** [PNW+16]. **Solved** [CD19]. **Solvent** [KC13b, PK19, AKK+16, BEM14, BRLS08, BRLS12, CAD16, CBG16, EK15, FZY+12, FD16, GA19, HDL+17, Has14, HPL+18, HYUS11, KJDB12, KB11b, KCPMG12, LHL+10, LC17b, LZL+16, LWZ+17, MBC11, MBC13, MS11, ML14, MCUJ15, MCC12, MNNK10a, MNNK10b, PDMT10, PS13, QQY+18,

[BMFG16, JZ17, Zim15]. **stringent** [DPOS16]. **strong** [Kan15, MLZZ12, SDF12, SS19, VVY17, Vik11, ZSLL17]. **stronger** [KSC16]. **Structural** [ESD18, FHG+19, GLF16, GBL+11, GTT10, GAMAC+14, GWX+12, HS17a, II10, KZK+12, KSD+12, LBTV11, MP19b, NC14, TS11, VSH19, ZWW10, AIGP15, AD10, AKK+16, ALH+10, BBOB16, BPC13, CD19, CPV+12, CDS16, CYI+10, DWL11, DH11, GWT+17, GNI18, HS17b, HVS16, KKPT11, KG11, KNE11a, KDT+12, LK13, LL13a, MCF10, OSA19, PHC13, PGY15, PNG10, RRF11, RKB+14, RSL16, SFA17, SS13c, TYX+18, VVW+18, WC11, XMSZ16, YVEI+17, ZYvIZ14, ZLW10, FAS+18, VPR10]. **structurally** [TZCK18]. **Structure** [BPPS19, BJP15, CGBK13, DXL+10, GPK+16, GWJJ12, GBGR16, HLB15, JLLW19, LAHS16, MM19, MHRR11, NC12, NC13, PMG+16, Rab12, SGH+16, VDVR14, WZK+13, AFPI13, AR15, AM19a, AM19b, AJR16, AC12, BPPS17, BFH+13, BDdS13, CPRS18, CD13, CvM19, CM13b, Clo15, DKE+17, DKT13, DSB+19, DDP16, DVVP14, DGSVGVM19, DLW12, EH13, EWK+13, EFOD13, FZY+12, FDH19, FSC+14, GLB16, GMSdG15, GRARO+14, GP12, GK10, GRD+10, GPdC+16, GBG+19, HASR+12, HNHR13, HSB+19, HNyH19, HS14a, HRB+17, HH15, HYMZ16, HZ13, HLWD15, Hua16, Ibr17, KYT+17, KKH19, KSM17, KT10, KS12, Kop19b, KKL+13, KLS10, KMLS10, LLBO12, LFB14, LKL10, LZJ+11, LMI+14, LYL16, LPE+10, LGL11, LHG11, LWWG12, LLFH16, Mat10, MDT10, Mau14, MAPB10, MV17, NGAS17, NCT18, OCL11, OL13, OLA15, PSS14, PdSC18, PML+12]. **structure** [PN13, RLG14, RCM+13b, RR11, SHMO11, SB10, SM11, SLP+12, SB19, SLIB12, SRS14, SYN+12, SKGB13, SPZP18a, SPZP18b, Tac19, TN12, TTB+11, TG12b, UNT16, VVP12, VHR16, VVBL17, VÅA14, VBMA13, VKC10, VI17, VLGK+17, WO15, WRM+12, WSGN11, YW12, YZZ16, ZRCC11, ZHHX11, CPR18, FDCJG18, OSF12, SA10]. **structure-** [HH15]. **structure-activity** [DXL+10]. **Structure-based** [CGBK13, DXL+10, DVVP14, GLB16, VKC10, YZZ16]. **structured** [GEP+14]. **Structures** [DLT17, HDM+19, NSN19, SNS16, SZL19, ZLX+19, AHK+19, BHNS14, BPM15, Ber17, CL16, CCOH14, CBDS19, CV12, DVVP14, DH14, DLC18b, DT19, DZA11, GS12, GSS13, HSY+11, HTS17, HPL+18, HS12, Hua16, IYK11, KNE11a, KOY+12, KTO11, KTO13, KDT+12, KSW16, LABSG17, uLhY11, LXZ+10, LLSW14, LL19b, Lüc14, MCS11, MTM14, MPA10, MPA12, MP13, Mau14, MN19, MH10, MCAY15, MP17b, NS18, PRP15, PNW+16, QZM11, RHRCH16, Rao11, RCR+16, RvL11, RHJ11, RVVK13, RSG+10, Sak18, SWA13, SFR+11, SJD11, SIT18, SPM+19, SKY+11, TN10, Tak11, TFQ+10, TFQ+11, Tsu19, UCFR16, WKC11, WD10, YNH+17, ZSL+11, ZLY+16, ZP13, ĆMD13, OSI+19, PGCT+12]. **studied** [Ish10, KRTB10, OLY17, RHPWS13, RI10, TS15b]. **Studies** [JW12, AALCM11, BŁS10, BRGN12, BLG10, BIL10, DMN15, DXL+10, FWS+18, GZZM16, GEP+14, JLS+10, KG15, KP11, LXFC17, LCWW10, LJL+11, LWD13, RCM+13b, SB10, SFA17, SLHW09, SZZ+18, TNI+19a,

TDP+12, VSD10, WCAH10, YKH+10, YPC+10, YDL+10, YXZZ17, ZZL+12, ZZL+10a, ZYG+15, ZX11]. **Study** [BHB19, JLH+14, LLX+19, MUGNVJ+18, VL17b, AARP17, AS11, AS15a, AMAA+11, ATP18, ASMS10, ANH+11, APA+14, APY+16, AHK+19, ALH+10, BEM14, BE14, BHB+17, BH19, BEEL14, BJSI12, BLG11, BMD19, BRLS08, BRLS12, BL12, BEL+11, CCLP12, CCCLRO14, CWHH11, CBG17, CC18c, CCJ+11, CKL+11, CXW14, CBTZ16, CL16, CSXZ17, CSC+18, cCVG+14, CBDS19, Chu10, CG12, CB11c, CPLL11, CXD+19, CB11d, DASA15, DR11, DK19, DI11, DLSD13, DSX+11, EHT19, EOA+11, EvRC+18, EV14, FCL+10, FF11, FCD10, FBEM11, FL15, FPB12, FB14b, GAI14, GG10, GYX+10, GKB+19, GC18, GVP+10, GD10, GTK10, GWZ15, GNGCA10, GGM+12, GKR13, GWPJ11, HZ11, HW19, HDB15, HHDC16, HRL11, HBR17, HVS16, Ibr11, ITY+19, IIF+10, INT18, IN19, IN13, IIHY15, II10, JA10, JAHS+19, JS17a]. **study** [JCG+10, JAH+17, JJAB16, JW16, JYS+12, KD10, KKPT11, KOP+14, KIOY19, KC13b, KSNT19, KB13, KT12, KG11, KMT+19, KNP+12, KS13b, KP10, LC10, LY10, uLhY11, LP11a, LL13a, LAM19, LLL+10, LDJ+10, LZL+10, LCL+10, LZJ+11, LZHH11, LWL+11, Li14a, Li14b, LGW12, LT13, LJW+11b, Lin18, LBTV11, LBTV12, LTP11, LYSS11, LHKS12, LH14b, LLSW14, LWXC16, LHT15, Lu11, LJG+11, LPMT17, MUN+19, MMS16, MSY19, MC10, MG15, MCF10, MJLV14b, MAPB10, MFM+12, MH11, MWJ+11, MS11, MPNS13, MAMF19, MN19, MHRR11, MBRC16, MO17, Mor15, MIS+15, NHF+10, NH19, NGAS17, NASH15, NC12, NC13, NC14, NS18, NJX+10, NFI+16, OPR16, ORZ11, OSS10, OSHG17, OSA19, OME16, OOK11, PVL+13, PGCT+12, PP10, PGC12, PGS+15, PH12, PG18, PAK17, PP19, PPH+14, QLYL10, QZ10b, RS17a, RAGLL11, RAR+11, Ray13, RS13, RS14]. **study** [RVCFF13, RSLML12, RKG11, RSKG14, SN16a, SSP+13, SGDT10, SJD14, SCM+15, SRF+17, SSC+19, SWM10, ŠBD+17, SNS16, SGS+16, SSNT19, SMiN+19, SCF+19, SE14, SCMA+17, SCSM19, Su10, SKY+11, STS+10, SKTT11, SZZS16, STS15, SGHL13, SIG+15, SPZP18a, SPZP19, TM16, TFYO19, TTC+18, TLA10, TSNC+17, TSR+16, TL16, UvSvdWK19, VKNT16, VPR10, VAR12, Vik11, VLGK+17, VED10, WKC10a, WHL+10, WCWW11, WDLG12, WLHZ12, WYL+15, WFL+19, WNM17, WHX+10, WD10, WMW+10, WZQW10, WS11, WHDL11, WCL+11, WYGW12, WDP+12, XDL+10, XZ11, XWW+11, XCLZ19, XBSS19, YZGS14a, YZWC11, YHG+11, YZN13, YR13, YZLZ19, YJXZ13, YLZ+10, YKH15, YSRSS10, YCGA10, YB11, YYT12, YZ15b, ZCK+16, ZWGO16, ZTH+15, ZPP+16, ZXS+10, ZZL+10b, ZZWT12, ZYLL12, ZLLL12, ZSZ+14, ZDX11, ZWY+10b, ZWY+10a, ZBP11, ZZ12, ZZWX11, ZGZ19, dSDdAR10, dSdS12a, dSdS12b, dSdLBNB17]. **study** [dALdS+15, vRET19, vADC+14, GMBM18]. **studying** [SDL14]. **styrene** [MG15, PXXW10]. **sub** [LTT16, YO19]. **sub-optimal** [LTT16]. **sub-permutation** [YO19]. **subdomain** [LKL10]. **subjected** [JMX+16]. **submarine** [WWKS16]. **Subspace** [FBKD19, SBB10, SM18]. **Substituent** [MGS+16, AS18, CWHH11, JMX+16, MLY+13, TYN15, TY10].

BSD18, BB11a, CCR18, CVT+11, CAP17, CSSB11, DK19, DWL11, DBK17, DFF+15, DJS+18, DCHL12, DLZ15, ESD18, EWK+13, FF11, FRC18, FLM11, FZL+19, FL15, Gar12, GRS15, GFPSD17, GMO16, GZM11, GRL+11, GRL+12, GMBX+16, GTZ+18, HASR+12, HNS16, HNyH19, HLW+17, HDL+17, HH17, Höf14, HBL12, HYUS11, HJKJ13, HZSS17, HHWL17, HLEM18, Hug14, HRH+17, Ish10, IHJ+13, JLH+14, JMS13, KV13, Kan15, KSO+19, KERY+16, KT10, KLOS10, KGJZ19, KTNN10, KP11, LBGS16, LPK16, LRvdSM15, LZ12, LCH10, LCL+10, LMR14, LHG11, LTA+11, LBDP12, MS17, MZZ11, MRB14, MJC14, MN15, MY17a]. **using** [MHO18, MSS+13, MK19, MKM+17, MCUJ15, MVKS10, MKB+13, MFR+17, MIOM13, MMJ10, MS15, NPG+18, NLP+16, Nav18, NASH15, NHN16, OHPR18, OCW+15, PGdO+16, PC11, PG15, Pie14, PJ13, RB13a, RD18, RLDJ17, RDDS10, RHJ11, RVM19, RS13, RRK14, Ric16, REL17, REV+17, Rui11, RFHG10, REH13, SHMO11, SSO19, SZdB19, SFM14, SDF+17, SBV10, SA13, SCW11, SEF+16, SHL19, SS19, SHL+11, SKKS13, SB18, SY11, SRS14, SH19a, SZZS16, STS15, TYZ+16, TYX+18, Tak14, TKNN10, Tsi17, TTn19, TJB12, UTM11, VKAM12, VECT12, VI17, WKLC12, WdVN12, WLC12, WZ17, WJX+10, WDHZ13, XTY+14, XYX17, XWW+11, YWJ+16, Yon16, YN15, YDX16, YFH+19, ZWLX11, ZL11, ZLT13, ZWX19, ZWS+10, ZP13, ZH12, ZZZ+19, ZHHX11, dLC17, AIM+18, JCHT18, LHL+10]. **utility** [YHVM12]. **utilizing** [BVY+12, BP18]. **UV** [GGM+12, KASH14, RDF+11, RVdMB16]. **UV-photoexcitation** [RVdMB16]. **UV/Vis** [GGM+12].

V [WWKS16, LZL+15b, MG11, PBE16, WRM+12, WYGW12]. **vacancies** [HRB+17]. **valance** [FF11]. **Valence** [FBKD19, SZL19, WM12, YWZ14, BH19, BEEL14, BACSCJ+10, FE14, GCW16, Hil13, HAI+16, Ibr17, KGR+16, LOB18, LLW12, LWW12, OLPB19, POB13, RHRCH16, RvL11, SSMW09, SCSW13, TM16, WWU12, XP13, XhD15, vLBBR12, FBKD19, GWF11, VV19]. **validation** [GMMH+16, GCP+13, HLEM18, PFVL14, WMW+10, ZSTI14, GMG+10, HM13]. **validity** [LP11b, PdSC18]. **value** [Les19, SG10a, YLS19]. **values** [BA11, GK15a, SK12, VRKT19, Zha12b, Zha12a]. **vanadia** [GNGCA10]. **vanadium** [WYGW12]. **vapor** [BDTP11, GWJR18, SISK10]. **variable** [CF18, KDB13]. **variant** [TKT11]. **variants** [SLY+10]. **Variation** [IMK+16, LvG13a, MTvG12, CKH19]. **Variational** [FBKD19, RAGLL11, TH13]. **Variationally** [YK13]. **variations** [LLHM16, SH15]. **Various** [Sch18, CC11, DSM+11, GVP+10, GMO16, MJBM12, PGC12, PL18, QLKI19, SOYC12, WDW12]. **varying** [CC12a, GC11]. **VASP** [BVHI17, HASR+12]. **VBSCF** [ZZMW19, vLBBR12]. **VC** [WKLC12]. **VCH** [Spr10]. **vDNA** [XLY12]. **vector** [GTZ+18, HLXH17, HLXH18, HL19, PL19, RLL+10, RMRBH+19, TYZ+16]. **vectorization** [PC16]. **Verification** [WKLC12, EOO+16]. **Verlag** [Spr10].

[Ano13-50, Ano14a, Ano14b, Ano14c, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14n, Ano14o, Ano14p, Ano14q, Ano14r, Ano14s, Ano14t, Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14-28, Ano14-29, Ano14-30, Ano14-31, Ano14-32, Ano14-33, Ano14-34, Ano14z, Ano14-35, Ano14-36, Ano14-37, Ano14-38, Ano14-39, Ano14-40, Ano14-41, Ano14-42, Ano14-43, Ano14-44, Ano14-45, Ano14-46, Ano14-47, Ano14-50, Ano14-51, Ano14-52, Ano14-53, Ano14-54, Ano14-55, Ano14-27, Ano14-48, Ano14-49, Ano14-56, Ano14-57, Ano14-58, Ano14-59, Ano14-60, Ano14-61, Ano14-62, Ano14-63, Ano14-64, Ano14-65, Ano14-66, Ano14-67, Ano14-68, Ano14-69, Ano14-70, Ano14-71, Ano14-72, Ano14d, Ano14e, Ano14f, Ano15a, Ano15b, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n, Ano15o].
Volume
[Ano15p, Ano15q, Ano15r, Ano15s, Ano15t, Ano15u, Ano15y, Ano15z, Ano15-27, Ano15-28, Ano15-29, Ano15-30, Ano15-31, Ano15-32, Ano15-33, Ano15-34, Ano15-35, Ano15-36, Ano15-39, Ano15v, Ano15-40, Ano15-41, Ano15-42, Ano15-43, Ano15-44, Ano15w, Ano15x, Ano15-37, Ano15-38, Ano15-45, Ano15-46, Ano15-47, Ano15-48, Ano15-49, Ano15-50, Ano15-51, Ano15-52, Ano15-53, Ano15-54, Ano15-55, Ano15-56, Ano15-57, Ano15c, Ano15d, Ano15e, Ano15f, Ano15g, Ano15h, Ano16a, Ano16b, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m, Ano16n, Ano16o, Ano16p, Ano16q, Ano16r, Ano16u, Ano16v, Ano16w, Ano16x, Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16-29, Ano16-30, Ano16-31, Ano16-32, Ano16-33, Ano16-34, Ano16-35, Ano16-36, Ano16c, Ano16-39, Ano16-40, Ano16-41, Ano16s, Ano16t].
Volume [Ano16-37, Ano16-38, Ano16-42, Ano16-43, Ano16-44, Ano16-45, Ano16-46, Ano16-47, Ano16-48, Ano16-49, Ano16-50, Ano16-51, Ano16-52, Ano16-53, Ano16-54, Ano16-55, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h, Ano16-75, Ano16-89, Ano16-80, Ano16-94, Ano16-81, Ano16-95, Ano16-82, Ano16-96, Ano16-83, Ano16-97, Ano16-84, Ano16-98, Ano16-85, Ano16-99, Ano16-86, Ano16-100, Ano16-87, Ano16-101, Ano16-88, Ano16-102, Ano16-76, Ano16-90, Ano16-77, Ano16-91, Ano16-78, Ano16-92, Ano16-79, Ano16-93, Ano16-129, Ano16-108, Ano16-109, Ano16-110, Ano16-130, Ano16-111, Ano16-112, Ano16-113, Ano16-114, Ano16-103, Ano16-104, Ano16-105, Ano16-106, Ano16-107, Ano16-115, Ano16-121, Ano16-122, Ano16-123, Ano16-124, Ano16-125, Ano16-126, Ano16-127, Ano16-128, Ano16-116, Ano16-117, Ano16-118, Ano16-119, Ano16-120, Ano17a, Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x]. **Volume**
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zirconocene/borate [OSA19]. **Zn** [GEP+14, SLIB12, GPdC+16, LBC+19, QLYL10, RRF11, XP13]. **Zn-metalloenzyme** [GPdC+16]. **ZnH** [HYD10]. **ZnO** [HSH15, VI17]. **ZnPh** [RDT14]. **Zns** [NNS15]. **ZnSe** [Lar12]. **ZnX** [SPS+12]. **Zone** [PBE16, BPE16]. **Zone-folding** [PBE16, BPE16]. **zones** [TDKT10]. **ZORA** [ARAG17, JKS+16]. **Zr** [MCK17a, WZH+18, YW12, TCPPC14]. **ZrN** [FAA15]. **ZrO** [RRC+15]. **ZrS** [BE14, BPE16]. **ZSM** [Mor15, Pon10]. **zwitterion** [DQ16, ZZWT12]. **zwitterions** [PVS12].

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Anonymous:2012:CIIc

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Anonymous:2012:CIIe

[Ano12e] Anonymous. Cover image: Inside cover, volume 33, issue 27. *Journal of Computational Chemistry*, 33(27):iii–iv, October 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIIf

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Anonymous:2012:CIIg

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Anonymous:2012:CIIh

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Anonymous:2012:CIVb

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Anonymous:2012:CIVc

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Anonymous:2012:CIVd

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Anonymous:2012:CIVe

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Anonymous:2012:CIVf

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Anonymous:2012:CIVg

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Anonymous:2012:CIVh

[Ano12r] Anonymous. Cover image, volume 33, issue 30. *Journal of Computational Chemistry*, 33(30):i–ii, November 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVi

[Ano12s] Anonymous. Cover image, volume 33, issue 31. *Journal of Computational Chemistry*, 33(31):i–ii, December 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVj

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Anonymous:2012:RPP

[Ano12u] Anonymous. Retracted: "Prediction of posttranslational modification sites from sequences with kernel methods" by Xiaobo Wang, Yongcui Wang, Yingjie Tian, Xiaojian Shao, Ling-Yun Wu, and Naiyang Deng, published online on 21 April 2010. *Journal of Computational Chemistry*, 33(17):1524, June 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIa

[Ano13a] Anonymous. Cover image: Inside cover, volume 34, issue 1. *Journal of Computational Chemistry*, 34(1):iii–iv, January 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIj

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Anonymous:2013:CIIk

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Anonymous:2013:CIIl

[Ano13d] Anonymous. Cover image: Inside cover, volume 34, issue 12. *Journal of Computational Chemistry*, 34(12):iii–iv, May 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIm

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Anonymous:2013:CIIn

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Anonymous:2013:CIIo

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Anonymous:2013:CIIp

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Anonymous:2013:CIIq

[Ano13i] Anonymous. Cover image: Inside cover, volume 34, issue 17. *Journal of Computational Chemistry*, 34(17):iii–iv, June 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIr

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Anonymous:2013:CIIs

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Anonymous:2013:CIIb

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Anonymous:2013:CIIt

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Anonymous:2013:CIIu

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Anonymous:2013:CIIv

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Anonymous:2013:CIIw

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Anonymous:2013:CIIx

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Anonymous:2013:CIIy

[Ano13r] Anonymous. Cover image: Inside cover, volume 34, issue 25. *Journal of Computational Chemistry*, 34(25):iii–iv, September 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIz

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Anonymous:2013:CIIba

[Ano13t] Anonymous. Cover image: Inside cover, volume 34, issue 27. *Journal of Computational Chemistry*, 34(27):iii–iv, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIbb

[Ano13u] Anonymous. Cover image: Inside cover, volume 34, issue 28. *Journal of Computational Chemistry*, 34(28):iii–iv, October 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIbc

[Ano13v] Anonymous. Cover image: Inside cover, volume 34, issue 29. *Journal of Computational Chemistry*, 34(29):iii–iv, November 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIc

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Anonymous:2013:CIIbd

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Anonymous:2013:CIIbe

[Ano13y] Anonymous. Cover image: Inside cover, volume 34, issue 32. *Journal of Computational Chemistry*, 34(32):iii–iv, December 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIId

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Anonymous:2013:CIIe

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Anonymous:2013:CIIf

[Ano13-28] Anonymous. Cover image: Inside cover, volume 34, issue 6. *Journal of Computational Chemistry*, 34(6):iii–iv, March 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIg

[Ano13-29] Anonymous. Cover image: Inside cover, volume 34, issue 7. *Journal of Computational Chemistry*, 34(7):iii–iv, March 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIh

[Ano13-30] Anonymous. Cover image: Inside cover, volume 34, issue 8. *Journal of Computational Chemistry*, 34(8):iii–iv, March 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIi

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Anonymous:2013:CIVa

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Anonymous:2013:CIVj

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Anonymous:2013:CIVk

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Anonymous:2013:CIVl

[Ano13-35] Anonymous. Cover image, volume 34, issue 12. *Journal of Computational Chemistry*, 34(12):i–ii, May 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVm

[Ano13-36] Anonymous. Cover image, volume 34, issue 13. *Journal of Computational Chemistry*, 34(13):i–ii, May 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVn

[Ano13-37] Anonymous. Cover image, volume 34, issue 14. *Journal of Computational Chemistry*, 34(14):i–ii, May 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVo

[Ano13-38] Anonymous. Cover image, volume 34, issue 15. *Journal of Computational Chemistry*, 34(15):i–ii, June 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVp

[Ano13-39] Anonymous. Cover image, volume 34, issue 16. *Journal of Computational Chemistry*, 34(16):i–ii, June 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVq

[Ano13-40] Anonymous. Cover image, volume 34, issue 17. *Journal of Computational Chemistry*, 34(17):i–ii, June 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVr

[Ano13-41] Anonymous. Cover image, volume 34, issue 18. *Journal of Computational Chemistry*, 34(18):i–ii, July 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVs

[Ano13-42] Anonymous. Cover image, volume 34, issue 19. *Journal of Computational Chemistry*, 34(19):i–ii, July 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVb

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Anonymous:2013:CIVt

[Ano13-44] Anonymous. Cover image, volume 34, issue 20. *Journal of Computational Chemistry*, 34(20):i–ii, July 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVu

[Ano13-45] Anonymous. Cover image, volume 34, issue 21. *Journal of Computational Chemistry*, 34(21):i–ii, August 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVv

[Ano13-46] Anonymous. Cover image, volume 34, issue 22. *Journal of Computational Chemistry*, 34(22):i–ii, August 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVw

[Ano13-47] Anonymous. Cover image, volume 34, issue 23. *Journal of Computational Chemistry*, 34(23):i–ii, September 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVx

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Anonymous:2013:CIVy

[Ano13-49] Anonymous. Cover image, volume 34, issue 25. *Journal of Computational Chemistry*, 34(25):i–ii, September 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVz

[Ano13-50] Anonymous. Cover image, volume 34, issue 26. *Journal of Computational Chemistry*, 34(26):i–ii, October 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVba

[Ano13-51] Anonymous. Cover image, volume 34, issue 27. *Journal of Computational Chemistry*, 34(27):i–ii, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVbb

[Ano13-52] Anonymous. Cover image, volume 34, issue 28. *Journal of Computational Chemistry*, 34(28):i–ii, October 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVbc

[Ano13-53] Anonymous. Cover image, volume 34, issue 29. *Journal of Computational Chemistry*, 34(29):i–ii, November 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVc

[Ano13-54] Anonymous. Cover image, volume 34, issue 3. *Journal of Computational Chemistry*, 34(3):i–ii, January 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVbd

[Ano13-55] Anonymous. Cover image, volume 34, issue 30. *Journal of Computational Chemistry*, 34(30):i–ii, November 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVbe

[Ano13-56] Anonymous. Cover image, volume 34, issue 30. *Journal of Computational Chemistry*, 34(30):iii–iv, November 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVbf

[Ano13-57] Anonymous. Cover image, volume 34, issue 31. *Journal of Computational Chemistry*, 34(31):i–ii, December 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVbg

[Ano13-58] Anonymous. Cover image, volume 34, issue 32. *Journal of Computational Chemistry*, 34(32):i–ii, December 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVd

[Ano13-59] Anonymous. Cover image, volume 34, issue 4. *Journal of Computational Chemistry*, 34(4):i–ii, February 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVe

[Ano13-60] Anonymous. Cover image, volume 34, issue 5. *Journal of Computational Chemistry*, 34(5):i–ii, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVf

[Ano13-61] Anonymous. Cover image, volume 34, issue 6. *Journal of Computational Chemistry*, 34(6):i–ii, March 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVg

[Ano13-62] Anonymous. Cover image, volume 34, issue 7. *Journal of Computational Chemistry*, 34(7):i–ii, March 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVh

[Ano13-63] Anonymous. Cover image, volume 34, issue 8. *Journal of Computational Chemistry*, 34(8):i–ii, March 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVi

[Ano13-64] Anonymous. Cover image, volume 34, issue 9. *Journal of Computational Chemistry*, 34(9):i–ii, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CII

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Anonymous:2014:CIVa

[Ano14b] Anonymous. Cover image, volume 35, issue 1. *Journal of Computational Chemistry*, 35(1):i–ii, January 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVb

[Ano14c] Anonymous. Cover image, volume 35, issue 1. *Journal of Computational Chemistry*, 35(1):iii–iv, January 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVx

[Ano14d] Anonymous. Cover image, volume 35, issue 10. *Journal of Computational Chemistry*, 35(10):i–ii, April 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVy

[Ano14e] Anonymous. Cover image, volume 35, issue 10. *Journal of Computational Chemistry*, 35(10):iii–iv, April 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVz

[Ano14f] Anonymous. Cover image, volume 35, issue 10. *Journal of Computational Chemistry*, 35(10):v–vi, April 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVba

[Ano14g] Anonymous. Cover image, volume 35, issue 11. *Journal of Computational Chemistry*, 35(11):i–ii, April 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbb

[Ano14h] Anonymous. Cover image, volume 35, issue 11. *Journal of Computational Chemistry*, 35(11):iii–iv, April 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbc

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Anonymous:2014:CIVbd

[Ano14j] Anonymous. Cover image, volume 35, issue 12. *Journal of Computational Chemistry*, 35(12):i–ii, May 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbe

[Ano14k] Anonymous. Cover image, volume 35, issue 12. *Journal of Computational Chemistry*, 35(12):iii–iv, May 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbf

[Ano14l] Anonymous. Cover image, volume 35, issue 12. *Journal of Computational Chemistry*, 35(12):v–vi, May 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbg

[Ano14m] Anonymous. Cover image, volume 35, issue 13. *Journal of Computational Chemistry*, 35(13):i–ii, May 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbh

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Anonymous:2014:CIVbi

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Anonymous:2014:CIVbj

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Anonymous:2014:CIVbk

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Anonymous:2014:CIVbl

[Ano14r] Anonymous. Cover image, volume 35, issue 16. *Journal of Computational Chemistry*, 35(16):i–ii, June 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbm

[Ano14s] Anonymous. Cover image, volume 35, issue 16. *Journal of Computational Chemistry*, 35(16):iii–iv, June 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbn

[Ano14t] Anonymous. Cover image, volume 35, issue 17. *Journal of Computational Chemistry*, 35(17):i–ii, June 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbo

[Ano14u] Anonymous. Cover image, volume 35, issue 17. *Journal of Computational Chemistry*, 35(17):iii–iv, June 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbp

[Ano14v] Anonymous. Cover image, volume 35, issue 18. *Journal of Computational Chemistry*, 35(18):i–ii, July 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbq

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Anonymous:2014:CIVbr

[Ano14x] Anonymous. Cover image, volume 35, issue 19. *Journal of Computational Chemistry*, 35(19):i–ii, July 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbs

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Anonymous:2014:CIVc

[Ano14z] Anonymous. Cover image, volume 35, issue 2. *Journal of Computational Chemistry*, 35(2):i–ii, January 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVd

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Anonymous:2014:CIVbt

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Anonymous:2014:CIVbu

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Anonymous:2014:CIVbv

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Anonymous:2014:CIVbw

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Anonymous:2014:CIVbx

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Anonymous:2014:CIVby

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Anonymous:2014:CIVbz

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Anonymous:2014:CIVca

[Ano14-35] Anonymous. Cover image, volume 35, issue 23. *Journal of Computational Chemistry*, 35(23):iii–iv, September 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcb

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Anonymous:2014:CIVcc

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Anonymous:2014:CIVcd

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Anonymous:2014:CIVce

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Anonymous:2014:CIVcf

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Anonymous:2014:CIVcg

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Anonymous:2014:CIVch

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Anonymous:2014:CIVci

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Anonymous:2014:CIVcj

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Anonymous:2014:CIVck

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Anonymous:2014:CIVcl

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Anonymous:2014:CIVcm

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Anonymous:2014:CIVe

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Anonymous:2014:CIVf

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Anonymous:2014:CIVcn

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Anonymous:2014:CIVco

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Anonymous:2014:CIVcp

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Anonymous:2014:CIVcq

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Anonymous:2014:CIVcr

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Anonymous:2014:CIVcs

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Anonymous:2014:CIVg

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Anonymous:2014:CIVh

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Anonymous:2014:CIVi

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Anonymous:2014:CIVj

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Anonymous:2014:CIVk

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Anonymous:2014:CIVl

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Anonymous:2014:CIVm

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Anonymous:2014:CIVn

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Anonymous:2014:CIVo

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Anonymous:2014:CIVp

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Anonymous:2014:CIVq

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Anonymous:2014:CIVr

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Anonymous:2014:CIVs

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Anonymous:2014:CIVt

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Anonymous:2014:CIVu

[Ano14-70] Anonymous. Cover image, volume 35, issue 9. *Journal of Computational Chemistry*, 35(9):i–ii, April 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVv

[Ano14-71] Anonymous. Cover image, volume 35, issue 9. *Journal of Computational Chemistry*, 35(9):iii–iv, April 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVw

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Anonymous:2015:CIVa

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Anonymous:2015:CIVb

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Anonymous:2015:CIVu

[Ano15c] Anonymous. Cover image, volume 36, issue 10. *Journal of Computational Chemistry*, 36(10):i–ii, April 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVv

[Ano15d] Anonymous. Cover image, volume 36, issue 10. *Journal of Computational Chemistry*, 36(10):iii–iv, April 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVw

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Anonymous:2015:CIVx

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Anonymous:2015:CIVy

[Ano15g] Anonymous. Cover image, volume 36, issue 11. *Journal of Computational Chemistry*, 36(11):iii–iv, April 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVz

[Ano15h] Anonymous. Cover image, volume 36, issue 11. *Journal of Computational Chemistry*, 36(11):v–vi, April 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVba

[Ano15i] Anonymous. Cover image, volume 36, issue 12. *Journal of Computational Chemistry*, 36(12):i–ii, May 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbb

[Ano15j] Anonymous. Cover image, volume 36, issue 12. *Journal of Computational Chemistry*, 36(12):iii–iv, May 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbc

[Ano15k] Anonymous. Cover image, volume 36, issue 13. *Journal of Computational Chemistry*, 36(13):i–ii, May 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbd

[Ano15l] Anonymous. Cover image, volume 36, issue 13. *Journal of Computational Chemistry*, 36(13):iii–iv, May 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbe

[Ano15m] Anonymous. Cover image, volume 36, issue 14. *Journal of Computational Chemistry*, 36(14):i–ii, May 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbf

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Anonymous:2015:CIVbg

[Ano15o] Anonymous. Cover image, volume 36, issue 15. *Journal of Computational Chemistry*, 36(15):i–ii, June 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbh

[Ano15p] Anonymous. Cover image, volume 36, issue 16. *Journal of Computational Chemistry*, 36(16):i–ii, June 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbi

[Ano15q] Anonymous. Cover image, volume 36, issue 16. *Journal of Computational Chemistry*, 36(16):iii–iv, June 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbj

[Ano15r] Anonymous. Cover image, volume 36, issue 17. *Journal of Computational Chemistry*, 36(17):i–ii, June 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbk

[Ano15s] Anonymous. Cover image, volume 36, issue 18. *Journal of Computational Chemistry*, 36(18):i–ii, July 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbl

[Ano15t] Anonymous. Cover image, volume 36, issue 18. *Journal of Computational Chemistry*, 36(18):iii–iv, July 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbm

[Ano15u] Anonymous. Cover image, volume 36, issue 19. *Journal of Computational Chemistry*, 36(19):i–ii, July 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVc

[Ano15v] Anonymous. Cover image, volume 36, issue 2. *Journal of Computational Chemistry*, 36(2):i–ii, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVd

[Ano15w] Anonymous. Cover image, volume 36, issue 2. *Journal of Computational Chemistry*, 36(2):iii–iv, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVe

[Ano15x] Anonymous. Cover image, volume 36, issue 2. *Journal of Computational Chemistry*, 36(2):v–vi, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbn

[Ano15y] Anonymous. Cover image, volume 36, issue 20. *Journal of Computational Chemistry*, 36(20):i–ii, July 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbo

[Ano15z] Anonymous. Cover image, volume 36, issue 21. *Journal of Computational Chemistry*, 36(21):i–ii, August 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbp

[Ano15-27] Anonymous. Cover image, volume 36, issue 22. *Journal of Computational Chemistry*, 36(22):i–ii, August 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbq

[Ano15-28] Anonymous. Cover image, volume 36, issue 22. *Journal of Computational Chemistry*, 36(22):iii–iv, August 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbr

[Ano15-29] Anonymous. Cover image, volume 36, issue 23. *Journal of Computational Chemistry*, 36(23):i–ii, September 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbs

[Ano15-30] Anonymous. Cover image, volume 36, issue 24. *Journal of Computational Chemistry*, 36(24):i–ii, September 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbt

[Ano15-31] Anonymous. Cover image, volume 36, issue 25. *Journal of Computational Chemistry*, 36(25):i–ii, September 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbu

[Ano15-32] Anonymous. Cover image, volume 36, issue 26. *Journal of Computational Chemistry*, 36(26):i–ii, October 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbv

[Ano15-33] Anonymous. Cover image, volume 36, issue 26. *Journal of Computational Chemistry*, 36(26):iii–iv, October 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbw

[Ano15-34] Anonymous. Cover image, volume 36, issue 27. *Journal of Computational Chemistry*, 36(27):i–ii, October 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbx

[Ano15-35] Anonymous. Cover image, volume 36, issue 28. *Journal of Computational Chemistry*, 36(28):i–ii, October 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVby

[Ano15-36] Anonymous. Cover image, volume 36, issue 29. *Journal of Computational Chemistry*, 36(29):i–ii, November 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVf

[Ano15-37] Anonymous. Cover image, volume 36, issue 3. *Journal of Computational Chemistry*, 36(3):i–ii, January 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVg

[Ano15-38] Anonymous. Cover image, volume 36, issue 3. *Journal of Computational Chemistry*, 36(3):iii–iv, January 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbz

[Ano15-39] Anonymous. Cover image, volume 36, issue 30. *Journal of Computational Chemistry*, 36(30):i–ii, November 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVca

[Ano15-40] Anonymous. Cover image, volume 36, issue 30. *Journal of Computational Chemistry*, 36(30):iii–iv, November 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVcb

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Anonymous:2015:CIVcc

[Ano15-42] Anonymous. Cover image, volume 36, issue 31. *Journal of Computational Chemistry*, 36(31):iii–iv, December 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVcd

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Anonymous:2015:CIVce

[Ano15-44] Anonymous. Cover image, volume 36, issue 32. *Journal of Computational Chemistry*, 36(32):i–ii, December 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVh

[Ano15-45] Anonymous. Cover image, volume 36, issue 4. *Journal of Computational Chemistry*, 36(4):i–ii, February 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVi

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Anonymous:2015:CIVj

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Anonymous:2015:CIVk

[Ano15-48] Anonymous. Cover image, volume 36, issue 5. *Journal of Computational Chemistry*, 36(5):iii–iv, February 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVl

[Ano15-49] Anonymous. Cover image, volume 36, issue 5. *Journal of Computational Chemistry*, 36(5):v–vi, February 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVm

[Ano15-50] Anonymous. Cover image, volume 36, issue 6. *Journal of Computational Chemistry*, 36(6):i–ii, March 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVn

[Ano15-51] Anonymous. Cover image, volume 36, issue 6. *Journal of Computational Chemistry*, 36(6):iii–iv, March 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVo

[Ano15-52] Anonymous. Cover image, volume 36, issue 7. *Journal of Computational Chemistry*, 36(7):i–ii, March 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVp

[Ano15-53] Anonymous. Cover image, volume 36, issue 7. *Journal of Computational Chemistry*, 36(7):iii–iv, March 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVq

[Ano15-54] Anonymous. Cover image, volume 36, issue 8. *Journal of Computational Chemistry*, 36(8):i–ii, March 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVr

[Ano15-55] Anonymous. Cover image, volume 36, issue 8. *Journal of Computational Chemistry*, 36(8):iii–iv, March 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVs

[Ano15-56] Anonymous. Cover image, volume 36, issue 9. *Journal of Computational Chemistry*, 36(9):i–ii, April 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVt

[Ano15-57] Anonymous. Cover image, volume 36, issue 9. *Journal of Computational Chemistry*, 36(9):iii–iv, April 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:ECS

[Ano15-58] Anonymous. Erratum: Corrigendum: A spherical harmonic transform spectral analysis of a localized surface plasmon on a gold nano shell. *Journal of Computational Chemistry*, 36(2): 136, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [BH14].

Anonymous:2015:ECG

[Ano15-59] Anonymous. Erratum to Csonka, G. I., Nguyen, N. A., & Kolossváry, I. (1997). Simple tests for density functional methods. Journal of Computational Chemistry, 18 (12), 1534–1545. (DOI: `c7rfjv`). *Journal of Computational Chemistry*, 36(30):2270, November 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [CNK97].

Anonymous:2015:OPS

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Anonymous:2016:CIVa

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Anonymous:2016:CIVb

[Ano16b] Anonymous. Cover image, volume 37, issue 1. *Journal of Computational Chemistry*, 37(1):ii, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVc

[Ano16c] Anonymous. Cover image, volume 37, issue 1. *Journal of Computational Chemistry*, 37(1):iii, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVv

[Ano16d] Anonymous. Cover image, volume 37, issue 10. *Journal of Computational Chemistry*, 37(10):i, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVw

[Ano16e] Anonymous. Cover image, volume 37, issue 10. *Journal of Computational Chemistry*, 37(10):ii, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVx

[Ano16f] Anonymous. Cover image, volume 37, issue 11. *Journal of Computational Chemistry*, 37(11):i, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVy

[Ano16g] Anonymous. Cover image, volume 37, issue 11. *Journal of Computational Chemistry*, 37(11):ii, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVz

[Ano16h] Anonymous. Cover image, volume 37, issue 11. *Journal of Computational Chemistry*, 37(11):iii, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVba

[Ano16i] Anonymous. Cover image, volume 37, issue 12. *Journal of Computational Chemistry*, 37(12):i, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbb

[Ano16j] Anonymous. Cover image, volume 37, issue 12. *Journal of Computational Chemistry*, 37(12):ii, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbc

[Ano16k] Anonymous. Cover image, volume 37, issue 13. *Journal of Computational Chemistry*, 37(13):i–ii, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbd

[Ano16l] Anonymous. Cover image, volume 37, issue 14. *Journal of Computational Chemistry*, 37(14):i–ii, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbe

[Ano16m] Anonymous. Cover image, volume 37, issue 15. *Journal of Computational Chemistry*, 37(15):i, June 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbf

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Anonymous:2016:CIVbg

[Ano16o] Anonymous. Cover image, volume 37, issue 16. *Journal of Computational Chemistry*, 37(16):i, June 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbh

[Ano16p] Anonymous. Cover image, volume 37, issue 17. *Journal of Computational Chemistry*, 37(17):i, June 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbi

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Anonymous:2016:CIVbj

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Anonymous:2016:CIVd

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Anonymous:2016:CIVe

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Anonymous:2016:CIVbk

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Anonymous:2016:CIVbl

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Anonymous:2016:CIVbm

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Anonymous:2016:CIVbn

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Anonymous:2016:CIVbo

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Anonymous:2016:CIVbp

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Anonymous:2016:CIVbq

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Anonymous:2016:CIVbr

[Ano16-28] Anonymous. Cover image, volume 37, issue 24. *Journal of Computational Chemistry*, 37(24):i, September 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbs

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Anonymous:2016:CIVbt

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Anonymous:2016:CIVbu

[Ano16-31] Anonymous. Cover image, volume 37, issue 25. *Journal of Computational Chemistry*, 37(25):ii, September 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbv

[Ano16-32] Anonymous. Cover image, volume 37, issue 26. *Journal of Computational Chemistry*, 37(26):i, October 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbw

[Ano16-33] Anonymous. Cover image, volume 37, issue 26. *Journal of Computational Chemistry*, 37(26):ii, October 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbx

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Anonymous:2016:CIVby

[Ano16-35] Anonymous. Cover image, volume 37, issue 28. *Journal of Computational Chemistry*, 37(28):i, October 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbz

[Ano16-36] Anonymous. Cover image, volume 37, issue 29. *Journal of Computational Chemistry*, 37(29):i, November 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVf

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Anonymous:2016:CIVg

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Anonymous:2016:CIVca

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Anonymous:2016:CIVcb

[Ano16-40] Anonymous. Cover image, volume 37, issue 31. *Journal of Computational Chemistry*, 37(31):i, December 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVcc

[Ano16-41] Anonymous. Cover image, volume 37, issue 32. *Journal of Computational Chemistry*, 37(32):i, December 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVh

[Ano16-42] Anonymous. Cover image, volume 37, issue 4. *Journal of Computational Chemistry*, 37(4):i, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVi

[Ano16-43] Anonymous. Cover image, volume 37, issue 4. *Journal of Computational Chemistry*, 37(4):ii, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVj

[Ano16-44] Anonymous. Cover image, volume 37, issue 5. *Journal of Computational Chemistry*, 37(5):i, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVk

[Ano16-45] Anonymous. Cover image, volume 37, issue 5. *Journal of Computational Chemistry*, 37(5):ii, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVl

[Ano16-46] Anonymous. Cover image, volume 37, issue 6. *Journal of Computational Chemistry*, 37(6):i, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVm

[Ano16-47] Anonymous. Cover image, volume 37, issue 7. *Journal of Computational Chemistry*, 37(7):i, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVn

[Ano16-48] Anonymous. Cover image, volume 37, issue 7. *Journal of Computational Chemistry*, 37(7):ii, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVo

[Ano16-49] Anonymous. Cover image, volume 37, issue 7. *Journal of Computational Chemistry*, 37(7):iii, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVp

[Ano16-50] Anonymous. Cover image, volume 37, issue 8. *Journal of Computational Chemistry*, 37(8):i, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVq

[Ano16-51] Anonymous. Cover image, volume 37, issue 8. *Journal of Computational Chemistry*, 37(8):ii, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVr

[Ano16-52] Anonymous. Cover image, volume 37, issue 8. *Journal of Computational Chemistry*, 37(8):iii, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVs

[Ano16-53] Anonymous. Cover image, volume 37, issue 9. *Journal of Computational Chemistry*, 37(9):i, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVt

[Ano16-54] Anonymous. Cover image, volume 37, issue 9. *Journal of Computational Chemistry*, 37(9):ii, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVu

[Ano16-55] Anonymous. Cover image, volume 37, issue 9. *Journal of Computational Chemistry*, 37(9):iii, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:EPR

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Anonymous:2016:IIa

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Anonymous:2016:IIb

[Ano16-58] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(16):1407–1412, June 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IId

[Ano16-59] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(17):1525–1530, June 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIf

[Ano16-60] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(18):1651–1656, July 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIg

[Ano16-61] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(19):1747, July 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIh

[Ano16-62] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(20):1855, July 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIi

[Ano16-63] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(21):1947–1952, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIj

[Ano16-64] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(22):2039–2043, August 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIk

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Anonymous:2016:IIl

[Ano16-66] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(24):2165–2169, September 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIm

[Ano16-67] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(25):2243–2247, September 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIn

[Ano16-68] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(26):2335–2339, October 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIo

[Ano16-69] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(27):2403–2407, October 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIp

[Ano16-70] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(28):2479–2483, October 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIq

[Ano16-71] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(29):2547–2551, November 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIr

[Ano16-72] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(30):2617–2621, November 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIs

[Ano16-73] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(31):2671, December 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIu

[Ano16-74] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(32):2743–2747, December 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICa

[Ano16-75] Anonymous. Issue information — coming soon, volume 37, issue 1. *Journal of Computational Chemistry*, 37(1):1, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICs

[Ano16-76] Anonymous. Issue information — coming soon: Volume 37, issue 10. *Journal of Computational Chemistry*, 37(10):871, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICu

[Ano16-77] Anonymous. Issue information — coming soon: Volume 37, issue 11. *Journal of Computational Chemistry*, 37(11):955, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICw

[Ano16-78] Anonymous. Issue information — coming soon: Volume 37, issue 12. *Journal of Computational Chemistry*, 37(12):1037, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICy

[Ano16-79] Anonymous. Issue information — coming soon: Volume 37, issue 13. *Journal of Computational Chemistry*, 37(13):1133,

May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICba

[Ano16-80] Anonymous. Issue information — coming soon: Volume 37, issue 14. *Journal of Computational Chemistry*, 37(14):1245, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICc

[Ano16-81] Anonymous. Issue information — coming soon, volume 37, issue 2. *Journal of Computational Chemistry*, 37(2):155, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICe

[Ano16-82] Anonymous. Issue information — coming soon, volume 37, issue 3. *Journal of Computational Chemistry*, 37(3):315, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICg

[Ano16-83] Anonymous. Issue information — coming soon, volume 37, issue 4. *Journal of Computational Chemistry*, 37(4):389, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICi

[Ano16-84] Anonymous. Issue information — coming soon, volume 37, issue 5. *Journal of Computational Chemistry*, 37(5):461, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICk

[Ano16-85] Anonymous. Issue information — coming soon: Volume 37, issue 6. *Journal of Computational Chemistry*, 37(6):543, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICm

[Ano16-86] Anonymous. Issue information — coming soon: Volume 37, issue 7. *Journal of Computational Chemistry*, 37(7):623, March

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Anonymous:2016:IICo

[Ano16-87] Anonymous. Issue information — coming soon: Volume 37, issue 8. *Journal of Computational Chemistry*, 37(8):695, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICq

[Ano16-88] Anonymous. Issue information — coming soon: Volume 37, issue 9. *Journal of Computational Chemistry*, 37(9):781, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICb

[Ano16-89] Anonymous. Issue information — copyright, volume 37, issue 1. *Journal of Computational Chemistry*, 37(1):2, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICt

[Ano16-90] Anonymous. Issue information — copyright: Volume 37, issue 10. *Journal of Computational Chemistry*, 37(10):872, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICv

[Ano16-91] Anonymous. Issue information — copyright: Volume 37, issue 11. *Journal of Computational Chemistry*, 37(11):956, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICx

[Ano16-92] Anonymous. Issue information — copyright: Volume 37, issue 12. *Journal of Computational Chemistry*, 37(12):1038, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICz

[Ano16-93] Anonymous. Issue information — copyright: Volume 37, issue 13. *Journal of Computational Chemistry*, 37(13):1134, May

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Anonymous:2016:IICbb

[Ano16-94] Anonymous. Issue information — copyright: Volume 37, issue 14. *Journal of Computational Chemistry*, 37(14):1246, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICd

[Ano16-95] Anonymous. Issue information — copyright, volume 37, issue 2. *Journal of Computational Chemistry*, 37(2):156, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICf

[Ano16-96] Anonymous. Issue information — copyright, volume 37, issue 3. *Journal of Computational Chemistry*, 37(3):316, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICh

[Ano16-97] Anonymous. Issue information — copyright, volume 37, issue 4. *Journal of Computational Chemistry*, 37(4):390, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICj

[Ano16-98] Anonymous. Issue information — copyright, volume 37, issue 5. *Journal of Computational Chemistry*, 37(5):462, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICl

[Ano16-99] Anonymous. Issue information — copyright: Volume 37, issue 6. *Journal of Computational Chemistry*, 37(6):544, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICn

[Ano16-100] Anonymous. Issue information — copyright: Volume 37, issue 7. *Journal of Computational Chemistry*, 37(7):624, March 15,

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Anonymous:2016:IICp

[Ano16-101] Anonymous. Issue information — copyright: Volume 37, issue 8. *Journal of Computational Chemistry*, 37(8):696, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICr

[Ano16-102] Anonymous. Issue information — copyright: Volume 37, issue 9. *Journal of Computational Chemistry*, 37(9):782, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEj

[Ano16-103] Anonymous. Issue information — editorial board: Volume 37, issue 10. *Journal of Computational Chemistry*, 37(10): 873, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEk

[Ano16-104] Anonymous. Issue information — editorial board: Volume 37, issue 11. *Journal of Computational Chemistry*, 37(11): 957, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEl

[Ano16-105] Anonymous. Issue information — editorial board: Volume 37, issue 12. *Journal of Computational Chemistry*, 37(12):1039, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEm

[Ano16-106] Anonymous. Issue information — editorial board: Volume 37, issue 13. *Journal of Computational Chemistry*, 37(13):1135, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEn

[Ano16-107] Anonymous. Issue information — editorial board: Volume 37, issue 14. *Journal of Computational Chemistry*, 37(14):1247,

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Anonymous:2016:IIEb

[Ano16-108] Anonymous. Issue information — Editorial Board, volume 37, issue 2. *Journal of Computational Chemistry*, 37(2):157, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEc

[Ano16-109] Anonymous. Issue information — Editorial Board, volume 37, issue 3. *Journal of Computational Chemistry*, 37(3):317, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEd

[Ano16-110] Anonymous. Issue information — Editorial Board, volume 37, issue 4. *Journal of Computational Chemistry*, 37(4):391, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEf

[Ano16-111] Anonymous. Issue information — Editorial Board: Volume 37, issue 6. *Journal of Computational Chemistry*, 37(6):545, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEg

[Ano16-112] Anonymous. Issue information — Editorial Board: Volume 37, issue 7. *Journal of Computational Chemistry*, 37(7):625, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEh

[Ano16-113] Anonymous. Issue information — Editorial Board: Volume 37, issue 8. *Journal of Computational Chemistry*, 37(8):697, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEi

[Ano16-114] Anonymous. Issue information — Editorial Board: Volume 37, issue 9. *Journal of Computational Chemistry*, 37(9):783,

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Anonymous:2016:IITa

[Ano16-115] Anonymous. Issue information — table of contents volume 37, issue 1. *Journal of Computational Chemistry*, 37(1):4–8, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITj

[Ano16-116] Anonymous. Issue information — table of contents: Volume 37, issue 10. *Journal of Computational Chemistry*, 37(10): 874–875, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITk

[Ano16-117] Anonymous. Issue information — table of contents: Volume 37, issue 11. *Journal of Computational Chemistry*, 37(11): 958–959, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITl

[Ano16-118] Anonymous. Issue information — table of contents: Volume 37, issue 12. *Journal of Computational Chemistry*, 37(12): 1040–1042, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITm

[Ano16-119] Anonymous. Issue information — table of contents: Volume 37, issue 13. *Journal of Computational Chemistry*, 37(13): 1136–1138, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITn

[Ano16-120] Anonymous. Issue information — table of contents: Volume 37, issue 14. *Journal of Computational Chemistry*, 37(14): 1248–1250, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITb

[Ano16-121] Anonymous. Issue information — table of contents, volume 37, issue 2. *Journal of Computational Chemistry*, 37(2):158–

161, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITc

[Ano16-122] Anonymous. Issue information — table of contents, volume 37, issue 3. *Journal of Computational Chemistry*, 37(3):318–319, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITd

[Ano16-123] Anonymous. Issue information — table of contents, volume 37, issue 4. *Journal of Computational Chemistry*, 37(4):392–393, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITe

[Ano16-124] Anonymous. Issue information — table of contents, volume 37, issue 5. *Journal of Computational Chemistry*, 37(5):464–465, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITf

[Ano16-125] Anonymous. Issue information — table of contents: Volume 37, issue 6. *Journal of Computational Chemistry*, 37(6):546–548, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITg

[Ano16-126] Anonymous. Issue information — table of contents: Volume 37, issue 7. *Journal of Computational Chemistry*, 37(7):626–627, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITh

[Ano16-127] Anonymous. Issue information — table of contents: Volume 37, issue 8. *Journal of Computational Chemistry*, 37(8):698–699, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITi

[Ano16-128] Anonymous. Issue information — table of contents: Volume 37, issue 9. *Journal of Computational Chemistry*, 37(9):

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Anonymous:2016:IIEa

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Anonymous:2016:IIEe

[Ano16-130] Anonymous. Issue information – Editorial Board, volume 37, issue 5. *Journal of Computational Chemistry*, 37(5):463, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVa

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Anonymous:2017:CIVj

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Anonymous:2017:CIVk

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Anonymous:2017:CIVl

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Anonymous:2017:CIVn

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Anonymous:2017:CIVo

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Anonymous:2017:CIVp

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Anonymous:2017:CIVq

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Anonymous:2017:CIVr

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Anonymous:2017:CIVs

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Anonymous:2017:CIVt

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Anonymous:2017:CIVbc

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Anonymous:2017:CIVbd

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Anonymous:2017:CIVbe

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Anonymous:2017:CIVbh

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Anonymous:2017:CIVd

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Anonymous:2017:CIVf

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Anonymous:2017:CIVg

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Anonymous:2017:CIVh

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Anonymous:2017:CIVi

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Anonymous:2017:IIb

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Anonymous:2017:IIc

[Ano17-38] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(3):127–131, January 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IId

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Anonymous:2017:IIe

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Anonymous:2017:IIf

[Ano17-41] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(6):313–317, March 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIg

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Anonymous:2017:IIh

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Anonymous:2017:IIi

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Anonymous:2017:IIj

[Ano17-45] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(10):639–644, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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Anonymous:2017:IIl

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Anonymous:2017:IIm

[Ano17-48] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(13):935–939, May 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIn

[Ano17-49] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(14):1017–1021, May 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIo

[Ano17-50] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(15):1103–1110, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIp

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Anonymous:2017:IIq

[Ano17-52] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(17):1489–1494, June 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIr

[Ano17-53] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(18):1561–1565, July 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIs

[Ano17-54] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(19):1655–1659, July 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIt

[Ano17-55] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(20):1741–1745, July 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIu

[Ano17-56] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(21):1819–1823, August 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIv

[Ano17-57] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(22):1891–1895, August 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIw

[Ano17-58] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(23):1981–1986, September 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIx

[Ano17-59] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(24):2057–2061, September 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIy

[Ano17-60] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(25):2135–2139, September 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIz

[Ano17-61] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(26):2207–2211, October 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIba

[Ano17-62] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(27):2283–2287, October 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIbb

[Ano17-63] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(28):2365–2369, October 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIbc

[Ano17-64] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(29):2453–2457, November 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIbd

[Ano17-65] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(30):2553–2557, November 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIbe

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Anonymous:2017:IIbf

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Anonymous:2018:CIVa

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Anonymous:2018:CIVb

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Anonymous:2018:CIVk

[Ano18c] Anonymous. Cover image, volume 39, issue 10. *Journal of Computational Chemistry*, 39(10):i, April 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVl

[Ano18d] Anonymous. Cover image, volume 39, issue 10. *Journal of Computational Chemistry*, 39(10):ii, April 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVm

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Anonymous:2018:CIVn

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Anonymous:2018:CIVo

[Ano18g] Anonymous. Cover image, volume 39, issue 13. *Journal of Computational Chemistry*, 39(13):i, May 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVp

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Anonymous:2018:CIVq

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Anonymous:2018:CIVr

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Anonymous:2018:CIVs

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Anonymous:2018:CIVt

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Anonymous:2018:CIVu

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Anonymous:2018:CIVc

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Anonymous:2018:CIVv

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Anonymous:2018:CIVw

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Anonymous:2018:CIVx

[Ano18q] Anonymous. Cover image, volume 39, issue 21. *Journal of Computational Chemistry*, 39(21):C1, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVy

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Anonymous:2018:CIVz

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Anonymous:2018:CIVba

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Anonymous:2018:CIVbb

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Anonymous:2018:CIVbc

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Anonymous:2018:CIVbd

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Anonymous:2018:CIVbe

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Anonymous:2018:CIVbf

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Anonymous:2018:CIVbg

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Anonymous:2018:CIVbh

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Anonymous:2018:CIVbi

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Anonymous:2018:CIVd

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Anonymous:2018:CIVbj

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Anonymous:2018:CIVbk

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Anonymous:2018:CIVbl

[Ano18-32] Anonymous. Cover image, volume 39, issue 32. *Journal of Computational Chemistry*, 39(32):C1, December 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVe

[Ano18-33] Anonymous. Cover image, volume 39, issue 4. *Journal of Computational Chemistry*, 39(4):i, February 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVf

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Anonymous:2018:CIVg

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Anonymous:2018:CIVh

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Anonymous:2018:CIVi

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Anonymous:2018:CIVj

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Anonymous:2018:IIa

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Anonymous:2018:IId

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Anonymous:2018:IIe

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Anonymous:2018:IIf

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Anonymous:2018:IIg

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Anonymous:2018:IIh

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Anonymous:2018:IIm

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Anonymous:2018:IIn

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Anonymous:2018:IIv

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Anonymous:2018:IIw

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Anonymous:2018:IIx

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Anonymous:2018:IIy

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Anonymous:2018:IIba

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Anonymous:2018:IIbe

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Anonymous:2019:CIVa

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Anonymous:2019:CIVj

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Anonymous:2019:CIVk

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Anonymous:2019:CIVl

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Anonymous:2019:CIVm

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Anonymous:2019:CIVn

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Anonymous:2019:CIVo

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Anonymous:2019:CIVp

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Anonymous:2019:CIVq

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Anonymous:2019:CIVr

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Anonymous:2019:CIVs

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Anonymous:2019:CIVb

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Anonymous:2019:CIVt

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Anonymous:2019:CIVu

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Anonymous:2019:CIVw

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Anonymous:2019:CIVx

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Anonymous:2019:CIVy

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Anonymous:2019:CIVz

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Anonymous:2019:CIVba

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Anonymous:2019:CIVbb

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Anonymous:2019:CIVbc

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Anonymous:2019:CIVc

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Anonymous:2019:CIVbd

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Anonymous:2019:CIVbe

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Anonymous:2019:CIVbf

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Anonymous:2019:CIVe

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Anonymous:2019:CIVf

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Anonymous:2019:CIVg

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Anonymous:2019:CIVh

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Anonymous:2019:CIVi

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Anonymous:2019:IIa

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Anonymous:2019:IIb

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Anonymous:2019:IIc

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Anonymous:2019:IId

[Ano19-36] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(4):625–629, February 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIe

[Ano19-37] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(5):707–711, February 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIf

[Ano19-38] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(6):763–767, March 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIg

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Anonymous:2019:IIh

[Ano19-40] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(8):911–915, March 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIi

[Ano19-41] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(9):959–964, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIj

[Ano19-42] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(10):1067–1072, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIk

[Ano19-43] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(11):1185–1189, April 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIl

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Anonymous:2019:IIm

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Anonymous:2019:IIn

[Ano19-46] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(14):1415–1419, May 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIo

[Ano19-47] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(15):1483–1487, June 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIp

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[Ano19-49] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(17):1609–1613, June 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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Anonymous:2019:IIs

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Anonymous:2019:IIt

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Anonymous:2019:IIv

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Anonymous:2019:IIw

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Anonymous:2019:IIy

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