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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]. $4d$ [Hil13]. $4f$ [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]. $\bar{1}_8$ [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 [RDT14]. ¹⁹ [DKE⁺17]. ¹ Δ_g [WLF19]. ¹ Σ [LWD13]. ¹ Σ^+
 [Kop15b]. ¹ Σ_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]. $\bar{2}_8$ [YLT⁺19]. ²⁹
 [HAI⁺16]. ^{2•-} [LGW12]. ² Π [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]. ¹²
 [BHP19, CC18c, DM15, LLLM11, LLB⁺12, LLD17, LCWW10, VIT⁺15]. ¹³
 [JCG⁺11, LAHS16, SC17]. $\bar{1}_3$ [OPR16]. $\bar{1}_5$ [OPR16]. ¹⁶ [WZH⁺18]. ¹⁸
 [DM15, TFQ⁺10, VIT⁺15]. ¹⁹ [DM15, VIT⁺15]. $\bar{1}_9$ [YLZ⁺19]. ²
 [AS15a, AR10, BE14, BPE16, BLF14, 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, MLC11, 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]. $\bar{2}_0$ [YLZ⁺19]. ²⁴ [GBGR16, YW12].
²⁶ [LAHS16]. ²⁸ [MCK17a]. $\bar{2}$ [CG12, EVR18, MH11]. $\bar{2}$ [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]. 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]. ₆₀ [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* [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]. *n*^{/0} [YLL11]. *n*^{/0} [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]. *ī* [HSH15]. *β* [AKMT11, BLS10, 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]. *.* [ATP18, BH13, LZL⁺15b, RAGLL11, TNY18, YKH15, ATP18, BZH14]. *...* [CROB16, TDT19, VVJ15, WvRSM14]. *...π* [BSF18, CCCLCGRO14]. *...π...π* [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, BLBG⁺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, BLBG⁺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]. $\pi \dots$ [YZZ⁺17]. $\pi \dots \pi$ [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]. $\tilde{A}^1 A'$ [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** [III10]. **-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** [BLBG⁺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**

[ZBP11, ZP13]. **-glycine** [DB12]. **-grafted** [DSB⁺19]. **-H** [LJW⁺11b, TKCN19]. **-hairpin** [LJW⁺11b]. **-helices** [KKK⁺19, HHT⁺13a, HHT⁺13b]. **-helix** [CCOH14, WXL⁺12]. **-heptane** [RRF11]. **-heterocyclic** [KYKR15, LXZ⁺10, RF15, dSdLBNB17]. **-hole** [BSF18, GZZM16, LZL⁺15b]. **-holes** [PM18a]. **-hydrogen** [GNC⁺18]. **-hydrogenase** [GS11]. **-hydroxy-dimethylnitrosamine** [FFA14]. **-hydroxybutyrate** [SJD14]. **-hydroxymethylfurfural** [APY⁺16, WFL⁺19]. **-hydroxyquinolin-imidazolinone-based** [CSC⁺18]. **-hydroxysteroid** [ZX11]. **-inhibitor** [LJL⁺11]. **-iodanes** [SLT14]. **-keto** [XLYZ10]. **-LEUS** [BH15]. **-LiCl** [LCL⁺18]. **-like** [WGN⁺16]. **-maltose** [SWM10]. **-metalloid** [MMS16]. **-methyl** [LZL⁺16]. **-methyl-Imidazolium** [MG15]. **-methylacetamide** [KSK11]. **-methylation** [QZM11]. **-methylbenzyl** [NDG14]. **-methylformamides** [JSW10]. **-Montmorillonite** [BHB19, BHB⁺17]. **-N-benzyl-N-** [NDG14]. **-naphthol** [CYY⁺17]. **-nearest** [Hug14, YS15]. **-nitroaniline** [ZTH⁺15]. **-nucleophile** [ZYR⁺15]. **-one** [YZLZ18]. **-ones** [YZ15b]. **-orbitals** [MCK17a]. **-organic** [AH10]. **-oxo** [VBMA13, RHPWS13]. **-oxoalkyl-substituted** [AARP17]. **-Pd** [dSdLBNB17]. **-pentane** [TCGNT18]. **-peptide** [LLvG10, LvG13a]. **-peptides** [LvG13c, ZKH⁺10]. **-peroxo** [RHPWS13]. **-phenyl-azacrown-5** [ZWY⁺10a]. **-phosphano** [KYKR15]. **-phosphoranes** [TR12]. **-pinene** [BLS10]. **-pleated** [WCAH10]. **-point** [BTB⁺11]. **-proline** [AS11]. **-propionic** [CM16]. **-pyridone** [AFSW16]. **-representability** [PM18b]. **-salen** [DSHLM18]. **-secretase** [YLCX10]. **-sextet** [KDS17]. **-sheet** [CCOH14, WS10]. **-substituted** [LZH16]. **-system** [SWW⁺19]. **-thiaphosphiranes** [TR12]. **-turn** [SZB19]. **-type** [SLY⁺19]. **-types** [SKY⁺11]. **-Unsaturated** [HPT16a]. **-X-** [SZBM13]. **-yl** [YZLZ18]. **-ZSM-5** [Pon10].

/AT [YZWC11]. **/aug** [Gil11]. **/aug-CC-pVTZ** [Gil11]. **/epoxide** [DSHLM18]. **/Fe** [DAdGR15]. **/GIAO** [OPR16]. **/GIAO-CCSD** [OPR16]. **/H** [WLF19]. **/metal** [BSF18]. **/MgO** [BS16b]. **/MM** [CZY11]. **/PDIxCN** [ZZL19]. **/TD** [TS15b]. **/X** [BSF18]. **/Zn** [GEP⁺14].

0 [KKH19].

1 [ZZWX11, CS17, DLZ15, GTK10, NHN16, SYH12, SRS14, TTB⁺10, UNT16, XLY12, ZsA10]. **1'-** [ZZWX11]. **1-14** [GNI18]. **1-16** [XWSW13]. **1-21** [GNI18]. **1-Methyluracil** [HvM17, HvM16]. **1-Octene** [MJLV14a]. **1-penten-5-yl** [LXFC17]. **1.0** [SWB⁺12]. **1.1** [KJM⁺17]. **1.3** [LSL⁺19]. **10-Phenanthroline-5** [SCSM19]. **10.1002/jcc.25747** [MT20]. **102** [ZDX11]. **11-cis-retinal** [ZLHH14]. **13** [CD19, LAHS16]. **13-13** [LAHS16]. **13-978-1-4987-1151-7** [CD19]. **13-dichloropentacene** [ZYG⁺15]. **132b** [RVdMB16]. **17** [KSM17]. **195** [PGdO⁺16]. **1D** [AWF⁺18]. **1D-charge** [AWF⁺18]. **1H** [YZ15b]. **1T** [RSK⁺15].

2 [DPNM11, MWJ⁺¹¹, THI⁺¹⁹, ATP18, DH17, HOM⁺¹⁶, LGW12, Lüc14, THI⁺¹⁹, YZGS14b, Yu12b, Yu12a]. **2-** [AMQ⁺¹⁴, YLZ⁺¹⁰]. **2-a** [LWL⁺¹¹, QQY⁺¹⁸]. **2-aminophenyl** [LZL⁺¹⁶]. **2-azaborine** [EFB16]. **2-benzoquinones** [GNDA⁺¹²]. **2-benzynes** [FC16]. **2'-Bipyridyl** [THI⁺¹⁹]. **2'-bipyridyl-3** [MWJ⁺¹¹]. **2-dioxetanone** [RSLML12, dSdS12a, dSdS12b]. **2'-hydroxyl** [DPNM11]. **2-migration** [KYKR15]. **2-naphthol** [GZL⁺¹²]. **2-phenylimidazo** [LWL⁺¹¹]. **2.0** [SJL18, Yes15]. **2.1.0** [KYG⁺¹⁵]. **2010** [Ano10b, Ano12u]. **2018** [KPF⁺¹⁹]. **2019-Automating** [SSP^{+19b}]. **263fb** [AR10]. **28** [HNWF12]. **2C9** [SLY⁺¹⁰]. **2D** [DAB16, DLC18b, YMY⁺¹⁹]. **2D-** [YMY⁺¹⁹]. **2D-/** [YMY⁺¹⁹]. **2G12** [UNT16]. **2Gau** [SH19a]. **2H** [RSK⁺¹⁵]. **2nd** [KKGW19]. **2nd-Quantized** [KKGW19]. **2P** [SGY⁺¹⁸]. **2X** [SIG⁺¹⁵].

3 [MWJ⁺¹¹, DH17, HPSK12, Spr10, YZGS14b]. **3-** [LZL⁺¹⁶, YZLZ18]. **3'-15-crown-5** [MWJ⁺¹¹]. **3-527-32442-9** [Spr10]. **3-6** [LZSM19]. **3-alternate** [ZWS⁺¹⁰]. **3-bis** [SB19]. **3-d** [YZ15b]. **3-dihydropyrido** [YZ15b]. **3-Dipolar** [YZN13]. **3-metal-carbon** [ZYW⁺¹⁶]. **3-methyl-7-azaindole** [YYT12]. **3-squaraines** [AMQ⁺¹⁴]. **3-thiophenic** [NHF⁺¹⁰]. **3.0** [HMO⁺¹⁸, SvLK18]. **31** [Kne11b, MSK⁺¹²]. **311G**** [TKN13]. **31G** [Mit13]. **31G**** [TKN13]. **33** [ABB⁺¹³, CHR^{+12b}, ICS⁺¹³]. **35** [SFCKK⁺¹⁵]. **36** [SMM15a]. **38** [HLXH18]. **3c** [KV14, LW16]. **3c/4e** [LW16]. **3D** [HSB⁺¹¹, SA10, YMY⁺¹⁹]. **3D-QSPR** [YMY⁺¹⁹]. **3D-space-based** [HSB⁺¹¹]. **3D-structure** [SA10]. **3z** [PTK11].

4 [YLZ⁺¹⁰, LZTV10]. **4'-** [YLZ⁺¹⁰]. **4-addition** [KSO⁺¹⁹]. **4-amino-1** [ZZWT12]. **4-aminophthalimide** [WHL⁺¹⁰]. **4-azaborinine** [RS17a]. **4-dihydro-1** [RS17a]. **4-hydroxyphenylpyruvate** [DGH⁺¹¹]. **4-methoxybenzyl** [YZLZ18]. **4-substituted** [SKGB13]. **4-triazol-3-one** [ZZWT12]. **4.5** [AG11]. **40** [MT20]. **43A1** [LGL11]. **4AP** [WHL⁺¹⁰, WHL⁺¹⁰]. **4D** [MdOdQ18, MdOdQ18]. **4D-QSAR** [MdOdQ18]. **4e** [KV14, LW16]. **4Fe** [PNI13]. **4S** [PNI13].

5 [SC18b, ZZWX11, cCVG⁺¹⁴, LL10c, Mor15, Pon10, SOvG12]. **5-b** [YLZ⁺¹⁰]. **5-biphosphate** [CKG18]. **5'-bridged** [ZZWX11]. **5-nitroiminotetrazolate-based** [ZYL⁺¹²]. **5'-phosphate** [SC18b]. **5-triazine** [WDLG12]. **5-triazines** [YPC⁺¹⁰]. **5-triene** [ABDGN12]. **53A6** [PFVL14, LGL11]. **54A7** [LvG13c]. **56A6** [PLH16].

6 [WDLG12, ABM⁺¹⁵, TKN13]. **6-311G**** [TKN13]. **6-31G**** [TKN13]. **6-bisphosphatase** [RAR⁺¹¹]. **6-Diimine** [SCSM19]. **6-fluoroquinolones** [MPNS13]. **6'-tetra** [WDLG12]. **6-trinitrotoluene** [SH14]. **6-triphenyl** [AS18]. **6.0** [GLW13a, GLW13b]. **60th** [HIS17].

7 [ADF⁺¹⁰, CD19, MBR⁺¹⁵]. **7-azaindole** [YYT12]. **7-diphenylamino-9**

[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, ŠSB⁺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]. **acetoxyhydroxyacid** [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, MSL10, 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].

adduct [KK19]. **adducts** [LC10, LS11b, ZRCC11]. **adenine** [BZH14, LLT12]. **adenosine** [SRA17, WZQW10]. **adhesion** [Won18]. **adhesive** [HTY19]. **adiabatic** [MT19b, UD12]. **adjacency** [GZH10]. **Adjacent** [JLLW19]. **adjusted** [HH15, KHLM19]. **Adjustment** [BLZ+13]. **ADMA** [MA17]. **AdNDP** [KDS17]. **adrenergic** [CV12, LLHM16, VKC10]. **adsorbate** [GBS+17]. **adsorbate-induced** [GBS+17]. **adsorbed** [MCF10, PXXW10, SLLL13, SIG+15, THI+19]. **adsorbents** [HVS16]. **adsorbing** [KGJZ19]. **Adsorption** [CCJ+11, FVP14, HB15, KD10, LH14b, PH12, AS15a, BS16b, CMM18, CR14, cCVG+14, Hei10, KMT+19, LL13a, LPK16, LPLS16, LZ14, LT14, LCM+14, NPP13, PGC12, PLZ17, RHNN10, SH14, SDB+16, SKTT11, SYZ+17, VS14, WSZW15, WYGW12, YDR13]. **Adsorption-induced** [HB15]. **Advanced** [DJS+18, WBN+13, Yan16]. **advancement** [PGK+19]. **affect** [SV15, UNT16]. **affected** [MCF+18, OHNK11]. **affecting** [GMSV14]. **affects** [CLK11]. **affinities** [ĆMD13, CTP13, GRS15, MGWR12, NHN16, NFG+13, PBLdS12, RJWW12, RMGB11, VCL18, VKC10, WNP+16, WLLH18, SDIP18]. **Affinity** [ZFOS19, CG15, CZAF17, DLZ15, MUGNVJ+18, MCK17a, SSP+13, VL17a, ZJZM13, ZYvIZ14]. **After** [WZK+13]. **Ag** [LLX+19, Rab12, AS15a, BBG+18a, IN13, LLTC12, MCF10, PGS+15, SLLL13, TNI+19a, THI+19, YXZZ17]. **Ag-nanocluster** [AS15a]. **against** [Gil11, MPNS13]. **Age** [Yan16]. **agents** [PSdPE+10]. **Aggregate** [NNT+19]. **aggregated** [BSL+16]. **aggregates** [LSH+11, LCK+18, SMDP18, SLP+12, Ber17]. **Aggregation** [PK19, RCM+13a, RML+15, WDP+12, ZSTRS+18]. **aggregators** [RLL+10]. **Agonist** [HK18]. **agonists** [CV12]. **AgX** [YS13]. **AHAS** [SJD14]. **aimed** [KS12]. **AIREBO** [HB19]. **AI** [LCWW10, Pon10, UT15, YR13, CC18c, GWJJ12, KKR+13, SH14]. **Al-hydroxylated** [SH14]. **Ala** [SZBM13]. **alanine** [IO13b, LL19a, MAMF19, MVKS10, SEM12]. **AIB** [MCAY15]. **albumin** [JAHS+19]. **alchemical** [BB11b, BB11c, BG12, GMSdG15, GRS15, HLW+17, KB11a]. **alcohol** [MS13, ZSZ+14]. **alcohol-based** [MS13]. **alcohols** [VVLG17]. **aldehyde** [ZZWT12]. **Alder** [CC18a, FB12, FB14a, GNDA+12, LZH16, ORZ11, ST13, dSVdM+16]. **Alder-ene** [FB12]. **Alderase** [BJSI12]. **aldol** [HJLV16]. **aldosterone** [RVP+11]. **algebraic** [GJMPAM+14, WWD14, YD17]. **algebraic-diagrammatic** [YD17]. **Algorithm** [WM12, AMGB10, AM10, AYYO17, BW11a, BYE+16, BDdS13, CM13a, CDBM11, CGA19, CVT+11, CM13b, CB11b, DS15, DJ13, DLSA14, DZA11, EVR18, FRLN10, GFG11, GPE13, GBFD12, HTS15, HEMCZE+14, HQC16, HKR+14, Hug14, Ish10, IHJ+13, JCPC11, KK17a, KNHN16, KN17, KD18, KDT+12, LZX16, LZL+13, LZLMP16, LZS+17, LLJ12, LTA+11, LMA15, MEH18, NYN17, NC12, NG10, dIRL11, PS17, RMPAM15, Ras17, RSL16, SSO19, SRSLO15, SYH12, SSMW09, SCSW13, SA11, UCRL18, WMW+10,

XHLH16, YVEI⁺17, ZSS⁺13, vLBBR12]. **algorithm-artificial** [WMW⁺10]. **Algorithmic** [LPS12]. **Algorithms** [BV14, KGHC15, AGR11a, AC12, CD13, Fom11, GBSE11, KJM⁺17, Leh15, LLZA12, MS16, MO15, NC14, NOKJ16, RFN15, TRA⁺16, ZVY⁺15, dACP12, vLBBR12]. **aligned** [KC14].

alignment
[BF15, HRK⁺10, HKRS11, HS11, MJM⁺15, RP15, RHJ11, Ran12].

alignments [CYI⁺10, Ran13]. **aliphatic** [CROB16, SB10]. **Alkali** [YHCS11, Ano11, AM19a, DDM⁺15, JHMB⁺09, JHMB⁺11, THP⁺15, ZWY⁺10a].

alkali-metal [ZWY⁺10a]. **alkalides** [WXS⁺12]. **Alkaline**
[XZ11, Ano11, JHMB⁺09, JHMB⁺11, WD10]. **alkaline-earth** [WD10].

alkane [JGS⁺17, ZST114]. **alkanes** [Jor17]. **Alkanethiol** [SJSS19]. **AlkB**
[PHC13]. **alkenes** [Jor17]. **alkenoyl** [YZL⁺15]. **alkoxy** [WFL⁺19].

alkoxy-catalyzed [WFL⁺19]. **alkyl** [Den12, RMGB11]. **alkylthiols**
[FVP14]. **alkyne** [WWTL19]. **alkynes** [Jor17, YXZZ17]. **All-atom**
[SM14b, CS14, DPNM11, HM13, JYC⁺16, KT18, LZZ14, MZZ11, OCW⁺15, VHA⁺10]. **all-atomistic** [FPH⁺19]. **All-electron** [KKA⁺18, PGdO⁺16].

all-organic [LZL⁺15a]. **all-siliceous** [Lar11]. **allene** [GRCL12]. **allenes**
[KV15b]. **allocation** [NOKJ16]. **allophycocyanin** [RML⁺15]. **allosteric**
[DBK17, ILKR11, MWJ⁺11, SRA17, ZDT18]. **Allotropes** [OSI⁺19].

allotropic [GKB⁺19]. **allowing** [MLC13]. **alloy** [NIIT15]. **alloys**
[GD10, vADC⁺14]. **ALMOST** [FSC⁺14]. **AIN** [wZbZ11]. **AIO** [GWPJ11].

along [ABDGN12, AC11b, CM13a, CX10]. **Alpha**
[MH10, MKB⁺13, SPZP18b, XTY⁺14]. **alphabets** [PHDH13]. **AIPO**
[LL10c]. **alter** [CBTZ16]. **alterations** [HHT⁺13a, HHT⁺13b]. **alternate**
[ZWS⁺10]. **alternation** [ASL⁺11]. **alternative**
[DSHLM18, MA17, NYN17, TF15, Wei12a]. **alumina** [SH14]. **Aluminum**
[Kop19a, SBGP18, WFL⁺19, GWJJ12, LK16a]. **always** [KSC16, MBFG15].

AM [FBY⁺17]. **AM05** [MMJ10]. **AM1** [KLS10, KMLS10]. **AMBER**
[MSK⁺12, RSR⁺12, MLN⁺18, GCW14, MSK⁺10, MJG⁺15, OYK⁺11, PGW⁺17, SOYC12, SJ16]. **AMBER-compatible** [SOYC12]. **AmberTools**
[RNSF⁺16]. **Ambident** [WBKS19]. **amide** [LJW11a, LW11, NDG14].

amidoborane [PMT16]. **amidoboranes** [DLT17]. **amination** [YZ17].

amine [AK10, BMB13]. **amines** [MRC⁺18]. **amino** [BSG⁺18b, CCCLCGRO14, CFC15, CB11d, DKE⁺17, FZL⁺15, FP17b, GRL⁺11, GRL⁺12, HCP15, KLS10, KMLS10, LXL⁺11, LP11b, MRO17, PHDH13, RSL16, SISK10, SZBM13, SST⁺18, WC14, ZZWT12, ZKH⁺10, ZHHX11].

amino-acid [KLS10, KMLS10]. **aminoacid** [MC10]. **aminophenyl**
[LZL⁺16]. **aminophthalimide** [WHL⁺10]. **aminopolycarboxylate**
[ĆMD13]. **aminotriethylene** [MSY19]. **ammine** [dCGCRN19]. **ammonia**
[BEPM14, CC12a, KT12, SNS16, SJZ⁺15, VS14]. **ammonia-borane**
[BEPM14]. **ammonium** [AvKSP16, DSHLM18]. **AMOEBa**
[HLW⁺17, MBE16, PZCL16, XP13]. **among**
[KYB13, SH15, TCGNT18, WGL⁺11]. **amorphous** [Fom13]. **amounts**
[FN12]. **amplitudes** [Les19]. **Amsterdam** [FPV13, SFG⁺17]. **amyloid**

[IO13b, LH11]. **amyloid-** [IO13b]. **amyloid-beta** [LH11]. **analog** [JBAM11]. **analogs** [DCHL12, LP11b, SISK10, VM11, WBT10]. **analogue** [PGW⁺17]. **analogues** [LPS⁺13, NK19, SGWA17, VVBL17, VM19, WS12, YLL11]. **analyses** [BSF18, CBDS19, KASH14, KP11, PZBA13, SKGB13, VVJ15, XWW⁺11]. **Analysis** [BMD19, CDM⁺15, ELKE19, HAI⁺16, JCGM18, KKGW19, LL19a, MOS12, SZL19, SvLK18, Spr18, XFG⁺16, AKMT11, AST⁺16, ASL⁺11, ARRC15, AAB⁺19, AS18, Ano15-58, AM19a, AM19b, BK15, BL19, BH14, BSPP⁺13, BBG⁺18b, CLFRO18, CMM18, CAF⁺13, CEBO15, CCC⁺11, CAT⁺13, CH14, DMJ17, DDP⁺18, DHF⁺11, DJD12, DBK17, DJS⁺18, DCŠ15, DN19, ESD18, EHSPT16, EB18, Fer17, FB12, FHW⁺11, FHK⁺12, GVP⁺10, GLW13a, GLW13b, GNDA⁺12, dCGCRN19, GCP⁺13, Han11, HSB⁺19, HCD⁺10, HPSK12, HHT⁺13a, HHT⁺13b, HGW18, HDHL15a, HDHL15b, HDHL15c, HHWL17, Hug12, IY18, Jan16, JHH⁺13, JJW⁺14, JZM14, JCX10, JLS18, KG13, KYG⁺15, LSL⁺19, LBC⁺19, LL13a, LCPS13, LMZ⁺11b, LFM12, LAHS16, LGKS17, MLG18, MDTD13, MJC14, MT19b, Mez10, MADWB11, MCLD10, MGS⁺16, MCK17b, NK19, NH19]. **analysis** [NIIT15, NS17, OXBW16, OC14, PTK11, PSP15, PRYI⁺17, PTB⁺15, PPUBGD10, PVS12, PS14, RDT14, RSSG18, RC18, REL17, RLG14, SFM⁺18, SLY⁺10, SBB10, SFR⁺11, SHFJ18, SSGS15, SEJ⁺18, SB18, SNDK16, SS13c, SB19, SPR⁺13, SH18b, SSP⁺19b, SH19b, TYN15, TCB16, TD10, TTB⁺10, TS10b, UKS11, VBMA13, WNP⁺16, WWW19, Wei12a, Wei12b, WDKT19, XFG⁺15, YK13, YNH⁺17, Yes12, Yes15, ZCS⁺15, ZBB16, ZH12, ZZZ⁺19, ZCWX18, dSH19, vSGP10, JCHT18, ZSB⁺11]. **Analytic** [Boz18, MDTD13, NF18, SZX13a, SZX13b, TSH⁺19, MY17b]. **Analytical** [CCR18, CCB15, HNWF07, HNWF12, HH17, LBG16, SFG⁺17, WOH18, CHC⁺13, FBY⁺17, GRN19, HH16a, KN17, KTSW11, MK13a, Pon11, Pop18, ZWF15]. **analytics** [JZL⁺17]. **analyze** [LP11c, OVPK15, QLQ11, RLG14, YKO⁺11, dVAG16]. **analyzer** [JJW⁺14, LC12, PVZ13]. **Analyzing** [BGS⁺19, BD11, MRB14, BCP⁺10, HPT17, LZS⁺17, PHT17, SWA13, WES13]. **anapole** [ZPP⁺16]. **anatase** [HRL11]. **and/or** [KB10, Pog10]. **androstenedione** [VCM15]. **angle** [CKP10, GBFD12, XML⁺15]. **angle-dependent** [CKP10]. **angles** [BKLA13, EJ13, FZY⁺12, GREA11, KTK17, LDH⁺14, OZ14, YZ16]. **angular** [BBG⁺18b, ENKK⁺17]. **anharmonic** [Kow11, SSWX14]. **anhydrase** [SSP⁺13]. **anhydrides** [RB12]. **aniline** [PLP⁺16]. **Anion** [TT18, CG15, KSNT19, LC10, uLhY11, LCC18, SC18a, SDF12]. **Anionic** [BHP19, AM19a, AM19b, GZZ12, GWPJ11, HPL13, JCP14, QZ10b, ZYR⁺15]. **anionic-water** [JCP14]. **anions** [PVS12, RDT14, RJS17, ZWY⁺10b, ZYL⁺12]. **anisotropic** [Ano10a, CAT⁺13, EPH⁺13, ENKK⁺17, NLP⁺16, SLX⁺15, SN10]. **anisotropy** [BP18, CGP12, LPLB16, ZLZ14]. **ANN** [XWW⁺11, ZDW18]. **ANN-based** [ZDW18]. **annealing**

[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, RKG10,
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].

approximations [CGPP11, HAGK10, MKH⁺13]. **April** [Ano12u]. **aprotic** [RK16a, RK16b]. **aqua** [GK15a]. **AquaBridge** [AIGP15]. **Aqueous** [ALK⁺15, BDTP11, CFC15, DR11, EOA⁺11, GAI14, HDK⁺12, HNN⁺17, JWST10, KKO⁺16, KVR10, MFM⁺12, MS11, OC19, OCW⁺15, PMC⁺17, PGW⁺17, RVM19, SC18b, UvSvdWK19, VSA11, WHL⁺10, WLF19, WZWW18, XP13]. **AR231453** [HK18]. **arbitrary** [CHC⁺13, EPD⁺11, GP12, HAL14]. **archetypical** [vSGP10]. **architectures** [MJB12, OPB⁺12, SOM⁺13]. **area** [FZY⁺12, GY10, HWLW11, KRSC12, KTSW11, MOS12, NW17, WXL⁺12, WBF17, dCLFGL13]. **areas** [MK13a, ZKE⁺17]. **arene** [BEM14, BEPM14, PRRT⁺10, ZCK⁺16, ZWY⁺10a, ZWS⁺10]. **arene-**[ZWY⁺10a]. **arene-substituted** [PRRT⁺10]. **arenes** [GMASBF16]. **armchair** [LPLS16, RRK14]. **aromatase** [NS10, VCM15]. **aromatic** [Alg17, CCCLCGRO14, CB11d, FVB10, JHH⁺13, Kar17, KDS17, MJM⁺15, MVKS10, PRJ⁺17, PL18, RSSG18, SSA⁺17, TTR⁺12, TDKT10, WSZW15, YCK16, YHCS11]. **Aromaticity** [CD16, AH10, AFSW16, Ano11, BY11, FC16, FNSF⁺11, GRD⁺10, HSB⁺11, JHMB⁺09, JHMB⁺11, KASH14, LZH16, MPSG11, RS17a, Ran19, YOPB16, FB12]. **aromatics** [YDR13]. **Arrhenius** [CSAdOM17]. **arsenic** [GWX⁺12, KSNT19]. **arsenic/phosphorus** [GWX⁺12]. **arsine** [OSF12]. **art** [YJ19, NJR18]. **ART-RRT** [NJR18]. **Articles** [GS16, MFEM16, XFG⁺16]. **artifact** [DP11]. **Artificial** [PC11, Aou16, AGM⁺13, DMN15, MTM14, MHT⁺18, PPM15, WMW⁺10]. **aryl** [FWB14]. **arylalkyne** [ZZL⁺12]. **arylamides** [LTP11]. **As-Rigid-As-Possible** [NJR18]. **AsCl** [MLCD11]. **ascorbate** [HHDC16]. **ASED** [BRP⁺12]. **ASED-MO** [BRP⁺12]. **Asp** [LY10]. **asparagine** [JDW⁺19]. **asparaginylnyl** [LBS10]. **asparaginylnyl-tRNA** [LBS10]. **aspects** [ABB⁺12, ABB⁺13, ECZWD17, NC13, NC14, OPR16, Tac19, VKNT16]. **Assembled** [SJSS19, KC13b]. **assemblies** [AKK⁺16]. **assembling** [AFSW16, CD11]. **assemblings** [CBTZ16]. **assembly** [AGR11b, HHNK19, Hei10, JM11, KLN16, uLhY11, Mau14, OAN15b, TBJ18]. **assess** [SJ16]. **Assessing** [HWLW11, KYB13, KSR⁺16, OCLM14, SNDK16, VL17a, FNSF⁺11]. **Assessment** [ARRC15, BF19a, FB10, GHK12, HDK⁺12, HJ10, KB10, KB13, LSH⁺11, OOT15, SB14, UCFR16, WL10, WYT17, YB16, Yu12b, ZZL⁺12, AR15, BG13, ED15, FCE15, FPRS14, FLM11, GAI13, ITIN15, LTT16, LZLC13, MS13, MFR⁺17, SZX13a, SZX13b, SWW⁺19, Tsi14, ZTH⁺15, HCB11, Sch12, YVEI⁺17]. **assigning** [LFB14]. **assignment** [Ben17, KKH19, MPBJ11]. **Assignments** [TT18]. **assist** [TS10a]. **Assisted** [DBGO⁺17, Dra19, LL13b, LL19b, SSGS15]. **Associated** [ZFOS19, WNM17, ZZ10, dLvNC18a]. **association** [DSF17, JA10, MBR⁺15, NC14, OCW⁺15, PD12]. **associations** [Ano10a, JLS18, SN10]. **associative** [RIJ⁺11]. **astatine** [SDM⁺16]. **asymmetric** [DLSA14, HAL14, KSO⁺19, NDG14, PBL19, QLYL10, WCDM11].

asymptotic [KIOY19]. **Asynchronous** [XFG⁺16, XFG⁺15]. **AT-rich** [YZWC11]. **Aten** [You10]. **atmospheric** [BCNH⁺11]. **atom** [ATP18, BS10b, CVT⁺11, CS14, DPNM11, DM15, FSC⁺14, GBVA11, HRK⁺10, HM13, JYC⁺16, JGS⁺17, Jor17, KV14, KT18, LC10, LZZ14, LKZM18, MZZ11, Niz13, OCW⁺15, ST11, SM14b, SYH12, Tsi17, VIT⁺15, VHA⁺10, VKAM12, VI17, VDVR14, YPKB12, YHCS11, ZFS18, dLC17, dVZ17, YMP14]. **atom-aromatic** [YHCS11]. **atom-based** [dVZ17]. **atom-centered** [VI17]. **atom-typing** [YPKB12]. **Atomic** [BMFG16, EPD⁺10, KGM12, VSP19, AYYO17, BLDK⁺13, BB11a, CCR18, CP15, EKH14, Elk16, EP12, EV14, HS12, HH18, JMLL13, JXSW15, KHLM19, KOP⁺14, KR12, LRVN18, Lar11, LZGS11, MK13a, MPA10, MPA12, Mat10, MPBJ11, NPG17, NOKJ16, OBW12, OV14, Pol13, RB13a, SS16b, SE14, SMP17b, TSH⁺19, VSA11, WWCL15, YOMT14, dLC18a, dLvNC18b, VV19]. **Atomic-resolution** [BMFG16, NPG17]. **Atomistic** [BH13, CHKR10, MTS⁺19, MBA14, SE14, BLKP12, CZNA11, DDP16, FPH⁺19, HDPM14, LZ12, MSC⁺10, MMZW14, RO14b, RSG⁺10, WSWD19, ZSTI14]. **atomization** [KSM17]. **Atoms** [BGS⁺19, ELKE19, JCHT18, VSP19, ZLX⁺19, ARAG17, ARLP13, BSF18, BSPP⁺13, CGA19, DC13, EV14, GAMAC⁺14, HSJ18, HSB⁺11, HGCCGR⁺16, IN13, Jab18a, KHE⁺19, LSH12, MP17a, Mit13, MvBD18, PNE18, Pop18, Pyy13, SFCCK⁺14, SFCCK⁺15, STS15, TY10, VGV⁺11, Vyb15, Vyb16, WZH⁺18, YWZ14, YKH15, ZYW⁺16]. **Atoms-in-Molecules** [ELKE19, BSF18, HSB⁺11, YKH15]. **ATP** [BMFG16, HYSF19, SYH12, YHH⁺13]. **ATP-binding** [YHH⁺13]. **ATP-Mg** [BMFG16]. **ATPase** [II10]. **ATPases** [HYSF19]. **atrazine** [BHB⁺17]. **attachment** [HBL12, SST⁺18, THP⁺15]. **attack** [JDW⁺19, MLY⁺13]. **attenuation** [SPH11]. **attract** [VVY18, CZAF17]. **Attracting** [ZSB⁺16, VVY18]. **Attraction** [WDS⁺19]. **Attractive** [MKH⁺13, IO13a, SNDK16]. **attractive/repulsive** [SNDK16]. **attributed** [CM16]. **Au-Ag** [THI⁺19]. **aufbau** [EKH14]. **aug-CC-pVTZ** [Gil11]. **augmented** [BVHI17]. **austenitic** [ZFS18, vADC⁺14]. **auto** [LDH⁺14]. **auto-encoder** [LDH⁺14]. **autoCAS** [SR19]. **autocorrelation** [IY18, LL13a]. **autoDIAS** [SH19b]. **AutoDock** [TO10, ZFOS19]. **Autodock4** [CSSB11]. **autoencoders** [CF18]. **AutoGridFR** [ZFOS19]. **Automated** [BHI19, BW15, EMD17, GMSdG15, KFT18, MYKO18, OZS⁺13, PBG17, SM11, SR19, TN18, Zim13, CCLP12, KG13, LLHM16, MN15, NKJ16, RRFV⁺18, SH18b, SH19b, FN12, JBAM11, JSD⁺11]. **Automatic** [AJR16, Leh15, ODB18, STF⁺19, UKS11, KSH⁺17]. **automatically** [SMDP18]. **automating** [IGK16, SSP⁺19b]. **automaton** [VBD11]. **automerization** [SFM14]. **autoxidation** [HHDC16]. **AuX** [Li14a, Li14b, YS13]. **Auxiliary** [Hil13, TKN13, HDL⁺17]. **availability** [HJ13]. **available** [SPR⁺13]. **averaged** [HCD⁺10, WLO⁺17]. **averaging** [DB12]. **avibactam** [LD18]. **Avoiding** [BB11a, dACP12]. **axial** [SNDK16]. **axis** [KGM12]. **Aza** [NDG14]. **azaborine** [EFB16]. **azaborinine** [RS17a].

azacrown [ZWY^{+10a}]. **azaindole** [YYT12]. **azetidine** [SHL⁺¹³]. **azido** [MLG18, WDLG12]. **azidolysis** [BCP⁺¹⁰]. **Azobenzene** [ZB18]. **Azobenzene-bridged** [ZB18]. **azulene** [WWKS16]. **azurin** [SOvG12].

B

[GNI18, MLQ⁺¹², RLZ⁺¹⁸, UT15, YLZ⁺¹⁹, YLT⁺¹⁹, YLZ⁺¹⁰, BWKW10a, GTZ⁺¹⁸, HJ13, HQC16, LLLM11, LLL⁺¹², SJD11, YLT⁺¹⁹, YLL11]. **B-Au-B** [YLL11]. **B-DNA** [HQC16]. **B-factor** [GTZ⁺¹⁸]. **B-site** [LLL⁺¹²]. **B3LYP** [DOM⁺¹¹, ZWX16]. **B97** [SPH11]. **BA** [KHLM19]. **BA-LCAO** [KHLM19]. **BACE** [CS17]. **BACE-1** [CS17]. **BACE1** [ETLS17]. **Bacillus** [CPK12]. **back** [GWT⁺¹⁷, REH13]. **back-bonding** [PKK17]. **Backbone** [DMD⁺¹⁸, AB10, CKP10, CHP11, FZY⁺¹², FTW12, HLH⁺¹², KLS10, KMLS10, LZZ14, LDH⁺¹⁴, MKB⁺¹³, OZ14]. **backward** [KZP^{+18a}]. **bacterial** [BHI19, HBJ⁺¹⁷]. **Bader** [TCB16, dLvNC18a]. **balance** [MO15, SNDK16, TTB⁺¹⁰]. **balanced** [MG14]. **Balancing** [FMG12]. **balls** [CVT⁺¹¹, KRSC12, OV14]. **band** [KT19, KLZ⁺¹⁸, QZ10b, QB10, QB11, SH11a, SLY⁺¹⁹, VLGK⁺¹⁷]. **bandgap** [VVMY18]. **bang** [KPF⁺¹⁵, KPF⁺¹⁹, MPA12]. **Baoshan** [JW12]. **BAR** [WTD⁺¹⁹]. **BAR-based** [WTD⁺¹⁹]. **bare** [SM17]. **barrel** [LJR⁺¹², yOaCG10, WXL⁺¹²]. **Barrier** [BS10b, ZW17, GAJ⁺¹⁷, HRID16, KG15, MSBF16, PG18, Yu12a]. **Barriers** [VL19, HH10, MJLV14a, SFM14, VV14, XLYZ10, dALdS⁺¹⁵]. **basal** [LL13b]. **Base** [GMBM18, BH13, BZH14, DKT13, DSB⁺¹⁹, FD14, GA18, HvM12, LZH⁺¹¹, LW11, ONTTL16, SZS16, VMPS17, WXY14, YKH⁺¹⁰, ZLL⁺¹⁰, ZLHH14]. **base-catalyzed** [WXY14]. **Based** [AIM⁺¹⁸, CSM16, CPK19, LI19, SN16b, YKNN19, AMGB10, ALK⁺¹⁵, AM10, AWF⁺¹⁸, AO10, BCSCJ⁺¹³, BAMR13, BPE16, BMPML⁺¹³, BHR15, BMD19, CFM⁺¹⁹, CC18c, CGA19, CGPP11, CSC⁺¹⁸, CDS16, COHI19, CH10, CGBK13, CB11b, DK11, DVVP14, DH14, Dil15, DJX^{+11b}, DJX^{+11a}, DFF⁺¹⁵, DPB⁺¹², DXL⁺¹⁰, DCŠ15, DDM⁺¹⁵, EFAC13, EHSPT16, EV14, EBK13, EP15, EBPK17a, EB18, FCL⁺¹⁰, FCOGM12, FCPJM14, FHZA⁺¹⁸, FMG12, Fra15, Fra16, GLB16, GHL17, Gar12, GJMPAM⁺¹⁴, GKJ⁺¹⁹, GBVA11, GC18, GVP⁺¹⁰, GWW19, GNI18, GSS13, GBSE11, GZ14, GK15b, HKRS11, HS11, HLS12, HH11, HTS15, HW19, HZY⁺¹⁰, HSW⁺¹⁹, HPL⁺¹⁸, HKR12, HB14, HEMCZE⁺¹⁴, HSB⁺¹¹, HYUS11, HM13, HLWD15, ISN13, IN19, ISM18, JJW⁺¹⁴, JLCA17, KS18, KGHC15, KZZ⁺¹⁶, KLZ⁺¹⁸, KNE11a, KC14, KSHP⁺¹⁹, KP11, KKH18]. **based** [LSL⁺¹⁹, LFB14, LZ11, LM18a, LDB⁺¹⁷, LMZ11a, LMZ^{+11b}, LWL⁺¹¹, LLZA12, LSH⁺¹¹, LZS⁺¹⁷, LZSM19, LTA⁺¹¹, LGKS17, MDTD16, MZZ11, MMM⁺¹⁶, Man19a, MSY19, MC10, MP19a, MA16, MS13, MdOdQ18, MGCC19, MPNS13, MMZW14, MAP18, MFR⁺¹⁷, MO15, MNNK10b, NB19, NC12, NC13, NC14, NMH19, NJX⁺¹⁰, NG10, OVPK15, OZLSBH12, PRP15, PLZ17, PC11, PSC11, PBBP11, PN13, PKIC11, PPJ14, PLH16, PBE16,

PPUBGD10, RLDJ17, RZG⁺¹³, RMRBH⁺¹⁹, RVP⁺¹¹, SZdB19, SM14b, SFG⁺¹⁷, SLP⁺¹², SLX⁺¹⁵, SGY⁺¹⁸, SFDE16, SLC⁺¹⁷, TYZ⁺¹⁶, Tak14, TTb⁺¹⁰, TS14, VGV⁺¹¹, VVJ15, VKC10, VSA11, Vor10, WXL⁺¹², WLLH18, WCDM11, Wei12b, WS19, WL14, WS13, WDHZ13, WZWW18, XCLZ19, YJN⁺¹¹, YZ16, YWJ⁺¹⁶, YZZ16, YZLZ19, YDL⁺¹⁰, YJ11, YN15, YS13, YS15, YS10, YZZ⁺¹⁷, ZSLL17, Zha12b, Zha12a, ZY14, ZW18, ZM10]. **based** [ZYL⁺¹², ZGZ19, ZT14, dCLFGL13, dSVdM⁺¹⁶, dVZ17, FAS⁺¹⁸, NKJ16, WTD⁺¹⁹, ZDW18, dLvNC18a, dLvNC18b]. **based-on** [CDS16]. **Bases** [WBKS19, CWZB10, KASH14, LRVM18, MSLS10, SC18b, SBW12, WGA18, ZLL⁺¹⁰, Zha12a, ZBMZH15]. **Basic** [CMvG10, WLF19]. **basin** [JLH⁺¹⁴, RDRC16]. **basin-hopping** [JLH⁺¹⁴]. **basins** [SBN13a, dLC18a, SBN13b]. **Basis** [BLF14, BRSL08, BRSL12, PHK14, SN16b, TKN13, ACD^{+13a}, ACD^{+13b}, BLFZ13, BLL13, BLBG⁺¹³, BS10a, BLG10, CC11, DBM⁺¹⁵, DLZ15, Fer13a, HSN14, Hil13, HBL12, IT19, KK17a, KT19, KNP⁺¹², LOB18, LBH⁺¹¹, LCW12, Leh15, LYC⁺¹³, LZ18, Mit13, OAN15a, OLPB19, PML⁺¹², PGdO⁺¹⁶, POB13, Pla11, PD11, RLD12, SWM10, SG10a, Sea10, SNKS10, SM18, Sun15, SG13, TH13, WX12, ZPP⁺¹⁶, ZLT13]. **Batch** [WHJH13, TJB12]. **bath** [CSEMB⁺¹⁶, MO15, Vor12, WAM17]. **BaTiO** [BE12, EB12, EBK13]. **batteries** [GNI18, YZLZ19]. **battery** [SMiN⁺¹⁹]. **bay** [QCR12, WvRSM14]. **Bay-type** [WvRSM14]. **Bayesian** [Fer17, GZ14, SKGP19, VZ14]. **BayesWHAM** [Fer17]. **BD_BOX** [DZT11]. **Be** [AM19b, GNI18, KKGW19, LDJ⁺¹⁰, LLX⁺¹⁹, EPH⁺¹⁵, IMSR18, KV15b, LZW⁺¹¹, NDG14, SMGB11, TH13, TCPPC14, Zha12b, BWKW10a, CC18c, CCM15, CM16, ZLY⁺¹⁶]. **Becke** [FPV13]. **become** [Tan19]. **BeH** [ZLY⁺¹⁶, ZLY⁺¹⁶]. **behavior** [AVHB18, BVY⁺¹², CME11, CSAAdOM17, FCD10, FTR15, KRTB10, LZY^{+12a}, PD11, TLdG⁺¹²]. **belief** [GFPSD17]. **Benchmark** [CXD⁺¹⁹, WSZW15, AF14, ANH⁺¹¹, CSXZ17, cCVG⁺¹⁴, DGSVGM19, GAI14, KG15, NH19, RS13, ZWGO16, IKN13]. **benchmarked** [XYW⁺¹⁴]. **Benchmarking** [Ben17, GAJ⁺¹⁷, Hug12, LCM⁺¹⁴, GP11b, HRJ⁺¹⁴, HRJ⁺¹⁵, HZ13, IY18, JRSH14, KSM17, RSG14]. **benchmarkings** [GPdC⁺¹⁶]. **benchmarks** [HLEM18, IT19, XKW18, ZDKM12]. **bending** [KB11c, Sch13]. **Bennett** [BB11b, KB11c, dRBO13]. **Benson** [VRKT19]. **benzaldehyde** [Lu11]. **benzannulation** [YZL⁺¹⁵]. **benzene** [BPM15, BRSL08, BRSL12, CR14, Fom13, FTR15, FPRS14, NK19, SNS16, SGS⁺¹⁶, TFYO19, Tak18, UGK18, VVJ15, YHCS11]. **benzenesulfonamide** [SSP⁺¹³]. **benzenesulfonamides** [ALK⁺¹⁵]. **benzenesulfonyl** [YZGS14b]. **Benzenoid** [Ran19]. **benzimidazole** [SJ16]. **benzo** [GKR13, Ray13, RKG11]. **benzo-** [GKR13, Ray13, RKG11]. **benzoquinones** [GNDA⁺¹²]. **benzotriazole** [dCGCRN19]. **benzyl** [NDG14, YZGS14b]. **benzyne** [FC16]. **Bergman** [DCHL12]. **Berne** [SLX⁺¹⁵]. **beryllium** [CME11, DLT17, Kop17a]. **Best** [KPF⁺¹⁵, AOW11, EK17, KM13, NG10]. **Best-First** [NG10]. **Beta**

[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, MSĀK12, 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,

JS17b, LPLA13, Mat14, MG11, SCF⁺¹⁹, VHA⁺¹⁰, WCJ⁺¹⁴, SDIP18].
biologically [BZH14, Mat10]. **biomass** [WFL⁺¹⁹]. **biomimetic** [ZRCC12].
biomolecular [BK17a, Hei10, HJ10, JCL⁺¹⁷, KAG⁺¹², KPF⁺¹⁵, MBA11,
 MSC⁺¹⁰, MPBJ11, NO16, PGY15, PRSG13, PBBP11, SSO19, SBV10,
 WSH10, XW15, XYX17, YHVM12, ZCS⁺¹⁵]. **Biomolecules** [HIS17, AO10,
 FGM11, FB10, Gri13, ISK14, ISM18, IO13a, LZX16, MK11, MK13a]. **BION**
 [PZA15]. **bioorganometallic** [SDL14]. **biophysical**
 [FN12, JND⁺¹⁹, Mat14, RTP⁺¹³]. **biophysics** [HRHI17]. **biosynthesis**
 [BEL⁺¹¹]. **biosynthetic** [GS11]. **biotin** [MLZZ12, ZJZM13]. **biphenyl**
 [EV14, JMX⁺¹⁶]. **biphosphate** [CKG18]. **bipyridinyl** [KPL15]. **Bipyridyl**
 [THI⁺¹⁹, MWJ⁺¹¹]. **bipyrimidyl** [ZLZ14]. **Biradicals** [SZL19]. **bird**
 [CvM19]. **birthday** [HIS17]. **Bis**
 [WWKS16, KGR⁺¹⁶, KTK17, SB19, YMY⁺¹⁹, RHPWS13]. **Bis-**
 [RHPWS13]. **bis-triarylamine** [KGR⁺¹⁶]. **bisphosphatase** [RAR⁺¹¹].
bisselenation [WCWW11]. **bit** [HRID16]. **Blastochloris** [IIF⁺¹⁰]. **blender**
 [MSSP17, RD18]. **blending** [KM13]. **Blind** [Vor10]. **Block**
 [BGR13, Car14, CAT⁺¹³, EWK⁺¹³, MCK17b, TDKT10]. **Block-adaptive**
 [BGR13]. **blockade** [AB10]. **blocked** [KLS10, KMLS10]. **blockers** [CV12].
blocks [VYV17]. **blue** [Jab14, LWL⁺¹¹]. **blue-green** [LWL⁺¹¹]. **BlueGene**
 [Abr11]. **BLUF** [GGM⁺¹², XBSS19]. **BLW** [BSPP⁺¹³]. **BLW-LOL**
 [BSPP⁺¹³]. **BM** [VL17b]. **BN** [Oht16]. **BO** [GWJJ12]. **Board**
 [Ano16-103, Ano16-104, Ano16-105, Ano16-106, Ano16-107, Ano16-129,
 Ano16-108, Ano16-109, Ano16-110, Ano16-130, Ano16-111, Ano16-112,
 Ano16-113, Ano16-114]. **Boca** [CD19]. **BODIPY** [LCC18, WJG⁺¹³].
BODIPY-linked [LCC18]. **Body**
 [SC17, Aou16, CGPP11, HRJ⁺¹⁴, HRJ⁺¹⁵, JRSHP14, LYC⁺¹³, NF17, PG14,
 PGK⁺¹⁹, RVM19, RHPWS13, VMPS17]. **boiling** [YHW17]. **Boltzmann**
 [ALRM18, BCCO10, BD12, CLA16, Coo19, FBY⁺¹⁷, FHMB15, FCE15,
 Fra15, Fra16, HWLW11, KB11c, NWW17, SK15a, WL10, WLQ19, XYX17,
 YOMT14, YLS19]. **Bond**
 [BVC13, FBKD19, Jab18a, NKD18, Pon11, SK13, WM12, ASL⁺¹¹, AFSW16,
 BK17a, BMD19, CFM⁺¹⁹, CPV⁺¹², CR19, CVT⁺¹¹, CD11, CKL⁺¹¹, CKP10,
 DR11, DBG11, DL19, EPH⁺¹⁵, FCPJM14, GREA11, GCCM15, GLW13a,
 GLW13b, GWW19, GCW16, dCGCRN19, GSMZ19, GC11, HS14a, HAI⁺¹⁶,
 HEM⁺¹⁷, JSW10, KTT16, KV14, KSNT19, KMT⁺¹⁹, KKA⁺¹⁸, KKK⁺¹⁹,
 KLS10, KMLS10, KSC16, LCPS13, LDJ⁺¹⁰, LLL⁺¹¹, LZJ⁺¹¹, LZY12b,
 LGKS17, MPST11, MLGB16, MS11, MvBD18, NHF⁺¹⁰, Niz13, PKK17,
 QZM11, RHRCH16, RvL11, RS17b, Rob13, RRR16, SZ17, SP13, SFA17,
 SSWX14, SB18, SSMW09, SCSW13, TM16, Tan19, TD11, VECT12, Wei12a,
 Wei12b, XP13, YK13, ZWLX11, ZLT13, ZZMW19, ZWF15, vLBBR12].
bond-order [ZWF15]. **bond-valence** [HAI⁺¹⁶]. **bonded**
 [BLFZ13, BSD18, BLDK⁺¹³, DKT13, JCP14, LJW11a, LHHW14, LZSM19,
 PAT⁺¹⁰, SSGS15, UT14, UT15, WHX⁺¹⁰, ZZL⁺¹², ZDX11, ZBMZH15].
Bonding [BSPP⁺¹³, GRD⁺¹⁰, HvM17, MCK17b, THP⁺¹⁵, WWCL15,

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, LZYL12b, 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]. **borafuorenes** [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**

[KOY⁺¹², GS12, QLKI19, WCJ⁺¹⁴]. **Building** [MB14, BHI19, CBP14, GS12, KSW16, MJB12, RLG14, Tak11, TJB12, VVY17]. **building-up** [Tak11]. **buildup** [SS13a]. **built** [FCPJ14, KOP⁺¹⁴]. **bulk** [BC13, KHL19, Man13, MBC13, NNS15, PAK15, QZ10b, RRC⁺¹⁵, VBV13a, VVB13]. **bulky** [SLC⁺¹⁷]. **butadiene** [MCC11]. **butane** [TCGNT18, WKC11]. **butane-like** [WKC11]. **butanol** [BS10b]. **Butene** [CSM16, MSBF16, WvRSM14]. **butterfly** [NDG14]. **butyl** [MG15]. **butylbenzene** [HCB11]. **BX** [YKH15].

C [LdSRR16, LTR18, LAHS16, LLD17, LCWW10, LWD13, MLQ⁺¹², MCK17a, MCK17b, NKD18, PMG⁺¹⁶, RLA⁺¹¹, Sak18, SKMS13, STS⁺¹⁰, SBW12, Tak11, UT15, WCY⁺¹¹, WWKS16, YZZ⁺¹⁷, ZYG⁺¹⁴, ZLY⁺¹⁶, ZLX⁺¹⁹, BS16a, VAMS14, AM19a, Ben17, BWKW10a, BS16b, BH13, CG12, ED15, FL15, GWT⁺¹⁷, GMSV14, GZZ12, HJ13, HVS16, IMK⁺¹⁶, JLS⁺¹⁰, JLLW19, KV14, KMT⁺¹⁹, KP10, LFB14, LLC17, LDH⁺¹⁴, MSV16, MH11, MSPC19, Niz13, OPR16, PTK11, Pie14, PZBA13, RWR⁺¹³, SNDK16, TFQ⁺¹⁰, TFQ⁺¹¹, TS15a, TKCN19, VAR12, VED10, WKC10a, WLW⁺¹⁰, WS10, WWTL19, WL14, WTH⁺¹⁶, Yes12, Yes15, YDGZ15, ZZZ⁺¹⁹, ZZL19]. **C-F** ··· [JLLW19]. **C-H** [KMT⁺¹⁹]. **C-terminal** [IMK⁺¹⁶]. **C2** [KYCL11]. **C2-methylation** [KYCL11]. **C60** [SBW12]. **c7rfjv** [Ano15-59]. **Ca** [LLX⁺¹⁹, BHB⁺¹⁷, BHB19, HBI⁺¹⁷, LZTV10, LPE⁺¹⁰, LBTV12]. **CABS** [LK11]. **CABS-NMR** [LK11]. **caffeine** [FF11]. **Cage** [LLX⁺¹⁹, Avd18, GLZ17, LZ14, OAN15b, WLW⁺¹⁰, WCY⁺¹¹, YLZ⁺¹⁹]. **cage-like** [OAN15b, YLZ⁺¹⁹]. **cages** [KSM16, KZK⁺¹², MKH15, WCY⁺¹¹]. **caging** [DPB⁺¹²]. **calbindin** [TJR19, PNG10]. **calcium** [Pla11, PD12, TJR19]. **calcium-binding** [TJR19]. **calcium-induced** [PD12]. **Calculate** [GH16b, BCSCJ⁺¹³, BACSCJ⁺¹⁰, HDK⁺¹², PSC11, SK17, Yap11, YFH⁺¹⁹]. **calculated** [CHP11, GY10, KJDB12, MJLV14a, MRK11, NMLD13, SKMS13, Yan11, YAO18]. **Calculating** [CPZ19, Hei18, PNI13, SK12, WNP⁺¹⁶, WWD14, CPK12, CXD⁺¹⁹, EFS16, EPD⁺¹¹, HAI⁺¹⁶, OK16, SM16a, WYT17, dRBO13]. **Calculation** [Fer13b, Fer13a, HQSZ19, KSH13, KPG18, MY17a, MMJ10, MS15, SH11b, SOD⁺¹¹, SOvG12, AC11a, Bac12, BW11a, BK17b, BD11, BL12, CPRS18, CCR18, CHG⁺¹⁶, CG15, CX10, DKE⁺¹⁷, DSX⁺¹¹, FD14, FGM11, FPH⁺¹⁹, GREA11, GCW16, Han11, JIS13, KNHN16, KN17, KB16, KDB13, KNR⁺¹⁸, LFN⁺¹⁰, LLW12, LZW⁺¹¹, MYT⁺¹⁴, MLC13, MS12, NYN17, NH19, NMH19, NFPD13, PDMT10, PAK15, Pie14, PW12, RO14b, RZ16, RB12, RRK16, SBV10, SH18a, SLIB12, SCSW13, SACdG14, SMM17, SR11, UT15, VVV^{+15a}, VVG13, WLLH18, WLF19, WDHZ13, ZHS⁺¹⁸, ZZ14, ZZL^{+10b}, ZLLL12, ZGZC19, HH10]. **Calculations** [HBI⁺¹⁷, HWB19, Jia19, MP19b, SR19, THI⁺¹⁹, AR10, AAC⁺¹⁶, BE12, BLL13, BS10a, BTMS12, BH15, Bou14, BS18, BG12, BLZ⁺¹³, CR14, CCJC10, CS17, CKKK16, CBDS19, CMvG10, CXS10, CHKR10, CKG18, DGH⁺¹¹, DSV⁺¹⁹, DGSVGM19, EFAC13, EK17, EWK⁺¹³, EP12, EB12,

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, LEdOLdIV17, LRV18, 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, PLAG11, 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].

carbonyls [SSX⁺14]. **carboranes** [HJ13]. **carboxybetaine** [DQ16].
carboxylates [AARP17, RVM19]. **carboxylation** [CKG18, DGSVGV19].
carboxylic [LPMT17, RB12, dSH19]. **card** [SR11]. **Carlo**
 [LHMM11, NQB19, Aou16, BFH⁺13, CLK11, CG12, CTP13, CAP17,
 DMN15, FFA14, GP12, GPM17, HFSSO12, Hes19, HMM10, HYUS11, HQC16,
 HHBY10, IHJ⁺13, LPK16, LMZ11a, LZ12, MS16, MBRC16, MOS12,
 NDW15, OPBR17, PSS14, PS13, Pon10, PHH⁺12, RHNN10, RdA12,
 SCOJ13, SAGC16, SMRM⁺17, SSP19a, SE14, UU12, YO19, ZLM⁺15, ZW17].
Carlo/Brownian [DMN15]. **Carlo/molecular** [RdA12]. **carotenoids**
 [PVAM16]. **carrabiose** [YSRSS10]. **carrier** [SFDE16]. **carriers**
 [GMASBF16, UGK18]. **Cartesian** [REH13, FHMB15, AlQ19, Elk16].
caryolene [ONTTL16]. **caryolene-forming** [ONTTL16]. **CAS**
 [KMS⁺19, MH11]. **cascade** [HS17b, ONTTL16, ZZWT12]. **cascaded**
 [LZL⁺15a]. **Case** [BMD19, Alg17, ASMS10, AM19a, AM19b, BM12, BG13,
 CCLP12, CB11c, DSB⁺19, DOM⁺11, DS12a, EFOD13, EOA⁺11, GH10,
 GKR13, GPdC⁺16, HSH15, KB13, LPAS11, LP11a, LT13, MIS⁺15, OME16,
 PG18, PVAM16, Ray13, RVM19, Rod13, RKG11, RCM⁺13b, RJS17, SRF⁺17,
 SC18a, SPZP18b, TLA10, VKNT16, WDS⁺19, ZTH⁺15, RAR⁺11]. **cases**
 [GREA11]. **CASPT2** [LWGZ15, SGWA17, VFRAR16, WGA18]. **Cassandra**
 [SMRM⁺17]. **CASSCF** [KSHP⁺19, KKL⁺13, LWGZ15, NH19, SGWA17].
CASSCF/CASPT2 [LWGZ15]. **CASSCF/MC** [KKL⁺13].
CASSCF/MC-XQDPT2 [KKL⁺13]. **CAST** [GBW⁺14]. **catalysis** [Can10,
 Can11, EvRC⁺18, GSMZ19, KK19, LHMM11, MG14, RNS19, WFL⁺19].
catalyst [BEM14, DK19, DSHLM18, LLC17, OSA19, RLZ⁺18, WWTL19,
 YZ15b, ZSWL12, ZX19, dSDdAR10, SSD19]. **catalysts**
 [AHK⁺19, BEPM14, GSMZ19, JJAB16, MPJ⁺19, NJX⁺10, WJX⁺10].
Catalytic [YMY⁺19, AHK⁺19, GHL17, GA19, KV15b, ONTTL16, SJD14,
 SLY⁺10, SOYC12, TM18, UKS11, WZQW10, dSDdAR10]. **catalyzed**
 [AS11, BF19b, CYY⁺17, CCJC10, CPLL11, HPT16a, HDB15, HJLV16,
 KSO⁺19, KB13, KT12, MUN⁺19, MRC⁺18, MG15, MTS⁺19, QLYL10,
 TLA10, Tsi17, VCM15, WCWW11, WFL⁺19, WWTL19, WXY14, XLYZ10,
 YXZZ17, YZ17, YZLZ18, dSDdAR10, dSdLBNB17, dCDP15]. **catastrophe**
 [ABDGN12, GNDA⁺12]. **catechol** [PBLdS12].
catechol-O-methyltransferase [PBLdS12]. **Catenanes** [LAHS16].
cathepsin [ETLS17]. **cathode** [SMiN⁺19]. **cation** [CCCLCGRO14,
 CGPP11, DLMH12, DDM⁺15, MUN⁺19, RMGB11, SSGS15, ZYL⁺12].
Cationic [HJ13, SC18a, WJX⁺10]. **Cations**
 [ND19, SB19, CC18b, KGR⁺16, LCL⁺10, LdSRR16, LTR18, PVS12,
 SBD⁺17, Tac17, THP⁺15, ZWY⁺10a, ZWS⁺10]. **cations/nucleobases**
 [CC18b]. **caused** [GDV17]. **caveolin** [PGI19]. **caveolin-1** [PGI19]. **cavitand**
 [CC18a]. **cavities** [HRB⁺17, ZSB⁺16]. **cavities/vacancies** [HRB⁺17].
cavity [KD18, ZWS⁺10]. **CAVS** [SDZ17]. **CB** [BTMS12, CC18a, ILKR11].
CBS [KG15]. **CBS-QB3** [KG15]. **CC** [Gil11, LLTC12]. **CC2** [SGWA17].
CC3 [LZ14]. **ccCA** [RJWW12]. **CCSD**

[BBI⁺11, MSPC19, CSGOA17, Gil11, KK17a, KKL⁺13, MVKS10, OPR16, PC14, RS13, SRR16, SB14, XKW18, YJ17]. **Cd** [SLIB12]. **cdftbmd** [NN19]. **CDOCKER** [GLB16]. **C** = [CROB16]. **CdS** [NS18]. **CdSe** [MP19a]. **CdSe-Dye-TiO** [MP19a]. **Ce** [Ibr17, YOPB16]. **CeF** [KKA⁺18]. **cefotaxime** [MFM⁺12]. **cell** [ACS12, CGBK13, Elk16, Fom11, Gon12, JMS14, SRL⁺15, VÅA14, dACP12]. **Cells** [FPV13, ACS12, DZA11, DGL⁺13, JYS⁺12, LZL⁺15a, MP19a, SV11, SLC⁺17, TZ12, YJN⁺11]. **cellular** [VBD11]. **cellulose** [GS12, LHT15, GS12]. **Cellulose-Builder** [GS12]. **cementite** [VED10]. **cementite-type** [VED10]. **cementitious** [TZ11]. **CENCALC** [SDMS13]. **census** [PPUBGD10]. **center** [CXD⁺19, IIF⁺10, LRER13, YLL11, Yu12b]. **centered** [FA18, VMV19, VI17]. **centers** [Gav12, GA19, WC14]. **central** [DGL⁺13, Yu12a]. **centrality** [RNVP13]. **centre** [SC18a]. **centric** [LABSG17]. **CeO** [LLLW19]. **CEPA** [Sch12, SB14]. **ceramics** [RKB⁺14]. **CERES** [CPRS18]. **cerium** [SRL⁺15]. **CF** [JCG⁺10, NMLD13, RVdMB16, ZLLL12, AR10, CROB16, NMLD13, ZZL⁺10a]. **CFCF** [NMLD13]. **CFCI** [JCG⁺10]. **CGenFF** [WS19]. **CGenFF-based** [WS19]. **CH** [AR10, ATP18, LWD13, LJG⁺11, OZLSBH12, TLdG⁺12, WLHZ12, ZZL⁺10b, ZYLL12, ZLLL12, BS16b, CK10, CXW14, GY12, HVS16, JCG⁺10, KBC12, KT19, LWW12, LGW12, LLTC12, LJG⁺11, MCUJ15, OOK11, RVCFF13, SSC⁺19, TCPPC14, VVY17, VDVR14, WLHZ12, ZZL⁺10a, dCRN18, DR11]. **CH/** [OOK11]. **chaff** [NMF⁺14]. **Chain** [vRWGS17, BFH⁺13, CHKR10, DMD⁺18, HAL14, KV14, KLS10, KMLS10, LPS⁺13, LZGS11, LP11b, LvG13a, LZLMP16, OZ14, PD12, PS10, QZM11, SA13, SISK10, SZBM13, TSN16, DKV18]. **chains** [AFSW16, FP17a, JSW10, LZZ14, NPP13, Pla11, PLH16, TLdG⁺12, TS15b]. **chalcogen** [CFM⁺19, DDP⁺18]. **chalcogenides** [SPS⁺12]. **chalcogens** [AM19b]. **chalcone** [CPLL11, YZ17]. **challenge** [SDM⁺16]. **Challenges** [HGY15, KHWB17, ASW19, HLvdV13]. **challenging** [CAP17, DSB⁺19, VT14, WLF11]. **change** [EMD17, OSA19]. **changes** [GDV17, GBS⁺17, HB15, LK13, MJLV14b, MO17, PdSC18, RO14b, YZGS14b]. **Changing** [XVN17, LLvG10]. **channel** [HYYZ13, PVL⁺13, SFBT17, SY16b, TCX⁺13]. **channels** [KC13a, LL10c, NSK18, OKIS17, TO19]. **character** [Ali18, BMB13, Cas14, Ibr17, LCK⁺18, RIJ⁺11, VSH19, YSSB12]. **characteristics** [DPSL16, Gav12, LT14, Mat14, RDT14, TZ11]. **Characterization** [DDP⁺18, VT14, XWSW13, CBP⁺15, DGL⁺13, GBW⁺14, GZZ12, Kop15b, MJB12, MPA10, RNP13, ZYG⁺14]. **characterize** [MGCC19]. **Characterizing** [LH11, PRSG13, She12, Yu12b]. **characters** [LSH⁺11, ZLL⁺10]. **Charge** [CMF⁺17, JM11, RDT14, SFDE16, VV19, AWF⁺18, AS15b, ANH⁺11, ALH⁺10, BCSCJ⁺13, BE16, CS14, CBTZ16, CMS13, Cor17, DS12a, DWR17, DAdGR15, EFAC13, ENKK⁺17, GMG⁺10, HLWD15, JCGVPHT17, JZZM14, Jia19, Kan15, KVR10, LLLM11, LPE⁺10, LBDP12, MSV16, MCF⁺18, MHRR11, MPBJ11, NN18, OBW12,

PL14, PTB⁺¹⁵, RSSG18, RO14b, Rez19, Ric16, REL17, SPS⁺¹², SFM⁺¹⁸, SSGS15, SMiN⁺¹⁹, SMP17a, SFLG⁺¹⁷, SLC⁺¹⁷, TN10, TKNN10, UT15, UGK18, VPR10, VAR12, VL17b, WCT⁺¹¹, WWCL15, YKO⁺¹¹, YWZ14, YLZ⁺¹⁰, YJ17, YFH⁺¹⁹, ZDZM13, ZZL19, dSH19, dLC17]. **charge-assisted** [SSGS15]. **charge-inverted** [UT15, YJ17]. **Charge-transfer** [JM11, ANH⁺¹¹, EFAC13, YLZ⁺¹⁰]. **charge-transport** [HLWD15]. **charged** [BK13, KD10, MRO17, NPP13, RJS17, Tsi14]. **Charges** [WFZ⁺¹⁸, CCB15, IM17, JMLL13, LRVM18, RB13a, SN15, TBSM12, VSA11, Yan14, ZBG11]. **Charles** [HIS17]. **CHARMM** [MSK⁺¹², AKMYB18, BF17, BAF18, DPNM11, GLB16, GZM11, HBJ⁺¹⁷, HC14, JCL⁺¹⁷, KLJ⁺¹⁷, KYB13, LZdL⁺¹⁰, MSK⁺¹⁰, MMZW14, QLKI19, RR14, VHA⁺¹⁰, WCJ⁺¹⁴, XVA⁺¹⁶, YHVM12]. **CHARMM-based** [MMZW14]. **CHARMM-compatible** [KYB13]. **CHARMM-GUI** [HBJ⁺¹⁷, KLJ⁺¹⁷, QLKI19]. **CHARMM27** [ST11]. **CHARMM36** [HM13]. **CHARMMing** [WPM⁺¹⁵]. **Charts** [SJL18]. **Chatt** [Bac12]. **CHCICH** [WLHZ12]. **CH**... [MVKS10]. **cheapest** [SA13]. **cheapest-path** [SA13]. **checkpoint** [DXL⁺¹⁰, DSX⁺¹¹]. **chelation** [KYCL11]. **Chem** [ABB⁺¹³, CHR^{+12b}, HNWF12, HLXH18, ICS⁺¹³, Kne11b, MT20, MSK⁺¹², RK16a, SFCK⁺¹⁵, SMM15a, GCC14, GKV⁺¹³]. **Chemical** [BLG10, BCP⁺¹⁰, BGS⁺¹⁹, JCGVPHT17, OSI⁺¹⁹, OM12, SLLL13, VGTL16, ALK⁺¹⁵, ASS⁺¹⁷, AAC⁺¹⁶, APA⁺¹⁴, Bac12, BPC19, Ben17, Bou14, Cam15, CKG18, CHP11, DKE⁺¹⁷, DDP⁺¹⁸, DS12a, DI11, DB12, Dra19, EOA⁺¹¹, FB10, FVB10, GH10, GLW19, GGM⁺¹², GPGSM11, GPGSM12, HPT^{+16b}, HHDC16, HJ13, Ihl12, JKS⁺¹⁶, KV12, KASH14, KP11, LK11, LZH⁺¹¹, Li14a, Li14b, MDTD13, MDTD16, Man19b, MN15, MTS⁺¹⁹, MAPB10, MSvG12, MSSP17, MFR⁺¹¹, MMJ10, MH10, NCV10, NC13, NC14, OKIS17, OKY18, OSHG17, ONTTL16, OC14, PTK11, PGdO⁺¹⁶, Pie14, PBG17, RRFV⁺¹⁸, RK15, RSKG14, SRA17, SLT14, SFM⁺¹⁸, SCOJ13, SEF⁺¹⁶, SKMS13, SHB17, TLA10, TG12b, TEDT18, TR12, UD12, VBD11, VBMA13, WBT10, WCT⁺¹¹, WF16, Wei12b, WL14, Wu10, WDP⁺¹², YZ15a, YB16, ZY14, ZBB16, ZT14]. **chemical** [dCDP15, Chu10]. **chemical-bonding** [MDTD13]. **Chemically** [EFAC13, ZZ12, JAHS⁺¹⁹, Zim13]. **chemist** [DHE⁺¹²]. **chemistries** [BS10b]. **Chemistry** [Ano10b, Ano15-59, Cam19, HJG09, KKGW19, Spr10, ZLX⁺¹⁹, All11, BRP⁺¹², BGR13, CBH14, CD19, DDM⁺¹⁵, FLM11, GHV17, HSN⁺¹⁸, IGK16, JBB⁺¹¹, KTNN10, LBC⁺¹⁹, LK16a, MP19c, OZLSBH12, PNW⁺¹⁶, PPUBGD10, RZG⁺¹³, Rez16, REL⁺¹⁴, TKNN10, TF15, UDK⁺¹⁸, VVP12, VV14, WDY13, ZVY⁺¹⁵, GS16, MFEM16, XFG⁺¹⁶]. **ChemNetworks** [OC14]. **chemoselectivity** [WWTL19]. **chemosensing** [LZHH11]. **chemosensor** [LZL⁺¹⁰]. **CheY** [Pet11]. **CHFCF** [NMLD13]. **chi** [EJ13]. **chignolin** [HTS15]. **Chiral** [KHE⁺¹⁹, KSO⁺¹⁹, LG14, PC14, ZPP⁺¹⁶]. **Chiral-selective** [KHE⁺¹⁹]. **chirality** [AS15a, DZA11, PBBP11]. **chirality-based** [PBBP11]. **Chloride** [KJ10, KLN16, Rab12, SG10b]. **chlorides** [RRF11, YZGS14b]. **chloridophenylacetohydroxamate** [CBDS19]. **chlorine**

[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]. **CI** [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]. **CIC** [KJ10]. **CICH** [RVdMB16]. **CICHO** [SS19]. **CICI** [LGW12]. **clean** [CCJ⁺11]. **cleaning** [YR13]. **cleavage** [HEM⁺17, MS11]. **click** [TKXT13]. **CLL** [dACP12]. **CINH** [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, RKG10]. **coding** [QLQ11, YS10]. **Codoped** [RLZ⁺18]. **coefficient** [FSD⁺18, WH11, WF16, WZWW18]. **coefficients** [AR10, JIS13, KCL⁺14, LRV18, 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, PLAG11, 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, RKG10, 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, BLF14, 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, EHSP16, GPdC⁺¹⁶, SvLK18, SKGB13, AvKSP16, AMK11, ASMS10, AK10, AM19a, BCSCJ⁺¹³, BLFZ13, 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].

component [CLA16, CSKH16, DMJ17, HSN⁺18, HKR⁺14, JKS⁺16, KM13, NK19, NASH15, PSP15, PW12, RK15, SV11]. **Components** [ELKE19, CHR⁺12b, CHR⁺12a, MBT14, Pil17, XTG⁺11]. **composed** [TFYO19, ZYL⁺12]. **composite** [KG15, SLG15, TNSS17]. **composites** [AS15a]. **Composition** [DH11, GRL⁺11, GRL⁺12, GC11, II18, LLH⁺19, ZHHX11].

Composition-induced [DH11]. **compound** [CQFC10, CJZS10, EH13, HLH⁺12, RLL⁺10, VBMA13]. **Compounds** [LLX⁺19, SZL19, AH10, AR15, ARLP13, BEEL14, CME11, CL16, CSSB11, DOM⁺11, DCOD13, DPB⁺12, EPH⁺13, FHT⁺15, FSD⁺18, GBPCC19, GRP⁺12, JSF19, LAM19, LWL⁺10, MMS16, NHN16, NFG⁺13, OCLM14, PMG⁺16, PSC11, SH15, SK12, SSNT19, SGHL13, TFQ⁺11, TD10, TTB⁺11, VVBL17, VFRAR16, WGL⁺11, WWKS16, XWW⁺11, YHVM12, YDX16, ZM10]. **Comprehensive** [BGL⁺18, HLS12, CCCLRO14, dCGCRN19, PS14, RRC⁺15, ZXS⁺10].

Compressing [HRID16]. **compression** [MKS⁺12]. **comprising** [FWS⁺18]. **Comput** [HLXH18, MT20, RK16a, SFCCCK⁺15, SMM15a]. **Computation** [PBLdS12, ŠB13, AO10, FCL⁺10, GMSV14, GJMPAM⁺14, HDL⁺14, HAP⁺12, JLS18, MTS⁺19, NNK⁺16, SM14a, XSZL11]. **Computational** [Alg17, Ano10b, Ano15-59, BF19a, Cam19, DKV18, DPB⁺12, ED15, ECZWD17, EOA⁺11, GS16, HYYZ13, HJG09, Hei10, HRL11, JS17a, JLS⁺10, KAR12, LI19, LGC19, LBS10, Lu11, MFM⁺12, MFEM16, MSÅK12, PGCT⁺12, SGM⁺13, TKXT13, VM19, XFG⁺16, XLYZ10, YKH⁺10, ZSTI14, ZPP⁺16, ZYW⁺16, ZZWX11, AARP17, All11, ABB⁺12, ABB⁺13, BCJC⁺14, BH13, CCCLRO14, CCJ⁺11, CSC⁺18, DK19, DPOS16, DZA11, DHE⁺12, EHT19, FMG12, GS14, GAI13, GD10, GHV17, HCB11, HS16b, HDH12, HZ13, HVS16, IY18, IIHY15, KC13b, KG11, KJM⁺17, KK19, KV15b, LC10, uLhY11, MS13, MS16, ME10, MP19c, OSHG17, OSA19, PGC12, PLZ17, PNW⁺16, PPUBGD10, PVS12, RCR⁺16, Řez16, RK15, SLY⁺10, SRR16, SNS16, SGS⁺16, Sie18, SNDK16, SY16a, Su10, SDMS13, SDL14, SIG⁺11, SIG⁺15, TF15, TLA10, TRA⁺16, VZ14]. **computational** [VRKT19, WDY13, WXL⁺12, WCDM11, WS11, XWSW13, YDX16, ZCK⁺16, dCLFGL13, FHW⁺11, Spr10]. **computationally** [JJAB16].

computations [AGB13, BLBG⁺13, CC12b, KKA⁺18, SRL⁺15, SPZP18b, VECT12, VAMS14, YB16, dACP12]. **compute** [HHNK19, HDM⁺15, KK17a, LM18b, OHPR18, QS19, YAS13, dVAG16].

computed [CCYL11, Fra15, Fra16, HJ13, JJH⁺13, RLDJ17, UKS11]. **Computer** [BBG⁺18b, CLC11, SCK18, BV14, CBP14, DSK17, GP12, KSH⁺17, PL19, SYN⁺12]. **Computerized** [NYH⁺17, VBDS⁺11].

computers [CSSB11, ESB13, TJB12]. **Computing** [Ano10a, GK15a, HDL⁺17, HRH⁺17, KHWB17, PBDW11, SN10, ACD⁺13a, ACD⁺13b, BK13, BZB⁺13, CHC⁺13, CKKK16, GM17, LPLA13, MK13a, MKO⁺13, OV14, OPB⁺12, Rod13, TF15, XYX17, Yan14, ZWL13].

concatenated [PSP15]. **concave** [CLFRO18]. **concentrating** [LLL⁺10].

concentration [IPAA11]. **concept** [GRL⁺11, GRL⁺12, dSVdM⁺16].
conceptual [DDP⁺18, vS18]. **concerted** [III10]. **concurrent** [HS14b].
condensation [KNE11a, XLYZ10]. **condensed** [BGL⁺18, BG17, HRB⁺17, MKK⁺19, RSLML12, VKAM12, dSdS12a, dSdS12b]. **condensed-matter** [BGL⁺18]. **condensed-phase** [MKK⁺19]. **condition** [AA18, IKN13, MTvG12, TTC⁺18, YAO18]. **conditional** [BMPML⁺13].
conditions [AA18, BRGN12, KB14a, MO15, MO17, NO16, SSP19a, Sie15, SKMS13, TCPPC14, VECT12]. **CONDON** [SvLK18, CHC⁺13, MCLD10, MLCD11]. **conducting** [SV11]. **conduction** [KJ10]. **conductivity** [ASL⁺11]. **Conductor** [KB14b, GRN19, KD18, SDF⁺17]. **Conductor-like** [KB14b, GRN19, KD18, SDF⁺17]. **conductors** [MRB14, NFI⁺16]. **cone** [BKLA13]. **confidence** [KSM17]. **Configuration** [KKGW19, SS13a, Cas13, CTP13, CAP17, EK17, FF11, FA18, GA14, GP11a, HPT17, HBL12, LCB10, MT19b, MIS⁺15, MCP18, ZRCC11].
configurational [RO14a, WTD⁺19, WDHZ13]. **Confined** [NSP15, CCR18, CDB10, FTR15, Vyb15, Vyb16]. **Confinement** [CC18a, DLC18b, TM16]. **Confining** [WRG⁺17]. **conformation** [AST⁺16, CR19, EJ13, FBvdB18, GKJ⁺19, PVJ10, SEF⁺16].
conformation-dependent [PVJ10]. **Conformational** [CDM⁺15, ETL17, KRTB10, LGL11, LTA⁺11, MO17, OGL10, vRWGS17, AD10, BLKP12, BD11, ĆMD13, DPSL16, DPNM11, DSHLM18, FCD10, FCOGM12, GDV17, GO13, GBSE11, HTS15, HYNS19, HDL⁺17, HKNH18, HCD⁺10, IMK⁺16, ISK14, JLS18, KB10, KNE11a, KGM12, LLHM16, LC17b, NMF⁺14, Pet11, PKIC11, PLH16, PVS12, PS14, RSL16, SBT17, SHL⁺11, SEM12, SDMS13, TJB12, VZ14, YZ16, YBS19, Yon16].
conformational-space [AD10]. **conformationally** [AFPI13, CP15].
conformations [CC12b, DJ13, ESD18, LC16, LZZ14, NR11, OCL11, PGI19, PH10a, RVP⁺11, ZC14, DKV18]. **Conformers** [SZZ⁺18, BHF⁺18, DBG11, HH10, HH11, LG11, MS17, TCGNT18, VP19].
congested [MvBD18]. **conjugate** [MSV16]. **Conjugated** [RVB⁺12, BLBG⁺13, HDHL15a, HDHL15b, HDHL15c, JYS⁺12, RSSG18, YJN⁺11, JCHT18]. **conjugating** [JDW⁺19]. **conjunction** [CGA19, LBH⁺11, NC13, RKG10]. **connected** [ACD⁺13a, ACD⁺13b, NR11, XTn18]. **connection** [Lüc14]. **connections** [CDC19]. **Connectivity** [ISP⁺10, ZYS⁺10]. **Conquer** [NN19, YKNN19, BRP⁺12, BGR13, KKNN11, KFT18, NYH⁺17, NN18, NNK⁺16, WX12, YN15]. **consensus** [DMJ17, SRA17, PLV⁺11].
consequences [KG15]. **conservation** [MB16]. **conserved** [JDW⁺19].
Conserving [PH17]. **considerable** [LLD17]. **Consideration** [Fom11].
considerations [SBGP18]. **Considering** [CSEMB⁺16]. **considers** [YBS19].
Consistent [LOB18, MKO⁺13, POB13, BKŠ⁺11, BY11, BK17b, DK11, GBVA11, Hil13, HKR⁺14, JSXH16, KT10, KFT18, LBH⁺11, LCW12, ON14, OLPB19, Rez19,

SPS⁺¹², SMP17b, SCSW13, TYN15, VGV⁺¹¹, YN15, ZBG11, BLKP12].
consistently [IM17]. **consolidate** [BK17c]. **constant**
 [AB16a, CS14, IN19, KSK11, KNP⁺¹², KB19, MK17, MK19, PLFS18, PS13,
 RAGLL11, Sak18, STM17, Vor12, WOH16, WOH18, dACP12].
constant-distance [dACP12]. **constants** [AAMD⁺¹¹, CBH14, CPK12,
 DSD⁺¹¹, ECZWD17, FD14, GAI13, GKR13, MG11, OZLSBH12, Ray13,
 RSG14, RKG11, Rui11, RRK16, SSC⁺¹⁹, SPHF⁺¹⁸, SH18a, SACdG14,
 TTR⁺¹², Tsi14, WL14, XWW⁺¹¹, YS13, ZZL^{+10b}, ZLLL12]. **Constrained**
 [SLG15, GREA11, GA12, VBV13b, WBN⁺¹³]. **Constraint** [HNyH19].
constraints [KB11a, OPBR17, OZS⁺¹³]. **construct** [HH10]. **constructed**
 [HDL⁺¹⁷, Tsi19, ZLY⁺¹⁶]. **Constructing**
 [Che17, LLH⁺¹⁹, HS16b, LG11, SWA13]. **Construction** [FZL⁺¹⁹, AGR11b,
 JCPC11, KD18, KSR17, LZX16, UIW⁺¹⁰, WWD14, YD17]. **contact**
 [DBK17, LL19b, MK13a]. **contact-assisted** [LL19b]. **contacting** [Mau14].
contacts [CCCLCGRO14, Ham11, Kri10, PRP15, SNDK16]. **containing**
 [AKMYB18, ACD^{+13a}, ACD^{+13b}, DT19, DGL⁺¹³, GP12, GPdC⁺¹⁶,
 HDPM14, KLN12, KGJZ19, LDZW17, MUGNVJ⁺¹⁸, VDVR14, YHVM12,
 YDX16, ZZL⁺¹², ZM10, MSPC19]. **contaminated** [YR13]. **content**
 [CGBK13, GWPJ11]. **Contents** [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]. **context**
 [CBG16]. **continuation** [PJ13]. **Continuous**
 [Dry14, LPLA13, PZBA13, BS19, FGM11, LBGS16]. **Continuum**
 [CCR18, JJJ16, ND19, ALRM18, Cam15, CZY11, GRN19, HZSS17, ISO⁺¹³,
 LFN⁺¹⁰, MCUJ15, SK12, SK17, TNG⁺¹⁰, WC13, WRHF10, XZ11].
Contracted [FC18, SM18]. **Contraction** [Hes19, HSN14, STM17].
contractions [KK17a]. **Contrasting** [TS15a]. **contribution** [Pro16].
Contributions
 [JJH⁺¹³, ARRC15, BCNH⁺¹¹, CGR16, CPN⁺¹⁷, ENKK⁺¹⁷, WS10]. **control**
 [BVY⁺¹², DPAB16, Hel13, HH16b, KFT18, LPLB16, SR10, XYW⁺¹⁴, ZQ14].
Controlled [PGK⁺¹⁹, VGTL16]. **Controlled-advancement** [PGK⁺¹⁹].
Controlling [FWB14, NPG⁺¹⁸, SS19]. **convective** [SBN13a, SBN13b].
convenient [ZGZC19]. **Conventional** [SHL⁺¹³, BKŠ⁺¹¹]. **conventions**
 [BCJC⁺¹⁴]. **converged** [FLM11, GR10a, KHWB17]. **Convergence**
 [GS16, LT13, ZH12, ASS10, BKŠ⁺¹¹, GS15, ON14, RFHG10, SL17, SLY⁺¹⁹].
converges [SH11a]. **Converging** [OSR16]. **Conversion**
 [AlQ19, DAP⁺¹⁸, LDB⁺¹⁷, LZL^{+15a}, LCB10, RVP⁺¹¹, TTC⁺¹⁸, WFL⁺¹⁹].
converted [ZB18]. **convex** [CLFRO18, GWW19]. **convolution** [SZTSM10].
convolutional [LHO17]. **cooperative** [DBG11, WFL⁺¹⁹]. **Cooperativity**
 [RS14, AFSW16, JSW10, KPH⁺¹⁹, SM16a]. **coordinate**
 [AMGB10, HSN14, Hel13, LL15, LL13a, MS10, WBN⁺¹³]. **coordinated**
 [Sak18]. **Coordinates** [AlQ19, BK15, LWK⁺¹⁴, MK19, NCV10, PH10a,
 Sch13, VBV13b, You10, ZT14]. **Coordination** [LBC⁺¹⁹, ASMS10, AHK⁺¹⁹,
 CRC13, GBPCC19, HS16b, HH18, KLZ⁺¹⁸, KJ10, Mor15, SB19].

copolymerization [DSHLM18]. **copper** [JRSHP14, KKPT11, SBC⁺11, SIT18, SPR⁺13, WC14, ASMS10, BSG⁺18b, CPK12, HRJ⁺14, HGHP14, HRJ⁺15, XWSW13]. **coprocessors** [WS13].

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CopZ [CPK12]. **Coral** [TTL⁺12, TTB⁺11, TTR⁺12]. **corannulene** [CLFRO18, CBTZ16, LdSRR16, WL14]. **corannulene-based** [WL14]. **Core** [TBSM12, BVHI17, BG12, CKKK16, CB11d, EK17, GA12, Hil13, JXSW15, JCG⁺11, KK17a, KNHN16, LGVA14, MIS⁺15, OOK11, RLD12, SJC11, WWU12, WWD14, WGN⁺16, WGLG⁺16, ZCWX18]. **core-hole** [GA12]. **core-level** [WWD14]. **Core-shell** [TBSM12, JCG⁺11]. **core-shells** [JXSW15]. **core-valence** [Hil13]. **cored** [RSSG18]. **cores** [JND⁺19].

Coriolis [LWD13, Wu10]. **coronene** [KDS17]. **Corrected** [SG13, AG12, BLBG⁺13, CLFRO18, CR14, GEG11, Han11, KSH13, KSSH13, MMS16, Rui11, SHL⁺18, ST13, SPH11, SH19a, STS15, VCL18]. **correcting** [vS18]. **Correction** [ND19, DAG19, HGHP14, NLP⁺16, OLPB19, RR12, SMGB11, TSH⁺19].

corrections [JKS⁺16, KB10, KLN12, LCM⁺14, MGWR12, PTK11, RJPB12, RRK16, SJZ⁺15, SSA⁺17, TG12a, VL17a]. **correctly** [ASMS10]. **correlate** [MJLV14a]. **correlated** [BWKW10a, BWKW10b, EWK⁺13, KSH⁺17, LLLM11, MP11, yOTn16, RRK16, SM17, Vyb16]. **Correlating** [TZCK18, SNKS10]. **Correlation** [ASL⁺11, CKH17, ELKE19, RLA18, SN16b, VSP19, Vyb16, CSKH15, CSKH16, ESM⁺12, FRSA14, Hil13, HGCCGR⁺16, HG10, KSH13, KNP⁺12, LBH⁺11, LKZM18, MKGA10, NYH⁺17, NLL19, OAN15a, PTB⁺15, SH18a, SPH11, SH19a, VL17a, WFS19, ZPP⁺16]. **correlations** [AHK⁺19, CSKH16, Hei18, SB10, TTB⁺10]. **corresponding** [PG14, RvL11].

Corrigendum [Ano15-58, Fra16, HHT⁺13a, HRJ⁺15, HvM17, SSB13, WHAS⁺16]. **COSMO** [DS12a, UvSvdWK19]. **COSMO-RS** [DS12a]. **COSMOmic** [JIS13]. **Cost** [PDG⁺16, BLDK⁺13, BYE⁺16, CBP14, Gil11, LCM⁺14, SRR16, TF15]. **cost-effective** [LCM⁺14]. **cost-efficient** [CBP14]. **Could** [EPH⁺13, EPH⁺15, TLA10]. **Coulomb** [FED17, GC18, IO13a, JKS⁺16, LMR14]. **Coulombic** [DPAB16]. **coumaric** [HNN⁺17]. **coumarin** [MS11, ZDX11]. **count** [KTK17]. **counterintuitive** [WDS⁺19]. **Counterpoise** [SMGB11, LCM⁺14]. **Counting** [QZ10a, RNP13].

couple [IYK11, Tsi17]. **Coupled** [DAB16, Höf14, SZL19, VV14, ACD⁺13a, ACD⁺13b, BYE⁺16, CAT⁺13, EVR18, FZY⁺12, GA18, HKNH18, HHNK19, HDM⁺15, HGCCGR⁺16, ILKR11, IYK11, JLH⁺14, KT19, Les19, MC12, PGS⁺15, RKDM14, SB14, SH18b, SM17, TTn19, XTn18, XBSS19].

Coupled-cluster [Höf14, VV14, BYE⁺16, HGCCGR⁺16, Les19, MC12, PGS⁺15, TTn19, XTn18]. **coupled-cluster/Kohn** [VV14].

coupled-electron [SB14]. **Coupling** [NNT⁺19, AMQ⁺14, BLZ⁺13, FD16,

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, MR17, 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,

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, Ano18a, Ano18b, Ano18t, Ano18u, Ano18v, Ano18w, Ano18x, Ano18y, 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]. **Cover** [Ano18i, Ano18j, Ano18k, Ano18l, Ano18m, Ano18o, Ano18p, Ano18q, Ano18r, Ano18s, Ano19a, Ano19l, Ano19t, Ano19u, Ano19v, Ano19x, Ano19y, Ano19z, Ano19w, Ano19-27, Ano19-28, Ano19-29, Ano19-30, Ano19-31, Ano19-32, Ano19b, Ano19c, Ano19d, Ano19e, Ano19f, Ano19g, Ano19h, Ano19i, Ano19j, Ano19k, Ano19m, Ano19n, Ano19o, Ano19p, Ano19q, Ano19r, Ano19s]. **Coxeter** [WTH⁺16]. **Cp*CoEt** [MLQ⁺12]. **CP2K** [MJG⁺15]. **CPB** [FHMB15]. **CPMD** [SN16a]. **CPMD/GULP** [SN16a]. **CPPTRAJ** [RC18]. **CPU** [DZT11, MEH18]. **CPUs** [KK17a]. **Cr** [WWKS16, SSX⁺14, ZFS18]. **Crabbé** [GRCL12]. **Crafts** [CYY⁺17]. **Crafts-type** [CYY⁺17]. **crambin** [YMP14]. **CRC** [CD19]. **creation** [JBAM11, You10]. **Crick** [BZH14]. **criteria** [MvBD18]. **criterion** [dLvNC18a]. **critical** [HEMCZE⁺14, KCK⁺15, LTT16, MLZZ12, Wei12a, Wei12b, dLvNC18a]. **CrMnAs** [LKZM18]. **cross** [HPT⁺16b, HBL12, Lun12, MY17a, MY17b, WMW⁺10, ZHS⁺18, dCLFGL13]. **cross-boundary** [Lun12]. **cross-platform** [HPT⁺16b]. **cross-section** [dCLFGL13]. **crossing** [LLSW14, QCR12]. **crossover** [CSS17, KV14, MK17, SHMO11, VFRAR16]. **crotonaldehyde** [KK19]. **crowded** [MH17]. **crown** [AvKSP16, HLB15, MWJ⁺11]. **crown/ammonium** [AvKSP16]. **CrWO** [WMW11]. **cryo** [MKM⁺17]. **cryo-EM** [MKM⁺17]. **cryptands** [EHT19]. **CRYSLOT** [BPC19]. **Crystal** [FDCJG18, Kri10, VM11, ASL⁺11, BCSCJ⁺13, BCJC⁺14, Elk16, GMG⁺10, HB14, HJ10, MCAG⁺16, NHF⁺10, NTNY15, SPZP18b, VMV19, OPB⁺12, CPR18]. **crystalline** [BPC19, DOM⁺11, DCOD13, DLSD13, DB12, EP12, EFOD13, GKB⁺19, GS12, RB13b, VMV19, WDLG12]. **crystallography** [MM18, Mat18, Tsi18, YW13]. **crystals** [BS18, DL19, HZSS17, KGHC15, KLN12, KB16, LPAS11, PLP⁺16, SFDE16, SPZP18a, VECT12, You10]. **CS** [TLdG⁺12, ZBB16, DDM⁺15, YLT⁺19, FMNC11]. **CSe** [ZBB16]. **Csonka** [Ano15-59]. **CTOCD** [PC14]. **Cu** [LLX⁺19, NGAS17, Rab12, RHT⁺15, SIT18, TS15b, WRG⁺17, AMK11, CR14, ĆMD13, GEP⁺14, HSH15, MLG18, Mor15, PGS⁺15, PXXW10, PH12, RHT⁺15, SB10, TNI⁺19a, WGN⁺16, WGLG⁺16, XP13, ZRCC11, ZSWL12]. **Cu-O** [ZRCC11]. **Cu-ZSM-5** [Mor15]. **Cu2II** [WGLG⁺16]. **Cuby** [Řez16]. **CuCN** [TS15b]. **CUDA** [SR11]. **CUDA-enabled** [SR11]. **CuE** [TG12b]. **curcumin** [AMK11]. **Curie** [WMW11]. **curing** [LPMT17, PPH⁺14]. **Current** [ATM18, NS17, ABM⁺15, ATIP18, BL19, FNSF⁺11, GWT⁺17, HLBLCCG15, PCLL11, PL18, PZM15, Vik11]. **current-density** [Vik11]. **currents** [CPN⁺17, RVB⁺12]. **Curvature** [LPLS16, RR12, NW17].

Curvature-dependent [LPLS16]. **curves** [BBI⁺¹¹, LSH⁺¹¹]. **Curvilinear** [JL19]. **Customizable** [AFBR17]. **cut** [DH14]. **cutoffs** [HH18]. **CuX** [YS13]. **CVD** [NIIT15]. **CX** [AM19a, LGW12, EPH⁺¹⁵, ZYLL12]. **CXH** [CKL⁺¹¹]. **CXHM** [LDJ⁺¹⁰]. **cyanide** [LZHH11, LLW12, TLY⁺¹², VVBL17]. **cyanide-chemosensing** [LZHH11]. **cyanides** [PGS⁺¹⁵]. **cyano** [PKK17, TS10b]. **cyanobacteria** [RCM^{+13a}, RML⁺¹⁵]. **Cyanovirin** [VM11]. **cycle** [HDL⁺¹⁷, SJD14, SOYC12, dSDdAR10]. **cycles** [UKS11]. **cyclic** [CZH12, HLI⁺¹⁹, LC10, PB14, RB12]. **Cyclization** [HPT16a, SMB18, APA⁺¹⁴, LZL⁺¹⁶]. **cyclizations** [AARP17, DCHL12]. **cycloadditions** [YZN13]. **Cyclobutadiene** [SFM14, MCC11]. **cyclocized** [QZ10a]. **cyclodextrin** [DBG11]. **cycloguanil** [APA⁺¹⁴]. **cyclohexane** [CROB16, SNDK16, SAVG15, TFYO19]. **cyclohexanes** [SNDK16]. **cycloocta** [ABDGN12]. **cycloocta-1** [ABDGN12]. **Cyclooctatetraene** [DP11, SP13]. **cyclopentadienes** [LZH16]. **cyclopropenylidene** [VVP12]. **cyclosporin** [QZM11]. **CYP11B2** [RVP⁺¹¹]. **CYP11B2-mediated** [RVP⁺¹¹]. **CYP19A1** [VCM15]. **CYP2A6** [ALW⁺¹⁰]. **cysteine** [CPK12, SDL14]. **Cytochrome** [EH13, BS16a, MRR11, SLY⁺¹⁰, SOYC12, TN10, TDP⁺¹², VCM15]. **cytochrome-P450-mediated** [MRR11]. **cytochromes** [APA⁺¹⁴]. **cytosine** [JS17a, LZH⁺¹¹, ZZY⁺¹⁶].

D [LWD13, OZLSBH12, RSKG14, SPHF⁺¹⁸, UT14, GBG⁺¹⁹, MP19b, YZ15b, AKMT11, BWKW10a, BWKW10b, CKH19, Chu10, DVVP14, ETLS17, GMMH⁺¹⁶, GSS13, GPK12, HSW⁺¹⁹, KTT16, LTT16, MA16, MYT⁺¹⁴, MH11, MSSP17, MH10, NN19, PSS14, PZBA13, Pop18, RSKG14, SWW⁺¹⁹, TFQ⁺¹⁰, TJR19, UT15, VVMY18, YJN⁺¹¹, YDL⁺¹⁰, ZLY⁺¹⁶, dLvNC18b, TS15b, YOPB16]. **D-** [YJN⁺¹¹]. **d-AO** [YOPB16]. **D-FFT** [MYT⁺¹⁴]. **D-galactosidase** [AKMT11]. **d-metal** [GBG⁺¹⁹]. **D-QSAR** [GMMH⁺¹⁶]. **D-RISM** [MYT⁺¹⁴]. **D-structures** [DVVP14]. **D/TIP3P** [SA10]. **D2** [LAHS16]. **D5Cost** [REL⁺¹⁴]. **d9k** [PNG10]. **damaged** [LZH⁺¹¹]. **damping** [GEG11]. **DAMQT** [KYG⁺¹⁵]. **dance** [JW16]. **dancing** [LL10b]. **Dancoff** [HH17]. **data** [BRGN12, BCP⁺¹⁰, FN12, Fom11, HPT^{+16b}, HM13, JZL⁺¹⁷, JS17b, LAS⁺¹⁴, MMB⁺¹⁷, MCC12, RO14a, RC18, REL⁺¹⁴, RCM^{+13b}, SB10, WDKT19, WSWD19, XW15]. **database** [PLAG11, XTG⁺¹¹, XMSZ16]. **databases** [CSSB11, MP19c, OHPR17, ZWL13]. **DataPipeline** [FN12]. **dataset** [HZ13, KSM17]. **datasets** [GCC14]. **Dative** [JSF19]. **days** [Tsi18]. **DBD** [YJXZ13]. **DBeH** [UT14]. **DBU** [YZ15b, YZL⁺¹⁵, YZ17]. **DBU-H** [YZ15b]. **DCMB** [WX12]. **DDPredictor** [HLS⁺¹³]. **deacetylases** [KC13a]. **dead** [SL10]. **dead-end** [SL10]. **dealing** [MFR10]. **deaminase** [WZQW10, ZZY⁺¹⁶]. **deamination** [ZZY⁺¹⁶]. **Debye** [GBFD12]. **DEC** [BK17c]. **DEC-RI-MP2** [BK17c]. **decamer** [DDP16]. **decarboxylase** [BEL⁺¹¹]. **decay** [DPAB16, LCH10, LLT12]. **Decoding** [MBT14]. **decoherence** [CSEMB⁺¹⁶]. **Decomposition** [DBGO⁺¹⁷, Spr18, AMAA⁺¹¹,

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]. **decomposition-based** [KNE11a]. **decouples** [FM10]. **decoy** [HYMZ16, LS11a, PHDH13, UCFR16]. **decoys** [BSZ⁺12, MP11]. **decrease** [DLZ15, SLY⁺10]. **dedicated** [CPRS18, ZRCC11]. **Deep** [GHV17, TO19, GFPSD17, HPL⁺18, LHO17, LDH⁺14, WZWW18]. **deeper** [VIT⁺15]. **DeepIon** [TO19]. **defect** [ZWP11]. **defective** [YZN13]. **defects** [HYL⁺11]. **deficient** [YLL11]. **defined** [JJAB16, Man19a, GY10]. **defining** [HH18]. **definitions** [JYC⁺16]. **Definitive** [TCGNT18]. **Deformation** [WYL⁺15, Gav12, MRB14, WCY⁺11, WCT⁺11, dLC17]. **deformations** [HRMAL⁺13]. **Deformed** [CSAdOM17, TFQ⁺10]. **degree** [Clo15]. **dehydrogenase** [ZX11]. **deiodinase** [CFM⁺19]. **Dejan** [CD19]. **delayed** [FWS⁺18, ZGZ19]. **deleterious** [LXL⁺11]. **delineate** [SBT17]. **Delineating** [JL19]. **delivery** [AJA⁺19]. **delocalization** [BK11, FVB10, HSB⁺11, Jan16, Mat14, SS13b, SSA⁺17]. **delocalized** [Alg17, GLW19, HSH15, dLC17]. **DelPhi** [DLSA14, JLCA17, LLZA12, LPLA13, LJC⁺19]. **DelPhiForce** [LCA17]. **deltahedra** [LK16b]. **deMon** [LZdIL⁺10]. **deMon2k** [BTT10]. **Demystifying** [KKGW19]. **Denaturation** [IPAA11, FMG12]. **Dendrimer** [MJB12]. **dendrimers** [CAD16, HDHL15a, HDHL15b, HDHL15c]. **Deng** [Ano12u]. **dense** [ASK18]. **Densities** [ATM18, ATP18, HGCCGR⁺16, LP11c, MA16, REL17, UCRL18, dLC17]. **Density** [AMK11, BS19, BHB19, CD13, CWHH11, CKH19, FPV13, FD16, GMBM18, GNGCA10, GWPJ11, INT18, JYS⁺12, KKPT11, LBGS16, LGW12, LLX⁺19, LBTV12, LPMT17, MP19b, MWJ⁺11, MAP18, NN19, Oht16, PPH⁺14, RB12, RSLML12, TS10b, UvSvdWK19, WDLG12, WGN⁺16, YJ11, YKNN19, ZLZ14, ZYG⁺14, ZWY⁺10b, ZWY⁺10a, dSdS12a, ALK⁺15, Ali18, ASW19, Ano15-59, AG12, ASS10, BY11, BLBG⁺13, BL19, Ben17, Boz18, BBI⁺11, BZB⁺13, BG13, CHG⁺16, CRZ⁺18, CDB10, CR14, CAA10, CEBO15, CC18c, CGR16, CKH17, CSXZ17, CC11, CAP17, CNK97, CPLL11, CXD⁺19, CB11d, DAP⁺18, DH17, DWC17, Dil15, DSAS19, ED15, EP12, FED17, FCPJM14, GAI14, GHL17, GZL⁺12, GWJR18, GMG⁺10, GSS13, Gra15, GEG11, GAJ⁺17, Han11, HNWF07, HNWF12, HPT17, HEMCZE⁺14, HLBLCCG15, HRMAL⁺13, HH16a, HH17]. **density** [Hil13, Höf14, HG10, HOK17, IKN13, IM17, JCP14, JLH⁺14, JW16, KD10, KB10, KSSH13, KOP⁺14, KGHK12, KB13, KZZ⁺16, KLN12, KYG⁺15, LL15, LRV18, LCW12, LAM19, LBTV11, LHKS12, LWWG12, LH14b, LLH17, LZS⁺17, LK16a, MRC⁺18, MLG18, MMH19, MSY19, MCF⁺18, MGCC19, MAK⁺14, Mat14, ME10, MKM⁺17, MFR⁺17, MMJ10, NS18, NF17, NN18, NO16, NNK⁺16, NFI⁺16, NS17, OHPR18, ORZ11, OM12, OVPK15, PAK17, Pie14, Pil17, PW12, PZM15, QZ10b, RJPB12, RS13, Rez19, RB13b, RSG14, Rod13, RHPWS13, RHT⁺15, RNS19, RR19, REV⁺17, Rui11, RSKG14, SPS⁺12, SGPJS⁺17, SH15, SS16a, SDF⁺17,

SFG⁺¹⁷, SHL⁺¹⁸, Sea10, SCW11, SDM⁺¹⁶, SEF⁺¹⁶, SE14, SH14, ST13, SHL⁺¹³, SPR⁺¹³, SZX13a, SZX13b, SMM15a, SMM15b, SMM⁺¹⁸, SKTT11, SZSS16, 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]. **Dependencies** [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, MR17, 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** [DFE⁺¹⁵, MA16, PRYI⁺¹⁷, TMJ15, WMW⁺¹⁰, Yap11]. **descriptor-based** [DFE⁺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** [BLL13]. **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, BLS10, 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, JRSH14, KG15, Kar17, KT12, KKL⁺13, KM13, KP10, LEdOLDIV17, 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, MR17, MAP18]. **DFTB/MM** [RN17]. **DFTB3** [IY18, KWG15, VHS⁺19]. **DGeCl** [MCLD10]. **DH** [SGPJS⁺17]. **DH2** [SBW12]. **di-mannose** [VM11]. **di-tetrazine-tetroxide** [MCAG⁺16].

diabatic [RGVC⁺19, YFH⁺19, DHOG13]. **diabetes** [PC11]. **Diagnosis** [MC12, TDKT10]. **diagonal** [BMBJ11, KTK17, WZ19]. **diagonalization** [BKŠ⁺11, HKR⁺14]. **diagonalization-free** [BKŠ⁺11, HKR⁺14]. **diagram** [OV14, VED10, ZY14]. **diagrammatic** [WWD14, YD17]. **diameter** [AS15a, KGHK12]. **diamond** [JWO15, WGN⁺16, WGLG⁺16, ZSL⁺11]. **diamond-like** [ZSL⁺11]. **dianion** [DP11, GRD⁺10, YZGS14a]. **diarylalkyl** [NS10]. **diarylalkyl-imidazole** [NS10]. **diarylalkyl-triazole** [NS10]. **Diarylbibenzofuranone** [SFA17]. **diaryldichalcogenides** [ZWGO16]. **diastereoselectivity** [AARP17]. **Diatomic** [ATM18, KKA⁺18, LS11b, Tsi14, WDKT19]. **diatomics** [TG12b]. **diatropic** [CPN⁺17]. **dicarbide** [Kop16, Kop18]. **dicationic** [GC18]. **dichalcogenides** [FZL⁺19]. **dichloropentacene** [ZYG⁺15]. **dichroism** [HNHR13, SEJ⁺18, ŠB13, ŠB15]. **Dickerson** [IPAA11]. **dicopper** [RHPWS13]. **dielectric** [DOM⁺11, DSF17, JLCA17, KCPMG12, PS13, WXL17, YHW17]. **Diels** [BJSI12, CC18a, FB14a, GNDA⁺12, LZH16, ORZ11, ST13, dSVdM⁺16]. **difference** [LLH17, WL10, Yon16, ZRCC11]. **difference-dedicated** [ZRCC11]. **differences** [BVC13, GO13, HDL⁺17, KHWB17, LGL11, PM18a]. **Different** [PH15, BRGN12, Dil15, DLC18b, FZL⁺15, GO13, GR11, GFPSD17, GMPB12, Kar17, KB19, MCS11, MC12, MPA12, NMLD13, NOKJ16, RHNN10, Rao11, SLP⁺12, SIG⁺15, TTC⁺18, TSNC⁺17, UT15, VVY18, ZR10]. **Differential** [HHT⁺13a, HHT⁺13b, CJL⁺13, MY17a, MY17b, WDKT19]. **Difficult** [RJS17, VDVR14]. **diffuse** [YCGA10]. **Diffusion** [NQB19, CPZ19, CPV⁺12, CC12a, GC11, KB19, RSL13, ZW17, WH11]. **diffusional** [MBR⁺15]. **Diffusive** [SM16b]. **digestion** [MEH18]. **digitized** [YNH⁺17]. **dihedral** [CYG⁺15, OZ14, SZBM13, WES13, ZRL⁺15]. **dihedrals** [LDH⁺14]. **dihydrated** [HvM19]. **dihydro** [RS17a]. **dihydrofolate** [RKDM14]. **dihydrogen** [PM13, UT14, WHX⁺10]. **dihydrogen-bonded** [UT14, WHX⁺10]. **dihydrogen/hydride** [PM13]. **dihydropyrido** [YZ15b]. **diimide** [MCC11]. **Diimine** [SCSM19]. **diiodide** [AARP17]. **diiodide-induced** [AARP17]. **diketopyrrolopyrrole** [HLWD15, RSSG18]. **diketopyrrolopyrrole-based** [HLWD15]. **diketopyrrolopyrrole-cored** [RSSG18]. **dilanthanide** [ZLZ14]. **Dilemma** [MM19]. **dilute** [KVR10]. **dimension** [HKRS11]. **dimensional** [BPLL12, FBvdB18, FZL⁺19, KYT⁺17, KRSC12, KTO13, MB16, PJ13, SG10a, SHL19, TYN15, TCX⁺13, TKC⁺11, XCLZ19, YZLZ19, ZWX16]. **dimensionless** [MS10]. **dimensions** [CHC⁺13, HAL14, SRL⁺15]. **Dimer** [BPPS19, LWL⁺16, ZQH19, ARRC15, ANH⁺11, BPPS17, CBTZ16, FCL⁺10, FMNC11, JT18, KCB⁺12, LCB10, Nav18, PD11, SKY⁺11, Tac17, WWKS16, YCGA10]. **Dimeric** [VL19, PS14]. **dimerization** [DSD⁺11, KAR12, TNI⁺19a, TLA10, WJX⁺10]. **dimerization/oligomerization** [KAR12]. **dimers** [AM19a, BCNH⁺11, BWKW10a, BWKW10b, CLFRO18, CK10, DT19, JKS⁺16, LJW11a,

LMI⁺14, PG18, PVS12, RS13, SZSS16, VT14, VMV19, YJ19, Zha11, dSH19].
Dimetallic [ZYG⁺14]. **dimethyl** [GC11, KPH⁺19, WLC12, ZSWL12].
dimethylacridine [FWS⁺18]. **dimethylaminoazobenzene** [KP10].
dimethylaminophenyl [YLZ⁺10]. **dimethylnitrosamine** [FFA14].
dimyristoylphosphatidylcholine [ML14]. **dinitrophenol** [MIS⁺15].
Dinuclear [SCSM19, ITY⁺19, OSS10, QLYL10]. **diodes** [FWS⁺18, ZGZ19].
diorganotin [CBDS19]. **dioxane** [GM17]. **dioxetanone**
 [RSLML12, dSdS12a, dSdS12b]. **Dioxide** [SC17, KPH⁺19, Kop17b, QZ10b].
dioxygen [DSM⁺11]. **dioxygenase** [DGH⁺11]. **dipeptide**
 [EJ13, IO13b, LL19a, MAMF19]. **dipeptides** [DHF⁺11, RSL16]. **diphenyl**
 [GKR13, Ray13, RKG11]. **diphenylalanine** [KLN16]. **diphenylamino**
 [FWS⁺18]. **diplatinum** [KT12]. **Dipolar** [YZN13, CSS17, LK11]. **Dipole**
 [Ali18, Cam19, GH16b, LIRL⁺16, ZBG11, AS15b, BLBG⁺13, DHOG13,
 GH16a, HBKL10, IY18, KCB⁺12, LHHW14, MNNK10a, MNNK10b, PC14,
 Yan11, dSH19]. **dipped** [IN13]. **Dirac** [JKS⁺16]. **diradical**
 [HWB19, VSH19, YSSB12, ZB18]. **diradicals** [SH18a]. **Direct**
 [LZY12b, SM18, WAM17, FF11, FSSW17, FSSW19, FZL⁺19, JCG⁺10,
 MMH19, RSB⁺13, Yu12a, LLHM16]. **directed** [CH14, HHBY10]. **direction**
 [PAK17]. **direction-dependent** [PAK17]. **directionality** [WGD⁺16].
diruthenium [CRC13]. **disaccharides** [GMSV14]. **discharge** [SMiN⁺19].
disconnectivity [SOJ14]. **discotic** [AWF⁺18]. **discover** [Hsu14]. **Discovery**
 [AKMT11, Aki16, CF18, FMG12, HYYZ13, Ibr11, IGK16, PVJ10, RRFV⁺18,
 Zim13]. **Discrepancy** [Yan11]. **discrete** [EJ13, MCUJ15, WAM17].
discretization [AD10, LLFH16]. **discriminate** [UCFR16]. **Discriminating**
 [FZL⁺15]. **discrimination** [YL13]. **discriminative** [KS12]. **discussion**
 [CDB10]. **disjoint** [BK13]. **dismutase** [GEP⁺14]. **disorder** [LLL⁺12].
Disordered [MYT18, GP12, LC16, LC17a, NDLW13, SJZ⁺15, ZC14].
Dispersion [HSJ18, AG12, BCNH⁺11, CLFRO18, cCVG⁺14, DAG19,
 GEG11, Han11, Has14, HGHP14, ITIN15, KB10, KSSH13, LCM⁺14, RJPB12,
 STS15, SSB11, SSB13, TG12a, WM17]. **dispersion-corrected** [CLFRO18].
Dispersive [TG12a, SDB⁺16]. **disproportionation** [DLP11]. **dissected**
 [FNSF⁺11]. **Dissecting** [CLFRO18]. **dissection** [BMFG16]. **dissimilarity**
 [HS17a, YDL⁺10]. **dissipation** [VVG13]. **Dissipative** [PH17, SCK18].
Dissociation [JL19, CR19, CCJ⁺11, GCCM15, Gil11, LBC⁺12, LL10c,
 MH11, Rob13, TNY18, WSH10, Won18, YPvD13, ZWLX11, ZZL19].
dissociative [FPH⁺19, HBL12, RIJ⁺11]. **dissolve** [SG10b]. **dissolved**
 [SIG⁺15]. **Distance** [PHDH13, DCŠ15, Hug14, JMS13, KCPMG12, LZ12,
 PPUBGD10, RPNP10, ŘRH12, UT14, Yon16, ZT14, dACP12].
distance-dependent [KCPMG12]. **distances**
 [BLDK⁺13, SSWX14, SMGB11]. **distant** [Jab18a]. **distinct** [JAHS⁺19].
distinction [ZY14]. **Distinguishing** [FD14, GMBX⁺16]. **distortion**
 [BMD19, INT18, LSL⁺19, SH19b]. **distortion/interaction**
 [LSL⁺19, SH19b]. **distortion/interaction-activation** [LSL⁺19].
Distributed [XFG⁺16, BMBJ11, KNR⁺18, UIW⁺10, XFG⁺15].

distribution [Bou14, COHI19, HDK⁺12, HNS16, JLCA17, KS18, MLG18, SK18, SYH12, TKNN10, YKO⁺11]. **distributions** [AS15b, BCSCJ⁺13, GWF11, GMG⁺10, LRER13]. **disulfide** [ZYS⁺10]. **DiTe2** [CPZ19]. **ditetrazaoles** [ZZWX11]. **dithiolate** [GS11]. **dithiolene** [KTK17]. **Divagations** [CDC19]. **Divalent** [WC14, BMB13]. **divergence** [PNG10]. **diverse** [KSM17, LLC⁺10]. **diversity** [WF16]. **Divide** [NN19, NNK⁺16, YKNN19, BRP⁺12, BGR13, BK17c, KKNN11, KFT18, NYH⁺17, NN18, WX12, YN15]. **Divide-and-Conquer** [NN19, YKNN19, NNK⁺16, BRP⁺12, BGR13, KKNN11, KFT18, NYH⁺17, NN18, WX12, YN15]. **divide-expand-consolidate** [BK17c]. **Dividing** [SLT⁺15]. **Diving** [SFM⁺18]. **division** [WWWW18]. **DLPNO** [MSPC19, CSGOA17]. **DLPNO-CCSD** [MSPC19, CSGOA17]. **DM** [KNR⁺18]. **DMF** [YZL⁺15]. **DMPC** [GBL⁺11, PS10, SLX⁺15]. **DMRG** [KMS⁺19]. **DMS** [RAGLL11]. **DNA** [AB10, BD11, BH13, BZH14, DMN14, DMN15, FPB12, GMBM18, GWX⁺12, HDK⁺12, HQC16, HvM12, IPAA11, KvdV14, LRVM18, LW11, LMZ⁺11b, LLT12, OHNK11, OLA15, QLQ11, SM14b, She12, SK18, SM15, SM16b, SPM⁺19, SZSZ16, YZWC11, YJXZ13, YS10, ZLL⁺10]. **DNA-backbone** [AB10]. **DNMR** [SR11]. **Do** [MJLV14a, QZ10b, VVY18, Jab18a, HJ13]. **docetaxel** [SZZ⁺18]. **DOCK** [ABM⁺15, AFBR17, BS10c]. **docking** [ABM⁺15, BMR11, BAMR13, BBOB16, BPB11, BCG10, BEL⁺11, CSSB11, DFF⁺15, DSX⁺11, ESB13, FM10, FTW12, FRLN10, GLB16, GSHM10, GPS10, GZM11, HDM⁺15, HWLW11, HZ13, KERY⁺16, Kri10, LS11a, LLC⁺10, LL10b, LZL⁺13, LJL⁺11, MMM⁺16, MPNS13, MP11, MFR10, NMF⁺14, NHK⁺13, NG10, OCLM14, OZS⁺13, PBLs19, PLAG11, PLV⁺11, Pro16, RTP⁺13, SA13, SPL⁺18, SHL⁺11, SKKS13, SZZ⁺18, TO10, VSD10, Vor10, WdVN12, WZ17, XML⁺15, XYZ18, YBS19, ZL11, ZWL13, ZSB⁺16, dVZ17, DKV18]. **docking*** [LZ11]. **docking-rescoring** [BMR11]. **DockoMatic** [JBAM11]. **dodecyl** [TFYO19]. **Does** [MBFG15, SPZP18b, MIS⁺15, SV15, SPZP19, Tan19]. **DOI** [Ano15-59, MT20]. **Domain** [KNE11a, AC11a, IMK⁺16, MBT14, RZ16, SFBT17]. **domains** [FCPJM14, OOK11]. **dominant** [Hua16, Jab18a]. **done** [LRvE17]. **Donor** [SB19, DGL⁺13, EHT19, FWS⁺18, Gil11, Lu11, MSV16, MIS⁺15, ZSTRS⁺18, ZZL19]. **donor-** [MIS⁺15]. **donor-acceptor** [ZZL19]. **donors** [KKK⁺19, LC10, TZ12]. **dopant** [Lin18, SRL⁺15]. **Doped** [LLLW19, GC18, GAMAC⁺14, LLC17, Lin18, PGC12, TN12, VS14, WMW11]. **doping** [HYL⁺11, LLD17, WMW11]. **DOT2** [RTP⁺13]. **dots** [DPAB16, WAB17]. **Double** [LLH⁺19, LLX⁺19, MEH18, Alg17, BE14, CCB15, CGR16, CC11, FC16, HLI⁺19, KM13, LOB18, LBH⁺11, LYC⁺13, LLL⁺12, OLPB19, PG18, SGPJS⁺17, SP13, Sea10, YYT12, ZLY⁺16]. **double-** [LOB18, OLPB19]. **Double-buffered** [MEH18]. **double-Hybrid** [CGR16, LBH⁺11, SGPJS⁺17, Sea10]. **double-stranded** [HLI⁺19]. **double-wall** [BE14]. **doubly**

[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, VLK⁺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, ŠSB⁺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, BLFZ13, BLBG⁺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, DGSVGM19, 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, SFCKK⁺¹⁴, SFCKK⁺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** [EEO⁺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, BLF14, BVHI17, BS16b, BE16, BS18, CHG⁺16, CMD13, 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, WWW18, 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** [HRH17, 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, RSL13, 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, BRSL12, CY13, Fra16, GLW13a, HNWF12, HvM17, HDHL15a, HDHL15b, HLXH18, ICS⁺¹³, JHMB⁺¹¹, Li14a, MT20, MSK⁺¹², RK16a, SFCK⁺¹⁵, SBN13b, SZX13b, SMM15a, WHAS⁺¹⁶]. **error** [HAGK10, Hua16, KFT18, PHK14, PD11, WNP⁺¹⁶, ZH12]. **errors**

[LEdOLdIV17, 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, RRH12, RB13b, WNM17, YD17, BMR11, BLFZ13, BLF14, DLT17, DS12b, GS11, HBI⁺17, ISO⁺13, Kid19, KLOS10, Kos16, KT18, KSC16, LJW11a, LW11, LHHW14, LZY12b, NN18, PW12, SF18, UM13, VBDS⁺11, VM11, WO15, PLAG11]. **evaluations** [HP10a]. **evaporation** [RSB⁺13]. **event** [BSL11, HNS16]. **event-driven** [BSL11]. **events** [LRvE17, Lum12, 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, IHHY15, 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, SZSS16, 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].

Extremely [ZM11].

F [ATP18, CXW14, CXS10, GPK⁺16, GTK10, HBL12, LZJ⁺11, Li14a, Li14b, MP19b, PMG⁺16, Rab12, STM⁺15, TFQ⁺10, TFQ⁺11, TCPPC14, WLW⁺10, WCY⁺11, YS13, ZYLL12, ZLLL12, BWKW10b, CCM15, Chu10, DKE⁺17, II10, JLLW19, KIOY19, LZL⁺15b, MLGB16, MSPC19, SMiN⁺19, SYH12, TCPPC14, Yu12a, ZWY⁺10b]. **F-ATP** [SYH12]. **F12** [BBG⁺11]. **F12a** [MLCD11]. **F130L** [ZJZM13]. **Fabi** [STM⁺15, SJ16]. **face** [GY10, Zha11, Zha11]. **Face-to-face** [Zha11]. **faces** [Gra18, PRJ⁺17]. **facile** [YDGZ15]. **facilitate** [MBFG15]. **Facilitating** [ESB13]. **facilitation** [CC18a]. **facilitator** [Mez10]. **facilities** [GP11b]. **Facing** [SLT14]. **factor** [BHF⁺18, GTZ⁺18, WLF11, WC11, XMSZ16]. **factorizations** [VKAM12]. **Factors** [GMSV14, EFOD13, LBH⁺11, LCW12, Pie14, VSA11]. **fail** [WCWV15]. **failure** [JWO15]. **FALDI** [dLC17, dLvNC18a, dLvNC18b]. **FALDI-based** [dLvNC18a, dLvNC18b]. **false** [LL19b]. **family** [PHC13, TJR19, ZLZ14]. **FAMSEC** [CSM16]. **Faraday** [Avd18]. **farming** [HPSK12]. **Fast** [AGR11b, BSZ⁺12, GZM11, HKR12, Kne11b, KDT⁺12, LAT10, LAT11, MLN⁺18, NHN16, PPJ14, RB13a, RDDS10, SM14a, SR11, TRA⁺16, VGV⁺11, VSP19, VRKT19, XSZL11, YZZ16, Yes12, dVZ17, BS19, DZA11, FGM11, GBFD12, Kan15, LFB14, LBSG16, MDT10, MS12, MPBJ11, OV14, dIRL11, Sch12, TJB12, WFS19, Yes15, YAO18, YFH⁺19, ZSS⁺13, ZCGM11, dSAdSL13, IY18, NZM18, YWJ⁺16]. **faster** [BG17, HC14, AM10]. **fate** [SIG⁺11]. **fathead** [TTL⁺12]. **FAU** [LZTV10]. **F...** [JLLW19]. **FE** [JJAB16, BTMS12, DAdGR15, LLLM11, LLSW14, VED10, WWKS16, Bac12, DAdGR15, GBGR16, KMT⁺19, PHC13, SCSM19, SSX⁺14, TNI19b, YPvD13, ZFS18, vADC⁺14, YMY⁺19]. **Fe-Doped** [LLLW19]. **Fe-embedded** [KMT⁺19]. **Fe-Ni-Cr** [ZFS18]. **Fe-S** [TNI19b]. **Fe/** [YMY⁺19]. **Feasibility** [DKV18]. **feasible** [VAMS14]. **Feature** [PL19, TD10, ZYS⁺10]. **Features** [FHMB15, ALW⁺10, AS11, ABM⁺15, DWL11, HMO⁺18, PLP⁺16, TYX⁺18, WC11]. **Featuring** [SJL18, Alg17, ZYW⁺16]. **feedback** [VHR16]. **FeFe** [GS11]. **Fehlberg** [AMGB10]. **Fenhexamid** [BHB19]. **FeO** [NH19, TLY⁺12]. **FEP** [MUGNVJ⁺18, HYUS11, LWZ⁺19]. **Fep1d** [BK15]. **FePO** [SMiN⁺19]. **FEREBUS** [DBDP16]. **Fermi** [SHL⁺18, STF⁺19, TSH⁺19]. **Fermi-Orbital** [STF⁺19]. **fermion** [EVR18]. **ferritic** [ZFS18]. **ferromagnetic** [ZB18]. **ferromagnetism** [HYL⁺11]. **ferromagnets** [ZA15]. **FeS** [TLY⁺12]. **Festschrift** [HIS17]. **FEW** [HG13]. **FF** [LGW12]. **FFLUX** [FP17a, FP17b]. **FFT** [MYT⁺14, WS13]. **FH** [TDT19, TDT19]. **Field** [LLH⁺19, AKMYB18, ALRM18, AJR16, ALH⁺10, BKŠ⁺11, BCSCJ⁺13, BCJC⁺14, BY11, BW15, BF17, BAF18, BK17b, BBG⁺18b, CRC13, CIKT13, CYG⁺15, CZAF17, COHI19, CLC11, CB11b, CB11c, CK17, DPNM11, DGPM14, DFF⁺15, DMAH15, DP15, DGB⁺13, DLZ15, EPD⁺11, FPH⁺19, Gar12, GSD10, GZM11, HH11, HKR12, HYSF19, HLH⁺12, HKR⁺14, HM13, HLEM18, HJLV16, HCP15, ISO⁺13, IHJ⁺13, JSXH16, KKH19, KMT⁺19,

Kid19, KLJ⁺¹⁷, KSK11, KT10, KFT18, KGJZ19, KMLS10, KVR10, Lar11, LvDH13, LC17b, LM18a, LPS⁺¹³, LPE⁺¹⁰, LN15, LLvG10, LvG13c, LL13b, LDG⁺¹⁵, LCL⁺¹⁸, MRO17, MBC11, MSS⁺¹³, MTvG12, MBE16, MLC13, MHR11, MP17b, NB19, NTNY15, ON14, PHC13, PLZ17, PdSC18, PG15, PZCL16, PLH16, PVM10, PS10, PNG10, Rod13, SH15, ST11, SM14b, SK17, SS19, SZBM13, Sie15, SGY⁺¹⁸, SS13c, SCSW13, SM15]. **field** [SYZ⁺¹⁷, SBvG14, Tak14, TYN15, VVW⁺¹⁸, VHA⁺¹⁰, VPR10, Vik11, VVLG17, WXL17, WS19, WTH⁺¹⁶, WC14, WZK⁺¹³, WDHZ13, XP13, XVA⁺¹⁶, XMA⁺¹⁹, Yan11, YWZ14, YJXZ13, YJ11, YN15, YCK16, YHVM12, ZSLL17, ZL11, ZSYH12, ZX19, ZDKM12, ZP13, ZM10, ZCGM11]. **field-based** [HKR12]. **field-dependant** [PNG10]. **field-dependent** [DP15]. **Fields** [Coo19, AS15b, BHI19, BVY⁺¹², BAS14, CCLP12, CPN⁺¹⁷, GCWS15, GMMH⁺¹⁶, HDPM14, HJ10, JYC⁺¹⁶, KT18, KWL⁺¹⁶, LZZ⁺¹¹, LZGS11, LGL11, LTP11, LBDP12, MSK⁺¹⁰, MSK⁺¹², MS15, ST11, SGY⁺¹⁸, SEM12, TTC⁺¹⁸, VVV^{+15b}, VHA⁺¹⁰, WKC^{+10b}, WLC12, WG12, YPKB12, ZRL⁺¹⁵]. **fifth** [KM13, LOB18]. **fifth-rung** [KM13]. **file** [SY16b]. **files** [MKS⁺¹²]. **filter** [MH10]. **find** [MN15, RVVK13, SB11]. **Finding** [Ber17, MLC13, ZQH19, GFG11, JZ17, Zim15]. **fine** [Hua16]. **fine-structure** [Hua16]. **fingerprints** [BHF⁺¹⁸, SS13b, Yap11]. **Finite** [ISO⁺¹³, ZQH19, BBG^{+18a}, BCCO10, BVC13, DJX^{+11b}, EPD⁺¹¹, Hsu14, LLH17, MLC13, MKK⁺¹⁹, NPP13, SK15a, TD11, TCX⁺¹³, WL10, XYX17]. **finite-difference** [LLH17, WL10]. **Finite-field** [ISO⁺¹³]. **finite-size** [DJX^{+11b}, Hsu14]. **Finite-Temperature** [ZQH19, MKK⁺¹⁹]. **FIPSDock** [LZL⁺¹³]. **firefly** [FD14, PE11]. **First** [BE12, BE14, BF19a, CCJC10, DBM⁺¹⁵, EB12, EBK13, EBPK17a, HFSO12, JCG⁺¹¹, LLLM11, LLB⁺¹², LCWW10, RRK16, THI⁺¹⁹, TKN13, UGK18, YPvD13, YR13, wZbZ11, BPE16, BCCO10, BEL⁺¹¹, EMD17, EB18, GD10, GA14, Ibr17, KLZ⁺¹⁸, LL10c, Lu11, MCF10, NNS15, OC19, PLZ17, RZG⁺¹³, SBGP18, SFA17, SK12, TKC⁺¹¹, TZ11, WXS⁺¹², WYL⁺¹⁵, WD10, WZK⁺¹³, YHCS11, Zha12b, Zha12a, ZWMW10, ZZ12, vADC⁺¹⁴, HYL⁺¹¹, NG10, SPZP18a]. **First-** [TKN13]. **first-order** [BCCO10, SK12]. **First-principle** [CCJC10, DBM⁺¹⁵, LLB⁺¹²]. **First-Principles** [HFSO12, BE12, BE14, EB12, EBK13, EBPK17a, JCG⁺¹¹, LLLM11, wZbZ11, BPE16, EMD17, EB18, GD10, KLZ⁺¹⁸, PLZ17, RZG⁺¹³, WYL⁺¹⁵, WD10, ZWMW10, ZZ12, vADC⁺¹⁴, HYL⁺¹¹, SPZP18a]. **First-to-Third-Row** [BF19a]. **Fission** [NNT⁺¹⁹]. **fit** [BHNS14, BCG10, GDV17, KGM12, WKC^{+10b}]. **fitted** [KGJZ19]. **Fitting** [SN16b, BS19, Boz18, DGPM14, FN12, Gra15, Hil13, LBGS16, MKH⁺¹³, MKM⁺¹⁷, SY11, VYM15, WOH16, WOH18, ZDZM13]. **five** [HCD⁺¹⁰, KJDB12]. **five-membered** [HCD⁺¹⁰]. **fix** [WCWV15]. **Fixed** [Jia19, AS15b, FSD⁺¹⁸]. **Fixed-charge** [Jia19]. **flake** [Lin18]. **flakes** [SDF12]. **flanks** [RSSG18]. **flash** [AGM⁺¹³]. **Flavins** [Ale19]. **flavonoids** [PC11, ZDW18]. **flavor** [PFAS⁺¹⁹]. **Fleksy** [WdVN12]. **Flexibility** [OXBW16, BCG10, FTW12, FMG12, GTZ⁺¹⁸, KL14, LZ11, NPG17,

PRSG13, PHH⁺¹², YBS19, dVZ17]. **Flexible** [GLB16, MKM⁺¹⁷, NG10, SC17, WdVN12, AFPI13, CPZ19, CZNA11, DVVP14, FRLN10, GBW⁺¹⁴, HDM⁺¹⁵, JC16, LS11a, LSH12, MLN⁺¹⁸, PL14, PS13, PJ13, RHJ11]. **flexible-boundary** [PL14]. **Flexible-Monomer** [SC17]. **flip** [ZLHH14]. **flooding** [HYNS19, HNTS15, HNS16]. **flow** [TCC⁺¹³]. **fluctuating** [CCB15, CMS13, GM17, IIHY15, KUDG12, YWZ14]. **fluctuation** [II10, OXBW16]. **fluid** [Hei18]. **fluid-state** [Hei18]. **fluids** [KGHC15]. **fluorene** [CH10, HXM⁺¹⁶, PH10b, YJN⁺¹¹]. **fluorene-phenylene** [CH10]. **fluorescence** [CH10, EJ13, FWS⁺¹⁸, LM18b, VM19, ZLL⁺¹⁰, ZGZ19]. **fluorescent** [CSC⁺¹⁸, LZL⁺¹⁰, NSO⁺¹⁴, PGW⁺¹⁷, SCF⁺¹⁹, WJG⁺¹³]. **Fluoride** [LCC18, LZL⁺¹⁰, MBRC16, NC12, Rab12, SBGP18, SRL⁺¹⁵]. **fluorides** [ASS⁺¹⁷, Sán17]. **fluorinated** [DKE⁺¹⁷]. **Fluorine** [VMV19]. **Fluorine-centered** [VMV19]. **fluorobenzene** [KS13b]. **Fluorophilic** [vRWGS17]. **fluoroquinolones** [MPNS13]. **flux** [AA18, LGOM⁺¹⁵, MT19b, Pol13, RLA18, VGTL16, dSH19]. **fluxes** [GNDA⁺¹²]. **Fluxional** [YLZ⁺¹⁹, YLT⁺¹⁹]. **Fly** [PAK15, CF18, MIOM13, PL14]. **FMO** [LFN⁺¹⁰, UIW⁺¹⁰]. **FMO/PCM** [LFN⁺¹⁰]. **FO** [Chu10, GTK10]. **focal** [Won18]. **Fock** [ACD^{+13a}, ACD^{+13b}, BY11, BP18, CKH19, CB11d, FRN15, GRN19, HJKJ13, IYK11, Mat10, PB14, PW12, ŘRH12, SG13, UIW⁺¹⁰, VL17a, VL19]. **Fock-space** [ACD^{+13b}]. **Focused** [MMM⁺¹⁶, CHR^{+12b}, CHR^{+12a}]. **focussing** [CB11c]. **fold** [LK11]. **Foldamers** [Spr18]. **Folding** [MFEM16, AD10, BPE16, CYI⁺¹⁰, CBG16, DMJ17, DAB16, GRL⁺¹¹, GRL⁺¹², HTS15, HNTS15, HTS17, HLH⁺¹², JCX10, KLS10, KMLS10, LKL10, LLvG10, LvG13a, MFEM15, PBE16, WNM17]. **foldons** [CYI⁺¹⁰]. **folds** [CDS16, CHP11, MV17]. **followed** [AKMT11, Mau14]. **Following** [GS16, MFEM16, XFG⁺¹⁶, Tac17]. **footprint** [BMR11, BAMR13]. **foray** [KK19]. **forbidden** [TN18]. **Force** [CYG⁺¹⁵, COHI19, Coo19, DBG0⁺¹⁷, DP15, GSD10, LZZ⁺¹¹, LLH⁺¹⁹, PS10, PNG10, Sak18, ZSYH12, AKMYB18, AOW11, ALRM18, AS15b, AJR16, BHI19, BW15, BF17, BAF18, BVY⁺¹², BMBJ11, BAS14, CCLP12, CRC13, CIKT13, CZAF17, CLC11, CB11b, CB11c, CK17, DPNM11, DGPM14, Dil15, DFF⁺¹⁵, DMAH15, DGB⁺¹³, DLZ15, FED17, FHZA⁺¹⁸, FPH⁺¹⁹, GCWS15, Gar12, GZM11, HH11, HKR12, HYSF19, HDPM14, HLH⁺¹², HJ10, HM13, HLEM18, HJLV16, HCP15, IHJ⁺¹³, JYC⁺¹⁶, KLJ⁺¹⁷, KERY⁺¹⁶, KGJZ19, KS12, KSR⁺¹⁶, KT18, KLS10, KMLS10, KWL⁺¹⁶, LvDH13, LC17b, LM18a, LPS⁺¹³, LCA17, LZGS11, LN15, LLvG10, LGL11, LvG13c, LTP11, LDG⁺¹⁵, LCL⁺¹⁸, LBDP12, MTM14, MHT⁺¹⁸, MSK⁺¹⁰, MSK⁺¹², MRO17, MJC14, MBC11, MSS⁺¹³, MTvG12, MBE16, MJG⁺¹⁵, MIOM13, MS15, NB19, PHC13, PLZ17, PG15, PZCL16, PLH16, PVM10, RI10, ST11]. **force** [SM14b, SK17, SZBM13, Sie15, SGY⁺¹⁸, SNDK16, SS13c, SR18, SM15, SYZ⁺¹⁷, SBvG14, TTC⁺¹⁸, VVV^{+15b}, VVW⁺¹⁸, VHA⁺¹⁰, VVLG17, Vor12, WKC^{+10b}, WLC12, WOH16, WOH18, WS19, WTH⁺¹⁶, WC14, WG12, WDHZ13, XP13, XVA⁺¹⁶, YWZ14, YJXZ13, YPKB12, YHVM12, ZRL⁺¹⁵,

ZL11, ZP13, ZM10, ZCGM11]. **force-constant** [WOH18]. **Force-field** [COH19, 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, SFCCCK⁺14, SFCCCK⁺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]. **fpm** [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, MSÁK12, 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, WWW18, 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, BLBG⁺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, LBGS16, 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, SZS16, 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_embed** [WHAS⁺¹⁶, WHAS⁺¹⁰]. **Ga** [UT15, Mit13]. **Gabedit** [All11]. **GAFF** [MPBJ11]. **galactosidase** [AKMT11]. **GALAMOST** [ZLL⁺¹³]. **GalaxyDock2** [SKKS13]. **GalaxyDock3** [YBS19]. **GalaxyTongDock** [PBL19]. **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**

[RSR⁺12, OYK⁺11, Bou14, CGA19, DLL⁺10, EPD⁺10, FRC18, IT19, JLCA17, LOB18, Leh15, MG11, MKB⁺13, OLPB19, POB13, SPH11, SH19a, Sun15, TH13, VKTRJ15, ZKE⁺17]. **Gaussian-based** [CGA19, JLCA17]. **gaussian09** [RS13]. **Gay** [SLX⁺15]. **GB** [OBW12, VM11]. **GBMV2** [LC17b]. **GBSA** [DSX⁺11, GR10a, IMSR18, RDDSD10, STM⁺15]. **GC** [GWX⁺12, YZWC11]. **GC-** [YZWC11]. **GC-/AT-rich** [YZWC11]. **GC-related** [GWX⁺12]. **GDP** [SS13c]. **Ge** [Cas14, MCK17b, PMG⁺16, Sak18, UT15, YW12, LYL16, WKC11]. **GeauxDock** [DFE⁺15]. **GeC** [HSY⁺11, Kop18]. **GeH** [Kop19b]. **gelatinases** [XDL⁺10]. **Gelessus** [Spr10]. **gene** [CQFC10]. **general** [AA18, BSL11, EWK⁺13, FNSF⁺11, HSN14, Ish12, NLP⁺16, PH17, RJR14, Sun15, VHA⁺10, YHVM12]. **general-contraction** [HSN14]. **Generalization** [Sah18]. **Generalized** [GH16b, KCMPMG12, MSPC19, AB16b, BSPP⁺13, DSF17, FCE15, GH16a, HWLW11, LL10a, MA16, NMH19, PS13, SZTSM10, SSBW14, VMPS17, WWKS11, WHM10, WBVE16]. **generally** [KKK⁺19]. **generate** [MPA12, MdOdQ18]. **generated** [HWLW11]. **Generation** [ADF⁺10, AIM⁺18, MPA10, RvL11, STF⁺19, CAD16, GMSdG15, GKJ⁺19, HGY15, KLJ⁺17, KSH⁺17, LTT16, RB13a, RGVC⁺19, TDP⁺12, WLF19, WHJH13, ZCGM11]. **Generator** [MYT18, Gar12, GPM17]. **generators** [CLK11, GPM17, HMM10]. **genes** [YS10]. **GENESIS** [KJM⁺17]. **genetic** [AC12, CB11b, FRLN10, LLJ12, NC12, RSL16, SHMO11, SSO19, WMW⁺10, YVEI⁺17, LMA15]. **GenIce** [MYT18]. **GenLocDip** [GH16b]. **GeO** [DLSD13]. **Geometric** [MK11, AM19a, AM19b, CDB10, CDBM11, EH13, FXC⁺13, HHT⁺13a, HHT⁺13b, LLFH16, REH13, TCC⁺13]. **geometric-quantum** [CDBM11]. **Geometrical** [DPAB16, HRJ⁺14, JRSHP14, NSN19, LCM⁺14, SPR⁺13, Tak10, Tsu19, UT14, HRJ⁺15]. **Geometrically** [RIJ⁺11]. **Geometries** [VL19, ZLX⁺19, Alg17, HCP15, SRA17, SIT18, Tak10, LXZ⁺10]. **Geometry** [MP13, BW11b, CGA19, EPD⁺10, ELP19, FB10, Kow11, LIRL⁺16, MCLD10, OZS⁺13, Pon10, RSSG18, RS13, REH13, SLG15, SMM17, Tak18, VBV13b, WAB17, WX12]. **geometry-dependent** [EPD⁺10]. **Germanium** [GSMM15, ALH⁺10, Kop18]. **germylene** [Kop19b]. **GeSbTe** [NIIT15]. **GFP** [UD12]. **GGA** [BG13, EH13]. **ghost** [CMF⁺17]. **ghost-hunter** [CMF⁺17]. **Giant** [JCG⁺11]. **GIAO** [PTK11]. **GIAO-CCSD** [OPR16]. **gibberellin** [HYYZ13]. **gibberellin-binding** [HYYZ13]. **Gini** [WF16]. **GIPAW** [SPZP18b, SPZP19]. **GIST** [RNSF⁺16]. **give** [AA18, JT18]. **glass** [GFGS18]. **glasses** [You10]. **Global** [LvDH13, OKIS17, PRSG13, Tak10, VL19, BK17b, CPN⁺17, CZZL19, DS15, DMAH15, FDH19, GPE13, LK11, LL11, MP13, MB14, MO15, MCAY15, SKKS13, SC15, TSZQ12, Vor10, WDHZ13, Xhd15, XCLZ19, ZL11, DH11]. **Glu** [EJ13]. **glucopyranose** [HH10]. **glucosamine** [ZBP11, ZP13]. **Glucose** [APY⁺16, WFL⁺19]. **GLYCAM06** [SA10]. **GLYCAM06/TIP3P** [SA10]. **Glycan** [JSD⁺11]. **glycine** [DB12, DP15, FCD10, MC10, SPZP18a, SPZP18b]. **glycoconjugate**

[LABSG17]. **glycol** [MSY19, TFYO19]. **glycoproteins** [JSD⁺11, PFVL14]. **glycosaminoglycan** [CHKR10, SZdB19, SA10]. **glycosidic** [HH11]. **glycosyltransferase** [RN17]. **GmbH** [Spr10]. **GMCT** [UU12]. **GneimoSim** [LWK⁺14]. **gold** [Ano15-58, BH14, CCJC10, FHT⁺15, FDH19, GAMAC⁺14, Li14a, Li14b, LHKS12, LH14b, MFR⁺11, MG14, MBFG15, SRR16, SKTT11, YLL11]. **gold-thiolates** [FHT⁺15]. **Goldberg** [WTH⁺16]. **Good** [SB10]. **GPCR** [LLHM16, MFR⁺17]. **GPGPU** [UM13]. **GPR119** [HK18]. **GPU** [AKK⁺16, AGB13, BK17c, CVT⁺11, DZT11, HAP⁺12, Kan15, KGHC15, KPF⁺15, KPF⁺19, MLN⁺18, MEH18, PZCL16, REV⁺17, SBV10, SOM⁺13, UTM11, YLGX14, YSG12, YKNN19, ZLL⁺13]. **GPU-Accelerated** [YKNN19, AGB13, CVT⁺11, HAP⁺12, YLGX14, ZLL⁺13]. **GPU-based** [KGHC15]. **GPU-enabled** [BK17c]. **GPUs** [GBL⁺11, HLW⁺17, HLEM18, KK17a, RŠRR15]. **Gradient** [DS15, CDM10, HHBY10, KN17, MN19, SH15]. **gradient-directed** [HHBY10]. **Gradients** [GP11a, WM12, Boz18, BWMSM10, CCB15, HH16a, HH17, LBGS16, LFN⁺10, RSG14, SFG⁺17, SSMW09, SLG15, TSH⁺19, vLBBR12]. **grafted** [DSB⁺19]. **grafting** [KKR⁺13]. **Grain** [CPK19, SOM⁺13]. **Grained** [MT20, BLKP12, CAD16, HYSF19, HHWL17, JC16, KCK⁺17, KVQC⁺11, KLS10, KMLS10, KZP⁺18a, LZ12, LZX16, LZZ14, LZLMP16, MSLS10, MT19a, MBC11, MBC13, NST14, RSG⁺10, SLX⁺15, SDZ17, SJ17, SGY⁺18, SM15, SAvG15, WBF17]. **graining** [BJP15, GMPB12, ML14]. **gram** [BHI19, GWW19, EVR18]. **gram-based** [GWW19]. **gram-negative** [BHI19]. **Grand** [HLvdV13, PHH⁺12]. **grand-canonical** [PHH⁺12]. **Graph** [WSH10, DH14, GPGSM11, GPGSM12, Ihl12, MCC12, PSdPE⁺10, Pog10, RPNP10, dLvNC18a]. **graph-based** [DH14]. **Graph-theoretical** [WSH10, PSdPE⁺10, Pog10]. **graphane** [YZZ⁺17]. **graphene** [BSD18, CMM18, dRCFGRB18, DJX⁺11b, DJX⁺11a, JWO15, KMT⁺19, Lin18, LWZK13, LCM⁺14, PL18, RRK14, RLZ⁺18, SDF12, WCT⁺11, WSZW15, WYL⁺15, WTH⁺16, YSSB12, YZZ⁺17]. **graphic** [HASR⁺12]. **Graphical** [SJL18, All11, GBL⁺11, HZY⁺10, HSW⁺19, LLLC11, LBB⁺15, PVZ13, SEF⁺16, STH⁺10, WSGN11, WS13, YWJ⁺16, YDL⁺10, YN15, YS10, ZKE⁺17]. **graphics** [AB16a, AB16b, BDTP11, CKKK16, EP10, HKR12, HEMCZE⁺14, MSSP17, SR11]. **graphite** [Fom13, IN19, LAM19]. **graphitic** [LL13b]. **graphs** [AGR11b, RNP13, RNVP13, SOJ14]. **Grätzel** [VÅA14]. **gravitational** [DS15]. **Grcarma** [KG13]. **green** [LWL⁺11, NSO⁺14, PGW⁺17, yOTn16]. **greener** [ZX19]. **Gregori** [Ihl12]. **Gregori-Puigjané** [Ihl12]. **Grid** [BAMR13, CPK19, HEMCZE⁺14, BPLL12, CGA19, CKKK16, FHMB15, KP11, KKH18, LZ11, LLZA12, MMM⁺16, NCT18, RLLHL12, dVZ17, CM13b]. **Grid-Based** [CPK19, BAMR13, HEMCZE⁺14, CGA19, KP11, KKH18, LZ11, LLZA12, MMM⁺16]. **grids** [DH17, Min18]. **Gro2mat** [DDK14]. **gromacs** [Nav18, AG11, Abr11, Gar12, GP11b, KPF⁺15, KPF⁺19,

LRvdSM15, PHH⁺¹², TKT11, KWG15, DDK14]. **GROMOS** [HH11, HLH⁺¹², KAG⁺¹², LGL11, LvG13c, MRO17, MSvG12, PLH16, PFVL14, SBV10]. **GromPy** [PHH⁺¹²]. **Ground** [GMBM18, Kop19a, BBI⁺¹¹, CCM15, FAA15, GCCM15, HH16a, HWB19, Kop15a, LLBO12, LYC⁺¹³, LX11, LS11b]. **Ground-State** [Kop19a, HH16a, Kop15a, LLBO12]. **group** [Alg17, CAP17, Dry14, EHSPT16, FC16, GZZM16, GPK⁺¹⁶, Gil11, GWZ15, HB14, JJJ16, LZL^{+15b}, LTR18, SSSM15, TG12b, Tsi14, VDVR14, VRKT19, WS12, WZH⁺¹⁸, Xhd15, LdSRR16]. **group-IV** [WZH⁺¹⁸]. **groups** [Kan15, KV15b, LPS12, TN10, WGL⁺¹¹, WZC⁺¹⁹]. **growing** [JZ17, Zim15]. **Grown** [SJSS19]. **growth** [BHF⁺¹⁸, DWZ⁺¹⁷, FCL⁺¹⁰, KHE⁺¹⁹, LL10c, LZLMP16, MZZ11, OME16, RS14, VMV19, WC11, XYW⁺¹⁴]. **GRRM17** [MHT⁺¹⁸]. **Grubbs** [RS17b]. **GSK3** [LJL⁺¹¹]. **GTKDynamo** [BTA⁺¹³]. **GTP** [SS13c]. **guanidine** [HRJ⁺¹⁴, HGHP14, HRJ⁺¹⁵, JRSHP14]. **guanidinium** [CCCLCGRO14]. **guanine** [BZH14, CBG17, KK19, LZH⁺¹¹, PDMT10]. **guanine-cytosine** [LZH⁺¹¹]. **guanines** [WGL12]. **guanylthiourea** [MAPB10]. **guest** [CC18b, OAN15b, YDGZ15]. **GUI** [WCJ⁺¹⁴, HBJ⁺¹⁷, JCL⁺¹⁷, KLJ⁺¹⁷, QLKI19]. **guide** [BS15, GKV⁺¹³]. **guided** [OCL11, Tak18, WBVE16, YVEI⁺¹⁷, Yon16, ZC14]. **guiding** [HS17a]. **GULP** [SN16a]. **gWEGA** [YLGX14].

H [BSF18, BS16b, CXS10, CG12, CSNCS⁺¹⁸, DM15, DT19, GPK⁺¹⁶, HZ11, HSY⁺¹¹, HVS16, JLS⁺¹⁰, JLH⁺¹⁴, LLL⁺¹¹, LdSRR16, LAHS16, LWD13, MLQ⁺¹², MCAY15, NMLD13, OKY18, OPR16, PMG⁺¹⁶, RMPAM15, Sak18, SNDK16, STS⁺¹⁰, TNY18, Tak11, TSJ⁺¹⁰, TFQ⁺¹¹, UT14, UT15, VIT⁺¹⁵, VV14, WKC10a, WKLC12, WHL⁺¹⁰, WWKS16, WLF19, WCL⁺¹¹, XFX⁺¹⁶, XCLZ19, YKH15, YZ15b, YZZ⁺¹⁷, ZYLL12, AS15a, Ben17, BS10b, CK10, CKL⁺¹¹, Chu10, DT19, DHE⁺¹², EVR18, GTK10, GS11, HZ11, HRL11, JLLW19, KTT16, KMT⁺¹⁹, LJW^{+11b}, LWD13, MSPC19, Niz13, OKIS17, PLFS18, PTK11, Pie14, Pon10, STS⁺¹⁰, TS15a, TKCN19, UT15, UvSvdWK19, WGL12, WWTL19, WvRSM14, Xhd15, XCLZ19, YHX19, YZ15b, YZZ⁺¹⁷, YZLZ18]. **H-** [Pon10]. **H-atom** [BS10b]. **H-bonding** [WGL12]. **H-C-C-H** [YZZ⁺¹⁷, YZZ⁺¹⁷]. **H-cluster** [GS11]. **H-F** [JLLW19]. **H-FORMS** [RMPAM15]. **H-indol-** [YZLZ18]. **H \dot{O}** [BS10b]. **H/D** [Chu10, KTT16, UT15]. **H4** [BEEL14]. **hafnia** [EBPK17a]. **hafnia-based** [EBPK17a]. **hafnium** [MTS⁺¹⁹]. **hairpin** [LJW^{+11b}]. **Half** [SWMW10, QS19, TS15a, WDZN16, YLT⁺¹⁹]. **half-lives** [QS19]. **half-sandwich** [TS15a, YLT⁺¹⁹]. **half-saturated** [WDZN16]. **halide** [Li14a, Li14b, NC13, ZWY^{+10b}]. **halides** [FWB14, PGS⁺¹⁵, RVM19, VVP12]. **halobenzene** [CvM19, EPH⁺¹⁵, HvM19]. **halocyclopentadiene** [CvM19]. **halofullerenes** [TFQ⁺¹⁰]. **Halogen** [CvM19, FPRS14, GSMZ19, HvM17, HvM19, VVMY18, WFZ⁺¹⁸, ASW19,

BT18, CFM⁺¹⁹, DGB⁺¹³, HDB15, HvM16, Ibr11, JW16, LDJ⁺¹⁰, LLL⁺¹¹, LZL^{+15b}, LZSM19, Rez19, SJ16, TY10, VVJ15, VVY18, VMV19, ZBMZH15].
halogen- [LZSM19]. **halogen-bonded** [LZSM19]. **halogen-bonding** [HDB15]. **Halogen-Bonds** [WFZ⁺¹⁸]. **halogen-centered** [VMV19].
halogenabenzene [CvM19]. **Halogenated** [HvM17, EPH⁺¹³, HvM16].
Hamiltonian
 [IO13b, KCK⁺¹⁷, LCK⁺¹⁸, MGWR12, OZ14, VFRAR16, WGA18, YS13].
handle [FRC18]. **Handling** [IO13a, MBC13]. **Happens** [SMB18]. **Hard** [WBKS19]. **Hardness** [SBR13]. **hardnesses** [YB16]. **HArF** [LZJ⁺¹¹, WZK⁺¹³]. **Harmonic** [LBH⁺¹¹, Ano15-58, BH14, CHC⁺¹³, LLH17, WAM17, WTH⁺¹⁶]. **Hartree** [BY11, BP18, CKH19, CKKK16, CB11d, FRN15, GRN19, HJKJ13, IYK11, Mat10, PB14, PW12, RRH12, SG13, VL17a, VL19]. **harvesting** [KDR⁺¹⁸]. **HBeH** [UT14]. **HBO** [LCL⁺¹⁰]. **HBr** [LGW12]. **HCCH** [Tak10]. **HCCX** [LDJ⁺¹⁰]. **HCFC** [RVdMB16]. **HCFC-132b** [RVdMB16]. **HCl** [CSNCS⁺¹⁸, LGW12, JT18, KVR10]. **HCN** [DBGO⁺¹⁷, SKGB13]. **HCN/CNH** [DBGO⁺¹⁷]. **HCV** [SBT17]. **HDAC** [GWZ15]. **HDFS** [NMH19]. **H···** [UT15]. **headgroup** [PS10]. **headpiece** [LKL10]. **heat** [MO15, NMH19]. **heat-of-formation** [NMH19]. **Heats** [KSM16, ZWX19, ZWX16]. **heavy** [Tru18, VKAM12, WS11]. **Heck** [dSdLBNB17]. **heights** [BS10b, GAJ⁺¹⁷, KG15, ZW17]. **Heine** [Spr10]. **Heisenberg** [AA18, CME11, KMS⁺¹⁹]. **helical** [FCD10, HLI⁺¹⁹, KB14a, LHKS12, LH14b, MCvdV13, MV17, PRP15]. **helices** [DSF17, HHT^{+13a}, HHT^{+13b}, KKK⁺¹⁹]. **helium** [TEDT18]. **helix** [CCOH14, HLI⁺¹⁹, LMI⁺¹⁴, WXL⁺¹²]. **helix-inversion** [HLI⁺¹⁹]. **heme** [FBEM11, INT18, LS11b, PHC13, SOYC12, SHB17, TN10]. **Henkelman** [QB11]. **Henry** [QLYL10, VKTRJ15]. **HEOM** [KNR⁺¹⁸, KNR⁺¹⁸]. **HEPT** [ZsA10]. **heptagon** [GZH10]. **heptagonal** [GLF16]. **heptane** [RRF11]. **Hess** [YS13]. **Hessian** [Car14, GMPB12, WOH16, WOH18]. **Hessians** [GVP⁺¹⁰]. **hetero** [DAP⁺¹⁸]. **hetero-metallic** [DAP⁺¹⁸]. **heteroatom** [NK19]. **heterobimetallic** [dSDdAR10]. **heterocyclic** [BSDP16, CWT⁺¹², KYKR15, LXZ⁺¹⁰, RF15, SGHL13, WS12, dSdLBNB17]. **heterodimer** [YYT12]. **Heterogeneous** [DSF17, AFPI13, CKKK16, MEH18, RNS19, TM18, YZZ⁺¹⁷]. **heterojunctions** [FZL⁺¹⁹]. **Heuristic** [Hel13, MS16, Tak10, Tak18]. **Heusler** [GD10]. **HeX** [SLIB12]. **hexa** [GK15a]. **hexa-aqua** [GK15a]. **hexaazatrinaphthylene** [AWF⁺¹⁸]. **hexaazatrinaphthylene-based** [AWF⁺¹⁸]. **hexabenzocoronene** [RVB⁺¹²]. **hexacoordinated** [MC10]. **hexafluoropropylene** [VMV19]. **Hexahalogenated** [VVJ15]. **hexameric** [RCM^{+13a}, RML⁺¹⁵]. **hexasilabenzene** [NK19]. **hexopyranose** [HH11, PLH16]. **hexopyranose-based** [HH11, PLH16]. **hextuple** [XTn18]. **HF** [BRLS12, LGW12, MCK17a, WZH⁺¹⁸, BRLS08, Chu10, JT18, LSH⁺¹¹, SKGB13, YZLZ19, YHX19]. **HF-based** [YZLZ19]. **HF/DF** [Chu10]. **HF/DFT** [BRLS12, BRLS08]. **HF/HCl** [JT18]. **HFC** [AR10]. **HFC-263fb**

[AR10]. **HFD** [AASP18]. **HFD-like** [AASP18]. **HfO** [HYL⁺11]. **Hg** [SLIB12, BBI⁺11, LLLW19]. **HGeCl** [MCLD10]. **HgHe** [BBI⁺11]. **HgXe** [BBI⁺11]. **HH** [LGW12]. **HI** [LGW12]. **hIAPP** [PP19]. **hidden** [DVVP14, LTT16]. **Hierarchical** [JYC⁺16, BCG10, GBFD12, KKNN11, RMPAM15, SNS13]. **High** [HB19, KLZ⁺18, MCLD10, MKB⁺13, RSL13, ZHS⁺18, BACSCJ⁺10, Cam15, CM13b, CSSB11, DH17, DLSD13, ESB13, EWK⁺13, FBvdB18, GKJ⁺19, GWPJ11, IPAA11, JBAM11, JC16, KSM16, KSM17, LL10a, LCK⁺18, MJLV14a, MO17, OHPR18, OPB⁺12, PVL⁺13, PVJ10, RVCFF13, RNS19, REH13, SHL19, SC15, SWW⁺19, WGL⁺11, WDLG12, ZWL13, dSAdSL13, SDIP18]. **high-accuracy** [RVCFF13, SDIP18]. **high-confidence** [KSM17]. **high-dimensional** [FBvdB18, SHL19]. **High-level** [MCLD10, EWK⁺13, KSM16, KSM17, PVL⁺13]. **high-order** [REH13]. **High-Performance** [HB19, RSL13, CSSB11, ESB13, EWK⁺13, LL10a]. **high-precision** [DH17]. **high-pressure** [WDLG12]. **High-quality** [MKB⁺13]. **high-resolution** [CM13b, JC16]. **high-temperature** [DLSD13]. **high-throughput** [ESB13, PVJ10, RNS19]. **higher** [NYH⁺17, PJ13, VKAM12, WHM10]. **higher-dimensional** [PJ13]. **higher-order** [NYH⁺17, VKAM12]. **Highlighting** [BRGN12]. **Highly** [CHG⁺16, DBDP16, HAL14, LLZA12, LWL⁺16, BWKW10a, BWKW10b, DSV⁺19, HYUS11, KOY⁺12, KZK⁺12, KV15b, OK16, TFQ⁺10, TJB12, LZZ14]. **hindrance** [MP17a]. **Hirshfeld** [Man13, VVB13, VGV⁺11, EV14, GBVA11, OVPK15, VBV13a]. **Hirshfeld-based** [OVPK15]. **Hirshfeld-I** [Man13, VVB13, VGV⁺11, VBV13a]. **histidine** [KFY⁺13, WC14]. **histogram** [Fer17, HHWL17, SH11b, ZH12]. **histone** [GHK12, GH10, GSD10, KC13a]. **HIV** [DLZ15, NHN16, OBW12, SYH12, TTB⁺10, UNT16, XLY12, ZsA10]. **HIV-1** [DLZ15, NHN16, SYH12, TTB⁺10, UNT16, XLY12]. **HIVgp41** [AFBR17, BAMR13]. **HMH** [LDJ⁺10]. **HNCN** [WHDL11]. **HNO** [BLG10]. **HOB** [LCL⁺10]. **HoF** [NMH19]. **hole** [BSF18, Cas13, CWHH11, EPH⁺13, GZZM16, GA12, LZL⁺15b, PAK17, PTB⁺15]. **holes** [PM18a]. **Holliday** [Ish10, She12]. **hollow** [AAMR18]. **holographic** [CDB10]. **HolT** [She12]. **HOMO** [CBDS19, NPG⁺18, RS17a]. **homoarginine** [MUGNVJ⁺18]. **homoarginine-containing** [MUGNVJ⁺18]. **Homocysteine** [AALCM11]. **homodesmotic** [NMH19]. **homologated** [ZLL⁺10]. **homologation** [GRCL12]. **Homology** [ZX11, BPB11, DJ13, KOY⁺12, WZWW18, XFTW15, YZZ16]. **homology-based** [WZWW18]. **homology-model** [KOY⁺12]. **homology/ab** [DJ13]. **homolysis** [SZ17]. **homonuclear** [BWKW10a, BWKW10b]. **homopeptides** [FCD10]. **HomoSAR** [BPC13]. **HONO** [BLG10]. **HOONO** [BLG11]. **hopping** [JLH⁺14, KT19, KV14, LZW⁺11, RDR16, SRSLO15, SKA19]. **Horizontal** [PC16]. **hormone** [HYYZ13, LLL⁺10, NS10, OME16]. **hormone-dependent**

[NS10]. **hormone-receptor** [OME16]. **horsetail** [MCRL17]. **Host** [CC18b, OAN15b, YDGZ15]. **hot** [HQSZ19, RFHG10]. **Hou** [JW12]. **HOX** [LZJ⁺11]. **HP** [LKL10]. **HP-36** [LKL10]. **HPCCS** [ZHS⁺18]. **HPt** [dSDdAR10]. **HRPA** [SPHF⁺18]. **HS** [XCLZ19]. **HSE** [VLGK⁺17]. **HSiCl** [LX11]. **HSiCl/DSiCl** [LX11]. **Hua** [JW12]. **Huang** [MT19b]. **Hückel** [FL15, SKTT11]. **Huffman** [QLQ11]. **Huge** [NN19, NNK⁺16, OHPR17]. **Huge-System** [NN19]. **huisgen** [ZZWT12]. **human** [JAHS⁺19, OME16, SLY⁺10, ZX11]. **hunter** [CMF⁺17, She12]. **Huzinaga** [Fer13b]. **HXeOXeF** [ARLP13]. **HXeOXeH** [ARLP13]. **Hybrid** [CGR16, KS15, NS18, VVY17, ZDKM12, BTA⁺13, BG13, CCB15, CBG17, CSKH15, CSXZ17, CC11, DR11, DJ13, ELP19, FHT⁺15, GRN19, GFG11, HZSS17, JAHS⁺19, JMS14, KN17, KKR⁺13, KJM⁺17, LBH⁺11, LT14, MIS⁺15, OK16, PW12, RSG14, SGPJS⁺17, Sea10, SH18a, SZX13a, SZX13b, VCL18, VI17, WNM17, ZWLX11, ZWL13, ZWX19, HPT17]. **hybrid-meta** [BG13]. **hybrid-parallel** [KJM⁺17]. **hybridized** [DC13]. **Hybridizing** [RDRC16, FZL⁺15]. **Hybrids** [VL19, KM13]. **hydratase** [LT13]. **Hydrated** [ALH⁺10, BMFG16, CGPP11, GBL⁺11, GNGCA10, LPE⁺10, LBDP12, VPR10]. **hydrates** [LZLC13]. **Hydration** [BSG⁺18b, HL14, AS14, DQ16, KB11b, KYB13, OK16, PP10, RZ16, SK12, SC18a, SWPR11, WBT10, WC13, WG12]. **hydrazine** [GZL⁺12]. **hydrazo** [WDLG12]. **hydrazo-1** [WDLG12]. **hydrazone** [HPT16a, ZZWT12]. **Hydride** [Jab18b, PM13, RKDM14]. **Hydride-Triel** [Jab18b]. **hydrides** [DM15, PGC12, RMGB11, WKC11]. **hydridic** [Jab14]. **hydroamination** [KT12]. **hydroazidation** [YXZZ17]. **hydroboration** [ZX19]. **hydrobromic** [CYY⁺17]. **hydrocarbon** [CB11d, IT19, KSM16, Kar17, MH17, SV15, WDW12]. **Hydrocarbons** [JCHT18, FVB10, NMH19, PL18, Ran19, SBvG14, ZWX19]. **hydrocyanation** [HDB15]. **hydrodynamic** [AKK⁺16]. **hydroformylation** [BF19b, dSDdAR10]. **Hydrogen** [AFSW16, EHT19, ELKE19, EV14, HvM17, JLLW19, JT18, KKK⁺19, MYT18, PNE18, PZM15, TD11, TL16, WKC10a, WLHZ12, WFZ⁺18, YZL⁺15, AAMD⁺11, ASK18, BEM14, BEPM14, BLFZ13, BK17a, BLDK⁺13, CK10, CSAAdOM17, CPV⁺12, CD11, CSXZ17, CKP10, DKT13, DLT17, DBG11, DL19, EHSPT16, GNC⁺18, GGM⁺12, GY12, GC11, HW19, HvM16, JCP14, JCG⁺10, JSW10, KTT16, KSNT19, KNP⁺12, KGJZ19, LC10, LZH⁺11, LJW11a, LZJ⁺11, LLW12, LHHW14, LCC18, LTP11, LYSS11, LZY12b, LAW⁺16, MPSG11, MK13b, MKO⁺13, MS11, MB14, NHF⁺10, OOK11, PGC12, PGI19, PAT⁺10, PD11, PMT16, QZM11, SZ17, SSGS15, SKGB13, Tan19, TDT19, UT15, VVP12, VVY17, VECT12, VDVR14, WKLC12, WHL⁺10, XMA⁺19, YR13, YLZ⁺10, YJ17, ZDX11, ZLY⁺16, ZW17, dCRN18, vADC⁺14, SK13, SMD18]. **Hydrogen-**[WFZ⁺18]. **hydrogen-abstraction** [GY12]. **Hydrogen-bond** [TD11, BK17a, CD11]. **hydrogen-bonded** [BLFZ13, DKT13, JCP14, LJW11a, LHHW14, PAT⁺10, UT15, ZDX11]. **hydrogen-bonding** [LCC18, PD11, WHL⁺10]. **hydrogen-bonds** [LZH⁺11].

hydrogen-bridged [ZLY⁺16]. **hydrogen-contaminated** [YR13].
Hydrogen-Disordered [MYT18]. **hydrogen-storage** [BEM14].
hydrogen-transfer [ZW17]. **hydrogenase** [GS11]. **hydrogenated**
 [MBRC16, wZbZ11]. **Hydrogenation** [GBG⁺19, JJAB16]. **hydrolase**
 [BHNS14, LD18]. **hydrolysates** [LWZ⁺19]. **hydrolyses** [YZGS14b].
Hydrolysis [JAHS⁺19, LHT15, MFM⁺12, XZ11, YZGS14a]. **hydroperoxyl**
 [AAMD⁺11]. **hydrophilic** [PAK15]. **hydrophobic**
 [ARRC15, GMMH⁺16, JGS⁺17, Jor17, MBC11, PAK15, SY16b, TM16].
hydrophobic/hydrophilic [PAK15]. **hydrophobicity** [CH14, SV15].
hydroquinone [PNE18]. **hydrosilylation** [DK19, SSD19]. **hydrostatic**
 [FCW⁺14]. **hydroxamate** [GWZ15, GPdC⁺16]. **hydroxamate-containing**
 [GPdC⁺16]. **hydroxy** [FFA14]. **hydroxyapatite** [XYW⁺14].
hydroxybutyrate [SJD14]. **hydroxycoumarin** [LZHH11]. **Hydroxyl**
 [BHP19, DPNM11, GKR13, JCG⁺10, KS13b, Ray13, RKG11, TTR⁺12,
 ZSZ⁺14, dSH19]. **Hydroxyl-** [BHP19]. **hydroxylated** [CCJ⁺11, SH14].
hydroxylation [TLY⁺12, VCM15]. **hydroxylations** [MRR11].
hydroxymethyl [HH11]. **hydroxymethylfurfural** [APY⁺16, WFL⁺19].
hydroxynaphthaldehyde [MPSG11]. **hydroxyphenylpyruvate** [DGH⁺11].
hydroxyquinolin [CSC⁺18]. **hydroxysteroid** [ZX11]. **hydroxysulfinyl**
 [TL16]. **Hyper** [FRN15, BLBG⁺13, BZB⁺13, RFN15]. **Hyper-parallel**
 [RFN15]. **Hyper-parallelism** [FRN15]. **hyperballs** [CVT⁺11].
hyperboloids [CVT⁺11]. **hyperbonding** [LW16]. **Hyperconjugative**
 [GNC⁺18, LZH16]. **hypercoordinate** [BSPP⁺13]. **hypercube** [CDC19].
hyperfine [CSEMB⁺16, MG11]. **hypermatrices** [BMPML⁺13].
Hypernetted [HAL14]. **hyperpolarizabilities**
 [MLC13, WYT17, XKW18, YHCS11]. **hyperpolarizability**
 [ISO⁺13, KBC12, Lu11, TKC⁺11, WXS⁺12, WZK⁺13]. **hyperpolarizability**
 [KSK11]. **hypersurfaces** [Ano10a, SN10]. **hypervalent**
 [ASS⁺17, SLT14, SLT⁺15]. **hypothesized** [LLB⁺12]. **hypoxanthine** [FF11].
HZSM [cCVG⁺14]. **HZSM-5** [cCVG⁺14].

I50V [DLZ15]. **I50V-induced** [DLZ15]. **IBIsCO** [KVQC⁺11]. **ICD**
 [WAB17]. **Ice** [MYT18, AASP18, LPAS11, TD11]. **ICI** [GSMZ19]. **ICN**
 [KIOY19]. **icosahedral** [FCW⁺14, GKSS14]. **ID** [LLHM16]. **Identification**
 [HRB⁺17, KYT⁺17, RLL⁺10, DL16, JSD⁺11, MPNS13, RLDJ17, WSH10,
 YZWC11, ZYvIZ14]. **identifier** [Ihl12]. **identifiers** [GPGSM11, GPGSM12].
identify [LLHM16, LHL⁺10]. **Identifying**
 [AC12, HAGK10, RNS19, XTY⁺14, LHO17, LLJ12, She12]. **identity**
 [Höf14, KN17, YN15]. **IE** [MLCD11]. **IEF** [GMMH⁺16]. **IEF/PCM**
 [GMMH⁺16]. **IEF/PCM-MST** [GMMH⁺16]. **Ihlenfeldt** [GPGSM12]. **II**
 [AMK11, ALH⁺10, BSG⁺18b, ĆMD13, CK17, FPB12, FB14b, GEP⁺14,
 HRJ⁺14, HRJ⁺15, JJAB16, KPL15, LGW12, LWXC16, MLG18, MMB⁺17,
 PHC13, SB10, TLA10, WGN⁺16, XP13, XWSW13, ZCK⁺16, vSGP10,
 AKMYB18, BWKW10b, BB11c, CB11c, FXC⁺13, Fer13a, FVB10,

dCGCRN19, HPT17, HRJ⁺14, HWLW11, HHWL17, KTT16, KT12, KTTNN10, KMLS10, MBC11, PPUBGD10, SOD⁺11, Tsi19, WH11, YK13, ZSYH12].

II/III [dCGCRN19]. **III**

[BP18, IKN13, KPL15, LWL⁺11, LXZ⁺10, SRL⁺15, BEL⁺11, CWT⁺12, DSHLM18, GZZM16, dCGCRN19, HIS17, SKA19, Zha12b, ZKH⁺10]. **III/II** [KPL15]. **IKP** [HLS12]. **illuminating** [NSO⁺14]. **illustrating** [RML⁺15].

illustration [RP15]. **im** [FHG⁺19]. **Image**

[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]. **Image** [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]. **Image** [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]. **Image** [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,

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impurities [SBC⁺11]. **IMSPeptider** [dCLFGL13]. **in-depth** [DDP⁺18].
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infantum [VSD10]. **inference** [BFH⁺13, VZ14]. **Infinite** [CC11, GK15b].
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inspection [KOY⁺12]. **inspired** [CYY⁺17, DSM⁺11]. **instability** [MMH19]. **instantaneous** [RO14a]. **Instanton** [MK17, MK19, MRK11]. **Insubria** [GCC14]. **Insulator** [LLL⁺12]. **Insulin** [MV17]. **INT** [YJXZ13]. **INT-DBD** [YJXZ13]. **Integral** [Coo19, VSP19, DL19, KSNT19, MEH18, RFN15, SS13b, Sun15, VKAM12, WXY14, YS18]. **integrals** [CHC⁺13, PS17, PC16, RLA18, SZTSM10, WDKT19]. **integrase** [XLY12]. **Integrated** [HSW⁺19, vRWGS17, CKKK16, MCC12, US11]. **Integrating** [APK14, LZZ14]. **Integration** [FPV13, AYYO17, BB11b, BB11c, DH17, LP11a, MOS12, NSK18, dRL11, Pol13, Pop18, SJC11, SJ16, dRBO13, MYKO18]. **integrative** [Řez16]. **integrator** [JS17b]. **intelligence** [Aou16]. **intelligent** [CDS16]. **intensity** [dSH19]. **Inter** [CROB16, SSB11, IIHY15, SSB13]. **Inter-** [CROB16, SSB11, SSB13]. **inter-residue** [IIHY15]. **Interacting** [CM16, VSP19, ATP18, EV14, HGCCGR⁺16, MP17a, PNE18, WL14, JCHT18]. **Interaction** [BHB19, CK10, CCCLCGRO14, CCCLRO14, Den12, NNS15, SBW12, YZWC11, ALW⁺10, AG12, BLFZ13, BLF14, BCNH⁺11, BSD18, BHB⁺17, BRLS08, BRLS12, BG17, CLFRO18, Cas13, CZH12, CYG⁺15, CTP13, CAP17, EK17, EV14, FF11, FCCP17, FA18, GA14, GP11a, HPT17, HBL12, HLH⁺12, HSZ⁺11, HLXH17, HLXH18, HQSZ19, HL19, JZZM14, Kan15, KTN10, LL10a, LMZ11a, LPS⁺13, Li14a, Li14b, LHHW14, LZL⁺15b, LPLB16, LCWW10, Min18, MSÁK12, MCP18, MvBD18, NGAS17, NN18, OHPR17, OHPR18, OAN15b, PRJ⁺17, RZG⁺13, RS13, SM16a, SS13a, SBGP18, SBV10, SHL⁺18, SPL⁺18, SHF11, SH19b, TYN15, Tan19, TSH⁺19, WSH10, WYL⁺15, YK13, YWJ⁺16, YAO18, YCK16, YHCS11, ZRCC11, ZY14, ZW18, ZZZ⁺19, dLvNC18b, vS18, KCB⁺12]. **interaction-activation** [LSL⁺19]. **interaction-based** [ZW18]. **interaction-induced** [BLFZ13]. **Interactions** [BGS⁺19, Hes19, Sch18, WCT⁺11, ZCK⁺16, Abr11, ARRC15, AKK⁺16, AO10, BSF18, BSG18a, CSS17, CC18b, CIKT13, cCVG⁺14, CKP10, CROB16, CB11a, CB11c, dRCFGRB18, DDP⁺18, DHF⁺11, DBG11, DLMH12, EP10, ER18, GWF11, GZZM16, GZ14, HSJ18, HLvdV13, HTY19, ICS⁺12, ICS⁺13, IIHY15, Jab18a, KSSH13, KCK⁺15, KPH⁺19, KGJZ19, LZLC13, LZSM19, MLGB16, MH17, MKH⁺13, MR17, MJM⁺15, MVKS10, MG14, MFR⁺17, MPBJ11, OHNK11, PPJ14, PLV⁺11, RTS⁺13, RVM19, RMRBH⁺19, SSGS15, SDF12, SB19, SWW⁺19, SSB11, SSB13, TNSS17, TG12a, TY10, TSR⁺16, TNG⁺10, VVJ15, VMV19, WS10, WGD⁺16, WDS⁺19, WZ19, WM17, XTY⁺14, XLY12, YKO⁺11, YZ15a, YW13, YZL⁺15, YDGZ15, YZLZ18, ZZL⁺12, Zha11, dLC17, dLvNC18b]. **Interactive** [BRP⁺12, BGR13]. **interactiveness** [CQFC10]. **interatomic** [DPAB16, FCCP17, RLA18, YKO⁺11, dLC17]. **intercalation** [LAM19]. **interconnections** [GLF16]. **interconversion** [HH10]. **interconversions** [TCGNT18]. **Interdependence** [WAB17]. **interest** [BCNH⁺11, OZLSBH12]. **Interface** [S JL18, All11, BDTP11, CSSB11, GRP⁺12, GCW14, HL14, JJW⁺14, KG13, LJR⁺12, LZdIL⁺10, LBB⁺15, MSSP17, NS18, OYK⁺11, PHH⁺12, PVZ13, RR14, RSR⁺12, SN16a, SYDS11, SISK10, STH⁺10,

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, BLF14, BLDK⁺¹³, CCLP12, KSNT19,
 KCL⁺¹⁴, LZY12b, LZLC13, RRH12, SN10, TY10, TNG⁺¹⁰, VVP12, VMV19,
 WGD⁺¹⁶, ZZL⁺¹², ZLT13]. **Internal** [AIQ19, 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, MSPG11, SSB11, SSB13, VVJ15, YK13, YLZ⁺¹⁰,
 dALdS⁺¹⁵, dLC17]. **intrapphase** [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, LEdOLdIV17, 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, LEdOLdIV17, 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].

ion-pairing [KTK17]. **ion/water** [SV11]. **Ionic** [FDCJG18, JXSW15, AFPI13, APY⁺16, CG15, CFC15, EK15, GC11, IN19, IM17, LEoLdIV17, MG15, NFI⁺16, PS14, SCM⁺15, WWKS11]. **ionicity** [SLY⁺19]. **ionisation** [CTP13]. **Ionization** [SHL⁺18, ACD⁺13a, ACD⁺13b, BG17, CG15, CBG17, GWF11, HNYH19, LGOM⁺15, LK13, yOTn16, ŠSB⁺16, SGHL13, Tac17, VL17a, VCL18]. **ionizations** [LGVA14]. **Ionized** [GMBM18]. **Ions** [WFZ⁺18, AS14, BDTP11, CCCLRO14, CC12a, EKH14, PRJ⁺17, PZA15, SNS16, SGH⁺16, VHS⁺19, WKC10a, XP13]. **IP** [BK17b]. **IP-tuned** [BK17b]. **IPRO** [PGL⁺15]. **IQA** [CSM16]. **IR** [DCOD13, CWT⁺12, LWL⁺11, LXZ⁺10, WJX⁺10]. **irGPU.proton.Net** [Kan15]. **iridium** [CWT⁺12, HDPM14, KB13]. **Iridium-catalyzed** [KB13]. **iridium-containing** [HDPM14]. **Iron** [HS14a, AKMYB18, BH19, BG13, CTR13, DK19, GBGR16, HSB⁺19, HS16b, KPL13, KPL15, MC10, NH19, SBC⁺11, TS10b, VBMA13, EH13]. **iron-containing** [AKMYB18]. **iron-porphyrin-carbonyl** [BH19]. **iron-sulfur** [CTR13, HSB⁺19, HS16b]. **irradiation** [WZC⁺19]. **Irregular** [Kan15, ALH⁺10]. **ISBN** [CD19, Sch10, Spr10]. **ISBN-10** [Spr10]. **ISBN-13** [Sch10]. **isocloso** [LK16b]. **isoconversional** [DCŠ15]. **isocyanide** [TLY⁺12]. **Isoelectronic** [ZLX⁺19]. **isoindolin** [YZLZ18]. **isoindolin-** [YZLZ18]. **Isolated** [FL15, DSB⁺19]. **Isomeric** [FL15]. **isomerism** [dCGCRN19, RS17b]. **Isomerization** [BW11b, DBG0⁺17, EFB16, BLG10, BMFG16, LL19a, MSBF16, OKIS17, SJD11, Su10, WCL⁺11, ZWZ11]. **Isomers** [CSM16, ZWZ11, DSHLM18, Kar17, OKIS17, WCL⁺11]. **isoselectivity** [OSA19]. **Isoster** [EdOdS18]. **Isothiirane** [MM19]. **isotope** [KTT16, MRK11, NASH15, ORZ11, UT14, UT15, VKAM12, WXY14]. **isotope-substituted** [UT14]. **isotopomers** [UT14]. **isotropic** [JKS⁺16, Tak14]. **isotropy** [Tru18]. **Issue** [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]. **Issue** [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]. **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,

Ano18l, Ano18m, Ano18o, Ano18p, Ano18q, Ano18r, Ano18s, Ano18-39, Ano18-40, Ano18-65, Ano18-66, Ano18-67, Ano18-68, Ano18-69, Ano18-41, Ano18-42, Ano18-43, Ano18-44, Ano18-45, Ano18-46, Ano18-47, Ano18-48, Ano18-49, Ano18-50, Ano18-51, Ano18-52, Ano18-53, Ano18-54, Ano18-55, Ano18-56, Ano18-57, Ano18-58, Ano18-59, Ano18-60, Ano18-61, Ano18-62, Ano18-63, Ano18-64, Ano19a, Ano19l, Ano19t, Ano19u, Ano19v, Ano19x, Ano19y, Ano19z, Ano19w, Ano19-27, Ano19-28, Ano19-29, Ano19-30, Ano19-31, Ano19-32, Ano19b, Ano19c, Ano19d, Ano19e, Ano19f, Ano19g, Ano19h, Ano19i, Ano19j]. **Issue** [Ano19k, Ano19m, Ano19n, Ano19o, Ano19p, Ano19q, Ano19r, Ano19s, Ano19-33, Ano19-34, Ano19-59, Ano19-60, Ano19-61, Ano19-62, Ano19-63, Ano19-64, Ano19-35, Ano19-36, Ano19-37, Ano19-38, Ano19-39, Ano19-40, Ano19-41, Ano19-42, Ano19-43, Ano19-44, Ano19-45, Ano19-46, Ano19-47, Ano19-48, Ano19-49, Ano19-50, Ano19-51, Ano19-52, Ano19-53, Ano19-54, Ano19-55, Ano19-56, Ano19-57, Ano19-58]. **Issues** [GS16, MFEM16, XFG⁺16]. **iteration** [SBB10]. **Iterative** [Hei18, VV19, Gra15, HLXH17, HLXH18, HL19, SM18, TTn19, VHR16, ZVY⁺15, PGL⁺15]. **IV** [CBDS19, EH13, KMS⁺19, MUN⁺19, MLGB16, MTS⁺19, VBMA13, WZH⁺18]. **iVI** [HLXH18, HLXH17, HL19]. **iVI-TD-DFT** [HL19].

J [ABB⁺13, CHR⁺12b, HCD⁺10, HNWF12, HLXH18, ICS⁺13, KSK11, Kne11b, MT20, MSK⁺12, RK16a, SFCK⁺15, SMM15a, LWD13]. **JACOB** [WDY13, Kar17]. **Jahn** [BMD19]. **Jan** [Spr10]. **Jan-Ole** [Spr10]. **January** [Ano10b]. **Janus** [EPH⁺15, ZB18]. **Janus-like** [EPH⁺15]. **Jarzynski** [ABS⁺19]. **jcc.25747** [MT20]. **JEFREE** [ZPF14]. **Jicun** [JW12]. **joining** [RVB⁺12]. **joint** [BMPML⁺13]. **Jones** [DPSL16, DH11, KGHK12, NW17]. **Jordi** [Ihl12]. **Joswig** [Spr10]. **Journal** [Ano15-59, Ano10b, GS16, MFEM16, XFG⁺16]. **Journey** [HB19]. **judging** [RCM⁺13b]. **Jumping** [MS17]. **junction** [Ish10]. **junctions** [LZW⁺11].

KCl [HB15]. **keeps** [Avd18]. **Kekulé** [RvL11]. **kemptide** [MUGNVJ⁺18]. **kernel** [Ano12u, PM18b, WHM10, WO15]. **kernels** [SK11]. **ketene** [YZL⁺15]. **ketene-** [YZL⁺15]. **keto** [FD14, XLYZ10]. **key** [GRCL12]. **KGaA** [Spr10]. **kinase** [AS10, BHF⁺18, DXL⁺10, DSX⁺11, MUGNVJ⁺18, RZG⁺13, WC11, Won18]. **kinematic** [NR11]. **Kinetic** [Hes19, ISN13, MRK11, CC18a, DWC17, DCŠ15, HLS12, Hel13, HFSO12, JCG⁺10, LLH14, LZLMP16, MMB⁺17, NCT18, NFI⁺16, ORZ11, PSS14, PGY15, SE14, SNS13, STS⁺10, TSJ⁺10, VKAM12, WLHZ12, WXY14, WSWD19]. **Kinetics** [CSNCS⁺18, GAI14, GY12, BRE16, CGVBAI19, ITY⁺19, IN19, JLS⁺10, KS13b, LPLB16, LJG⁺11, RS12, RRFV⁺18, SB14, TCGNT18, ZSWL12, dCRN18]. **KiSThelP** [CBH14]. **kit** [BJP15]. **knowledge** [GZ14]. **knowledge-based** [GZ14]. **KoBra** [KB19]. **Kohn** [BWMSM10, ŠSB⁺16, VV14]. **Kolossváry** [Ano15-59]. **Koopmans** [KSH13, YB16]. **KQ** [FHK⁺12]. **Kr** [Mit13]. **Kramers** [QS19]. **kriging**

[CBP14, DDP16, DBDP16, KFY⁺¹³]. **Kroll** [YS13]. **Kutta** [AMGB10].

L [HIS17, vSGP10, EOA⁺¹¹, GWF11, GSMZ19, LK16a, PDG⁺¹⁶, PVS12]. **L-edge** [PDG⁺¹⁶]. **L-lactide** [GSMZ19]. **L-phenylalanine** [GWF11, PVS12]. **L-tryptophan** [EOA⁺¹¹]. **La-doped** [WMW11]. **labeling** [HRK⁺¹⁰]. **Labile** [SCSM19]. **LabVIEW** [PPM15]. **LaCoO** [LLBO12]. **lactide** [GSMZ19]. **lactose** [OHNK11]. **ladder** [Kar17]. **ladders** [Tsi19]. **Lagrange** [GREA11]. **Lagrangian** [AA18, FXC⁺¹³, HGCCGR⁺¹⁶, IN19, LRvdSM15, RHJ11, SDF⁺¹⁷]. **Lagrangian-based** [IN19]. **Laigang** [WZC⁺¹⁹]. **Lamarckian** [FRLN10]. **lambda** [ISK14]. **Landau** [SA11]. **Landscape** [PK19, CF18, HDM⁺¹⁵, IMK⁺¹⁶, ZSB⁺¹⁶]. **landscapes** [BRE16, CDM⁺¹⁵, HHNK19, JCPC11, PJ13, RDRC16, SOJ14, SH11b, SC18b, WSH10]. **Langevin** [OCL11, SSWX14, WBVE16]. **language** [LMR14]. **lanthanide** [CPRS18, DBF14, HW19, Hua16, TS11]. **lanthanide-based** [HW19]. **lanthanides** [JXSW15]. **lanthanoid** [BCSCJ⁺¹³]. **Laplacian** [TEDT18]. **Large** [HSN⁺¹⁸, JBSQG11, XFG⁺¹⁵, XFG⁺¹⁶, YKNN19, AF14, AGR11a, CSGOA17, CHG⁺¹⁶, CEBO15, CSSB11, CKG18, DSV⁺¹⁹, DZA11, DDM⁺¹⁵, FN12, GRS15, GBW⁺¹⁴, GP11b, GWZX12, HLXH17, HLXH18, JSXH16, JS17b, JND⁺¹⁹, KG15, KNE11a, LS11a, LCPS13, LZX16, LWL⁺¹⁰, LCM⁺¹⁴, MK11, Man19a, MDT10, MEH18, NYN17, NH19, NLL19, NFG⁺¹³, OPB⁺¹², RLL⁺¹⁰, RS12, RC18, RSB⁺¹³, SZdB19, SCOJ13, SAGC16, Sch12, SRR16, SC18a, SG13, SMM17, TSR⁺¹⁶, TTn19, WLW⁺¹⁰, WFS19, WX12, WZH⁺¹⁸, Xhd15, YHCS11, ZWL13, ZLL⁺¹³]. **large-gap** [WZH⁺¹⁸]. **Large-Scale** [XFG⁺¹⁶, YKNN19, HSN⁺¹⁸, JBSQG11, XFG⁺¹⁵, DDM⁺¹⁵, JND⁺¹⁹, LCM⁺¹⁴, MDT10, RSB⁺¹³, Xhd15, ZLL⁺¹³]. **large-time-step** [RS12]. **laser** [SS19]. **LaSrVMoO** [SWMW10]. **lateness** [MS10]. **Lateral** [Hes19]. **Lattice** [RSL13, BS18, EFOD13, Pon10]. **layer** [MBA11, PP10, SE14, YZZ⁺¹⁷]. **layer-layer** [YZZ⁺¹⁷]. **lazy** [LLL⁺¹⁰]. **LC** [SH19a]. **LC-BOP** [SH19a]. **LCAO** [KHLM19]. **LCgau** [SPH11]. **LCgau-B97** [SPH11]. **Lck** [AC11a]. **LDA** [DOM⁺¹¹]. **lead** [SPZP19, VVMY18]. **leading** [SJD14, TCPPC14]. **leads** [dLvNC18b]. **LEAP** [LZZ14]. **learned** [FP17a]. **Learning** [HJG09, Aou16, Dra19, FZY⁺¹², FSD⁺¹⁸, GHV17, HPL⁺¹⁸, LHO17, LTA⁺¹¹, NB19, TO19, TM18, YLCX10, ZDT18]. **least** [BCCO10, Bow16, HGW18]. **least-squares** [BCCO10]. **leave** [WMW⁺¹⁰]. **leave-one-out** [WMW⁺¹⁰]. **leaving** [KV15b]. **lectins** [MSÅK12]. **Legacy** [HB19, vW11]. **Leishmania** [VSD10]. **length** [ASL⁺¹¹, KKA⁺¹⁸, KSC16, RAR⁺¹¹]. **lengths** [GREA11]. **Lennard** [DPSL16, DH11, KGHK12, NW17]. **Lennard-Jones** [DPSL16, DH11, KGHK12, NW17]. **Less** [SA10]. **Letters** [BCJC⁺¹⁴, Cor17, GKR13, GPGSM12, Ihl12, JW12, KR14, Man13, Ray13, RSLML12, SFLG⁺¹⁷, VVB13, WM12, dSdS12b, vLBBR12]. **LEUS** [BH15]. **level** [BVHI17, DMJ17, EWK⁺¹³, FFA14, HJKJ13, JCG⁺¹⁰, KSM16,

KSM17, KKNN11, LCK⁺¹⁸, MSC⁺¹⁰, MCLD10, OSR16, PVL⁺¹³, PTK11, PML⁺¹², PB14, VAMS14, WWD14, ZMMM12]. **Levels** [Kop19a, AC12, BCSCJ⁺¹³, BY11, BACSCJ⁺¹⁰, HYD10, Hua16, KIOY19, KHWB17, Kop15a, Kop16, Kop17a, Kop17b, Kop18, MK13b, dSAdSL13]. **leveraged** [EPH⁺¹⁵]. **Lewis** [EHSPT16, KASH14, Lüc14]. **LH1** [KPG18]. **Li** [AM19a, AM19b, DDM⁺¹⁵, JW12, RLA⁺¹¹, YCGA10, YHCS11, BWKW10a, GNI18, RLA⁺¹¹, TN12, YZLZ19, YCGA10, SBW12]. **Li-based** [GNI18]. **Li/Na** [YZLZ19]. **Li/Na-ion** [YZLZ19]. **Libcint** [Sun15]. **LIBEFP** [KS13a, KS15]. **libKEDF** [DWC17]. **Libra** [Aki16]. **libraries** [LG11, RLL⁺¹⁰, WF16]. **Library** [KSD⁺¹², Aki16, DWC17, EWK⁺¹³, FRN15, KS13a, KS15, LRvE17, LMZ11a, LAS⁺¹⁴, MZZ11, RFN15, SC15, Sun15, VAR12, Yes12, Yes15, ZCWX18]. **library-based** [MZZ11]. **LICHEM** [KWL⁺¹⁶]. **LiCl** [LCL⁺¹⁸]. **LiCN** [LLL⁺¹¹]. **LIE** [CZY11, VLB⁺¹⁰]. **life** [RHT⁺¹⁵]. **lifetimes** [CH10]. **Ligand** [DPOS16, KKH19, KC13a, LI19, MNNK10a, VKC10, ABD11, AG12, BKLA13, BPB11, BCG10, BBG^{+18b}, BS10c, ĆMD13, CIKT13, CHR^{+12b}, CHR^{+12a}, DFF⁺¹⁵, FTW12, FBEM11, FRLN10, GHK12, GDV17, GKJ⁺¹⁹, GS11, GZ14, HKR12, HG13, ITY⁺¹⁹, KLJ⁺¹⁷, KL14, KYB13, KTO11, KTO13, LZ11, LLC⁺¹⁰, LL10b, LWL⁺¹¹, LBS10, MC10, MGWR12, MG14, MFR⁺¹⁷, NST14, NJR18, NFG⁺¹³, NMF⁺¹⁴, OBW12, OHNK11, OGL10, OSR16, OCLM14, OOT15, PGCT⁺¹², PKK17, PPJ14, PLV⁺¹¹, RLDJ17, RZG⁺¹³, RCR⁺¹⁶, RO14b, RVP⁺¹¹, SPL⁺¹⁸, SKKS13, STM⁺¹⁵, TLY⁺¹², TNSS17, VVG13, Vor10, WdVN12, WNP⁺¹⁶, WZ17, WWW19, YZZ16, YBS19, dRBO13, AIM⁺¹⁸, YZZ16, SHL⁺¹¹]. **ligand-based** [RVP⁺¹¹]. **ligand-binding** [GDV17, MGWR12, OSR16, RO14b, WWW19]. **ligand-field** [BBG^{+18b}]. **ligand-induced** [KL14]. **ligand-receptor** [FRLN10, VKC10]. **ligand-sized** [OGL10]. **ligands** [CS17, GPdC⁺¹⁶, HRC13, KSO⁺¹⁹, LBC⁺¹⁹, LL10b, LXZ⁺¹⁰, LS11b, SSP⁺¹³, TS10b, ZRCC12, ZWY^{+10b}]. **ligated** [EH13, WC14]. **ligating** [BAD⁺¹⁹]. **LigDockCSA** [SHL⁺¹¹]. **light** [FWS⁺¹⁸, GNI18, HXM⁺¹⁶, KDR⁺¹⁸, PE11, REL17, XBSS19, ZGZ19]. **light-driven** [HXM⁺¹⁶, REL17]. **light-emitting** [FWS⁺¹⁸, ZGZ19]. **light-harvesting** [KDR⁺¹⁸]. **lighter** [WD10]. **Lightweight** [RLG14]. **like** [AASP18, Che17, EPH⁺¹⁵, GRN19, KOY⁺¹², KD18, KB14b, MP17b, OAN15b, SDF⁺¹⁷, SM15, UCFR16, VHA⁺¹⁰, VVY18, WFZ⁺¹⁸, WKC11, WGN⁺¹⁶, ZSL⁺¹¹, VVY18, YLZ⁺¹⁹]. **Limit** [SN16b, Fra15, Fra16, LW16, LYC⁺¹³, OAN15a, SLT14, WTH⁺¹⁶]. **Limitations** [LvG13a, VL19, HH18]. **limiting** [SLT⁺¹⁵]. **limits** [GC18, II18, NSK18, PdSC18]. **line** [dLvNC18b]. **Linear** [BG12, NNT⁺¹⁹, XKW18, YN15, ZLY⁺¹⁶, ARLP13, CPV⁺¹², DSAS19, EP12, FBY⁺¹⁷, FCE15, GZZ12, JZZM14, JMS13, KHLM19, Kid19, LP11b, MA17, MSĀK12, NYH⁺¹⁷, PH17, RS17a, RLA⁺¹¹, RR11, SS16a, Tak14, VBDS⁺¹¹, WL10, YDX16, ZZZ⁺¹⁹]. **linear-combination-based** [Tak14]. **Linear-scaling** [BG12, YN15, NYH⁺¹⁷, RR11]. **Linearity** [IKN13].

linearized [Fra15, Fra16, XTn18]. **Ling** [Ano12u]. **Ling-Yun** [Ano12u]. **link** [HH15]. **linkage** [dCGCRN19, HH11, OZS⁺13]. **linked** [Fom11, dACP12, LCC18]. **linked-cell** [Fom11]. **linked-lists** [dACP12]. **linker** [NPG17]. **Lipid** [BPPS19, BPPS17, MOS12, PGCT⁺12, ST11, WHAS⁺10, WHAS⁺16]. **lipids** [HM16, ML14, PGI19]. **lipopolysaccharide** [BHI19, DLSA14]. **lipopolysaccharide-rich** [BHI19]. **lipopolysaccharides** [HBJ⁺17]. **Liquid** [WLC12, AASP18, APY⁺16, BDTP11, CC12a, EK15, GWJR18, IN19, IM17, KGHC15, KT18, Lar12, MG15, NTTY15, RJS17, SBvG14, SAvg15, WCWV15, ZSTI14]. **liquid/lithium** [EK15]. **liquids** [AFPI13, CG15, CFC15, CVG14, DASA15, LEdOldIV17, SCM⁺15, SHF11, You10, FDCJG18]. **lists** [Gon12, dACP12]. **lithiated** [KZK⁺12]. **lithium** [EK15, GMG⁺10, KOP⁺14, KYCL11, LAM19, LLL⁺11, MBRC16, NDG14, NFI⁺16, PGC12, PMT16, SKY⁺11, TN12, ZZL⁺12]. **lithium-bonded** [ZZL⁺12]. **lithium-doped** [PGC12]. **lithium-graphite** [LAM19]. **lives** [QS19]. **load** [Fom11]. **loadings** [KB19]. **LOBSTER** [MDTD16]. **Local** [CHP11, GH16a, GH16b, HJKJ13, ITIN15, CPN⁺17, DDP16, Fer13a, HH10, KSSH13, KDT⁺12, KGM12, Lar12, LLL⁺10, LZS⁺17, MKH⁺13, NLL19, PH17, PRSG13, PRYI⁺17, PW12, Ran19, RVM19, Sch12, SEF⁺16, ŠB15, WM17]. **locality** [Gon12]. **localizability** [Bar14, BLG11, BWKW10a, BWKW10b]. **Localization** [Sax12, ABDGN12, BK11, BLG11, GNDA⁺12, HJJ13, Mat14, Pil17, dLC18a, vSGP10]. **localized** [Ano15-58, BH14, GLW19, KKH18, ŠB15, ZM11, dLC17]. **locate** [AMGB10]. **location** [PTB⁺15]. **locked** [GA18, XVN17]. **locking** [XVN17]. **locus** [NR11]. **logarithmic** [MIOM13]. **LOL** [BSPP⁺13]. **lone** [BSF18, BSG18a, ENKK⁺17, SSGS15, WCY⁺11]. **lone-pairs** [ENKK⁺17]. **Long** [BCNH⁺11, KSH13, KSSH13, AO10, BLBG⁺13, BZH14, JBSQG11, KB10, KV14, MMS16, MBC13, PNG10, SMGB11, ST13, SPH11, SH19a, SZB19, SSA⁺17, TSN16, VL17a, VCL18, Rui11]. **long-bond** [KV14]. **long-chain** [TSN16]. **Long-range** [BCNH⁺11, KSH13, KSSH13, KB10, MMS16, ST13, SPH11, SH19a, SZB19, SSA⁺17, VCL18, Rui11]. **long-range-corrected** [BLBG⁺13]. **long-term** [JBSQG11]. **look** [ACS12]. **Looking** [WGL⁺11, ZPF14]. **lookup** [JMS13]. **loop** [CYI⁺10, FTW12, LZZ14, NR11, OCL11, TJB12]. **loops** [PJ13]. **loss** [GBVA11, MH11]. **Low** [BPM15, BLDK⁺13, Gra15, AC12, CM13a, DH14, KKA⁺18, LG14, MPA10, MPA12, MJLV14a, RRC⁺15, SN15, SG10a, SM11, She12, TF15, TSN17, UGK18, Vor10, YW12, BS10c, BBI⁺11, SGP18]. **low-cost** [TF15]. **Low-density** [BBI⁺11]. **low-druggability** [LG14]. **Low-energy** [BPM15, DH14, MPA10, MPA12, SGP18]. **low-index** [RRC⁺15]. **low-lying** [AC12, KKA⁺18, TSN17]. **Low-memory** [Gra15]. **low-resolution** [SM11, Vor10, BS10c]. **low-strain** [She12]. **Löwdin** [SHL⁺18, TSH⁺19]. **lowest** [GFG11]. **LOX** [BG13]. **LPol** [BLBG⁺13]. **LPol-** [BLBG⁺13]. **LS** [ZCS⁺15]. **luciferin** [VM19]. **luminescence** [DBF14, SEJ⁺18]. **luminescent** [HW19]. **LUMO**

[CBDS19, NPG⁺¹⁸, RS17a]. **LUMPAC** [DBF14]. **lyase** [CJZS10]. **lying** [AC12, KKA⁺¹⁸, TSN17]. **lysine** [FHK⁺¹², GH10, TYX⁺¹⁸]. **lysine-malonylation** [TYX⁺¹⁸]. **lysozyme** [ZP13].

M [AM19b, LDJ⁺¹⁰, LLL⁺¹¹, MCK17a, Rab12, TLdG⁺¹², WWKS16, YW12, YHCS11, JJAB16, CCCLCGRO14, MCK17a, TLdG⁺¹², YHCS11, JJAB16]. **M05** [SIG⁺¹⁵]. **M05-2X** [SIG⁺¹⁵]. **M06** [LK16a]. **M06-L** [LK16a]. **m4** [VM11]. **m6** [Mit13]. **m6-31G** [Mit13]. **Machine** [ZDT18, Aou16, Dra19, FP17a, FSD⁺¹⁸, NB19, RMRBH⁺¹⁹, TYZ⁺¹⁶, TM18, YLCX10].

machine-learned [FP17a]. **machines**

[GTZ⁺¹⁸, RJBH18, RLL⁺¹⁰, ZWL13]. **macrocycles** [CMM18, GMASBF16].

macrocyclic [ZRCC12]. **macrolide** [PG15]. **macromolecular**

[Kne11b, LCA17, LAT10, LAT11, PG14, UU12, RTP⁺¹³]. **macromolecules**

[DGC14, DZA11, FXC⁺¹³, OHPR17, RZ16, ZKE⁺¹⁷]. **macrotricyclic**

[ZWY^{+10b}]. **Magnetic** [BHP19, LKZM18, MP19b, Avd18, BCSCJ⁺¹³, BP18, BACSCJ⁺¹⁰, CPRS18, CPN⁺¹⁷, CJPTC18, FNSF⁺¹¹, GTT10, GBG⁺¹⁹, HAI⁺¹⁶, Ibr17, JCG⁺¹¹, KNP⁺¹², LLLM11, LLB⁺¹², PLFS18, SH18a, SIT18, SACdG14, ŠB13, ŠB15, Vik11, wZbZ11, ZLZ14, ZB18].

Magnetically [ATM18, ATIP18]. **magnetizabilities** [ZPP⁺¹⁶].

Magnetochemical [SvLK18]. **magnetoresponse** [TDKT10, TS11].

magnets [BP18]. **main** [ACD^{+13a}, ACD^{+13b}, JJJ16, Xhd15]. **maingroup**

[RMGB11]. **maingroup-element** [RMGB11]. **make** [NH19]. **Maker**

[HBJ⁺¹⁷]. **Making** [Man19b]. **malaria** [FZL⁺¹⁵]. **maleimide** [LXFC17].

malonylation [TYX⁺¹⁸]. **maltose** [HYSF19, SWM10]. **man** [HDH12].

managed [LMA15]. **manganese** [GHL17, KMS⁺¹⁹]. **manganese-based**

[GHL17]. **manifold** [RGVC⁺¹⁹]. **Mannich** [AS11]. **mannose** [VM11].

Many [CGPP11, BDdS13, CKKK16, HRJ⁺¹⁴, HRJ⁺¹⁵, JRSH14, KNHN16, LYC⁺¹³, RHPWS13, VMPS17, WCWV15]. **Many-body**

[CGPP11, HRJ⁺¹⁴, HRJ⁺¹⁵, JRSH14, LYC⁺¹³, RHPWS13, VMPS17].

many-core [KNHN16]. **map** [MKM⁺¹⁷]. **mapper** [BJP15]. **mapping**

[EMD17, KZP^{+18b}, MMM⁺¹⁶, RNSF⁺¹⁶, TD10]. **Maps**

[ZFOS19, GJMPAM⁺¹⁴, YSRSS10]. **Marburg** [OLY17]. **Marcus** [WBKS19].

Marjana [CD19]. **marker** [JAH⁺¹⁷]. **Markov** [BFH⁺¹³, LTT16, WWW19].

Martini [HBJ⁺¹⁷, MT20, SM15, MT19a]. **MARTINI-like** [SM15]. **mass**

[NPTS16, PGY15]. **massive** [GP11b, TNYN16]. **Massively**

[FBKD19, KNHN16, KZZ⁺¹⁶, KCC⁺¹⁸, MYT⁺¹⁴, SHL19, BWMSM10, KN17, NNK⁺¹⁶, OPB⁺¹², WHK⁺¹²]. **Master** [NNT⁺¹⁹, RSL13]. **match**

[TZ12, YPKB12]. **matched** [KSR⁺¹⁶]. **matching** [AOW11, GPS10, HS12].

Material [JW12, DGL⁺¹³, HLWD15, JBSQG11, LL13b, MCAG⁺¹⁶, NGAS17, SHL19, SMiN⁺¹⁹, SLHW09]. **materials**

[BSL⁺¹⁶, CD11, DLT17, ECZWD17, EMD17, GNI18, KLZ⁺¹⁸, KB19, Man13, NDD⁺¹⁰, SB18, SYZ⁺¹⁷, VBV13a, VVB13, VVY17, VVMY18, YZLZ19].

MATLAB [DDK14, SKA19]. **matrices** [Car14, LHO17, Mat14, Yon16].

matrix

[CAP17, CWZB10, Kne11b, LAT10, LAT11, PW12, RPNP10, RNP13, RR11, SS13a, STM17, TCPPC14, UIW⁺¹⁰, VGV⁺¹¹, VKNT15, VKNT16, ZVY⁺¹⁵]. **matrix-based** [VGV⁺¹¹]. **matrix-free** [ZVY⁺¹⁵]. **matter** [BGL⁺¹⁸, HRB⁺¹⁷]. **Maxima** [Lüc14]. **Maximal** [DN19]. **maximum** [MLC13]. **may** [SMGB11]. **MB** [EdOdS18]. **MB-Isoster** [EdOdS18]. **MBJLDA** [SRS14]. **MC** [HYUS11, BF19a, LH14a, ATIP18]. **MC-DFT** [LH14a]. **MC-XQDPT2** [KKL⁺¹³]. **MCN** [LLL⁺¹¹]. **MCQDPT** [LLSW14]. **MCSCF** [ZZZ⁺¹⁹]. **MD** [HCD⁺¹⁰, RSR⁺¹², BM12, FB14b, GMASBF16, LWZ⁺¹⁹, LJL⁺¹¹, MTvG12, OYK⁺¹¹, RAR⁺¹¹, SISK10, SMP17a, WTD⁺¹⁹, WWW19]. **MD-FEP** [LWZ⁺¹⁹]. **MDAnalysis** [MADWB11]. **MDLab** [CCW⁺¹⁰]. **MDM2/** [HQSZ19]. **MDMX** [HQSZ19]. **MDockPeP** [XYZ18]. **MDTRA** [PVZ13]. **Me** [KKR⁺¹³]. **mean** [HDL⁺¹⁴, Kid19, KERY⁺¹⁶, KT10, KS12, KLS10, KMLS10, MIOM13, MP17b, RI10, VBDS⁺¹¹, Vor12]. **mean-field** [Kid19]. **mean-force** [MIOM13]. **meaning** [PSP15]. **Means** [Sch18, KSM16, TTB⁺¹⁰, dSH19]. **measure** [TZCK18, WF16]. **measurement** [MPSG11]. **measures** [CDB10, CAA10, Dry14, MK11, PZBA13]. **Mechanical** [NN19, AC11a, APY⁺¹⁶, ACS12, ALH⁺¹⁰, BTT10, BEL⁺¹¹, CXW14, DR11, DLW12, ECZWD17, FL15, GMMH⁺¹⁶, HYUS11, Ibr11, JWO15, JSXH16, KVR10, LPE⁺¹⁰, MHRR11, NNK⁺¹⁶, NDD⁺¹⁰, OSR16, PML⁺¹², PGW⁺¹⁷, PVAM16, Rez19, ŠBD⁺¹⁷, TZ11, VVW⁺¹⁸, VPR10, WKC^{+10b}, WLLH18, WCAH10, YKO⁺¹¹, ZSTI14, ZWMW10, ZKH⁺¹⁰]. **mechanical/effective** [DR11]. **mechanical/molecular** [BEL⁺¹¹, YKO⁺¹¹]. **mechanically** [SOYC12]. **Mechanics** [Ale19, AS10, AGB13, AS15b, BGR13, CGPP11, CXW14, Chu10, CHKR10, Cor17, CB11b, CB11c, DDM⁺¹⁵, EPH⁺¹³, ENKK⁺¹⁷, Fer13b, Fer13a, GEP⁺¹⁴, GPdC⁺¹⁶, HWLW11, KGHK12, LAHS16, LTP11, Lüc14, Mat18, Min18, MS12, NLP⁺¹⁶, NHK⁺¹³, PSC11, PGW⁺¹⁷, SFLG⁺¹⁷, VYM15, WOH16, WOH18, WCDM11, YPKB12, HWLW11]. **mechanics-based** [WCDM11]. **mechanics/dynamics** [DDM⁺¹⁵, EPH⁺¹³, GPdC⁺¹⁶]. **mechanics/generalized** [HWLW11]. **mechanics/molecular** [Fer13b, Fer13a]. **mechanics/Poisson** [HWLW11]. **Mechanism** [GZL⁺¹², SLY⁺¹⁰, SSC⁺¹⁹, VKNT15, WCWW11, WLF19, BHNS14, BMFG16, BEL⁺¹¹, CPV⁺¹², CPLL11, CKG18, FWS⁺¹⁸, FB14b, GYX⁺¹⁰, GRCL12, GSMZ19, HYYZ13, HLI⁺¹⁹, HDHL15a, HDHL15b, HDHL15c, JCG⁺¹⁰, JLS⁺¹⁰, JW16, KV14, KT12, KGJZ19, KS13b, KK19, LZL⁺¹⁰, LZHH11, LLB⁺¹², LCC18, LWZ⁺¹⁹, LWXC16, LD18, LHT15, LPMT17, NJX⁺¹⁰, Oht16, PMT16, RLG11, RSK⁺¹⁵, SLLL13, SBW12, SZZ⁺¹⁸, VMTL10, WWW19, WZQW10, WCL⁺¹¹, XLY12, YPC⁺¹⁰, YHG⁺¹¹, YXZZ17, ZSWL12, ZX19, vRET19]. **Mechanisms** [CGVBAI19, WJX⁺¹⁰, ZZWT12, DWZ⁺¹⁷, GG10, KC13a, MH11, MLY⁺¹³, PPH⁺¹⁴, RRFV⁺¹⁸, SLT14, SLT⁺¹⁵, SSP^{+19b}, TNY18, Won18, WSWD19, YB11]. **Mechanistic** [CYY⁺¹⁷, LZL⁺¹⁶, QQY⁺¹⁸, TSJ⁺¹⁰, WFL⁺¹⁹, YZ17, YZLZ18, ABB⁺¹²,

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, LBGS16, 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, PLV⁺¹¹, PM18b, Pon10, QLQ11, QB10, QB11, RHRCH16, RKG10, RSL13, 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, LEdOLdIV17, LZLC13, LLSW14, MS13, MY17b, MHO18, MŘ17, MVKS10, MOS12, NYH⁺¹⁷, NASH15, NC13, NC14, NTNY15, OSHG17, PN13, PVAM16, RZG⁺¹³, ŘRH12, Rez19, SRF⁺¹⁷, ŠSB⁺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, LLLFH16, 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,

PLZ17, PGY15, RRF11, SS13c, SLY⁺19, ZZ10]. **Mg-porphyrin-based** [PLZ17]. **MgO** [BS16b]. **MH** [HHT⁺13a, HHT⁺13b]. **MHC** [HHWL17]. **MIA-QSAR** [BF15]. **MIBPB** [CCC⁺11]. **Micellar** [SCK18]. **micelles** [TFYO19, WWKS11]. **Michael** [NDG14]. **microbes** [RSL13]. **microclusters** [NC12]. **microelectrostatic** [SMP17b]. **microhydrated** [SM17, ZYR⁺15]. **microhydration** [OSS10, ŠBD⁺17]. **microiteration** [SMM17]. **microiterative** [RR12]. **micromolecular** [XTG⁺11]. **microscopic** [HLWD15]. **microscopy** [LLJ12]. **Microsecond** [DMN14]. **microseconds** [Bow16]. **microstructures** [DASA15]. **microwave** [BLF14, WZC⁺19]. **MIDAS** [GJMPAM⁺14]. **Midpoint** [JMS14]. **migration** [FBEM11, Ish10, KYKR15, RSB⁺13, TN10]. **Milan** [CD19]. **milestoning** [BRE16]. **mimetic** [MV17]. **mimetics** [CFM⁺19]. **mimic** [GRP⁺12, ZWS⁺10]. **mineral** [TZ11]. **mini** [CFC15, HTS15, HTS17]. **mini-protein** [CFC15, HTS15]. **mini-proteins** [HTS17]. **minima** [AC12, GFG11, HvM12, MAMF19, SGWA17]. **minimal** [CGBK13, CG12, OYK⁺11, RSR⁺12, RVVK13, WHAS⁺10, WHAS⁺16]. **minimization** [GBVA11, Rao11, TJB12, XHLH16]. **minimized** [ZA15]. **minimizing** [KS12]. **Minimum** [RAR⁺11, CY09, CY13, CZZL19, HNYH19, LLSW14, MP13, MCAY15, PRP15, PHDH13, SRSLO15, SG10b, Tak10, MYKO18]. **mining** [BCP⁺10, MCC12]. **miniprotein** [MDT10]. **minnesota** [LH14a]. **minnesota-type** [LH14a]. **minnow** [TTL⁺12]. **misfolding** [LH11]. **mismatched** [BH13]. **mispair** [BZH14]. **Mixed** [RdA12, SZL19, BRGN12, BEEL14, BACSCJ⁺10, DH11, DFF⁺15, Fer13b, Fer13a, GMASBF16, GG10, Ibr17, JT18, KGR⁺16, LYL16, MP13, PSdPE⁺10, RB12, TFYO19, TS10b, VVJ15, WX12, YLL11]. **mixed-basis** [WX12]. **mixed-QSPR** [BRGN12]. **mixed-resolution** [DFF⁺15]. **Mixed-Valence** [SZL19, BEEL14, KGR⁺16]. **mixing** [LCH10, ZA15]. **mixture** [BBI⁺11, MKB⁺13, RHNN10]. **mixtures** [GM17, GC11, JA10, KGHC15, SV11, TKYN17]. **Mizoroki** [dSdLBNB17]. **MLatom** [Dra19]. **MLCT** [BF19a]. **MLR** [GCP⁺13, XWW⁺11]. **MM** [BM12, JAHS⁺19, LWZ⁺19, AALCM11, BTA⁺13, BD11, CZY11, CS17, CJZS10, DSK17, DSX⁺11, FLM11, FPB12, FB14b, GR10a, GRS15, GWZ15, GCW14, HH15, HBR17, IMSR18, JJH⁺13, JWST10, KTNN10, KWL⁺16, KWG15, LZdlL⁺10, LFM12, LT13, LHT15, LJL⁺11, MCRL17, MTvG12, MJG⁺15, NO16, OBW12, PMC⁺17, PDMT10, PL14, RDDS10, RFN15, RR14, RN17, RR12, SN16a, SGDT10, SJD14, SCM⁺15, STM⁺15, SSAS10, TSC⁺13, VKNT15, VKNT16, VCM15, VKTRJ15, VM11, WDP⁺12, ZZY⁺16, vRET19]. **MM-GBSA** [RDDS10]. **MM-MD** [RSR⁺12, OYK⁺11]. **MM-PB** [OBW12]. **MM-PBSA** [RDDS10]. **MM-QMC** [UTM11]. **MM-type** [Kid19]. **MM/GBSA** [GR10a, IMSR18]. **MM/PB** [VM11]. **MM/PBSA** [BD11]. **MM2QM** [NHK⁺13]. **MMGBSA** [GS14]. **MMPBSA** [WNP⁺16]. **MMX** [CRC13]. **Mn** [FHG⁺19, JCG⁺11, VED10, WWKS16, BHP19, DLW12, KMS⁺19, LLLW19, vADC⁺14]. **Mn/Fe** [LLLW19]. **Mn/Fe-Doped**

[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, BLS10, 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, TTh19, UIW⁺¹⁰, VV14, VHS⁺¹⁹, WWKS11, WXL⁺¹², WC13, WWW19, WNM17, WRHF10, WKC11, WCAH10, XZ11, XTY⁺¹⁴, XP13, YS18, YOMT14, YB13, YSG12, ZST14, ZKH⁺¹⁰, ZM10, dSDdAR10, dSH19, CCR18, FAS⁺¹⁸, MJB12]. **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, QLK19, 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, LBG16, 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]. **MolecularRnetworks** [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, BLBG⁺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, LJJ⁺11, LG14, MA16, MS13, Mat10, MSS⁺13, MH17, MBE16, MPBJ11, NIIT15, OGL10, OT12, PZBA13, Pyy13, RSSG18, RSG14, RK15, SFCK⁺14, SFCK⁺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]. **Molybdatricarboranes** [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].

monosaccharides [UNT16]. **monosubstituted** [SNDK16]. **monovalent** [TJR19]. **monoxide** [GYX⁺10, GPK⁺16, KKH19, YHG⁺11, YB11]. **Monte** [Pon10, Aou16, BFH⁺13, CLK11, CG12, CTP13, CAP17, DMN15, FFA14, GP12, GPM17, HFSO12, Hes19, HMM10, HYUS11, HQC16, HHBY10, IHJ⁺13, LPK16, LMZ11a, LZ12, MS16, MBRC16, MOS12, NQB19, NDW15, OPBR17, PSS14, PS13, PHH⁺12, RHNN10, RdA12, SCOJ13, SAGC16, SMRM⁺17, SSP19a, SE14, UU12, YO19, ZLM⁺15, ZW17]. **Montmorillonite** [BHB19, BHB⁺17]. **Moon** [MTS⁺19]. **MOR** [LZTV10]. **morphologies** [NDLW13]. **morphometric** [HRC13]. **MoS** [EB18, RSK⁺15, SB11]. **motif** [OOK11]. **motifs** [DAP⁺18]. **motion** [AA18, FBvdB18]. **motions** [II10, PG14]. **motor** [HXM⁺16]. **moves** [NDW15]. **Moving** [GKSS14]. **MoViPac** [WHK⁺12]. **MP2** [BK17c, BBG⁺11, BW11a, BK17c, CCB15, CGR16, HDM⁺19, KNHN16, LH14a, MKGA10, Mat10, MVKS10, RKGN10, SWW⁺19, TKN13, YJ17, Yu12b]. **MP2-F12** [BBG⁺11]. **MP2.5** [Boz18]. **MP2C** [YJ17]. **MP3** [Boz18, ISM18]. **MPI** [JMS14, KS15, KN17]. **MPI/OpenMP** [KS15, KN17]. **MPn** [VSP19]. **MR** [dALdS⁺15]. **MRCI** [LSD⁺10]. **MRMP2** [TNI⁺19a]. **MRPT** [SACdG14]. **MS** [BGL⁺18]. **MSINDO** [KB14b]. **MSL** [KSD⁺12]. **MST** [GMMH⁺16]. **much** [Cas14]. **Mulliken** [BVC13, VVY17]. **Multi** [FFA14, HH16b, YSSB12, Ali18, KK17a, MCRL17, OZLSBH12, PSG⁺17, Tak18, VBV13b, WZWW18]. **multi-core** [KK17a]. **multi-fragment** [VBV13b]. **Multi-level** [FFA14]. **multi-nanosecond** [MCRL17]. **multi-objective** [PSG⁺17]. **multi-reference** [Ali18, OZLSBH12]. **multi-seed** [Tak18]. **multi-state** [OZLSBH12]. **multi-task** [WZWW18]. **Multi-user** [HH16b]. **Multi-zinc-expanded** [YSSB12]. **Multicanonical** [JWST10, IUK⁺11]. **multicatalysis** [LZL⁺16]. **multicenter** [US11, dLvNC18b]. **multichromophoric** [SEJ⁺18]. **multicompartmental** [VBDS⁺11]. **Multicomponent** [BPPS19, BPPS17, HH18, UT15]. **multiconfiguration** [LCL⁺10]. **Multiconfigurational** [SR19, AAC⁺16, DSV⁺19, DCHL12, FRSA14, FD16, ON14, RGVC⁺19, VDL⁺13]. **multicore** [BWMSM10, KN17]. **multideterminant** [SAGC16]. **Multideterminantal** [PHT17]. **Multidimensional** [HHNK19, LMI⁺14, XW15, XFG⁺16, Che17, CJPTC18, XFG⁺15, dCRN18]. **Multidimensionality** [FVB10]. **multieffects** [YZL⁺15]. **multifrequency** [LBB⁺15]. **multifunctional** [LC12]. **Multigrid** [SHF11]. **multijunction** [MP19a]. **multilayered** [CXW14]. **multilevel** [LL19a, NMH19, TNYN16]. **multilinear** [GJMPAM⁺14]. **multimer** [HHNK19]. **multimolecular** [CD16]. **Multiobjective** [BDdS13]. **Multiparticle** [NDW15]. **multiphase** [BVY⁺12]. **Multiple** [JL19, JS17b, LL10b, YZ17, AYYO17, CD11, CL16, DGC14, DSX⁺11, ESB13, FBEM11, FSSW19, GA12, KPH⁺19, KJM⁺17, LZY12b, Rob13, RFHG10, TNSS17, YDX16, PPUBGD10]. **Multiple-Walker** [JL19]. **multipliers** [GREA11, RHJ11]. **multiply** [RJS17]. **Multipolar** [YMP14, FCCP17, HCP15, KFY⁺13, KWL⁺16, NLP⁺16]. **Multipole**

[NOKJ16, SWPR11, BS19, BLDK⁺¹³, CP15, CTP13, EPD⁺¹⁰, EPD⁺¹¹, Kan15, KR12, KSK11, Lar11, LBGS16, SF18, SLX⁺¹⁵, Tru18, YAO18]. **multipoles** [Elk16, KGM12, SMP17b]. **multiprocess** [MB16]. **multiprocessing** [GP11b]. **Multireference** [GA14, SP13, CCM15, CF14, GCCM15, GA18, MCC11, MC12, SSSM15]. **multiresolved** [DGC14]. **Multiscale** [BLKP12, FXC⁺¹³, LC16, LZ14, JBB⁺¹¹, MBC13, SYN⁺¹², WLO⁺¹⁷]. **multisite** [CK17, HS14b, MMB⁺¹⁷]. **multistart** [MS16]. **Multistate** [TM16, AM10]. **Multistep** [DWZ⁺¹⁷, FZY⁺¹², WZDN16]. **Multistructural** [SMM17]. **Multisubstate** [PBLdS12]. **multithreading** [TO10, ZWL13]. **multivalent** [AS14, FVP14]. **Multiwfn** [LC12]. **Mus** [WZQW10]. **muscarinic** [SRA17]. **musculus** [WZQW10]. **mutagenic** [BZH14]. **mutant** [FHK⁺¹², LMA15]. **Mutantelec** [VMRSH⁺¹⁷]. **mutants** [CSC⁺¹⁸, RKDM14]. **mutation** [BA11, VMRSH⁺¹⁷, ZJZM13]. **mutations** [BH15, GMO16, KYT⁺¹⁷, SL10, SY16a, WC11]. **mutual** [BMPML⁺¹³]. **MVPACK** [BACSCJ⁺¹⁰]. **MX** [Sch13]. **MXenes** [YZLZ19]. **mycobacterium** [MPNS13]. **MyMolDB** [XTG⁺¹¹]. **myoglobin** [SHB17].

N [ATIP18, Ano15-59, BLF14, BCNH⁺¹¹, KBC12, KCL⁺¹⁴, LPLB16, NDG14, PVL⁺¹³, RLZ⁺¹⁸, ZLX⁺¹⁹, GNI18, LZSM19, BCNH⁺¹¹, BWKW10b, BMB13, BSDP16, CWT⁺¹², CCM15, DCHL12, DLW12, GMASBF16, GZL⁺¹², HLH⁺¹², KV14, KCL⁺¹⁴, LZL^{+15b}, MLGB16, MSPC19, MS15, OZLSBH12, PVL⁺¹³, QQY⁺¹⁸, RHNN10, RWR⁺¹³, ŠBD⁺¹⁷, SGHL13, TSJ⁺¹⁰, VM11, WS10, WGL⁺¹¹, WCL⁺¹¹, WYGW12, WS12, Yu12b, YXZZ17, ZP13, HPSK12]. **N-** [BMB13]. **N-Bromosuccinimide-promoted** [QQY⁺¹⁸]. **N-Codoped** [RLZ⁺¹⁸]. **N-heterocyclic** [BSDP16, CWT⁺¹², SGHL13, WS12]. **N-methyl-N-phenyl-hydrazine** [GZL⁺¹²]. **N-methylacetamide** [HLH⁺¹²]. **N-substituted** [DCHL12]. **Na-ion** [SMiN⁺¹⁹, YZLZ19]. **NABs** [SBW12, SBW12]. **NABs-Li** [SBW12]. **NaCl** [HB15, PK19, TNY18]. **NaI** [OCW⁺¹⁵]. **Naïve** [JL19]. **Naiyang** [Ano12u]. **NAMI** [LWZ⁺¹⁹]. **NAMI-A** [LWZ⁺¹⁹]. **nano** [Ano15-58, BH14, QZ10b]. **nano-clusters** [QZ10b]. **Nanoalloy** [THI⁺¹⁹]. **nanobiotechnology** [Fel10]. **nanochannels** [TM16]. **nanocluster** [AS15a, AAMR18, AHK⁺¹⁹, RVVK13]. **nanoclusters** [AASP18, LLJ12]. **nanocrystal** [KC13b]. **nanodisc** [QLKI19, QLKI19]. **nanoflakes** [GNI18, Lin18]. **nanographene** [DWZ⁺¹⁷]. **nanographenes** [TSN17]. **nanolayers** [EBK13]. **nanoparticle** [CCJC10, NNS15]. **nanoparticle-PMMA** [NNS15]. **nanoparticles** [EOO⁺¹⁶, KHLM19, LZZ⁺¹¹]. **nanopore** [SM16b]. **nanopores** [DMN14, MJC14, SM15]. **nanoporous** [KB19]. **nanoribbon** [DJX^{+11b}, DJX^{+11a}, RRK14]. **nanoribbon-based** [DJX^{+11b}, DJX^{+11a}]. **nanoribbons** [LWZK13]. **nanorings** [TS15b, YDGZ15]. **nanorods** [LHKS12, LH14b]. **nanoscale** [Hei10, SWB⁺¹²]. **nanosecond** [Bow16, MCRL17]. **nanosheets** [wZbZ11]. **nanospheres** [AAMR18].

nanostructure [LLD17]. **nanostuctures** [YZZ⁺17]. **nanosystems** [PGK⁺19, Tia12]. **nanotube** [AJA⁺19, AS15a, FTR15, JWO15, KHE⁺19, OCW⁺15, RHNN10].

nanotubes [ASL⁺11, BE14, BPE16, DI11, Den12, DZA11, EBK13, EP15, EBPK17a, EBPK17b, EB18, GBS⁺17, KGHK12, KGJZ19, LPLS16, LL10c, LT14, MSY19, NDD⁺10, PBE16, TD11, TSR⁺16, VS14, WYL⁺15, WDZN16, YZN13].

nanowires [AJA⁺19, EP15]. **Nantong** [WZC⁺19]. **naphthalenediimides** [MGS⁺16]. **naphtho** [ZLL⁺10]. **naphtho-homologated** [ZLL⁺10]. **naphthodithiophene** [DGL⁺13]. **naphthol** [CYY⁺17, GZL⁺12]. **naphthoquinone** [HWB19]. **naphthyl** [CFM⁺19]. **naphthyl-based** [CFM⁺19]. **NARES** [SGY⁺18]. **NARES-2P** [SGY⁺18]. **native** [DJ13, HYL⁺11, UCFR16, YL13]. **native-like** [UCFR16]. **Natural** [AIQ19, dCGCRN19, KKGW19, LCPS13, MBFP15, SZL19, Spr18, Wei12a, Wei12b, AO10, BMD19, GMZ12, GWW19, NC14, Sch12, GLW13a, GLW13b].

naturally [XVA⁺16]. **Nature** [ABDGN12, ELKE19, MJM⁺15, SC18a, VMV19, WFZ⁺18, GPK⁺16, GA19, HBR17, Kri10, LZJ⁺11, LYL16, LdSRR16, LTR18, MLGB16, PKK17, RKDM14, YK13, YJ17, YJ19, ZRCC12, dLvNC18b]. **Navigating** [HB19].

navigation [SLG15]. **NBe** [UT14]. **NBO** [GLW13a, GLW13b, GLW19, WvRSM14]. **NBS** [YZ17]. **NCCH** [MLGB16]. **NCI** [REV⁺17, VVJ15]. **NCX** [LZL⁺15b, LZL⁺15b]. **NCY** [LZL⁺15b].

near [DJ13, NPG⁺18, SISK10, Yan11]. **near-infrared** [NPG⁺18]. **near-native** [DJ13]. **near-solute** [Yan11]. **nearest** [Hug14, YS15]. **nearly** [LPS12]. **necessarily** [Jab18a]. **Necessity** [JC16]. **necks** [CC12a]. **Negative** [PG18, BHI19, KV13]. **neglect** [WDKT19]. **neighbor** [AGR11a].

neighboring [HSJ18]. **neighbors** [Hug14, YS15]. **NEMO** [HBKL10].

nesting [HSB⁺19]. **Net** [RO14b, CS14]. **netropsin** [HDK⁺12]. **network** [AD10, GFPSD17, GGM⁺12, HNHR13, HAI⁺16, IHHY15, JCX10, LDH⁺14, NSK18, OC14, PC11, PPUBGD10, RKDM14, SHL19, WMW⁺10, XTY⁺14].

network-based [PC11, PPUBGD10]. **networks** [AGM⁺13, Clo15, Kan15, KUDG12, LHO17, PPM15, PPUBGD10, TD11, WZWW18]. **neural** [AGM⁺13, HNHR13, LHO17, LDH⁺14, PC11, SHL19, WMW⁺10, WZWW18].

Neutral [BHP19, AM19a, AM19b, GC11, GWPJ11, JM11, KD10, Tsi14, GMBM18].

new-type [HLWD15]. **newly** [CBDS19]. **News** [AIGP15, Aki16, APK14, AAC⁺16, BTA⁺13, BHB12, BCSCJ⁺13, BSZ⁺12, Ber17, BJP15, BFH⁺13, BBG⁺18b, CBH14, CSEMB⁺16, CZAF17, CAT⁺13, 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, IKG16, JHH⁺13, JJW⁺14, JLCA17, JP15, JCGM18, KS13a, KS15, KK17a, Kan15, KB16, KDR⁺18, KLJ⁺17, KJM⁺17, KDT⁺12, Kos16, KG13,

KWL⁺¹⁶, KK17b, KWG15, KYG⁺¹⁵, KAG⁺¹², KSW16, KPF⁺¹⁵, LPS12, LJR⁺¹², LSH12, Leh15, LRvdSM15, LRvE17, LDB⁺¹⁷, LLZA12, LBB⁺¹⁵, LWZ⁺¹⁷, LC12, LAS⁺¹⁴, MHT⁺¹⁸, MDTD16, MBR⁺¹⁵, MYT18, MSSP17, MB14, MB16, NKJ16, OV14, OPB⁺¹², OZS⁺¹³, OC14]. **News** [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, SWB⁺¹², SDMS13, TNYN16, TSC⁺¹³, TTR⁺¹², TTL⁺¹², UU12, VMRS⁺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, ZDKM12, ZLL⁺¹³, dVAG16, KKR⁺¹³]. **Next** [ADF⁺¹⁰, HGY15]. **next-generation** [HGY15]. **NF** [ABB⁺¹³, ABB⁺¹²]. **NGuaS** [WGN⁺¹⁶, WGLG⁺¹⁶, WRG⁺¹⁷]. **Nguyen** [Ano15-59]. **NH** [CG12, HDM⁺¹⁹, KSK11, LLX⁺¹⁹, LBTV12, VVY17, CCJ⁺¹¹, Kop15a, LYC⁺¹³, LBTV11, ONTTL16, UT14, Yu12a]. **NHC** [GA19, SB19]. **NHCHCO** [KMS⁺¹⁹]. **NH**... [MVKS10]. **NHN** [LZH⁺¹¹]. **NHOC** [LHHW14]. **Ni** [Ibr17, MP19b, TLdG⁺¹², Tsi17, WWKS16, ZFS18, MMB⁺¹⁷, SIT18, SSD19, SSX⁺¹⁴, TLA10, ZRCC12]. **Ni-NO** [Tsi17]. **Nickel** [SMB18, ED15, FCW⁺¹⁴, VHS⁺¹⁹]. **nicotine** [PMC⁺¹⁷]. **NICSzz** [AVHB18]. **Nine** [AAB⁺¹⁹]. **nitrate** [OSS10, SPZP19]. **nitric** [AM19b, BS16a]. **nitride** [GLF16, LT14]. **nitrides** [TS11]. **nitrioltri** [CM16]. **nitrioltri-** [CM16]. **nitrioltriacetic** [CM16]. **nitro** [YPC⁺¹⁰, ZWZ11, FAS⁺¹⁸]. **Nitro-Porphyrin** [FAS⁺¹⁸]. **nitro-substituted** [YPC⁺¹⁰]. **nitroaldol** [QLYL10]. **nitroaniline** [ZTH⁺¹⁵]. **nitroarenes** [MRC⁺¹⁸]. **nitroaromatic** [PSC11, SB18, TD10]. **nitrobenzenes** [ZGS⁺¹⁰]. **nitrocompounds** [SIG⁺¹⁵, SGH⁺¹⁶]. **nitrodibenzofuran** [DPB⁺¹²]. **nitroethane** [YZL⁺¹⁵]. **Nitrogen** [LLC17, BEPM14, KV14, Lin18, ZZWX11, ZYL⁺¹², SMD18]. **nitrogen-atom** [KV14]. **Nitrogen-doped** [LLC17, Lin18]. **nitrogen-rich** [ZZWX11, ZYL⁺¹²]. **nitrogen-substituted** [BEPM14]. **nitrogenase** [Sie18]. **nitroiminotetrazolate** [ZYL⁺¹²]. **nitromethane** [MCUJ15]. **nitrosamine** [dALdS⁺¹⁵]. **nitroso** [TDP⁺¹²]. **nitrosothiol** [TKXT13]. **NMR** [Ben17, CHP11, EOA⁺¹¹, HJ13, HBI⁺¹⁷, HM13, KASH14, LK11, OPR16, PTK11, PGdO⁺¹⁶, PC14, Pie14, RK15, SPHF⁺¹⁸, SEF⁺¹⁶, SKMS13, SPZP18b, SPZP19, Tsi19, TEDT18, WL14, YS13]. **NNO** [WGL⁺¹¹]. **NO** [MCUJ15, Tsi17, ZZ10, WYGW12, BS16a, GY12, LWZ⁺¹⁹, MN19, OSHG17, RGVC⁺¹⁹, TNI^{+19a}]. **Noble** [BGS⁺¹⁹, SMD18, ARLP13, GC18, JKS⁺¹⁶, PGS⁺¹⁵, PMG⁺¹⁶]. **Noble-Gas** [BGS⁺¹⁹]. **NOCV** [CSM16, DBGO⁺¹⁷]. **node** [KK17a]. **nodes** [FSSW19, KPF⁺¹⁵, KPF⁺¹⁹]. **NOEs** [LK11]. **Non** [KB11c, LCH10, BSD18, CSKH15, GMZ12, GA19, HOK17, MR17, NHN16, PHC13, RS13, VCL18, YWJ⁺¹⁶]. **Non-Boltzmann** [KB11c]. **non-bonded** [BSD18]. **Non-Born** [LCH10]. **non-classical** [GA19]. **non-covalent** [MR17, RS13]. **non-electrostatic** [HOK17]. **non-empirically** [VCL18].

non-equilibrium [NHN16]. **non-heme** [PHC13]. **non-hybrid** [CSKH15].
non-natural [GMZ12]. **non-uniform** [YWJ⁺16]. **nonadditive** [RTS⁺13].
Nonadiabatic
 [HZ11, RGVC⁺19, JBSQG11, KIOY19, MT19b, SRSLO15, WLF19].
nonadiabaticity [Wu10]. **Nonbonded** [ND19, Abr11, EP10]. **Noncatalytic**
 [SGS⁺16]. **Nonclassical** [GZH10, DM15]. **Noncovalent**
 [BGS⁺19, dRCFGRB18, Sch18, RRH12, RLA18, SM16a, SWW⁺19, SBW12,
 TSR⁺16, VT14, WGD⁺16, WDS⁺19, YW13, YZLZ18, SMD18]. **noncyclic**
 [SM16a]. **nonempirical** [BK17b, WYT17]. **nonequilibrium**
 [ASL⁺11, KHWB17]. **Nonfitting** [RZG⁺13]. **nongeometric** [KB11a].
nonheme [BG13]. **Nonideality** [GC11]. **nonionic** [WWKS11].
noniterative [Kid19, MS12]. **Nonlinear** [LLX⁺19, ARLP13, KOP⁺14,
 LLD17, MLQ⁺12, MIS⁺15, RLA⁺11, TFQ⁺10, Tia12, YCGA10].
nonlinear-optical [KOP⁺14]. **nonlocal** [LPAS11]. **nonlocality** [FVB10].
Nonmetal [ZLX⁺19]. **nonorthogonal** [ZM11]. **nonparametric** [RB13a].
nonperiodic [MS15]. **nonplanar** [KG11]. **nonpolar**
 [LvG13b, MPSA17, PAT⁺10, WWW18]. **nonpolarizable**
 [AOW11, WG12, ZRL⁺15]. **Nonrandom** [NPP13]. **nonredundant**
 [HZ13, MK19]. **nonresonant** [BZB⁺13]. **nonspecific** [CBP⁺15].
Nonstatistical [Yu12a]. **nontemplate** [OL13]. **Nontotally** [HOM⁺16].
nonuniform [BD12]. **norbornadiene** [Ant13, WJX⁺10]. **Normal**
 [IY18, GVP⁺10, GMPB12, KKH18, MS17, SBB10]. **Notes** [CD13]. **Novel**
 [FCL⁺10, KKO⁺16, RPNP10, AIGP15, BEPM14, BPM15, DWL11, DMN14,
 DFF⁺15, JYS⁺12, LLC11, LLJ12, MPNS13, PSdPE⁺10, RNP13, WFS19,
 WKC11, YJN⁺11, YHCS11, YDGZ15, dCLFGL13]. **Novic** [CD19]. **novo**
 [AFBR17, BAMR13, LK11, MDT10]. **Nuclear**
 [ASK18, DKT13, ECZWD17, KNP⁺12, CSEMB⁺16, HH16a, HH17, JKS⁺16,
 MT19b, NASH15, PLFS18, RSG14, SPHF⁺18, SS13b]. **Nuclear-relaxed**
 [ECZWD17]. **nuclearity** [BACSCJ⁺10]. **Nucleic**
 [HGY15, ZWP11, Fel10, FCE15, GREA11, MSLS10, OXBW16, SCF⁺19,
 SGY⁺18, SBW12, WG12, XVN17, ZSB⁺11]. **nucleic-acid** [SGY⁺18].
nucleobase [ANH⁺11]. **nucleobases** [CC18b, WG12, ZB18]. **nucleophile**
 [ZYR⁺15]. **Nucleophiles** [WBKS19]. **nucleophilic**
 [JDW⁺19, MA16, MLY⁺13]. **nucleophilicity** [TMJ15]. **nucleotide**
 [CBG17, MJC14, Ran13]. **nucleotides** [DMN14]. **Nucleus**
 [ZBB16, FVB10, TH13]. **Nucleus-independent** [ZBB16, FVB10]. **nudged**
 [QB10, QB11, SH11a]. **null** [TTn19]. **null-space** [TTn19]. **Number**
 [Ano10b, ASMS10, CLK11, DSV⁺19, GPM17, HMM10, MEH18, SL10, SG10b].
numeric [VI17]. **Numerical**
 [WXL17, CKKK16, KEMP17, KP11, MBA11, SKA19, SLG15, YSG12].
numerically [ZDZM13]. **NUPACK** [ZSB⁺11]. **NWChem** [PGW⁺17].
nylon [BHNS14]. **nylon-oligomer** [BHNS14].

O [AM19a, BCNH⁺11, CXS10, CSNCS⁺18, DHE⁺12, GBGR16, HRL11,

JM11, JLH⁺¹⁴, KMS⁺¹⁹, LZTV10, LLLM11, LLB⁺¹², LLSW14, MG11, PLFS18, PBE16, RHT⁺¹⁵, SPS⁺¹², ŠBD⁺¹⁷, TNY18, VV14, WHL⁺¹⁰, WLF19, WRM⁺¹², XFX⁺¹⁶, YW12, YR13, YOPB16, ZRCC12, ZLX⁺¹⁹, Tsi17, BCNH⁺¹¹, BWKW10b, CK10, Chu10, CROB16, CPLL11, DT19, DHE⁺¹², HZ11, LZL^{+15b}, LCWW10, MH11, MSPC19, MS15, PBLdS12, PP19, RHNN10, RAGLL11, SZ17, SJD11, SSX⁺¹⁴, TKCN19, WLF19, YZ15b, ZRCC11, ZSWL12, dCRN18). **o-atom** [Tsi17]. **O-H** [TKCN19]. **O-loss** [MH11]. **O-methyltransferase** [CPLL11]. **O/** [DT19]. **OBC** [FCE15]. **OBGMX** [Gar12]. **Obituary** [Ano15-60]. **object** [RLG14, SK15b]. **object-oriented** [SK15b]. **objective** [PSG⁺¹⁷]. **observables** [VZ14]. **observed** [XML⁺¹⁵]. **obtain** [GR10a, GR11, MA16]. **obtained** [LRVM18, OSR16, SISK10, Tak10]. **obtaining** [STM17]. **occlusion** [BK17a]. **occupancy** [MP13]. **occupied** [HJJ13, MRB14]. **occupied-virtual** [MRB14]. **occurring** [XVA⁺¹⁶]. **ocean** [SSNT19]. **OCF** [ZLLL12]. **OCHO** [dCRN18]. **octa** [ABDGN12, CC18b]. **octa-1** [ABDGN12]. **octaethylene** [TFYO19]. **Octahedral** [BF19a]. **Octene** [MJLV14a]. **OCXR** [FCOGM12]. **OD** [Chu10]. **off** [RGVC⁺¹⁹, WZ19]. **off-diagonal** [WZ19]. **offsets** [KRSC12]. **OFLOOD** [HNS16, HNTS15]. **OH** [CXW14, Chu10, GTK10, HZ11, LLSW14, AR10, CK10, CSNCS⁺¹⁸, GK10, LJW^{+11b}, LJG⁺¹¹, RAGLL11, SST⁺¹⁸, TSJ⁺¹⁰, VDVR14, WLHZ12, ZZL^{+10a}]. **OH/OD** [Chu10]. **OH··** [MVKS10]. **OHHGe** [WHX⁺¹⁰]. **oils** [ZSTI14]. **Ole** [Spr10]. **olefin** [KSO⁺¹⁹, MUN⁺¹⁹, MJLV14b, MTS⁺¹⁹, RS17b]. **olefins** [BF19b]. **olfactory** [DR14]. **oligo** [KSW16, TZ12]. **oligo-** [KSW16]. **oligoacene** [HZSS17]. **oligomer** [BHNS14]. **oligomerization** [KAR12, ZQ14]. **oligomers** [DP15, HLI⁺¹⁹, PH10b, ZSLL17, ZYW⁺¹⁶]. **oligopeptides** [RSL16]. **omit** [LL19b]. **On-the-Fly** [PAK15, CF18, MIOM13, PL14]. **On-the-path** [CY09, CY13]. **One** [MBFP15, CCOH14, GAMAC⁺¹⁴, HRID16, KPL13, LLvG10, LGL11, LvG13b, LvG13a, PSC11, RRK16, SM16a, SH19a, SJC11, SGHL13, WMW⁺¹⁰, YZLZ18, ZZWT12, ZGZC19, ZGS⁺¹⁰]. **one-** [SJC11]. **one-bit-per-sample** [HRID16]. **one-bond** [RRK16]. **One-electron** [MBFP15, PSC11, SGHL13, ZGS⁺¹⁰]. **one-parameter** [SH19a]. **one-step** [LLvG10, LGL11, LvG13b, LvG13a]. **ones** [YZ15b]. **ONETEP** [LCPS13, WS13]. **ONIOM** [JAHS⁺¹⁹, AALCM11, CR19, FRC18, Gil11, GWZX12, Lun12, Mor15, PFAS⁺¹⁹, RJWW12, TS10a]. **ONIOM-ccCA** [RJWW12]. **online** [Ano12u, BJP15]. **only** [LT13]. **ONO** [WGL⁺¹¹]. **onto** [LL13a]. **ontology** [CQFC10]. **OOH** [LJG⁺¹¹]. **OP** [CSKH16]. **Open** [HMO⁺¹⁸, HLS⁺¹³, Aki16, APK14, BG13, FBY⁺¹⁷, HPT17, ISO⁺¹³, KNR⁺¹⁸, KSD⁺¹², NS17, PHT17, RJR14, SRR16, SMRM⁺¹⁷, XTG⁺¹¹, Yap11, Yes12, ZCWX18, CZH12]. **open-ended** [RJR14]. **open-shell** [BG13, ISO⁺¹³]. **Open-source** [HMO⁺¹⁸, HLS⁺¹³, Aki16, APK14, FBY⁺¹⁷, HPT17, KSD⁺¹², PHT17, Yes12]. **opening** [GMBX⁺¹⁶, GSMZ19, LGC19, WCL⁺¹¹, ZQ14]. **OpenMM** [HLW⁺¹⁷, HLEM18]. **OpenMP** [JMS14, KS15, KN17]. **operation** [Bac12]. **operational** [MA16]. **operations** [WS13]. **operator**

[LMR14, SH19a, SNS13, YLS19]. **operators** [Car14, NCT18]. **Oppenheimer** [BLZ⁺13, LCH10, RSB⁺13]. **opportunities** [KHWB17]. **opposed** [WWKS16]. **opposite** [ŠSB⁺16]. **opsin** [RLG11]. **Optical** [LLX⁺19, WGLG⁺16, ARLP13, BLL13, BLS10, CJPTC18, DSB⁺19, GTT10, HB15, HRJ⁺14, HRJ⁺15, JRSHP14, KRTB10, KKPT11, KOP⁺14, LLBO12, LLD17, MLQ⁺12, MIS⁺15, MGS⁺16, MCK17a, TFQ⁺10, TFQ⁺11, TS15b, YB13, YCGA10]. **optically** [RJBH18]. **optics** [Tia12]. **Optimal** [DBK17, VSA11, HS12, Kne11b, LTT16, LAT10, LAT11, MLC13, SM17, Tak11, TTB⁺10, WGA18, CKH19]. **optimally** [Ali18, SZS16]. **Optimization** [AG11, CB11b, CB11c, HOK17, LC17b, MY17b, TKN13, WM12, BW11b, BSD18, BHR15, BW15, BS15, BC13, CY09, CY13, CJL⁺13, DS15, DH11, DMAH15, Elk16, FDH19, GKJ⁺19, GWW19, HNYH19, HKR12, HJKJ13, KSHP⁺19, LvDH13, Leh15, LZL⁺13, LLJ12, NB19, Pon10, PGK⁺19, SA13, SZBM13, SKKS13, SSMW09, SLG15, SR10, SMM17, Tak18, TSZQ12, TO10, Vor10, VBV13b, YS15, ZWP11, ZsA10, vLBBR12, PGL⁺15]. **optimization-based** [YS15]. **optimizations** [RR12, WX12]. **optimized** [Boz18, CX10, GA12, HH10, LZZ14, NDW15, NLL19, ŠSB⁺16, SB14, WO15]. **Optimizing** [SYDS11]. **optimum** [KTNN10, SB11, TKNN10, WTD⁺19]. **ORAC** [MSC⁺10]. **orange** [LWL⁺11]. **orbit** [AMQ⁺14, ATIP18, FAA15, FD16, GP11a, JKS⁺16, KT19, KKA⁺18, MG11, MCP18, PS17, YB11]. **Orbital** [STF⁺19, SZL19, WM12, ASL⁺11, BMD19, Boz18, BVC13, CIKT13, CPN⁺17, CGPP11, DHF⁺11, DN19, FE14, GWF11, GLW13a, GLW13b, dCGCRN19, IIF⁺10, IKN13, ISM18, KSHP⁺19, KTNN10, LCPS13, LFN⁺10, LTP11, MFR⁺17, MGS⁺16, NF18, NPG⁺18, NF17, OHNK11, OOT15, OOK11, PRYI⁺17, PH15, RKGN10, RR19, SGPJS⁺17, Sch12, SHL⁺18, SSMW09, SB14, ŠB15, TKNN10, TSH⁺19, TS14, TSN16, US11, UM13, Wei12a, Wei12b, WCWV15, WM17, ZA15, ZZZ⁺19, vLBBR12]. **orbital-based** [CGPP11, MFR⁺17, Wei12b]. **orbital-dependence** [SGPJS⁺17]. **orbital-free** [RR19]. **orbital-optimized** [Boz18, SB14]. **orbital-weighted** [PRYI⁺17]. **orbital/local** [ŠB15]. **orbitals** [AVHB18, CAF⁺13, CCM15, Dil15, EP12, Fer13b, Fer13a, GCCM15, HJKJ13, HJJ13, JXSW15, KHLM19, MRB14, MY17a, MBFP15, MCK17a, Sax12, TZ12, VI17, YFH⁺19, ZR10, ZM11]. **ORBKIT** [HPT⁺16b]. **ORCA** [MG11]. **Orchestrated** [LL10b]. **order** [BCCO10, DCHL12, FSSW17, FSSW19, Hil13, KKNN11, KN17, LCL⁺10, LPS⁺13, MLQ⁺12, MCC11, NYH⁺17, yOTn16, RBOH11, REH13, SK12, ŠSB⁺16, TAG16, VKAM12, VFRAR16, WLQ19, WHM10, WGA18, ZWF15]. **ordered** [LPAS11, LC17a, LLB⁺12, SJZ⁺15]. **ordering** [LKZM18, MNNK10a, MNNK10b]. **ordering-based** [MNNK10b]. **orders** [GWW19]. **Org27569** [ILKR11]. **organic** [AH10, BBG⁺18a, Ben17, BE16, BS18, CWHH11, CYG⁺15, CLK11, DGL⁺13, ED15, FWS⁺18, FNSF⁺11, GLZ17, GAJ⁺17, KLZ⁺18, LZ14, LZL⁺15a, LWL⁺10, NPG⁺18, NDLW13, PLZ17, PNW⁺16, Pog10, PPM15, RSG14, RNS19, SRR16, SH18a, SSNT19, SFDE16, SSAS10, SIG⁺11, TTR⁺12,

TTB⁺¹¹, VVV^{+15b}, VVW⁺¹⁸, VVY17, WFS19, WZC⁺¹⁹, XWW⁺¹¹,
 YJN⁺¹¹, YNH⁺¹⁷, Zha12a, ZA15, ZGZ19, ZCGM11]. **organization**
 [AO10, FDH19, MCC12]. **organo** [MMS16]. **organo-metallic** [MMS16].
organocatalytic [ORZ11]. **organocuprates** [KYCL11]. **Organofluorine**
 [JLLW19]. **organometallic** [OCLM14, ZYW⁺¹⁶]. **organometallics**
 [GMG⁺¹⁰, dCDP15]. **organophosphorus** [VRKT19]. **organoselenium**
 [RK15]. **orientation** [AST⁺¹⁶, LZ12, LZGS11, RI10, SJZ⁺¹⁵].
orientation-dependent [LZ12, LZGS11]. **orientations** [WWKS16].
oriented [HPSK12, KG13, RLG14, SCM⁺¹⁵, SK15b]. **origami** [SPM⁺¹⁹].
Origin [FB14a, ŠB15, CD13, FCOGM12, dLvNC18a]. **Origin-independent**
 [ŠB15]. **origins** [CB11d, NSO⁺¹⁴, WGD⁺¹⁶]. **Ornstein** [Hei18]. **ORP**
 [BLL13]. **ortho** [LTP11]. **ortho-substituted** [LTP11]. **Orthogonal**
 [BH15, DCŠ15, LAW⁺¹⁶]. **orthogonality** [GA12]. **OsC** [ZWW10].
oscillator [LRvdSM15, LM18a, Ric16, SM14b, ZM10]. **oscillators** [CHC⁺¹³].
Osmosis [LLH⁺¹⁹]. **OsO** [ZXS⁺¹⁰]. **OSPNEY** [HMO⁺¹⁸]. **other**
 [AFBR17, SK12]. **out-of-plane** [Gav12]. **outcome** [WCDM11]. **Outer**
 [TEDT18, BHI19, HS16b, KT12]. **outer-sphere** [KT12]. **outlier**
 [CLX⁺¹⁰, HNS16, HYS19, YS15, ZLM⁺¹⁵, HNTS15]. **Outline** [GPE13].
outlook [MP19a]. **output** [DDK14]. **outputs** [DJD12]. **overall**
 [FZL⁺¹⁹, LZL^{+15a}]. **overcome** [BRGN12, GMO16]. **Overcoming**
 [HH18, VVG13]. **overcrank** [GFGS18]. **overestimation** [FHK⁺¹²]. **overlap**
 [BBG^{+18b}, SFDE16, WDKT19]. **overlapping** [Mau14]. **overly** [BLDK⁺¹³].
oversubscription [FSSW17, FSSW19]. **overview** [Wei12a].
oxadiazoylbenzoyl [FCL⁺¹⁰]. **oxadiazoylbenzoyl-ureas** [FCL⁺¹⁰].
oxaziridine [PC14]. **OXe** [MLGB16]. **oxidant** [WWTL19]. **oxidase** [TN10].
oxidation
 [CCJC10, DSB⁺¹⁹, GHL17, GNGCA10, HFSO12, KB13, LZTV10, LLC17,
 MBFG15, NH19, PXXW10, SFA17, SO_vG12, SGHL13, SIG⁺¹⁵, WWTL19].
oxidation/C [WWTL19]. **oxidative** [FWB14]. **oxide**
 [BS16a, BS16b, GBGR16, GBG⁺¹⁹, MG15]. **oxides**
 [Hua16, OSF12, VLGK⁺¹⁷, VRKT19, YK13]. **oxidized** [WRG⁺¹⁷]. **oxo**
 [RHT⁺¹⁵, SBGP18, SSX⁺¹⁴, VBMA13, EH13, RHPWS13]. **oxo-fluoride**
 [SBGP18]. **oxo-metal** [SSX⁺¹⁴]. **oxoalkyl** [AARP17]. **Oxoiron** [MUN⁺¹⁹].
Oxygen [LT14, LLLW19, OSF12, GWPJ11, IN13, KD10, LL13b, LWXC16,
 LK16a, MBFG15, PXXW10, RLZ⁺¹⁸, SL17, WC14, YJ11].
oxygen-adsorbed [PXXW10]. **oxygen-ligated** [WC14]. **oxygenated**
 [YDR13]. **oxyluciferin** [FD14, PE11].

P [ATIP18, GTK10, HZ11, LCWW10, VT14, dCRN18, PG18, BE16, ED15,
 HAI⁺¹⁶, RVCFF13, WZWW18]. **P-type** [BE16]. **P3HT** [NS18, YFH⁺¹⁹].
P3HT-CdS [NS18]. **P3HT-PbS** [NS18]. **P450**
 [EH13, MRR11, SLY⁺¹⁰, SOYC12, TDP⁺¹², VCM15]. **P51G** [VM11].
P51G-m4-Cyanovirin-N [VM11]. **p53** [IMK⁺¹⁶, HQSZ19]. **p53/PMI**
 [HQSZ19]. **p53/PMI-MDM2/** [HQSZ19]. **PACE** [WNM17]. **Package**

[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, LSH12, 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, LEOLdIV17, 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, PBL19, 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**

[LRVM18, HGCCGR⁺¹⁶, JIS13, LRER13, WG12, WDHZ13, WZWW18, YAS13]. **Partitioning** [VSP19, DK11, EV14, FCOGM12, FHZA⁺¹⁸, LZS⁺¹⁷, REL17, SS13a, TMJ15, VGV⁺¹¹, ZW18, VV19]. **partner** [dVZ17]. **pass** [SR18]. **passing** [CSSB11, ZWL13]. **Past** [GS16, MFEM16, XFG⁺¹⁶]. **patches** [OME16, YSSB12]. **Path** [MA17, VKAM12, CY09, DL19, HXM⁺¹⁶, Ish10, JZ17, KSNT19, MvBD18, SRSLO15, SA13, SS13b, SMM17, TN18, TNY18, WXY14, ZT14, MYKO18, CY13]. **path-based** [ZT14]. **Path-integral** [VKAM12, WXY14]. **path-search** [Ish10]. **PathOpt** [GPE13]. **Paths** [SH11a, AMGB10, Ant13, CX10, Jab18a, NMLD13, RVP⁺¹¹]. **pathway** [BHB12, HOM⁺¹⁶, LKL10, SJD14, TDP⁺¹², XLYZ10]. **Pathways** [JL19, CM13a, EFB16, GS11, HNTS15, KGR⁺¹⁶, KDR⁺¹⁸, MTM14, NJR18, QSW⁺¹⁰, QB16, RCM^{+13a}, RML⁺¹⁵, SJD11, SH18b, Tsi17, WSH10, Yon16, BHB12]. **pattern** [CXS10, LZSM19, WGL12]. **Patterned** [SJSS19]. **Patterns** [KKGW19, FZL⁺¹⁵, RS14]. **Paul** [Ano15-60, Ano16-56]. **Pauli** [JH⁺¹³]. **PAW** [LGKS17, MDTD13]. **PAW-based** [LGKS17]. **Pb** [MCK17b, PMG⁺¹⁶, vSGP10, FBY⁺¹⁷, OBW12, VM11, vSGP10]. **PB-AM** [FBY⁺¹⁷]. **PBE** [DOM⁺¹¹, PTK11, LK16a, SGPJS⁺¹⁷, TG12a]. **PBE-QIDH** [SGPJS⁺¹⁷]. **PBE/3z** [PTK11]. **PBE0** [DOM⁺¹¹, LK16a, SGPJS⁺¹⁷]. **PBE0-DH** [SGPJS⁺¹⁷]. **PBESOL** [DOM⁺¹¹]. **PbI** [VVY17, VVMY18]. **PbS** [NS18]. **PBSA** [BD11, CS17, RDDS10, STM⁺¹⁵]. **PBSS** [DVVP14]. **PC** [VL17b]. **PCASSO** [LFB14]. **PCCP** [VT14]. **pCCSD** [Sch12]. **PCM** [LFN⁺¹⁰]. **PCM-MST** [GMMH⁺¹⁶]. **PD** [HLS⁺¹³, Hil13, KD10, Niz13, YDR13, dSdLBNB17, GA19]. **PD-PK-T** [HLS⁺¹³]. **Pd/** [GA19]. **PDB2PQR** [UHH⁺¹¹]. **PDBbind** [PLAG11]. **PDECO** [CJL⁺¹³]. **PDielec** [KB16]. **PDIxCN** [ZZL19]. **peaks** [LZS⁺¹⁷]. **PEG** [EOO⁺¹⁶]. **PEG-PLA** [EOO⁺¹⁶]. **penalty** [GZH10, LL19b]. **penetration** [NLP⁺¹⁶]. **penta** [dCGCRN19, LBC⁺¹⁹, Sak18]. **penta-coordinated** [Sak18]. **penta-coordination** [LBC⁺¹⁹]. **Pentaatomic** [XhD15]. **Pentacene** [NNT⁺¹⁹, CWHH11, ZYG⁺¹⁵]. **pentacoordinated** [TS10b]. **pentagon** [FL15, GZH10]. **pentane** [TCGNT18]. **pentaprismane** [PCLL11]. **pentathienoacene** [ZYG⁺¹⁵]. **penten** [LXFC17]. **peptide** [FP17a, HHNK19, HPL13, HLH⁺¹², ICS⁺¹², ICS⁺¹³, JBAM11, JWST10, LTT16, LW11, LLvG10, LJW^{+11b}, LvG13a, LMA15, MDT10, MV17, OZ14, QZM11, SV15, SEM12, SZB19, TYZ⁺¹⁶, WS19, XHLH16, XYZ18, YZ15a, dCLFGL13]. **peptide-backbone** [HLH⁺¹²]. **peptide-design** [XHLH16]. **peptides** [BLKP12, BPC13, CR19, CCOH14, CZNA11, GFG11, HSB⁺¹⁹, HLH⁺¹², HHWL17, IO13b, JCX10, KB10, LvG13c, MZZ11, MUGNVJ⁺¹⁸, OLY17, WNM17, XHLH16, XWSW13, ZKH⁺¹⁰]. **peptoid** [MMZW14]. **peptoids** [WS19]. **perception** [AJR16, HYYZ13]. **Performance** [Abr11, BZB⁺¹³, CSKH16, CKKK16, DAP⁺¹⁸, DOM⁺¹¹, GWJR18, HSB⁺¹¹, HB19, JCP14, LK16a, RKB⁺¹⁴, SF18, SH18a, SGWA17, ZZMW19, ABM⁺¹⁵, BLBG⁺¹³, CLFRO18, CXS10, CSSB11, CJZS10, ESB13,

EWK⁺¹³, GAI14, GRARO⁺¹⁴, GSS13, HWLW11, KZZ⁺¹⁶, KLZ⁺¹⁸, LL10a, LRBB12, LLC⁺¹⁰, MHT⁺¹⁸, MC12, MG11, OPB⁺¹², RRH12, RSL13, SRF⁺¹⁷, SPR⁺¹³, SJ16, TF15, XMA⁺¹⁹, YPC⁺¹⁰, YMY⁺¹⁹, ZHS⁺¹⁸, ZSTRS⁺¹⁸, ZSLL17, ZWL13, SBW12]. **Pericyclic** [HPT16a, KG15, ZZMW19]. **period** [LOB18]. **Periodic** [Sce07, Sch10, AAC⁺¹⁶, BBG^{+18a}, BS19, BS18, CMM18, CDC19, CEBO15, FCD10, Gar12, HSH15, HBI⁺¹⁷, ITIN15, KB14a, LBGS16, Man13, MGS⁺¹⁶, NN18, NO16, NTNY15, RJPB12, RLZ⁺¹⁸, RNS19, SN16a, SSP19a, Sie15, SPZP18b, TLdG⁺¹², Tak14, VBV13a, VVB13, VECT12, VI17, YAO18]. **Perlin** [HLBLCCG15]. **permeation** [DMN15]. **permutation** [IO13b, YO19]. **pernitrides** [WD10]. **perovskite** [LLB⁺¹², LLL⁺¹², VVY17, VVMY18]. **peroxide** [HW19, KNP⁺¹², MK13b, SZ17]. **peroxo** [RHPWS13, RHT⁺¹⁵, ZRCC12]. **peroxo/superoxo** [ZRCC12]. **Peroxyl** [CGVBAI19]. **peroxynitrous** [BLG11]. **persistence** [XW15]. **Persistent** [WZWW18, XFTW15]. **personal** [Tsi18]. **perspective** [ABDGN12, Dil15, Hsu14, JCGVPHT17, JMX⁺¹⁶, LGOM⁺¹⁵, MM18, MP17a, Niz13, PZM15, TNY18, XLY12]. **Perspectives** [NSK18, DR14, Wei12a]. **Perturbation** [ELKE19, CCM15, CF14, DCHL12, FRSA14, FSSW17, FSSW19, FE14, GRS15, GCCM15, GA18, Hil13, HRJ⁺¹⁴, HRJ⁺¹⁵, HYUS11, JRSHP14, KKN11, KN17, KSHP⁺¹⁹, KM13, LCL⁺¹⁰, LLvG10, LGL11, LvG13b, LvG13a, MCC11, MUGNVJ⁺¹⁸, RLDJ17, RAR⁺¹¹, RHPWS13, SSSM15, TAG16, VDL⁺¹³, WHAS⁺¹⁰, YKH15, ZZ14, WHAS⁺¹⁶]. **perturbation-based** [KSHP⁺¹⁹]. **perturbation-selection** [FE14]. **perturbations** [GMSdG15, OSR16, Tak10, WWCL15]. **Perturbative** [SSWX14]. **perylene** [BSL⁺¹⁶, SLP⁺¹²]. **perylene-based** [SLP⁺¹²]. **perylenebisimide** [LCK⁺¹⁸]. **perylenediimides** [QCR12]. **pesticide** [BHB⁺¹⁷]. **peta** [KNHN16]. **peta-scale** [KNHN16]. **petascale** [SCOJ13, ZWL13]. **PH** [LZL^{+15b}, dSDdAR10, LBC⁺¹⁹, LZL^{+15b}, AB16a, CS14, CAD16, HS14b, MBA14, PZA15, PS13, SY16a, SOvG12, Vor12]. **pH-dependent** [SY16a]. **pH-responsive** [MBA14]. **Phage** [MP17b]. **Phage-like** [MP17b]. **PHAISTOS** [BFH⁺¹³]. **pharmacokinetics** [VBDS⁺¹¹]. **Pharmacophore** [HRK⁺¹⁰, HKRS11, HS11, TD10, AKMT11]. **Phase** [ATM18, ZMW10, ABB⁺¹², BE12, BG17, Coh18, DLSD13, DLW12, EMD17, FC18, GYX⁺¹⁰, Hsu14, KD10, LJW11a, LPLB16, LGKS17, MFM⁺¹², MKK⁺¹⁹, NIIT15, PSC11, RWR⁺¹³, RSLML12, RJS17, SJZ⁺¹⁵, SPZP18a, VKAM12, VED10, YHG⁺¹¹, YSG12, ZSZ⁺¹⁴, ZWW10, ZYR⁺¹⁵, ZLHH14, dSdS12a, dSdS12b, ABB⁺¹³]. **phase-change** [EMD17]. **phase-space** [FC18]. **phases** [EB12, LPAS11]. **Phen** [FD16, FHG⁺¹⁹]. **Phenanthroline** [SCSM19, MRC⁺¹⁸]. **phenol** [AAMD⁺¹¹, AK10, IYK11, PPH⁺¹⁴, TFYO19, WHX⁺¹⁰, YKH⁺¹⁰, AK10]. **phenol-imidazole-base** [YKH⁺¹⁰]. **phenol-triethylgermanium** [WHX⁺¹⁰]. **phenolates** [SKGB13]. **phenols** [SK12]. **phenomena** [JBSQG11, WDP⁺¹²]. **phenoxy** [IYK11]. **phenoxy/phenol** [IYK11].

phenyl [GZL⁺12, ZWY⁺10a]. **phenylacetylene** [ZZL⁺12].
phenylacetylene-containing [ZZL⁺12]. **phenylalanine** [GWF11, PVS12].
phenylaziridines [KYCL11]. **phenylene** [CH10]. **phenylhydrazine** [Lu11].
phenylimidazo [LWL⁺11]. **PHI** [CAT⁺13]. **philicity** [Tsi19]. **Phonon**
[EBPK17b, EP15, WZ19]. **phosphaalkene** [TR12]. **phosphano** [KYKR15].
phosphate [MRO17, SC18b, XZ11, YZGS14a]. **phosphatidylcholine**
[PVM10]. **phosphetane** [SHL⁺13]. **phosphine**
[KSO⁺19, MG14, VRKT19, YK13]. **phosphine-olefin** [KSO⁺19].
phosphines [VRKT19]. **phospholipid** [PS10, RBOH11, SDZ17, WLO⁺17].
phospholipid/cholesterol [RBOH11]. **phosphopeptide** [AC11a].
phosphoranes [TR12]. **phosphorescence** [LWL⁺11, LXZ⁺10]. **phosphoric**
[HPT16a, KSNT19]. **phosphorous** [KLN12]. **phosphorus**
[GWX⁺12, RB12, YDX16]. **phosphorus-containing** [YDX16].
phosphorylation [RIJ⁺11]. **Photo** [HNN⁺17, ZB18]. **photo-converted**
[ZB18]. **photocatalysts** [FZL⁺19]. **photochemical** [Su10].
photocycloaddition [LXFC17]. **Photodeactivation** [Ant13].
photodetachment [MLCD11]. **photodetectors** [DPAB16].
photodissociation [KT19, KIOY19]. **photodynamic** [ZZ12].
Photoelectron [MN19, TT18, FF11, MLCD11]. **photoemission** [RJS17].
photoexcitation [RVdMB16]. **photoexcited** [MS11]. **photoinduced**
[CGP12, MSV16]. **photoionization** [MY17a, MY17b]. **photoisomerization**
[ZLHH14]. **photon** [DPB⁺12, ZTH⁺15]. **photooxidation** [LWXC16].
Photophysical [SCF⁺19, CWT⁺12, ZGZ19]. **photoreceptor** [XBSS19].
photoresponse [MP19a]. **photoresponsive** [YDGZ15]. **photosensitizers**
[ZZ12]. **photosynthetic** [IIF⁺10]. **photosystem**
[AKMYB18, KTT16, ZSYH12]. **photovoltaic** [NS18]. **photovoltaics**
[VVMY18]. **phthalocyanine** [SKY⁺11]. **phycocyanin** [RCM⁺13a].
phylogenetic [CCYL11]. **Physical** [BGS⁺19, CB11d, YJ19, BPC19,
FCOGM12, JJH⁺13, LHG11, VVP12, YJ17, WCT⁺11]. **physicochemical**
[CCYL11, HZY⁺10, LHL⁺10, RI10]. **physiological** [HM16]. **phytochrome**
[FD13]. **piano** [FPB12, FB14b, ZCK⁺16]. **piano-stool**
[FPB12, FB14b, ZCK⁺16]. **Picture** [KKGW19, ASS⁺17]. **pictures** [MA16].
PICVib [dSAdSL13]. **piezoelectric** [ECZWD17]. **pillar** [uLhY11]. **pillars**
[NNK⁺16]. **pilot** [SSSM15]. **Pimephales** [TTL⁺12]. **pinane** [BLS10].
pincer [ED15, JJAB16]. **pincers** [KJDB12]. **pinene** [BLS10]. **Pipek**
[HJJ13]. **Pivotal** [ZLX⁺19]. **pivoting** [PS17]. **PK**
[HLS⁺13, GK15a, SK15a, SK12, SK17, YDX16, Zha12b, Zha12a]. **PKA**
[MUGNVJ⁺18]. **PKA17** [CPK19]. **PLA** [EOO⁺16]. **Placevent** [SYH12].
planar [BSPP⁺13, EV14, KSO⁺19, Tsi19, Xhd15, YS18, YLT⁺19, ZYW⁺16,
ZLY⁺16, YLZ⁺19]. **planar-chiral** [KSO⁺19]. **planarity** [NK19].
planarization [NK19]. **Plane**
[SH14, BTB⁺11, EH13, Gav12, IT19, LL13b, MDTD13, MDTD16, TCB16].
Plane-wave [SH14, BTB⁺11, MDTD13, MDTD16]. **planewave**
[ASW19, SM18]. **planning** [FBvdB18]. **plasmepsin** [SOD⁺11].

plasminogen [BM12]. **plasmon** [Ano15-58, BH14]. **plastocyanin** [HBR17]. **PLATform** [TNYN16, BTMS12, HPT⁺16b, PSG⁺17, PZCL16, VMRS⁺17]. **platforms** [KJM⁺17, SCOJ13]. **platinum** [ITY⁺19, Tsi19]. **platonic** [KSM16]. **PLATYpus** [TNYN16]. **plausible** [KV14]. **Plavsić** [CD19]. **pleated** [WCAH10]. **Plesset** [FSSW17, FSSW19, Hil13, KKNN11, KN17, MCC11, YKH15]. **PlmII** [VLB⁺10]. **PlmII-inhibitors** [VLB⁺10]. **plot** [MP17a]. **plug** [BTA⁺13, KLOS10]. **plug-in** [BTA⁺13, KLOS10]. **plugin** [FRC18, RD18, BHB12]. **plumbacyclopentadienylidenes** [KASH14]. **PM3** [SA10]. **PM3-CARB1** [SA10]. **PM3-CARB1/TIP3P** [SA10]. **PM6** [SBW12]. **PM6-DH2** [SBW12]. **PMF** [ZLX⁺13]. **PMI-MDM2** [HQSZ19]. **PMMA** [NNS15]. **pmx** [GMSdG15]. **pnicoen** [LDG⁺15]. **Pocket** [AIM⁺18]. **pockets** [MK11, Man19a, TNSS17]. **Point** [Lar11, AS15b, AGM⁺13, BHR15, BEL⁺11, BTB⁺11, EPD⁺10, LPS12, LLSW14, OHPR17, SN15, Tac17, TBSM12, Wei12b, YHW17, dLvNC18a, NQB19]. **Points** [ZQH19, HDL⁺17, HEMCZE⁺14, OHPR18]. **Poisson** [ALRM18, BCCO10, BD12, CLA16, Coo19, FBY⁺17, FHMB15, FCE15, FBvdB18, Fra15, Fra16, GRARO⁺14, NWW17, SK15a, WL10, WLQ19, XYX17, YOMT14, HWLW11]. **polar** [BK17a, CVG14, GMG⁺10, LvG13b, PAT⁺10, WWWW18]. **polar-nonpolar** [WWW18]. **polarizabilities** [BLBG⁺13, BZB⁺13, KR12, KNP⁺12, LIRL⁺16, MLC13, PLFS18, RLA⁺11, SS16b, XKW18]. **polarizability** [CPK12, EPD⁺11, HBKL10, KSK11, NYN17, OVPK15, PC14, YB13]. **polarizability/reaction** [KSK11]. **Polarizable** [CCR18, Coo19, GEP⁺14, LM18a, LPS⁺13, LCL⁺18, NS11, SAvg15, ZM10, ALRM18, BSL⁺16, Cam15, CCB15, CGPP11, DGPM14, DGB⁺13, DDM⁺15, ENKK⁺17, ESM⁺12, FP17a, GRN19, GRS15, GPdC⁺16, HOK17, HZSS17, HLEM18, HCP15, ISO⁺13, KFY⁺13, KR12, KWL⁺16, LRvdSM15, LFN⁺10, LHHW14, LDG⁺15, MBC11, MBC13, MBE16, NLP⁺16, ODB18, PMC⁺17, PZCL16, Ric16, SM14b, SK17, SBvG14, VVLG17, WRHF10, WLO⁺17, XZ11, XP13, ZRL⁺15, ZP13]. **Polarization** [Mit13, CD11, IN19, JZ12, LOB18, LCW12, MLZZ12, OLPB19, POB13, RF15, TNG⁺10, WWD14, YD17, ZJZM13, ZBG11, ZBP11]. **polarizeable** [SS16b]. **Polarized** [BS10a, Jia19, BLBG⁺13, DLZ15, JZM14, NHF⁺10, SFM14, SEJ⁺18, VHS⁺19, YJXZ13]. **pole** [NYN17]. **pole-search** [NYN17]. **pollutants** [GCC14, SIG⁺11, TTR⁺12]. **pollution** [LZ14]. **Poly** [KKGW19, CH10, PRRT⁺10]. **Poly-Electron** [KKGW19]. **polyacenes** [KAR12, RS17a]. **polyacetylenic** [ZZZ⁺19]. **Polyamide** [LLH⁺19]. **polyamidoamine** [CAD16]. **polyatomic** [OT12]. **polybrominated** [GKR13, Ray13, RKG11]. **polycyclic** [CB11d, FVB10, Kar17, PL18, ZWX19]. **polyelectrolyte** [DLP11, NPP13]. **polyelectrolytes** [NSP15]. **polyethyleneimine** [BAF18]. **Polyethyleneimine** [MT20, BF17, MT19a]. **polyglutamine** [CCOH14]. **Polygonal** [PL18]. **polyguluronate** [Pla11]. **polyhedra** [CD16].

polyhedral [CL16]. **Polymer** [HP10b, PH10a, AHK⁺19, KZP⁺18b, MZZ11, SCMA⁺17, YCGA10, YFH⁺19]. **polymer-growth** [MZZ11]. **polymer-stabilized** [AHK⁺19]. **polymerase** [SBT17]. **polymerization** [GSMZ19, KZP⁺18a, MTS⁺19, OSA19, SCK18, YMY⁺19]. **polymers** [BPC19, CRC13, FPH⁺19, GREA11, KLZ⁺18, SA11]. **polymorph** [SPZP18b]. **polymorphic** [SLY⁺10, XWSW13]. **polymorphisms** [LXL⁺11]. **polymorphs** [RRC⁺15, WRM⁺12]. **polynomial** [SY11]. **Polynuclear** [SvLK18, CAT⁺13]. **polyoxometalate** [JAHS⁺19]. **polyoxometalates** [CB11a, CB11b, CB11c, GLZ17, RDF⁺11]. **polyoxy** [SC18a]. **polyoxy-anion** [SC18a]. **Polypeptide** [AD10, IUK⁺11]. **polyphenacenes** [QZ10a]. **Polyphilic** [vRWGS17]. **polypropylene** [OSA19]. **polysaccharide** [KSW16]. **polyspherical** [PH10a]. **polyuronate** [PD12]. **poor** [HDH12]. **popular** [CXD⁺19]. **populated** [CBP⁺15]. **Population** [KKGW19, LTA⁺11]. **population-based** [LTA⁺11]. **Populational** [DK11]. **populations** [BVC13, KV13, OGL10, VZ14, WES13]. **pore** [KJ10, SFBT17, WNM17]. **pores** [DMN15, Fom13, HPL13, LJR⁺12]. **porous** [LZ14, PLZ17, SYZ⁺17]. **porphin** [SMDP18]. **porphyrin** [BH19, BEL⁺11, EH13, INT18, KCK⁺15, MUN⁺19, PLZ17, VBMA13, FAS⁺18]. **porphyrins** [DSB⁺19, MLQ⁺12, TSNC⁺17]. **portable** [KS13a]. **Porting** [WS13]. **pose** [Vor10]. **poses** [HWLW11]. **position** [LHO17, VDVR14, BEEL14]. **positions** [AVHB18, JDW⁺19]. **Positive** [SJSS19, SRA17, VVY18]. **positron** [SST⁺18]. **positronation** [BL12]. **Possible** [NJR18, Oht16, FHK⁺12, GNI18, RB12, Tsi17]. **POSSIM** [LPS⁺13, SK17]. **Post** [SJL18, BY11, CGR16, CB11d, MRO17, RRH12]. **post-Hartree** [CB11d, RRH12]. **post-MP2** [CGR16]. **post-self-consistent** [BY11]. **post-translationally** [MRO17]. **Post-treatment** [SJL18]. **postprocessing** [HPT⁺16b]. **posttranslational** [Ano12u]. **potassium** [SG10b]. **potent** [NS10, XDL⁺10]. **Potential** [Jia19, KIOY19, Kop19a, OSI⁺19, SC17, VSP19, Vor12, AMGB10, AS18, BTA⁺13, BLF14, BT18, BPM15, BSF18, BBI⁺11, CM13a, CG15, Car14, CSXZ17, CKP10, CKKK16, DR11, DLT17, DS12b, DLSA14, EFS16, EPH⁺13, FMNC11, FED17, GKV⁺13, GLM⁺17, GKSS14, GA12, GFG11, HDL⁺17, HBKL10, HYD10, INT18, IN19, KS13a, KS15, KTT16, KPL13, KPL15, KERY⁺16, KS12, Kop15a, Kop16, Kop17a, Kop17b, Kop18, KGM12, KYG⁺15, KCL⁺14, uLhY11, Lar11, LYC⁺13, LDZW17, LX11, LSH⁺11, LCM16, MK13b, Mat14, MK19, MPNS13, MB14, MLCD11, NNS15, NGAS17, NW17, OKIS17, OHPR18, PRRT⁺10, RLD12, RI10, SBR13, SN15, SRF⁺17, SHL19, SC15, ŠSB⁺16, SRS14, SLG15, SJ16, TBSM12, TNI19b, VMRSH⁺17, VT14, VVY18, VL17a, VGTL16, Vyb15, Vyb16, WKC⁺10b, WLO⁺17, XFX⁺16, XCLZ19, Yu12b]. **potential** [ZDZM13, ZLT13, ZWF15, ZFS18, ZGS⁺10]. **potential-derived** [TBSM12]. **Potentials** [Sch18, ACD⁺13a, ACD⁺13b, AS18, BK13, CVG14, DMN14, DMN15, Gpdc⁺16, HH10, Hei18, Ish12, KOY⁺12, KLS10, KMLS10, MCS11, MPA12, MKO⁺13, NOKJ16, PHDH13, PNI13, PSC11, PVJ10, RTS⁺13,

SHL⁺¹⁸, SLX⁺¹⁵, ŚSB⁺¹⁶, SJC11, SGHL13, VCL18, YB16, ZL11].
powdered [KB16]. **Power** [Min18, LZL^{+15a}]. **powerful**
 [CAT⁺¹³, HMO⁺¹⁸]. **powers** [WZ17]. **pp** [CD19, Spr10]. **PPI**
 [RMRBH⁺¹⁹]. **PPI-Detect** [RMRBH⁺¹⁹]. **PR** [TTB⁺¹⁰]. **Practical**
 [GR10b, SLG15, BB11b]. **pre** [RLDJ17]. **pre-computed** [RLDJ17].
preadsorbed [KD10]. **prebiotic** [SSNT19]. **precatalyst** [MJLV14a].
precatalysts [MJLV14a, MJLV14b]. **precision** [DH17, MLC13, SWW⁺¹⁹].
predict [ASMS10, CBH14, DLC18b, HWB19, LLvG10, LLSW14, SEF⁺¹⁶,
 SPZP18a, WJG⁺¹³]. **predictability** [BBOB16]. **predictable** [GDV17].
predicted [DWL11, LZW⁺¹¹, TYX⁺¹⁸, WKLC12, YZ16, Zha12b, ZWX19].
Predicting
 [AS14, AS18, BVHI17, BPB11, cCVG⁺¹⁴, CPK19, ELKE19, GC18, GRL⁺¹¹,
 JGS⁺¹⁷, Jor17, LZSM19, LDH⁺¹⁴, PGdO⁺¹⁶, RDF⁺¹¹, SJWE10, TYX⁺¹⁸,
 VL19, YZ15a, DBM⁺¹⁷, Kar17, KTO13, RB13b, SMDP18, SIG⁺¹¹,
 WCDM11, Yon16, Zha12b, Zha12a, ZLX⁺¹³, ZYS⁺¹⁰, GRL⁺¹²]. **Prediction**
 [Ano12u, AIM⁺¹⁸, CP15, CQFC10, FSD⁺¹⁸, HZSS17, KPL15, LDZW17,
 MCAG⁺¹⁶, yOaCG10, PRP15, SRA17, SPL⁺¹⁸, WDW12, YHW17, ZYL⁺¹²,
 AGM⁺¹³, BLDK⁺¹³, Ben17, BDdS13, BA11, CZAF17, DWL11, DDP16,
 EOA⁺¹¹, FZY⁺¹², GK10, GFPSD17, GTZ⁺¹⁸, HLS⁺¹³, HPL⁺¹⁸, HYMZ16,
 HL14, JSW10, KL14, KT10, KTO11, KB19, LXL⁺¹¹, LMI⁺¹⁴, LZL^{+15a},
 LZZ14, LLH11, LWL⁺¹⁰, LSH⁺¹¹, MDT10, Mau14, MG11, MSÅK12,
 PML⁺¹², PN13, PPJ14, PLV⁺¹¹, RCR⁺¹⁶, RMRBH⁺¹⁹, RKB⁺¹⁴, SM11,
 SYH12, SSD19, TYZ⁺¹⁶, VKC10, WLF11, WH11, WXS⁺¹², WXL⁺¹²,
 WWW18, XFTW15, YVEI⁺¹⁷, YLCX10, YHH⁺¹³, YDX16, YDGZ15,
 ZsA10, wZbZ11, ZYvIZ14, ZLW10, ZHHX11, ZDW18, MSPC19, SDIP18,
 VVBL17]. **predictions** [ALK⁺¹⁵, BCP⁺¹⁰, CLA16, CS17, EOO⁺¹⁶, GAI13,
 KZK⁺¹², PdSC18, RDDs10, RCM^{+13b}, SHMO11, SA10, WZWW18].
predictive [LLL⁺¹⁰, WKC11]. **predictor** [CDS16]. **predictors** [GHK12].
predissociation [YB11]. **Preface** [GS18]. **preference**
 [DSHLM18, LKZM18]. **preferences** [FCOGM12, LGL11]. **preferential**
 [TKYN17]. **preorganized** [CM16]. **preorganized-interacting** [CM16].
preparation [JSD⁺¹¹]. **present** [Cas14]. **presenting** [ZGZ19]. **preserving**
 [ZBG11]. **Press** [CD19]. **Pressure**
 [YAO18, AYYO17, Cam15, CCR18, FCW⁺¹⁴, HYNS19, HRHI17, II18,
 LLL⁺¹², MO17, NFPD13, SMM⁺¹⁸, SPZP18a, WDLG12, CCR18].
pressures [RHNN10]. **primary** [ALK⁺¹⁵, GAI13, VVLG17, KTNN10].
prime [DSX⁺¹¹]. **prime/MM** [DSX⁺¹¹]. **primitive** [HAL14]. **principal**
 [PSP15]. **Principle**
 [WBKS19, CCJC10, DBM⁺¹⁵, LLB⁺¹², MCF10, SBGP18, Tak11, YPvD13].
Principles
 [HFSO12, BE12, BE14, BPE16, EMD17, EB12, EBK13, EBPK17a, EB18,
 GD10, HYL⁺¹¹, Ibr17, JCG⁺¹¹, KLZ⁺¹⁸, LLLM11, LCWW10, NNS15,
 OC19, PLZ17, RZG⁺¹³, SFA17, SPZP18a, TZ11, UGK18, WYL⁺¹⁵, WD10,
 YR13, wZbZ11, Zha12b, Zha12a, ZWMW10, ZZ12, vADC⁺¹⁴, THI⁺¹⁹].

principles-based [Zha12b, Zha12a]. **Prion** [TTC⁺18]. **prismane** [DM15, VIT⁺15]. **pristine** [Avd18]. **Pro** [RB12]. **Pro-Tide** [RB12]. **probe** [LCC18, MvBD18, RN17, Tsi19, TEDT18]. **probes** [HW19, Man19a, SCF⁺19]. **Probing** [HH15, KG11, KKH18, LPK16, TG12b, ZYR⁺15, BSG18a]. **ProBiS** [KDT⁺12]. **problem** [BB11a, Coh18, GA14, KV13]. **problems** [CD19, CJPTC18, HLXH17, HLXH18, PNW⁺16, vS18]. **procedure** [AD10, BKŠ⁺11, BY11, CJZS10, HKR⁺14, MG14, MS12, SA13, dSAdSL13]. **procedures** [AC11b, CKH17, KSM16, PW12]. **process** [ABDGN12, BM12, DPAB16, HBL12, NIIT15, ZZ10]. **processes** [BPLL12, FBEM11, HTS17, JM11, KV15b, LPLB16, PAK17, PTB⁺15, REL17, SSNT19, TNI⁺19a]. **processing** [CKKK16, EP10, GBL⁺11, HASR⁺12, HEMCZE⁺14, WSGN11, WS13, YWJ⁺16, YN15, ZKE⁺17]. **processor** [HKR12, JND⁺19]. **processors** [AB16a, AB16b, BDTP11, Fom11]. **PROCOS** [FHW⁺11]. **produced** [LS11a, SIG⁺15]. **Producing** [RN17]. **product** [CC12b, ZQ14]. **production** [GYX⁺10, SSNT19]. **products** [KIOY19, TR12]. **profile** [AK10, BS16a, GTZ⁺18, KTT16, XML⁺15]. **profiles** [MIOM13, RBOH11, SISK10, Yu12b]. **profiling** [VMRSH⁺17]. **profit** [KB11c]. **Program** [FPV13, GH16b, NN19, SWA13, SR19, BBG⁺11, BBG⁺18b, CBH14, CZZL19, CAT⁺13, Dra19, FM10, GLW13a, GLW13b, GBW⁺14, HS16a, HSN⁺18, HL14, JS17b, KWL⁺16, KK17b, LSH12, MHT⁺18, MSC⁺10, MSvG12, Mez10, MSSP17, MAP18, MB14, NMH19, SMDP18, SFG⁺17, SFR⁺11, SYN⁺12, TNYN16, TSC⁺13, UDK⁺18, VVV⁺15b, WCDM11, WHK⁺12, ZL11]. **program/multiple** [JS17b]. **programming** [GWW19, LMR14]. **programs** [LLC⁺10, PGL⁺15, PLAG11, vW11]. **progressive** [SH19a]. **proguanil** [APA⁺14]. **Projected** [EFS16, TTn19]. **projection** [MDTD13, RHRCH16, TTn19]. **projector** [BVHI17]. **prolapse** [TH13]. **proline** [AS11, HJLV16, OOK11]. **proline-catalyzed** [HJLV16]. **proline-recognition** [OOK11]. **promelas** [TTL⁺12]. **Promising** [CGVBAI19, KSSH13, RNS19, ZSLL17]. **promolecular** [REV⁺17]. **promoted** [LPLB16, QQY⁺18]. **promoters** [MPJ⁺19]. **Proof** [FVB10]. **propagator** [WWD14, YLS19, YD17]. **propane** [WKC11]. **propane-** [WKC11]. **propargyl** [ZSZ⁺14]. **propellant** [WGL⁺11]. **propene** [HSL⁺11, QSW⁺10, dSDdAR10]. **Properties** [LLX⁺19, MP19b, SFCCK⁺14, TY10, AWF⁺18, ARAG17, ASS10, Avd18, ARLP13, ALH⁺10, BCSCJ⁺13, BE12, BPE16, BLFZ13, BS10a, BPC19, BAD⁺19, BP18, BACSCJ⁺10, BC13, CPRS18, CBH14, CWT⁺12, CWHH11, CBTZ16, CH10, CCYL11, CXS10, CLC11, CJPTC18, DSB⁺19, DDP16, DOM⁺11, DMD⁺18, DBM⁺15, DPNM11, DJX⁺11b, DJX⁺11a, DP15, DLW12, DQ16, EPH⁺15, EBPK17b, FB10, GBL⁺11, GTT10, GK10, GNI18, GWJJ12, GBGR16, GBG⁺19, HZY⁺10, HRB⁺17, HLH⁺12, HZSS17, HLWD15, Ibr17, JBSQG11, JJH⁺13, KKPT11, KDB13, KZK⁺12, KPG18,

uLhY11, LHL⁺¹⁰, LSH12, LLLM11, LZJ⁺¹¹, LLD17, LBTV11, LBTV12, LXZ⁺¹⁰, LWWG12, MC10, MCF10, MJLV14b, Mat10, Mat14, MIS⁺¹⁵, MGS⁺¹⁶, MCK17a, NSO⁺¹⁴, NC14, NS18, PHC13, PGY15, PKK17, PGW⁺¹⁷, Pog10, PH10b, Pop18, PBE16, PS10, RR14, RRF11, RI10, SDF⁺¹⁷]. **properties** [SCF⁺¹⁹, SB11, SIT18, SLIB12, SWMW10, SZB19, SZZ⁺¹⁸, SIG⁺¹⁵, SGH⁺¹⁶, TN12, TFQ⁺¹⁰, TFQ⁺¹¹, TS11, TS15b, VVW⁺¹⁸, VPR10, VECT12, WLC12, YW12, YCGA10, wZbZ11, ZYG⁺¹⁵, ZWMW10, ZB18, ZLX⁺¹³, ZBP11, ZYL⁺¹², ZGZ19, FDCJG18, SFCK⁺¹⁵]. **property** [CD13, GPS10, GBS⁺¹⁷, GWX⁺¹², PH15, VAA14, WH11]. **propionate** [TN10]. **propionic** [CM16]. **Proposal** [PRYI⁺¹⁷]. **proposed** [GS11]. **protease** [DLZ15, NHN16, OBW12, SYH12]. **protection** [SBW12]. **protective** [JAH⁺¹⁷]. **Protegrin** [RI10]. **Protegrin-1** [RI10]. **Protein** [CIKT13, CDS16, CPK19, DPOS16, GPS10, HNTS15, HS16b, JL19, LZGS11, MFEM16, MFR10, PGL⁺¹⁵, Ran12, RP15, Rao11, SHMO11, SKKS13, YBS19, AIGP15, AKK⁺¹⁶, AM10, AG12, BSZ⁺¹², BFH⁺¹³, BPB11, BPC13, BCG10, Bow16, BDdS13, BA11, CSC⁺¹⁸, CZAF17, CFC15, CHR^{+12b}, CHR^{+12a}, CM13b, CCYL11, CKP10, CH14, CC12b, CBG16, CHP11, DWL11, DJ13, DVVP14, DLMH12, ESD18, FZY⁺¹², FHW⁺¹¹, FCE15, FLM11, FSC⁺¹⁴, GS14, GDV17, GMSdG15, GRP⁺¹², GZ14, GRL⁺¹¹, GRL⁺¹², HAGK10, HNHR13, HMO⁺¹⁸, HTS15, HTS17, Has14, HZY⁺¹⁰, HPL⁺¹⁸, HKR12, HYMZ16, HJ10, HHBY10, HM13, HZ13, HQSZ19, ILKR11, IHHY15, JZ12, JZZM14, JZL⁺¹⁷, KYT⁺¹⁷, Kan15, KNE11a, KOY⁺¹², KL14, KERY⁺¹⁶, KJ10, KTO11, KTO13, KDT⁺¹², KLS10, KMLS10, LS11a, LFB14, LHL⁺¹⁰, LH11, LCPS13, LC16, LC17b, LZ11, LLC⁺¹⁰, LL10b, LFM12, LPS⁺¹³]. **protein** [LZZ14, LLLC11, LHG11, LBS10, LM18b, LL19b, LDH⁺¹⁴, MS17, MMM⁺¹⁶, MJC14, Mau14, MUGNVJ⁺¹⁸, MA17, MFEM15, MS16, MP11, MKB⁺¹³, MOS12, MNNK10a, NSK18, NST14, NS11, NFG⁺¹³, NG10, OHNK11, OCL11, OL13, OXBW16, OCLM14, OK16, OME16, OOT15, PGCT⁺¹², PBLs19, PGW⁺¹⁷, PLV⁺¹¹, RZG⁺¹³, RCR⁺¹⁶, RMRBH⁺¹⁹, SZdB19, SPL⁺¹⁸, SBB10, SYDS11, SK17, SGY⁺¹⁸, SGM⁺¹³, SY16a, Sti15, TYZ⁺¹⁶, TNYN16, TJR19, TTC⁺¹⁸, TNSS17, TRA⁺¹⁶, TJB12, UNT16, UCFR16, VMPS17, WdVN12, WNP⁺¹⁶, WZ17, WLLH18, WES13, WHAS⁺¹⁰, WHAS⁺¹⁶, XML⁺¹⁵, XYZ18, YZ15a, YZ16, YDL⁺¹⁰, Yon16, YS10, YL13, ZL11, ZC14, ZYvIZ14, ZLW10, ZLX⁺¹³, ZDT18, ZSB⁺¹⁶, dRBO13, AIM⁺¹⁸, DKV18, LGL11, SL10, SHL⁺¹¹]. **protein-bound** [FLM11]. **protein-coding** [YS10]. **protein-coupled** [ILKR11]. **protein-glycosaminoglycan** [SZdB19]. **protein-ligand** [AG12, CHR^{+12b}, CHR^{+12a}, LLC⁺¹⁰, OOT15, SPL⁺¹⁸, WdVN12, dRBO13, AIM⁺¹⁸]. **protein-like** [KOY⁺¹²]. **protein-lipid** [PGCT⁺¹²]. **protein-peptide** [XYZ18]. **Protein-protein** [GPS10, HQSZ19, NG10, PBLs19, RMRBH⁺¹⁹, WLLH18, ZL11, DKV18]. **protein-RNA** [HZ13]. **Protein-specific** [CIKT13, JZZM14]. **proteins** [ABD11, CTR13, CGBK13, DMJ17, FZL⁺¹⁵, FP17b, FBEM11, HS16a, Ham11, HTS15, HTS17, HS17b, HYNS19, HRC13, HS14b, HRH⁺¹⁷, JC16,

JCX10, KCK⁺¹⁷, KDR⁺¹⁸, LHO17, LC17a, MBT14, Man19a, NSO⁺¹⁴, NR11, OCLM14, yOaCG10, PGCT⁺¹², PRP15, PHC13, PNI13, PZBA13, PS13, SK15a, SPL⁺¹⁸, SA11, TYX⁺¹⁸, TO19, VMRS⁺¹⁷, Vor12, WWW19, XSZL11, YZWC11, YMP14, DZA11, GREA11]. **proteochemometric** [NSO⁺¹⁴]. **proteoglycans** [NPG17]. **proteolysis** [VKNT15]. **Proteus** [SGM⁺¹³]. **protic** [RK16a, RK16b]. **protocol** [KPL13, RCR⁺¹⁶, SDL14, VVW⁺¹⁸, WdVN12, dCLFGL13]. **protocols** [CLA16, EOA⁺¹¹, GR11, ZKH⁺¹⁰]. **profibrillation** [PP19]. **Proton** [AK10, IYK11, RJWW12, RK16b, CG15, LPAS11, LBC⁺¹², LZL⁺¹⁰, LWGZ15, MPSG11, PG18, RSB⁺¹³, SRF⁺¹⁷, ŠBD⁺¹⁷, SV11, TM16, VMTL10, Vor12, WG14, XBSS19, YZGS14a, YKH⁺¹⁰, YYT12, dALdS⁺¹⁵, RK16a]. **Proton-coupled** [IYK11]. **proton-ordered** [LPAS11]. **protonatable** [Kan15]. **protonated** [BF17, BAF18, GA18, RSB⁺¹³, US11, WGA18, ZLHH14, dALdS⁺¹⁵]. **protonation** [DMD⁺¹⁸, OBW12, PBG17, SB10, THP⁺¹⁵]. **prototropic** [SC18b]. **prototype** [VMV19]. **prototypes** [dRCFGRB18, VVJ15]. **prototypical** [DT19]. **prototyping** [CCW⁺¹⁰]. **provide** [HRMAL⁺¹³]. **provides** [DSF17]. **proximal** [RVB⁺¹²]. **proximity** [ESD18]. **ps** [SWM10]. **Pseudo** [BF19a, BMD19, FZL⁺¹⁵, GLB16, GRL⁺¹¹, GRL⁺¹², LMZ^{+11b}, ZHHX11]. **pseudo-entropy** [LMZ^{+11b}]. **pseudo-explicit** [GLB16]. **Pseudo-Octahedral** [BF19a]. **pseudoclassical** [EKH14]. **pseudomolecular** [MH10]. **pseudopotential** [BTB⁺¹¹, EH13]. **Pseudopotentials** [DC13, ZCWX18]. **pseudorandom** [GPM17]. **pseudospectral** [CHG⁺¹⁶]. **Pseudosymmetry** [CAF⁺¹³]. **PSII** [SL17]. **Pt** [TLdG⁺¹², AAMR18, CK17, NJX⁺¹⁰, PKK17, PGdO⁺¹⁶, YDR13]. **Pt-195** [PGdO⁺¹⁶]. **Pt-based** [NJX⁺¹⁰]. **Pt-Co** [AAMR18]. **PTCDA** [BBG^{+18a}, HB15]. **PTCDA/KCl** [HB15]. **PTCDA/NaCl** [HB15]. **Pteros** [Yes12, Yes15]. **Publishable** [SJL18]. **Published** [GS16, MFEM16, XFG⁺¹⁶, Ano12u]. **Puigjané** [Ihl12]. **pull** [MLQ⁺¹²]. **pulses** [SS19]. **PUPIL** [BTT10]. **pure** [BG13, GC18, LBH⁺¹¹, SN15, SIT18]. **purely** [BDdS13]. **purine** [WBT10]. **purposes** [MP19c]. **push** [MLQ⁺¹²]. **put** [GKJ⁺¹⁹]. **Putting** [PNW⁺¹⁶]. **pVTZ** [Gil11]. **PyADF** [JBB⁺¹¹]. **PyDEF** [SJL18]. **pyEFP** [ODB18]. **PyFrag** [SSP^{+19b}]. **PyFREC** [KDR⁺¹⁸, Kos16]. **PyGlobal** [NKJ16]. **PyMOL** [BTA⁺¹³, HL14]. **PyMOL360** [HH16b]. **pyMolDyn** [HRB⁺¹⁷]. **PYP** [UD12]. **PyPES** [SC15]. **pyramidalization** [Gav12]. **pyramidalized** [EHT19]. **pyrazine** [WDP⁺¹²]. **PyRETIS** [LRvE17]. **pyridin** [BMB13]. **pyridin-2-yl** [BMB13]. **pyridine** [LWL⁺¹¹, MFR⁺¹¹, PMC⁺¹⁷, QQY⁺¹⁸, SSD19, SLLL13, YMY⁺¹⁹, YLZ⁺¹⁰, CCLP12, FDCJG18]. **pyridone** [AFSW16]. **pyridoxal** [SC18b]. **pyridylamido** [MTS⁺¹⁹]. **pyrimidin** [YZ15b]. **pyrimidin-4** [YZ15b]. **pyrimidine** [ZGZ19]. **pyrimidine-based** [ZGZ19]. **Pyrite** [RD18]. **pyrolysis** [HSL⁺¹¹, LGC19, QSW⁺¹⁰]. **pyrophyllite** [BHB⁺¹⁷]. **pyrrole** [YCGA10, YHCS11]. **pyruvate** [CJZS10].

python [SH19b, HPT^{+16b}, LRvE17, PHH⁺¹², SHFJ18, TBJ18, Yes15].
Pytim [SHFJ18]. **PYX** [LWWG12].

Q [WPM⁺¹⁵, BS10c, GKV⁺¹³]. **Q-CHEM** [GKV⁺¹³]. **Q-Dock** [BS10c].
Q2MM [LN15]. **Q5** [REL⁺¹⁴]. **Q5/D5Cost** [REL⁺¹⁴]. **QB3** [KG15]. **QC**
 [BTA⁺¹³]. **QC/MM** [BTA⁺¹³]. **QCT** [BLG10]. **QIDH** [SGPJS⁺¹⁷].
QikProp [LP11a]. **QM** [BM12, Lun12, RSR⁺¹², Lun12, PLP⁺¹⁶, AALCM11,
 BH13, BZH14, CBG17, CJZS10, DSK17, FRC18, FLM11, FPB12, FB14b,
 GRS15, GWZ15, GCW14, HH15, HYUS11, HBR17, JJH⁺¹³, JWST10, Kid19,
 KTNN10, KWL⁺¹⁶, KWG15, LZdL⁺¹⁰, LFM12, LT13, LHT15, LJL⁺¹¹,
 MCRL17, MTvG12, MJG⁺¹⁵, NO16, OYK⁺¹¹, PMC⁺¹⁷, PP10, PDMT10,
 PL14, PLP⁺¹⁶, RR14, RR12, SN16a, SGDT10, SJD14, SCM⁺¹⁵, STM⁺¹⁵,
 SSAS10, TSC⁺¹³, UTM11, VKNT15, VKNT16, VCM15, VKTRJ15,
 WDP⁺¹², vRET19, GRS15, JAHS⁺¹⁹, LWZ⁺¹⁹, RFN15, ZZY⁺¹⁶].
QM-only [LT13]. **QM/** [GRS15, JAHS⁺¹⁹, LWZ⁺¹⁹, RFN15]. **QM/EFP**
 [CBG17]. **QM/MC/FEP** [HYUS11]. **QM/MM**
 [BM12, RSR⁺¹², AALCM11, CJZS10, DSK17, FLM11, FPB12, FB14b,
 GWZ15, GCW14, HH15, HBR17, JJH⁺¹³, JWST10, Kid19, KTNN10,
 KWL⁺¹⁶, KWG15, LFM12, LT13, LHT15, LJL⁺¹¹, MCRL17, MTvG12,
 MJG⁺¹⁵, NO16, OYK⁺¹¹, PMC⁺¹⁷, PDMT10, PL14, RR14, RR12, SN16a,
 SGDT10, SJD14, SCM⁺¹⁵, STM⁺¹⁵, SSAS10, TSC⁺¹³, UTM11, VKNT15,
 VKNT16, VCM15, VKTRJ15, WDP⁺¹², vRET19]. **QM/MM-MD**
 [RSR⁺¹², OYK⁺¹¹]. **QM/MM-QMC** [UTM11]. **QM/MM-type** [Kid19].
QM/QM' [PLP⁺¹⁶]. **QMC** [UTM11]. **QMX** [KKR⁺¹³]. **QSAR**
 [GKR13, Ray13, AKMT11, BF15, CLX⁺¹⁰, FCL⁺¹⁰, GMMH⁺¹⁶, GCP⁺¹³,
 GCC14, LLL⁺¹⁰, LZL^{+15a}, MdOdQ18, PKIC11, PPUBGD10, RKG11,
 TTb⁺¹⁰, TTL⁺¹², WMW⁺¹⁰, ZDW18]. **QSAR/QSPR** [CLX⁺¹⁰, GCC14].
QSARINS [GCP⁺¹³, GCC14]. **QSARINS-chem** [GCC14]. **QSPR**
 [CD13, BRGN12, CLX⁺¹⁰, CD13, CD16, GCC14, KKO⁺¹⁶, TTR⁺¹²,
 XWW⁺¹¹, YMY⁺¹⁹]. **QTAIM** [BH13, BZH14, FCOGM12, FCPJM14,
 GMBX⁺¹⁶, HXM⁺¹⁶, JMX⁺¹⁶, dIRL11, Rod13, RSKG14, VVJ15, Wei12b,
 WvRSM14, XFX⁺¹⁶, ZZL⁺¹², ZCW18, dLC18a]. **QTAIM-** [VVJ15].
QTAIM-based [FCOGM12, FCPJM14, Wei12b]. **quadrupolar**
 [CSEMB⁺¹⁶]. **quadrupole** [HBKL10, LIRL⁺¹⁶]. **quadrupoles** [NLP⁺¹⁶].
Qualitative [YK13]. **Quality** [CLK11, KCK⁺¹⁷, KYB13, LOB18, MCF⁺¹⁸,
 MKB⁺¹³, OLPB19, POB13, RB13a, RCM^{+13b}, SC15]. **QuanPol** [TSC⁺¹³].
quantification [Fer17, Ham11, PC14, SKGP19, YNH⁺¹⁷]. **quantify**
 [LLHM16]. **Quantifying** [TMJ15, GMBX⁺¹⁶, MS10]. **Quantitative**
 [DZA11, RDT14, VAA14, Wei12b, BPC13, CD13, DXL⁺¹⁰, NPG⁺¹⁸,
 NFG⁺¹³, REL17, RCM^{+13b}, XFTW15, TTb⁺¹¹]. **Quantized** [KKGW19].
Quantum [ALK⁺¹⁵, AC11a, APA⁺¹⁴, Chu10, CG12, DDM⁺¹⁵, FRN15,
 GH10, HHDC16, JCHT18, KASH14, Li14a, Li14b, LWD13, MM18, Mat18,
 MBRC16, MS12, NNT⁺¹⁹, NN19, OKY18, RFN15, SCOJ13, SAGC16,
 ŠBD⁺¹⁷, SOYC12, SR10, SHB17, TR12, UD12, VP19, VSP19, WCAH10,

WDP⁺¹², YHX19, Aki16, ATP18, ASS⁺¹⁷, ARAG17, AAC⁺¹⁶, APY⁺¹⁶, ACS12, ASK18, ALH⁺¹⁰, Bac12, BTT10, BRP⁺¹², BGR13, BEL⁺¹¹, Cam15, CBH14, CDM10, CDB10, CDBM11, CD13, CD16, CDC19, CXW14, CHKR10, CSNCS⁺¹⁸, CM16, CKG18, DR11, DKT13, DDP⁺¹⁸, DPAB16, Dra19, ECZWD17, EV14, Fer13b, Fer13a, FB10, FFA14, FC18, FLM11, GPM17, GMMH⁺¹⁶, GTK10, GGM⁺¹², HZ11, HSN⁺¹⁸, HLvdV13, HPT^{+16b}, HGCCGR⁺¹⁶, HMM10, HYUS11, HGY15, JBB⁺¹¹, JSXH16, KP11, KNR⁺¹⁸, KVR10, KKH18, LPE⁺¹⁰, Lüc14, Man19b]. **quantum** [MP17a, MAPB10, MSvG12, ME10, MSSP17, MHRR11, MFR⁺¹¹, NC13, NC14, NNK⁺¹⁶, NDD⁺¹⁰, NHK⁺¹³, NS17, OKIS17, OSR16, PML⁺¹², PNE18, PSC11, PGW⁺¹⁷, PBG17, PVAM16, RLLHL12, Rez19, REL⁺¹⁴, SLT14, SKA19, SS13b, SPZP19, Tac19, Tsi18, UDK⁺¹⁸, VPR10, VBMA13, WKC^{+10b}, WBT10, WLLH18, WAB17, XCLZ19, YKO⁺¹¹, YLS19, YW13, YKH15, ZW17, ZVY⁺¹⁵, dCDP15, BLG10, OSI⁺¹⁹, SKA19].

Quantum-chemical [KASH14, FB10, MSvG12, MFR⁺¹¹].

Quantum-chemistry [DDM⁺¹⁵]. **quantum-classical** [HLvdV13, SKA19].

quantum-mechanical [ACS12, ECZWD17, PGW⁺¹⁷, Rez19]. **quasi**

[YLT⁺¹⁹]. **quasi-planar** [YLT⁺¹⁹]. **quasiclassical**

[Chu10, LWD13, dSVdM⁺¹⁶]. **quaternary** [DSHLM18]. **QuBiLS**

[GJMPAM⁺¹⁴]. **quest** [AOW11, EK17]. **question** [BZH14]. **questions**

[AAB⁺¹⁹]. **quick** [VVV^{+15b}]. **QuickFF** [VVV^{+15b}, VVW⁺¹⁸]. **quickly**

[vW11]. **quinacridone** [HSZ⁺¹¹]. **quinoline**

[HRJ⁺¹⁴, HGHP14, HRJ⁺¹⁵, JRSHP14, SSD19]. **quinolone** [ZCK⁺¹⁶].

quinone [GLM⁺¹⁷, VSD10]. **quinones** [uLhY11, SDIP18].

R [LdSRR16, LTR18, NDG14, Sch10, DJS⁺¹⁸, GA19, LdSRR16, LTR18].

R-C [LdSRR16, LTR18]. **R-Group** [LdSRR16, LTR18]. **R-NHC** [GA19].

Radial [ME10, COHI19]. **Radial-template** [ME10]. **radiation** [LZH⁺¹¹].

radiation-damaged [LZH⁺¹¹]. **radical**

[AAMD⁺¹¹, GAI14, GKR13, JCG⁺¹⁰, KGR⁺¹⁶, KV14, LJG⁺¹¹, MUN⁺¹⁹,

PNE18, Ray13, RKG11, SJD11, TTR⁺¹², TL16, WHDL11, ZZL^{+10b}, ZLZ14,

ZSZ⁺¹⁴, dLC17, CPR18]. **radical-bridged** [ZLZ14]. **radical-formic** [TL16].

radical-molecule [GAI14]. **Radicals**

[CGVBAI19, Den12, KS13b, LGC19, SRR16, WCT⁺¹¹, WLHZ12, ZZL^{+10a}].

radii [STM⁺¹⁵, YOMT14]. **radio** [AB10]. **Ragué** [Ano16-56].

Ramachandran [KS12, MP17a]. **Raman** [EB18, PAK15, SLLL13, YB13].

Randić [CD19]. **Random**

[HMM10, AC11b, CY09, CY13, CLK11, GPM17, OLA15, RDRC16, WZ17].

Randomized [JCPC11]. **Range** [CKH19, Ali18, AO10, BLBG⁺¹³,

BCNH⁺¹¹, BK17b, CSKH15, ELP19, HH15, HZSS17, Jan16, KKH19, KB10,

KSH13, KSSH13, MMS16, NLP⁺¹⁶, RSG14, Rui11, SMGB11, SH18a, ST13,

SPH11, SH19a, SZB19, SZZS16, SSA⁺¹⁷, VL17a, VCL18, WYT17].

range-separated [Ali18, BK17b, HZSS17, RSG14, SH18a, SZZS16, WYT17].

range-separation [VCL18]. **ranges** [MPA12]. **rank** [EPD⁺¹¹]. **Ranking**

[KERY⁺16, HWLW11, MP11, PBG17]. **Rapid**
 [LJW11a, LW11, LAT11, MZZ11, MRR11, MSS⁺13, MFR⁺17, NO16, PG14, RZ16, TM18, JSW10, KLOS10, LK11, WBF17]. **rapidly** [OPR16, RDRC16].
RAQET [HSN⁺18]. **rare** [HNS16, LRvE17, MP13, Sea10, STS15]. **rare-gas**
 [MP13, Sea10]. **RASPT2** [BH19]. **Rate**
 [AR10, AAMD⁺11, CSNCS⁺18, NMLD13, CBH14, GAI13, GKR13, HSL⁺11, JWO15, KB19, KCL⁺14, MSV16, MK17, MK19, NDW15, OZLSBH12, RAGLL11, Ray13, RKG11, SSC⁺19, STM17, TTR⁺12, ZZL⁺10b, ZLLL12].
rates [BL12, CSAdOM17, GRL⁺11, GRL⁺12, QB16, SHB17, WAB17]. **ratio**
 [BB11b, KB11c, STM17, dRBO13]. **Rational**
 [CSC⁺18, NPG⁺18, Spr18, SCSM19]. **rational** [AARP17]. **Rationalization**
 [TLdG⁺12, SLC⁺17]. **ratios** [OZLSBH12]. **Raton** [CD19]. **rats** [TTB⁺11].
Ray
 [CPR18, FLM11, LLBO12, LSH12, MKK⁺19, PDG⁺16, WWD14, XML⁺15].
Rayne [GKR13]. **Rb** [YLT⁺19, ZWY⁺10a]. **RbLi** [DHOG13]. **RC** [YKH15].
RDG [VVJ15]. **RDG-based** [VVJ15]. **Re** [FD16, KSC16, DLW12].
Re-evaluation [KSC16]. **reach** [QZ10b]. **Reaching** [MCRL17]. **Reaction**
 [DBGO⁺17, FB14b, HSL⁺11, IT19, LWL⁺16, LWZ⁺19, NJX⁺10, QSW⁺10, QB16, ST13, AMGB10, AS11, Alg17, AR10, APA⁺14, BK15, CYY⁺17, CSAdOM17, CXW14, CSNCS⁺18, FB12, GYX⁺10, GZL⁺12, GTK10, GKR13, GAJ⁺17, HOM⁺16, Hel13, HJLV16, ITY⁺19, IIF⁺10, JZ17, JLS⁺10, JW16, KV12, KV13, KG15, KB13, KSK11, KK19, LGOM⁺15, LZY⁺12a, LJW⁺11b, LZL⁺16, LWD13, LPMT17, MTM14, MHT⁺18, MPSG11, MS10, MJLV14a, MJLV14b, MTS⁺19, MT19b, MB16, MMJ10, NH19, NMLD13, NMH19, NTNY15, OSA19, OZLSBH12, PVL⁺13, PG18, PNE18, PPH⁺14, QLYL10, RAGLL11, Ray13, RLZ⁺18, RSL13, RRFV⁺18, RN17, RKG11, RSKG14, RSK⁺15, SLT14, SLT⁺15, SJD14, SRF⁺17, ŠBD⁺17, STS⁺10, SSP⁺19b, SMM17, SM17, Tac17, Tak14, TN18, TNY18, TSJ⁺10, TDP⁺12, TCPPC14, Tsi17, VBD11, VV14, VGTL16, VMTL10, Wu10, WHDL11, WCL⁺11, XCLZ19]. **reaction**
 [XBSS19, YHG⁺11, YJ11, Yu12a, ZYLL12, ZSZ⁺14, ZX19, ZYR⁺15, Zim13].
reaction-diffusion [RSL13]. **Reactions**
 [CC18c, ATP18, AAMD⁺11, ABB⁺12, ABB⁺13, APA⁺14, Cam15, CC18a, CSXZ17, Chu10, DSD⁺11, DS12a, DGSVGVM19, FB14a, FC16, FFA14, GAI14, GH10, GNDA⁺12, GMBX⁺16, GSMZ19, HLS12, HYUS11, HRL11, JZ17, JCG⁺10, KG15, KZP⁺18a, LLH14, LGW12, LT13, LXFC17, LJG⁺11, MC10, MSV16, ORZ11, OSHG17, RWR⁺13, RB12, SSC⁺19, ST13, Su10, SSX⁺14, TM18, TN18, TKXT13, TTR⁺12, Tsi17, UvSvdWK19, VKAM12, VKTRJ15, VGTL16, WLHZ12, WCDM11, WSWD19, XLYZ10, YZGS14a, YNH⁺17, Yu12b, ZZL⁺10b, ZZL⁺10a, ZWZ11, ZLLL12, ZZMW19, ZW17, dSdLBNB17, dCRN18, dSvdM⁺16, SMB18]. **reactive**
 [DMAH15, HJLV16, IHJ⁺13, LvDH13, MB14, NB19, RLLHL12, TDP⁺12].
reactivities [WS11, WS12]. **Reactivity**
 [FHG⁺19, QQY⁺18, TS14, WBKS19, BCP⁺10, CRZ⁺18, CBDS19, DI11,

HGY15, JS17a, LZH16, MAPB10, OSF12, OM12, PML⁺¹², PRYI⁺¹⁷, SIT18, Sti15, YB16, ZYR⁺¹⁵, ZT14]. **read** [DDK14]. **reader** [GHK12, JSD⁺¹¹, KLJ⁺¹⁷]. **READY** [MB14]. **reagent** [SLT⁺¹⁵]. **reagents** [SLT14]. **Real** [NCT18, VHR16, JCGVPHT17, MBFP15, RHT⁺¹⁵]. **real-life** [RHT⁺¹⁵]. **Real-space** [NCT18]. **Real-time** [VHR16]. **Realistic** [HCP15, WCJ⁺¹⁴]. **reality** [SFM⁺¹⁸]. **realizes** [YHCS11]. **really** [MP17a]. **Reannotation** [YS10]. **rearrangement** [ABDGN12, BIL10, OPR16, SFM⁺¹⁸]. **rearrangements** [BIL10, RSKG14]. **reason** [SJWE10]. **reasonable** [Zim13]. **ReaxFF** [HJLV16, JWO15, LvDH13, YPvD13]. **Recasting** [RHRCH16]. **receive** [JT18]. **Receptor** [HK18, BHF⁺¹⁸, CV12, ESB13, FTW12, FRLN10, HYYZ13, ILKR11, LZ11, LLL⁺¹⁰, OME16, PPJ14, SSP⁺¹³, VKC10, WC11, YZZ16]. **receptor-ligand** [FTW12]. **receptors** [DR14, SRA17, UU12]. **Recognition** [ZDT18, CXS10, EPH⁺¹⁵, HS12, Hsu14, ISP⁺¹⁰, LG14, OME16, OOK11]. **recognized** [CDS16]. **recognizers** [uLhY11]. **recombination** [DS12a, SLC⁺¹⁷, ZZL19]. **Reconsideration** [MS11]. **Reconstruction** [RSG⁺¹⁰, DWZ⁺¹⁷, MKB⁺¹³, MIOM13]. **reconstructions** [WDZN16]. **recrossing** [Yu12a]. **rectification** [LWZK13]. **recurrence** [HSN14]. **recursive** [RJR14]. **Red** [Jab14, CSC⁺¹⁸, MTS⁺¹⁹]. **redesign** [CGBK13, HMO⁺¹⁸, SL10, PGL⁺¹⁵]. **Redesigned** [XHLH16]. **redistribution** [JCGVPHT17]. **Redox** [LCB10, GLM⁺¹⁷, INT18, KPL13, LZY^{+12a}, MLQ⁺¹², MKO⁺¹³, TN10, Tsi17]. **Redox-induced** [LCB10]. **redox-switchable** [MLQ⁺¹²]. **Reduced** [BYE⁺¹⁶, BLBG⁺¹³, SWM10, SRR16, SLC⁺¹⁷, VI17, WRG⁺¹⁷]. **Reduced-cost** [BYE⁺¹⁶]. **reduced-size** [BLBG⁺¹³]. **reduces** [ZJZM13]. **reducing** [HAGK10]. **reductase** [BS16a, RKDM14, STM⁺¹⁵, SJ16, VSD10]. **Reduction** [SST⁺¹⁸, TNI19b, AS18, BS16a, GMPB12, KPL15, LDZW17, PNI13, PSC11, RLZ⁺¹⁸, SIG⁺¹⁵, YJ11, ZGS⁺¹⁰]. **reductive** [MRC⁺¹⁸, dCDP15]. **Reevaluating** [PKK17]. **Reexamination** [CKL⁺¹¹]. **Reference** [AlQ19, Jia19, Ali18, FHZA⁺¹⁸, KGM12, LvG13b, OZLSBH12, SHF11, SMM15a, SMM15b, SMM⁺¹⁸, TYN15, dLC17]. **reference-free** [FHZA⁺¹⁸]. **reference-modified** [SMM15a, SMM15b, SMM⁺¹⁸]. **references** [EK17]. **refined** [KD18]. **Refinement** [LvG13c, BCG10, BS10c, CM13b, FLM11, KT18, LFM12, LZZ14, LHG11, OCL11, OL13, PN13, Vor10]. **reflectance** [DCOD13]. **Reformulating** [Pro16]. **Refractive** [MMS16]. **regime** [CSAdOM17]. **region** [MTvG12, MNK10a]. **regions** [KIOY19, MP17a, Pol13, TZ12]. **Regioselective** [WDZN16, BCP⁺¹⁰]. **regression** [DCŠ15, LLL⁺¹⁰, RB13a, YNH⁺¹⁷, YDX16]. **regular** [SWA13]. **Regularized** [YNH⁺¹⁷]. **regularly** [NPP13]. **regulated** [PGI19]. **regulators** [FCL⁺¹⁰]. **reHISS** [CKH19]. **reHISSB** [CKH19]. **reHISSB-D** [CKH19]. **related** [BP18, FCOGM12, GWX⁺¹², LEdOLDIV17, NDD⁺¹⁰, SRA17, TZCK18, TY10, WvRSM14, SMB18]. **Relating** [EJ13]. **Relation** [KTT16, CSKH16, HSN14, SBR13]. **Relations** [BMPML⁺¹³]. **Relationship**

[ACS12, TSN16, BPC13, DXL⁺¹⁰, Gav12, OSA19, RCM^{+13b}, TTB⁺¹¹, VÅA14]. **relationships** [CD13, Sti15, Wei12a, Wei12b]. **relative** [BLDK⁺¹³, CSS17, CM16, EOA⁺¹¹, HH10, HH11, HDK⁺¹², HLW⁺¹⁷, Kar17, NHN16, PBLdS12, PPJ14, RLDJ17, RAR⁺¹¹, RO14b, SOvG12, ZRCC11, ZZ14, dALdS⁺¹⁵, dRBO13]. **Relativistic** [ARAG17, BBI⁺¹¹, GCCM15, RRK16, SNKS10, HSN⁺¹⁸, HKR⁺¹⁴, JKS⁺¹⁶, KKA⁺¹⁸, LHKS12, LH14b, MCK17a, MCK17b, NASH15, OSHG17, PLFS18, PGdO⁺¹⁶, Pyy13, RK15, TH13, VI17, ZXS⁺¹⁰, ZCWX18]. **relativity** [JXSW15, SKMS13]. **relaxation** [GBPCC19, GA18, KSH13]. **Relaxed** [YSRSS10, ECZWD17, KB14b]. **relaying** [SZB19]. **release** [KC13a, MBA14, PMT16, YDGZ15]. **releasing** [GMASBF16]. **Relevance** [TSNC⁺¹⁷, HSB⁺¹⁹, ZSTRS⁺¹⁸]. **relevant** [ISP⁺¹⁰, KAR12, Mat10]. **reliability** [LLSW14]. **Reliable** [JZ17, LHG11, Kar17, NWW17, OV14, PTK11, RAR⁺¹¹, RK15, SHL⁺¹³, TSR⁺¹⁶, Zha12b, Zha12a]. **relocalisation** [dCDP15]. **Remarkable** [TKCN19, BIL10]. **REMD** [PNW⁺¹⁶]. **remote** [BSDP16, RKDM14]. **Removal** [LLLW19, LL13b, YS15]. **rendering** [RD18]. **renormalization** [CAP17]. **renormalized** [ZMMM12]. **Reoptimized** [HLH⁺¹², HH11]. **reorganization** [BE16, DAdGR15, RJS17]. **Reparameterizations** [DPSL16]. **reparametrization** [DH11, FCE15]. **replacement** [YHW17]. **Replacing** [ZSB⁺¹⁶]. **Replica** [GS15, GS16, XFG⁺¹⁶, YO19, ZC14, CH16, CCOH14, IO13a, IO13b, KCK⁺¹⁷, KTO11, KTO13, LC17a, LMI⁺¹⁴, MS16, OGL10, OL13, OLY17, OZ14, RFHG10, SBN13a, SBN13b, TKT11, XFG⁺¹⁵]. **replica-exchange** [CCOH14, IO13a, KTO11, KTO13, LMI⁺¹⁴, OLY17, OZ14, SBN13a, SBN13b]. **replica-permutation** [IO13b]. **replicas** [LL11]. **Reply** [Can11, Cor17, GKR13, QB11, VVB13, WM12, LAT11]. **representability** [PM18b]. **Representation** [SK18, CXW14, CWZB10, DSAS19, FXC⁺¹³, HZY⁺¹⁰, KCPMG12, KDS17, LLLC11, MT19b, ME10, NCT18, YLS19, YDL⁺¹⁰, YS10, YHH⁺¹³, dLvNC18b]. **representations** [OVPK15, dVZ17]. **representative** [KV12, KV13, VLGK⁺¹⁷]. **representing** [TY10]. **repressor** [OHNK11]. **reproduced** [Zha12b]. **reproducibility** [GKR13, Ray13, RKG11]. **reproducing** [KTNN10, MAK⁺¹⁴]. **reproduction** [OPBR17]. **repulsion** [BBOB16, CGPP11, ENKK⁺¹⁷, HOK17, PS17, PC16]. **repulsions** [JJH⁺¹³]. **repulsive** [IO13a, SNDK16]. **required** [RAR⁺¹¹, SG10b]. **requirement** [BF15]. **requirements** [TS15a]. **requires** [Bow16]. **resampling** [MMM⁺¹⁶]. **rescaling** [LL10a]. **rescoring** [BMR11]. **research** [Dra19]. **reservoirs** [RFHG10]. **residence** [VBDS⁺¹¹]. **residual** [LK11]. **Residue** [LABSG17, BH15, BA11, GMO16, IIHY15, JLS18, NR11, SL10, SEF⁺¹⁶, WC14, YHH⁺¹³]. **Residue-centric** [LABSG17]. **residue-residue** [JLS18]. **residues** [FHK⁺¹², KLS10, KMLS10, RKDM14, SK17, WXL⁺¹², WC14, ZDT18]. **resin** [HTY19]. **resistivity** [AB10]. **resolution** [BMFG16, BS10c, CM13b, DFF⁺¹⁵, Höf14, JC16, KN17, NPG17, SM11, Vor10, WNM17, YN15]. **resolution-of-identity** [YN15]. **Resolutions** [LMR14]. **Resolved**

[MM19, KNR⁺¹⁸]. **resolving** [AVHB18]. **resonance** [EFS16, GWW19, KNP⁺¹², PLFS18, Ran19, YB13]. **resource** [Gil11]. **respiratory** [TNI19b]. **Response** [GPGSM12, dSdS12b, BZH14, DSAS19, DHE⁺¹², ESM⁺¹², ITIN15, KSSH13, Kid19, KZK⁺¹², LP11b, MRB14, RJR14, RCM^{+13b}, SS16a, SDF⁺¹⁷, WGLG⁺¹⁶]. **responses** [GWX⁺¹², MLQ⁺¹²]. **responsive** [MBA14]. **restrained** [ER18, HCD⁺¹⁰, KCK⁺¹⁷, SR18, ZDZM13]. **restraining** [KOY⁺¹²]. **restraint** [RO14a]. **restraints** [LL19b, SM11]. **Restricted** [SL10, Cas13, PDG⁺¹⁶, YD17]. **restriction** [FSD⁺¹⁸]. **result** [PH15]. **resulting** [MvBD18]. **Results** [XKW18, Ber17, CBH14, CLK11, GR10a, KERY⁺¹⁶, PLAG11, RAR⁺¹¹, SHL⁺¹³, SPZP18b, WDHZ13, KMLS10]. **retinal** [CG12, GA18, SGWA17, WGA18, ZLHH14]. **retinoic** [LFM12]. **Retracted** [Ano12u, GRL⁺¹²]. **retro** [GRCL12]. **retro-imino-ene** [GRCL12]. **reveal** [MA16, RKDM14]. **revealed** [ALH⁺¹⁰, KKK⁺¹⁹, PNG10, VKNT15, YZGS14b, YJ19]. **Revealing** [VVY17, YW13, YJ17, Bac12, GFGS18]. **reveals** [NR11, WC11]. **Reverse** [KZP^{+18b}, LWL⁺¹⁶, LLH⁺¹⁹, ASL⁺¹¹, Aou16, GP12, OPBR17]. **reversible** [RIJ⁺¹¹]. **Review** [CD19, DR14, FRSA14, GHV17, JCL⁺¹⁷, LJC⁺¹⁹, CMvG10, Sch10, Spr10]. **Reviews** [HLvdV13, ZZWT12]. **Revised** [AKMYB18, CKG18]. **Revising** [Pla11]. **Revision** [PLH16]. **Revisit** [WZH⁺¹⁸]. **Revisited** [KR14, ASS⁺¹⁷, CYI⁺¹⁰, Dil15, HZ11, HFSO12, MSBF16, YW13, vSGP10]. **Revisiting** [OAN15a, Sán17, dSVdM⁺¹⁶]. **Revitalizing** [SZL19]. **reweighted** [SH11b]. **reweighting** [Fer17, OGL10]. **Rh** [KSO⁺¹⁹, SN16a, WJX⁺¹⁰]. **Rh-catalyzed** [KSO⁺¹⁹]. **rhenium** [TS15a, ZWMW10]. **Rhodium** [BF19b, GYX⁺¹⁰, RLD12]. **rhodopsin** [RLG11]. **rhodopsins** [HRMAL⁺¹³]. **rhombohedral** [BE12]. **Rhorix** [MSSP17]. **rhOver** [BP18]. **RI** [BK17c, BK17c, ISM18, KNHN16, TKN13, RKG10]. **RI-MP2** [BK17c, KNHN16, TKN13, RKG10]. **RI-MP3** [ISM18]. **ribonucleotides** [XVA⁺¹⁶]. **ribozyme** [BJSI12]. **ribulose** [CKG18]. **ribulose-1** [CKG18]. **rich** [BHI19, ZZWX11, ZYL⁺¹², YZWC11]. **right** [SJWE10]. **Rigid** [NJR18, Aou16, AGR11a, CZNA11, DBM⁺¹⁷, HDL⁺¹⁴, ODB18, PG14, PGK⁺¹⁹, dACP12]. **rigid-body** [PGK⁺¹⁹]. **Rigid-CLL** [dACP12]. **Rigidity** [NPG17, OXBW16, PRSG13]. **rigorous** [WO15]. **ring** [ABDGN12, CPN⁺¹⁷, CB11d, FNSF⁺¹¹, GWT⁺¹⁷, GMBX⁺¹⁶, GSMZ19, HH10, HH11, HCD⁺¹⁰, LGC19, PCLL11, PLH16, SP13, WCL⁺¹¹, XVN17, YHCS11, ZQ14, OSI⁺¹⁹]. **ring-closure** [ABDGN12]. **ring-conformational** [PLH16]. **ring-opening** [GMBX⁺¹⁶, GSMZ19, LGC19, WCL⁺¹¹, ZQ14]. **ring-polycyclic** [CB11d]. **rings** [FNSF⁺¹¹, GLF16, JHH⁺¹³, PRJ⁺¹⁷, Ran19, TDKT10, ZSTRS⁺¹⁸]. **RISM** [HNN⁺¹⁷, MYT⁺¹⁴]. **RM1** [VSA11]. **RM1-based** [VSA11]. **RMC_POT** [GP12]. **RMSD** [CW19]. **RMSDs** [PG14]. **RNA** [Clo15, DPNM11, GTZ⁺¹⁸, HZ13, KT10, LM18a, SM11, WXY14, XHLH16]. **RNA-binding** [XHLH16]. **roaming** [CSNCS⁺¹⁸]. **robust**

[LLC17, MKH⁺¹³, NWW17, RGVC⁺¹⁹, SIG⁺¹¹, WHK⁺¹²]. **Robustness** [VYM15, BD11]. **ROCS** [HP10a]. **Role** [AS11, Cam19, CAD16, LPAS11, LLLW19, LYL⁺¹¹, MCK17a, VL19, ZLX⁺¹⁹, ZT14, AALCM11, CFM⁺¹⁹, EJ13, GLF16, GFPSD17, HLBLCG15, LEdOLDIV17, OME16, PML⁺¹², RF15, SGPJS⁺¹⁷, SDB⁺¹⁶, SKMS13, SSA⁺¹⁷, VL17a, VMTL10, YDR13, ZRCC12]. **roles** [CC12a, CSNCS⁺¹⁸, YZ17]. **room** [TLdG⁺¹²]. **root** [HDL⁺¹⁴]. **rooted** [CM16]. **roots** [HL19]. **Rotamer** [WES13, KLS10, KMLS10]. **rotamers** [HH11]. **rotary** [HLI⁺¹⁹, HXM⁺¹⁶]. **Rotation** [Kop19a, BLL13, BLS10, GG10, GK10, Hug14, KRTB10, KIOY19, Kop15a, Kop16, Kop17a, Kop17b, Kop18, Kop19b, MK13b, MSBF16, SFM14]. **rotational** [HS12, Kne11b, LAT10, LAT11, MN19, RSG14]. **rotationally** [MK19]. **rotaxane** [LCM16]. **rough** [BRE16, ZSB⁺¹⁶]. **route** [BG17, NFPD13, NFG⁺¹³]. **Row** [BF19a, TKN13]. **RPA** [SPHF⁺¹⁸, SWW⁺¹⁹]. **RPBE** [TG12a]. **RRKM** [OZLSBH12]. **RRKM-based** [OZLSBH12]. **RRT** [NJR18]. **RS** [DS12a]. **RTAM** [Pyy13]. **Ru** [GTT10, JJAB16, LWXC16, FA18, FPB12, FB14b, OSHG17]. **ru-centered** [FA18]. **Rubisco** [CKG18]. **RuC** [ZWW10]. **rule** [FB14a, FL15, GZH10, KSC16, LW16, TLA10]. **rules** [HS16b, KB11c]. **rung** [KM13]. **Runge** [AMGB10]. **rungs** [Kar17]. **RuO** [HFSO12]. **Rut** [Ihl12]. **ruthenium** [BEM14, BEPM14, dCGCRN19, KKPT11, LWXC16, ZCK⁺¹⁶]. **ruthenium-copper** [KKPT11]. **rutile** [CCJ⁺¹¹, HRL11]. **RuvA** [Ish10]. **Rydberg** [LLW12, LWW12].

S

[AM19a, AM19b, CXS10, DT19, GTK10, LWD13, PLFS18, SPS⁺¹², WGN⁺¹⁶, WGLG⁺¹⁶, XCLZ19, YZGS14b, ZYG⁺¹⁴, PRRT⁺¹⁰, AS11, Alg17, ATP18, DT19, HOM⁺¹⁶, LGW12, MH11, MSPC19, MLY⁺¹³, RWR⁺¹³, TKXT13, TNI19b, WJX⁺¹⁰, WZWW18, YZGS14b, Yu12b, Yu12a, YZL⁺¹⁵, ZYR⁺¹⁵]. **S-loss** [MH11]. **S-nitrosothiol** [TKXT13]. **S**. [GKR13]. **S100** [TJR19]. **S100-family** [TJR19]. **S371** [MV17]. **SA** [OBW12, VM11]. **SAC** [EFAC13, FE14, IN13, MN19, PH10b, SRF⁺¹⁷, SCF⁺¹⁹]. **SAC-CI** [EFAC13, EFS16, IN13, MN19, SRF⁺¹⁷, SCF⁺¹⁹]. **SAC/SAC** [IN13]. **SAC/SAC-CI** [IN13]. **saccharide** [LABSG17]. **Saddle** [ZQH19]. **Sal** [LBC⁺¹⁹]. **salen** [DSHLM18]. **salicylidene** [PLP⁺¹⁶]. **Salpeter** [KK17b]. **salt** [EK15, IPAA11, OCW⁺¹⁵, PZA15]. **salts** [Ano11, DSHLM18, JHMB⁺⁰⁹, JHMB⁺¹¹, LCL⁺¹⁸, ZYL⁺¹²]. **samarium** [AARP17]. **same** [CSKH16]. **same-spin** [CSKH16]. **sample** [HRID16]. **sampled** [AST⁺¹⁶, CDM⁺¹⁵]. **Sampling** [AKN16, JL19, Yan16, BLKP12, BH15, BG17, CY09, CY13, CF18, CS17, DPNM11, DJ13, FM10, FBEM11, FB14b, GFPSD17, GMO16, HH10, HDK⁺¹², HTS15, HNS16, HS17a, HYNS19, HKNH18, HDM⁺¹⁵, HCP15, IMK⁺¹⁶, ISK14, Ish10, KvdV14, KJM⁺¹⁷, KTO11, KB11c, LTT16, LC16, LC17a, LL11, LMI⁺¹⁴, LZZ14, LAW⁺¹⁶, MZZ11, MCRL17, OL13, PBDW11, SSO19, SEM12, SBN13a,

SBN13b, STM⁺¹⁵, TJB12, WTD⁺¹⁹, YZ16, ZZ14, ZC14, ZGZC19, DAB16]. **sandwich** [TS15a, WWKS16, YLT⁺¹⁹]. **SAPT** [CLFRO18, DWR17, YJ17]. **SAR** [WPM⁺¹⁵]. **satellite** [ACD^{+13a}, ACD^{+13b}]. **satisfy** [KSH13]. **saturated** [WDZN16, ZWX19]. **saturation** [LW16, RLDJ17]. **Saturn** [RMM16]. **Saving** [FSSW17]. **Sb** [ATIP18, RDT14, SLY⁺¹⁹]. **Scalable** [NLP⁺¹⁶]. **scalar** [Rod13]. **Scale** [XFG⁺¹⁶, YKNN19, AH10, CKG18, DDM⁺¹⁵, FRSA14, HSN⁺¹⁸, JBSQG11, JND⁺¹⁹, KNHN16, LCW12, LCM⁺¹⁴, MDT10, RC18, RSB⁺¹³, XFG⁺¹⁵, XhD15, ZLL⁺¹³, LBH⁺¹¹]. **scaled** [CSGOA17, KM13, ŠSB⁺¹⁶]. **scaled-opposite-spin** [ŠSB⁺¹⁶]. **scales** [GMPB12]. **Scaling** [JND⁺¹⁹, BG12, II18, MA17, NPTS16, NYH⁺¹⁷, Pie14, RCM^{+13b}, RR11, SS13a, VSA11, YN15]. **scanning** [LLJ12]. **scattering** [GBFD12, RLLHL12, RGVC⁺¹⁹, SLLL13, XML⁺¹⁵]. **Scavengers** [CGVBAI19]. **scavenging** [RAGLL11, CPR18]. **SCC** [FHT⁺¹⁵, MŘ17, RN17, SA10]. **SCC-DFTB** [MŘ17, RN17]. **SCC-DFTB-D** [SA10]. **SCC-DFTB-D/TIP3P** [SA10]. **SCC-DFTB/MM** [RN17]. **Scents** [DR14]. **Scerri** [Sch10]. **SCF** [HNN⁺¹⁷]. **SCH** [ZZL^{+10a}]. **Scheme** [SN16b, BK17b, BG12, DK11, DGC14, HKR⁺¹⁴, ISN13, JSW10, MKO⁺¹³, MPBJ11, NB19, NN18, OLPB19, RK15, TCPPC14, UM13, WWD14, WDHZ13, YD17, YFH⁺¹⁹, dLC17, FPV13, FZL⁺¹⁹].

Schemes
[CSM16, Hes19, KYB13, LPLA13, MC12, WOH18, WDW12, XSZL11]. **Schiff** [GA18, SC18b, WGA18, ZLHH14]. **Schleyer** [Ano15-60, Ano16-56, LZH16]. **Schmidt** [EVR18]. **Schrödinger** [FC18, Sah18]. **ScO** [GWPJ11]. **Scope** [KMS⁺¹⁹]. **scores** [LZZ14]. **scoring** [FM10, GSHM10, GZ14, HS11, LHO17, PHDH13, Pro16, RZG⁺¹³, TO10, WZ17]. **scoring-docking-screening** [WZ17]. **screened** [CKH17]. **screened-exchange** [CKH17]. **screening** [AKMT11, CV12, GRP⁺¹², Hei10, JBAM11, KD18, KC14, KB14b, LG11, LMA15, MNNK10b, MH10, SDF⁺¹⁷, WZ17, Won18, YLCX10, YZZ16]. **screenings** [VKC10]. **script** [BK15]. **scripting** [JBB⁺¹¹]. **Scrutinizing** [SDM⁺¹⁶]. **SCS** [LH14a, YJ17]. **SCS-MP2** [LH14a, YJ17]. **SDA** [MBR⁺¹⁵]. **sDFIRE** [HYMZ16]. **SDOCK** [ZL11]. **SDOVS** [MNNK10b]. **Se** [AM19a, AM19b, PLFS18, SPS⁺¹², MLY⁺¹³, NGAS17, RK15]. **seamless** [TSC⁺¹³]. **Search** [ACD^{+13b}, MCAY15, Ran12, AIGP15, AGR11a, AC11b, DS15, GBSE11, GPE13, HRK⁺¹⁰, HKRS11, HS11, HEMCZE⁺¹⁴, Ish10, KM13, MS16, NYN17, NG10, Ran13, TNY18, TRA⁺¹⁶, Vor10, XHLH16, XhD15, YZZ16, HTS15, ACD^{+13a}, DKV18, MYKO18]. **searches** [Pet11, RSL16, TN18]. **searching** [CZZL19, GK15b, HRK⁺¹⁰, HKRS11, HS11, LTA⁺¹¹, ZYvIZ14]. **Second** [MCC11, TKN13, DCHL12, FSSW17, FSSW19, GRN19, Hil13, ISO⁺¹³, KKNN11, KN17, LCL⁺¹⁰, LPS⁺¹³, MLQ⁺¹², NF18, yOTn16, ŠSB⁺¹⁶, TAG16, WYT17, WLQ19, XKW18]. **Second-** [TKN13]. **Second-order** [MCC11, DCHL12, FSSW19, Hil13, KKNN11, KN17, LCL⁺¹⁰, MLQ⁺¹², yOTn16, ŠSB⁺¹⁶, TAG16, WLQ19]. **Secondary** [HSB⁺¹⁹, Clo15, DWL11, FZY⁺¹², HNHR13, HTS17, HPL⁺¹⁸, KT10, KS12,

LFB14, LGL11, Mau14, QZM11, SM11]. **secretase** [YLCX10]. **secretory** [FZL⁺15]. **section** [HBL12, ZHS⁺18, dCLFGL13]. **sections** [MY17a, MY17b]. **SEDD** [HNN⁺17]. **Seebeck** [FSD⁺18]. **seed** [Tak18]. **Segmentation** [TSR⁺16, LCM16]. **segments** [yOaCG10]. **selected** [ICS⁺12, ICS⁺13, KCL⁺14, SGM⁺13, VSD10, dSAdSL13]. **selection** [FE14, HS17a, HS17b, KDB13, LZ18, WMW⁺10, ZYS⁺10]. **selections** [HYMZ16]. **Selective** [PXXW10, KHE⁺19, LZTV10]. **Selectivity** [LPLB16, dSdLBNB17]. **selenium** [WGL12, ZWGO16]. **Self** [JSXH16, SJSS19, WBVE16, AFSW16, BKŠ⁺11, BY11, BK17b, CD11, DK11, FDH19, GBVA11, HS17a, Hei10, HKR⁺14, IM17, KC13b, KT10, KFT18, KLN16, MJLV14a, ON14, OCL11, Rez19, SPS⁺12, SHL⁺18, SCSW13, TYN15, TSH⁺19, WMW⁺10, YN15, ZSTRS⁺18, vS18, uLhY11]. **self-adaptive** [WMW⁺10]. **self-aggregation** [ZSTRS⁺18]. **Self-Assembled** [SJSS19, KC13b]. **self-assembling** [AFSW16, CD11]. **self-assembly** [Hei10, KLN16, uLhY11]. **Self-consistent** [JSXH16, BK17b, DK11, GBVA11, HKR⁺14, KT10, KFT18, ON14, Rez19, SPS⁺12, SCSW13, TYN15, YN15]. **self-consistent-field** [BKŠ⁺11]. **self-consistently** [IM17]. **Self-guided** [WBVE16, OCL11]. **self-guiding** [HS17a]. **self-interaction** [SHL⁺18, TSH⁺19, vS18]. **self-metathesis** [MJLV14a]. **self-organization** [FDH19]. **semi** [DAG19, FSSW17, FSSW19, SC15]. **semi-direct** [FSSW17, FSSW19]. **semi-empirical** [DAG19]. **semi-global** [SC15]. **semiclassical** [YLS19]. **semiconducting** [VS14, ZSLL17]. **semiconductor** [LCH⁺15, SFDE16, VVMY18]. **semiconductors** [BE16, NDLW13]. **Semiempirical** [FA18, SRL⁺15, BP18, GKJ⁺19, GP11a, HGY15, KTNN10, KB14b, LSD⁺10, MGWR12, Rez19, SPH11, SDL14, TKNN10, TG12a, UCFR16, WCWV15]. **semiexperimental** [VDVR14]. **Seminumerical** [PW12]. **sense** [DR14, ICS⁺12, ICS⁺13, NH19]. **sensing** [LZL⁺10, LCC18, RRK14]. **Sensitivity** [Han11, LL11, LWWG12, PDG⁺16, Sea10]. **sensitized** [ACS12, JYS⁺12, LZL⁺15a, MP19a, YJN⁺11]. **sensitizer** [YJN⁺11]. **sensitizers** [SLC⁺17]. **sensors** [DHE⁺12]. **separable** [WWU12]. **separated** [Ali18, BK17b, ELP19, HZSS17, RSG14, SH18a, SZSS16, WYT17]. **separation** [CSKH15, DS12a, NMH19, VCL18, VL17b, YSG12]. **Sequence** [TYZ⁺16, DLL⁺10, DWL11, HPL⁺18, LXL⁺11, MP17b, RMRBH⁺19, Sti15, TYX⁺18, WXL⁺12, YZWC11, YS10, ZWP11, HYMZ16]. **Sequence-based** [TYZ⁺16, RMRBH⁺19, WXL⁺12]. **sequence-reactivity** [Sti15]. **Sequence-specific** [HYMZ16]. **sequences** [Ano12u, CCYL11, Fel10, HZY⁺10, LMZ⁺11b, LLLC11, LDH⁺14, OLA15, QLQ11, YDL⁺10]. **Sequential** [CBP14]. **sequestration** [CC18c]. **Ser** [LY10]. **Serenity** [UDK⁺18]. **serial** [BB11a]. **series** [AWF⁺18, AM19b, AC11b, DDM⁺15, FWS⁺18, LZGS11, MCK17b, SRA17, SB10, TD10, ZGZ19, AM19a]. **serine** [LD18]. **serious** [BRGN12]. **SERS** [THI⁺19]. **serum** [JAHS⁺19]. **server** [PBL19, PZA15, SPM⁺19, XML⁺15, XYX17, XYZ18, dVAG16]. **servers** [UHH⁺11]. **services** [LP11a, UHH⁺11]. **Set**

[SN16b, BLL13, BLG10, BRLS08, BRLS12, CC11, HS16b, KNP⁺¹², LS11a, LLC⁺¹⁰, LYC⁺¹³, LZ18, LWL⁺¹⁰, Mat10, OAN15a, PML⁺¹², PGdO⁺¹⁶, PHK14, PD11, Pog10, PFVL14, RLD12, SPS⁺¹², Sch13, SWM10, SG10a, SG13, VLGK⁺¹⁷, VVLG17, WX12, YOMT14, ZPP⁺¹⁶, FL15]. **Sets** [TKN13, BLFZ13, BLBG⁺¹³, BLF14, BS10a, DBM⁺¹⁵, HSN14, Hil13, LOB18, LBH⁺¹¹, LCW12, Leh15, Mit13, OLPB19, POB13, Sea10, SNKS10, STM⁺¹⁵, TH13, UCFR16, ZLT13]. **Setschenow** [XWW⁺¹¹]. **setting** [AA18]. **seven** [PLAG11]. **sextet** [KDS17]. **SG** [DH17]. **SG-2** [DH17]. **SG-3** [DH17]. **SH** [XCLZ19]. **SH2** [AC11a]. **Sham** [BWMSM10, ŠSB⁺¹⁶, VV14]. **Shao** [Ano12u]. **Shape** [KC14, Zha11, GPS10, HCB11, Hsu14, MNK10a, OAN15b, XTY⁺¹⁴, YLGX14]. **Shape-based** [KC14]. **shape-complementarity** [GPS10]. **shaped** [LWZK13, PGI19]. **shapes** [KC14, PL18]. **Shared** [vW11, UIW⁺¹⁰]. **Shared-memory** [vW11]. **sharing** [JSF19]. **shed** [GNI18]. **sheet** [CCOH14, Hug12, WS10]. **sheets** [PL18, WCAH10, YZZ⁺¹⁷]. **shell** [BH14, BG13, GKSS14, ISO⁺¹³, JCG⁺¹¹, KSR17, MBA11, MA16, MS12, SRR16, TBSM12, TEDT18, WWD14, Ano15-58]. **shell-wise** [KSR17]. **shells** [GPK12, JXSW15, SC18a]. **Sheppard** [QB11]. **shielding** [GMSV14, HAI⁺¹⁶, PC14, VAMS14, YS13]. **shieldings** [JKS⁺¹⁶]. **Shift** [KZZ⁺¹⁶, CK10, CD13, DB12, HRMAL⁺¹³, PGdO⁺¹⁶, RLG11, SKMS13, TEDT18, ZZMW19, ZBB16]. **Shift-and-invert** [KZZ⁺¹⁶]. **shifted** [CSC⁺¹⁸, Jab14]. **shifting** [SP13]. **Shifts** [CPK19, BVHI17, Ben17, CHP11, DKE⁺¹⁷, EOA⁺¹¹, FVB10, HJ13, JKS⁺¹⁶, KASH14, LK11, LZH⁺¹¹, LS11b, MKH15, PTK11, Pie14, RK15, SEF⁺¹⁶, SK17, TKCN19, WL14]. **Short** [LL13a, BLDK⁺¹³, DH14, KTT16, LZJ⁺¹¹, NLP⁺¹⁶, SMGB11, SEM12, SPH11]. **short-cut** [DH14]. **short-range** [NLP⁺¹⁶, SPH11]. **Short-time** [LL13a]. **shorter** [KSC16, UT14]. **shuffled** [HS17b]. **shuffling** [HYNS19]. **Si** [DM15, Ibr17, LCWW10, MCK17b, Sak18, TN12, UT15, AC11b, Cas14, DM15, HAI⁺¹⁶, JM11, LL13a, LLD17, LGKS17, SRS14, UGK18, VIT⁺¹⁵, WKC11, WZH⁺¹⁸, YVEI⁺¹⁷, ZSL⁺¹¹]. **SIBFA** [DGPM14]. **Si** — [LYL16]. **SiC** [Kop16]. **Side** [vRWGS17, DMD⁺¹⁸, KLS10, KMLS10, LPS⁺¹³, LZGS11, LZZ14, LP11b, LvG13a, OZ14, QZM11, SA13, SISK10, SZBM13, DKV18]. **side-chain** [KLS10, KMLS10, LPS⁺¹³, SZBM13, DKV18]. **side-chain-rotamer** [KLS10, KMLS10]. **sidechains** [GMZ12, PS13]. **SIESTA** [KCC⁺¹⁸]. **sigma** [EPH⁺¹³]. **sign** [AVHB18, BLS10]. **signal** [HYYZ13]. **signaling** [FB10]. **Signatures** [BHP19, QZM11]. **Significance** [Sce07, ICS⁺¹², ICS⁺¹³, Sch10]. **Significant** [KOP⁺¹⁴]. **significantly** [CLK11]. **SiH** [ABB⁺¹³, ZYLL12, ABB⁺¹², ZZL^{+10b}]. **sil** [DM15, VIT⁺¹⁵]. **silabi** [DM15, VIT⁺¹⁵]. **silane** ··· [YJ19]. **silica** [HTY19, KKR⁺¹³, SIG⁺¹⁵]. **silicalite** [cCVG⁺¹⁴]. **silicene** [BMD19]. **siliceous** [Lar11, SN15]. **Silico** [VMRSH⁺¹⁷, AKMT11, AS11, DR14, EOO⁺¹⁶, GS11, HS14b, LXL⁺¹¹, MPNS13, PVJ10, YLCX10, GMASBF16, CV12]. **silicon** [AC11b, BIL10, DM15, EFOD13, GSMM15, KOP⁺¹⁴, Kop16, KZK⁺¹²,

TN12, THP⁺¹⁵, VIT⁺¹⁵, XhD15]. **silicon-doped** [TN12].
silicon-germanium [GSMM15]. **Silver** [NSN19, Tsu19, YXZZ17]. **silylene** [BIL10]. **Similarities** [PM18a]. **Similarity** [HS12, LMZ^{+11b}, YDL⁺¹⁰, CDM10, CDB10, CDBM11, CDC19, CQFC10, GWT⁺¹⁷, GK15b, HRK⁺¹⁰, HKRS11, HS11, HSW⁺¹⁹, RMPAM15, TZCK18, YZZ16, ZYvIZ14].
Similarity/dissimilarity [YDL⁺¹⁰]. **SIMONA** [SWB⁺¹²]. **Simple** [Ano15-59, CNK97, GM17, MPSA17, AB16b, BS10b, BD12, CWZB10, KRTB10, NSP15, PHC13, PRY⁺¹⁷, RHRCH16, RGVC⁺¹⁹, SEF⁺¹⁶, SS13c, YS18, dSAdSL13, KTSW11]. **simplified** [KOY⁺¹²]. **simplify** [BLZ⁺¹³].
Simplifying [BL19]. **SIMPRE** [BCSCJ⁺¹³, BCJC⁺¹⁴, KR14].
SIMULAI2 [CSEMB⁺¹⁶]. **Simulaid** [Mez10]. **simulate** [SLX⁺¹⁵].
Simulated [LBC⁺¹², MO15, LLvG10, MO17, NPTS16, RHJ11, SHMO11].
Simulating [HIS17, SS13c, FHT⁺¹⁵, PVM10, SA10]. **Simulation** [BVY⁺¹², CRC13, Yan16, YKNN19, AASP18, AJA⁺¹⁹, AG11, AST⁺¹⁶, BEM14, BPLL12, Ber17, BLKP12, BFH⁺¹³, Bow16, CBP14, CLC11, CCW⁺¹⁰, CHKR10, CZNA11, DOM⁺¹¹, EdOdS18, Fom13, FSC⁺¹⁴, GLZ17, GFGS18, GSD10, HM16, HYSF19, HQC16, HBJ⁺¹⁷, ISK14, IN19, Ish10, IM17, JA10, JJW⁺¹⁴, JAH⁺¹⁷, JSD⁺¹¹, JCL⁺¹⁷, JWST10, JGS⁺¹⁷, Jor17, JP15, KV12, KVQC⁺¹¹, KT18, KVR10, KAG⁺¹², LL15, Lar12, Lar11, LWK⁺¹⁴, LJR⁺¹², LC17b, LMZ11a, LZ14, LWZ⁺¹⁹, LBDP12, MCvdV13, MSC⁺¹⁰, MBR⁺¹⁵, MTS⁺¹⁹, MSvG12, Mez10, MMZW14, MLCD11, MCC12, NPG17, NFG⁺¹³, NDD⁺¹⁰, OYK⁺¹¹, ON14, PLZ17, PP19, QLK119, RHNN10, RAR⁺¹¹, RO14a, RO14b, RSR⁺¹², RSL13, SWM10, SK15b, SMRM⁺¹⁷, SSP19a, SHL19, SS19, SJZ⁺¹⁵, SBvG14, SAvG15, TNYN16, UTM11, UU12, VMRSH⁺¹⁷, Vor12, WC11, WLF19, WWW19, WSWD19, YAS13, ZX11].
simulation [ZSS⁺¹³, ZKH⁺¹⁰, ZLL⁺¹³, dCLFGL13, SGP18]. **Simulations** [BRE16, Hes19, JL19, MFEM16, NN19, PK19, RJBH18, RKDM14, XFG⁺¹⁶, Aki16, BTA⁺¹³, BM12, BDTP11, BW15, BF17, BJP15, BMBJ11, BB11b, BB11c, BBI⁺¹¹, CTR13, CCOH14, CVG14, CLK11, DGH⁺¹¹, DMN14, DSD⁺¹¹, DHF⁺¹¹, DZT11, DSK17, DLZ15, DDM⁺¹⁵, ER18, EK15, FTW12, GBL⁺¹¹, GR11, GPM17, GCW14, GP11b, Has14, HCD⁺¹⁰, HFSO12, HPSK12, HDPM14, HMM10, HYUS11, HJ10, HHWL17, HLEM18, II18, IPAA11, JIS13, JWO15, JMS14, JND⁺¹⁹, KV13, KCK⁺¹⁷, KCK⁺¹⁵, KvdV14, KGHK12, KGHC15, KLOS10, KB11a, KTO11, KSR⁺¹⁶, KLS10, KMLS10, KZP^{+18a}, KWL⁺¹⁶, KV15a, KPF⁺¹⁵, LH11, LC17a, LRvdSM15, LZ12, LPS⁺¹³, LMI⁺¹⁴, LZLMP16, LCL⁺¹⁸, LM18b, LL19b, LAS⁺¹⁴, MPJ⁺¹⁹, MMH19, MN15, MCRL17, MTvG12, MFEM15, MADWB11, MAP18, MKM⁺¹⁷, MB14, NST14, NFPD13, NNK⁺¹⁶, NTNY15, Oht16, OC19].
simulations [OCL11, OLY17, OZ14, OCW⁺¹⁵, PGY15, PH17, PL19, PZCL16, PL14, PM13, PS13, PS10, PNG10, RD18, RdA12, RLG14, RŠRR15, SSO19, SBV10, SKA19, SS13b, SHFJ18, SBT17, SISK10, SCK18, SJ17, SMP17a, SYN⁺¹², SK13, SFLG⁺¹⁷, ŠB15, SWB⁺¹², SDMS13, SPM⁺¹⁹, SV11, VSA11, VKTRJ15, VM11, WKLC12, WAM17, WH11, WWKS11, WLC12, WBF17, WS19, WG14, Won18, WCJ⁺¹⁴, XFG⁺¹⁵, XWSW13,

YKO⁺¹¹, YO19, YSG12, Yon16, YHVM12, YFH⁺¹⁹, ZZY⁺¹⁶, ZDKM12]. **simulator** [BSL11, KJM⁺¹⁷, RLLHL12, TCX⁺¹³]. **simultaneous** [LL10b, WZWW18]. **Single** [HPL⁺¹⁸, LP11c, PM18b, SR18, Zim15, AS15a, BE14, BP18, BK17b, Den12, FTR15, GCCM15, KK17a, KGJZ19, LXL⁺¹¹, MSY19, MT19b, MCLD10, MEH18, PBE16, RHNN10, RLDJ17, SY16b, SPM⁺¹⁹, TSR⁺¹⁶, VS14, WLW⁺¹⁰, WYL⁺¹⁵, YZN13]. **single-** [BE14]. **single-bond** [GCCM15]. **single-configuration** [MT19b]. **Single-ended** [Zim15]. **single-excitation** [MEH18]. **single-file** [SY16b]. **single-ion** [BP18]. **Single-pass** [SR18]. **Single-sequence-based** [HPL⁺¹⁸]. **single-step** [RLDJ17]. **single-vibronic-level** [MCLD10]. **single-wall** [KGJZ19, TSR⁺¹⁶]. **single-walled** [AS15a, PBE16, VS14, WYL⁺¹⁵, YZN13]. **singles** [EK17]. **Singlet** [NNT⁺¹⁹, SZL19, BSDP16, HWB19, ISO⁺¹³, RS17a, SSC⁺¹⁹, THP⁺¹⁵, TCPPC14, ZZL19]. **singlet-triplet** [RS17a]. **Singlet/** [ZZL19]. **singular** [Les19, SG10a]. **singular-value** [Les19]. **SiO** [DOM⁺¹¹, HEM⁺¹⁷]. **SiOH** [LvDH13]. **SIPs** [KCC⁺¹⁸]. **Site** [CH14, LJW^{+11b}, CVG14, DAP⁺¹⁸, GEP⁺¹⁴, GPdC⁺¹⁶, HL14, ISP⁺¹⁰, LLB⁺¹², LKZM18, LLL⁺¹², MP13, MNNK10a, OHPR17, OHPR18, RLDJ17, SHF11, SB11, SC18b, TYN15, ZLX⁺¹³]. **Site-directed** [CH14]. **site-identification** [RLDJ17]. **sites** [AIGP15, Ano12u, DVVP14, DBK17, JAHS⁺¹⁹, KDT⁺¹², LZTV10, LHL⁺¹⁰, LL10b, LZX16, LG14, MA16, PHC13, PBG17, TYZ⁺¹⁶, TYX⁺¹⁸, Vor10, YZ15a, YHH⁺¹³, ZZL⁺¹²]. **situ** [JZL⁺¹⁷, LZY12b]. **six** [DOM⁺¹¹, XhD15]. **Size** [NNT⁺¹⁹, Tak18, AS15a, BLBG⁺¹³, BD12, CC12a, CF14, DJX^{+11b}, FE14, GZZ12, Hsu14, MTvG12, SL17, SB11, XYX17, Zha11]. **Size-guided** [Tak18]. **size-modified** [BD12]. **sized** [LRvE17, OGL10, RK15, WWD14]. **sizes** [Lin18]. **SKATE** [FM10]. **slab** [BBG^{+18a}]. **Slater** [Dil15, LRER13, MY17b, SFG⁺¹⁷]. **Slater-function-based** [SFG⁺¹⁷]. **Slater-type** [Dil15, MY17b]. **slices** [AKN16]. **slicing** [KCC⁺¹⁸]. **SLIM** [SSBW14]. **slit** [Fom13]. **slope** [Zha12b]. **Slowing** [SGP18]. **SM** [XMSZ16]. **SM-TF** [XMSZ16]. **Small** [XYW⁺¹⁴, ASS10, BTMS12, BLKP12, BS16b, CQFC10, DT19, DGL⁺¹³, ETLS17, GAMAC⁺¹⁴, GBFD12, KKPT11, KGHK12, KLJ⁺¹⁷, KB11b, LK13, LHKS12, LH14b, Man19a, Man19b, MSS⁺¹³, MBE16, MBRC16, MPBJ11, NHN16, RLL⁺¹⁰, RSSG18, RS13, SG13, STS15, TNY18, VT14, WF16, WTH⁺¹⁶, XML⁺¹⁵, XMSZ16, ZCGM11]. **small-molecule** [ETLS17, WF16]. **smaller** [MCK17b]. **smallest** [PMT16]. **SMD** [ALK⁺¹⁵]. **smearred** [ENKK⁺¹⁷]. **SMILES** [TTB⁺¹⁰]. **SMILES-based** [TTB⁺¹⁰]. **Smoluchowski** [KS18, SG10a]. **smooth** [AG11, EFS16, JLCA17, ZSB⁺¹⁶]. **smoothed** [LZ12]. **SMPBS** [XYX17]. **Sn** [MCK17b, PMG⁺¹⁶, RDT14, YW12, ASS10, PKK17]. **SnCl** [dSDdAR10]. **SnO** [DHE⁺¹²]. **Sodium** [KLN16, OC19, TFYO19]. **Soft** [SJC11, WBKS19, Ben17, BG12]. **Soft-core** [SJC11, BG12]. **Software** [AIGP15, Aki16, APK14, AAC⁺¹⁶, BTA⁺¹³, BHB12, BCSCJ⁺¹³, BSZ⁺¹², Ber17, BJP15, BFH⁺¹³, BBG^{+18b}, CBH14, CSEMB⁺¹⁶, CZAF17, CAT⁺¹³,

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, LSH12, 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, dRL11, 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, WWW18, 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,

RVM19, RdA12, RRK16, SLT14, SBV10, SK17, SLX⁺¹⁵, SYH12, SCMA⁺¹⁷, SKMS13, TYN15, WWKS11, WXL⁺¹², WBF17, YOMT14, Yan14, YJ11, BK17a]. **solvent-dependent** [HYUS11]. **Solvent-driven** [KC13b]. **solvent-induced** [AKK⁺¹⁶]. **Solvents** [LHT15, ISO⁺¹³, Pie14, Pog10, RK16a, RK16b]. **solver** [FBY⁺¹⁷, FHMB15, Kan15, RR19, SHF11]. **solvers** [GRARO⁺¹⁴, WL10, XYX17]. **Solving** [KV13, SG10a, BYE⁺¹⁶, GA14, RRFV⁺¹⁸, SK15a]. **solvolysis** [OSS10]. **SOMA** [BMFG16]. **Some** [RCM^{+13b}, CME11, CC18a, CC18c, CCYL11, CXS10, MJLV14b, Vyb16, ZPF14]. **sometimes** [VDVR14]. **Song** [JW12]. **Soon** [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]. **soot** [KAR12]. **SOP** [AKK⁺¹⁶]. **SOP-GPU** [AKK⁺¹⁶]. **Sorafenib** [GMASBF16]. **sorbates** [KB19]. **Sorting** [NMF⁺¹⁴]. **Source** [GMBM18, TCB16, Aki16, APK14, BZH14, CD13, FBY⁺¹⁷, HMO⁺¹⁸, HLS⁺¹³, HPT17, KSD⁺¹², MLG18, PHT17, SMRM⁺¹⁷, XTG⁺¹¹, Yap11, Yes12]. **Source-Function** [GMBM18]. **sources** [BK13]. **Space** [vRWGS17, ACD^{+13a}, ACD^{+13b}, AD10, Cas13, CH16, CXS10, Coh18, DK11, DSHLM18, FC18, GA14, GK15b, HB14, HP10b, HSB⁺¹¹, JCGVPHT17, LMZ11a, LLFH16, LAW⁺¹⁶, MBFP15, NH19, NCT18, PDG⁺¹⁶, SS13a, SHL⁺¹¹, SCSW13, TTn19, TJB12, WDHZ13, XTn18, YD17]. **space-group** [HB14]. **spacer** [JYS⁺¹²]. **spaces** [CD13, FBvdB18, TTn19, WM17]. **spanning** [yOaCG10]. **sparse** [LK11, LDH⁺¹⁴, VZ14, YHH⁺¹³]. **sparsely** [CBP⁺¹⁵]. **Sparsity** [HNS16, BYE⁺¹⁶, RR11]. **sparsity-exploiting** [BYE⁺¹⁶]. **Sparsity-weighted** [HNS16]. **Spatial** [PTB⁺¹⁵, HAL14, MTvG12]. **SPC** [GM17]. **SPC/E** [GM17]. **SPC/E-I** [GM17]. **special** [Alg17, ZZZ⁺¹⁹]. **species** [MAK⁺¹⁴, MG11, OSS10, RHT⁺¹⁵, SSA⁺¹⁷, TCPPC14, Tsi14, VRKT19, WvRSM14, ZZ10, ZLY⁺¹⁶]. **Specific** [DHF⁺¹¹, OHNK11, CIKT13, CCM15, GCCM15, HNYH19, HYMZ16, JZM14, KR12, LHO17, LGL11, LXFC17, MCC11, MC12, SSSM15]. **specificity** [LJW^{+11b}, LBS10, ZX11]. **Spectra** [PAK15, TT18, AMQ⁺¹⁴, BG17, DCOD13, EBPK17b, FD13, FF11, GWF11, GGM⁺¹², GZZ12, HRH⁺¹⁷, KASH14, Kow11, LBC⁺¹², LX11, MAK⁺¹⁴, MCLD10, MKK⁺¹⁹, NHF⁺¹⁰, PMC⁺¹⁷, PDMT10, PDG⁺¹⁶, RS17a, RJS17, SGDT10, ŠB15, SR11, TYN15, TZCK18, TG12b, Tsi14, WGL12, WWD14]. **spectral** [Ano15-58, BH14, CBDS19, HRMAL⁺¹³, KZZ⁺¹⁶, NSO⁺¹⁴, QZM11, RLG11, SFDE16]. **spectrometer** [LBB⁺¹⁵]. **Spectroscopic** [SS13b, GK10, KDB13, Kop15b, NC13, NC14, TZCK18, Tsi14, ZLL⁺¹⁰]. **spectroscopy** [DMD⁺¹⁸, HDM⁺¹⁹, HPSK12, IY18, KNR⁺¹⁸, LLBO12, Lin18, NC12, OC19, WHK⁺¹², FAS⁺¹⁸]. **spectroscopy-oriented** [HPSK12]. **spectrum** [BLF14, KCC⁺¹⁸, MN19, MLCD11, RDF⁺¹¹, SLLL13, TSC⁺¹³, ZDX11].

spectrum-slicing [KCC⁺18]. **sped** [IMSR18]. **speed** [TO10, VM11, YD17]. **speed-up** [YD17]. **speeding** [AO10]. **sphalerite** [SBC⁺11]. **sphere** [KT12, MH10, Pop18, TH13]. **spheres** [HS16b]. **spherical** [Ano15-58, BH14, YOPB16]. **spherically** [Vyb15, Vyb16]. **spheroidal** [ZWY⁺10b]. **spider** [Che17]. **SPILLO** [DVVP14]. **Spin** [ATIP18, DSM⁺11, JKS⁺16, KM13, MLG18, SZL19, TT18, AB10, AMQ⁺14, CSEMB⁺16, CSS17, CSKH16, CAP17, FAA15, FD16, GP11a, KT19, KIOY19, KSK11, KKA⁺18, LXFC17, MG11, MCP18, PLFS18, PS17, RRK16, SFM14, SPHF⁺18, ŚSB⁺16, SH18b, TN18, TTn19, VFRAR16, VHS⁺19, YB11, ZLHH14, ZZZ⁺19]. **Spin-component-scaled** [KM13]. **spin-coupled** [SH18b]. **Spin-driven** [DSM⁺11]. **spin-flip** [ZLHH14]. **spin-forbidden** [TN18]. **Spin-orbit** [ATIP18, JKS⁺16, AMQ⁺14, FAA15, FD16, GP11a, KT19, KKA⁺18, MG11, MCP18, PS17]. **spin-orbital** [ZZZ⁺19]. **spin-polarized** [SFM14, VHS⁺19]. **spin-rotation** [KIOY19]. **spin-spin** [PLFS18, SPHF⁺18]. **spin-symmetry** [TTn19]. **SPINE** [FZY⁺12]. **Spinor** [CC12b, Bar14]. **spins** [ZR10]. **Spiral** [SK18]. **Splitting** [Rob13, EHSPT16, EHT19, FZL⁺19, LL19a, OT12]. **SPME** [NLP⁺16]. **SPOT** [YZZ16]. **SPOT-Ligand** [YZZ16]. **spots** [HQSZ19]. **Spread** [BEEL14]. **squaraines** [AMQ⁺14]. **square** [HDL⁺14, HGW18, ISK14, Tsi19]. **squared** [JMS13]. **squares** [BCCO10]. **SR** [ARAG17, WMW11]. **SR-ZORA** [ARAG17]. **SrO** [BL12]. **SSC** [LG11]. **SSThread** [Mau14]. **ST** [JJW⁺14]. **ST-analyzer** [JJW⁺14]. **STAAR** [JHH⁺13]. **Stabilities** [BF19a, ZLX⁺19, BLDK⁺13, SIT18, TFQ⁺11]. **Stability** [BPPS19, CSM16, EK15, GWT⁺17, LdSRR16, Lin18, OME16, PP10, BPPS17, CSS17, CFC15, CM16, CB11d, DLT17, DLW12, GPK⁺16, GC18, Ham11, HLB15, LTR18, LHKS12, MC10, MS15, PMG⁺16, PAT⁺10, Rab12, SBGP18, SY16a, SPZP18a, TN12, TKCN19, VP19, XFTW15, ZRCC11, ZWMW10, ZWW10]. **Stabilization** [KSR17, BSDP16, DBK17]. **stabilize** [KG11]. **stabilized** [AHK⁺19, KASH14]. **stabilizing** [MvBD18]. **stable** [NPTS16, PBDW11, ZDZM13]. **stacked** [ANH⁺11, HvM12, LDH⁺14]. **stacking** [HvM12, YZZ⁺17]. **stages** [CBP⁺15]. **staircase** [SK18]. **Stalis** [LI19]. **Standard** [DH17, BCJC⁺14, MKO⁺13, PNI13, RD18, REL⁺14, SRR16, VVG13, WHK⁺12, WGA18]. **standing** [TS11]. **staple** [SV15]. **Star** [MA17]. **State** [CCM15, FHG⁺19, GS16, Kop19a, MP19b, TT18, YKNN19, Alg17, AR10, ASS10, BS15, BBI⁺11, CSAAdOM17, CH10, CV12, ESM⁺12, FD14, GS15, GBPCC19, GCCM15, GA18, GPE13, HLS12, Hei18, HNWF07, HNWF12, HH16a, HH17, HBI⁺17, HWB19, HZSS17, HBR17, JZ17, KT19, KLN12, Kop15a, Kop15b, KKL⁺13, KKH18, KCL⁺14, LL15, LLBO12, LOB18, LZL⁺10, LYC⁺13, LWGZ15, LN15, LGL11, LvG13b, LLFH16, LXFC17, MTM14, MPSG11, MCC11, MC12, MCLD10, NYN17, NMLD13, OBW12, OLPB19, OZLSBH12, POB13, PGW⁺17, PH10b, QZ10c, RAGLL11, RIJ⁺11, RCM⁺13a, RML⁺15, RR14, RGVC⁺19, RSK⁺15, SRF⁺17, SSSM15, Sie18, SGWA17, VZ14, VL17b, WHL⁺10, WWW19, WHX⁺10, XCLZ19, XBSS19, YWZ14, YD17, YJ19, YYT12, YL13, ZZZ⁺19, Zim15].

state-of-the-art [YJ19]. **state-selected** [KCL⁺14]. **State-specific** [CCM15, GCCM15, LGL11, LXFC17, MCC11, MC12]. **state-to-state** [XCLZ19]. **States** [GMBM18, AST⁺16, ANH⁺11, BSL⁺16, BH19, DHOG13, DSV⁺19, EFS16, EK17, EVR18, EP15, FAA15, FD16, GO13, GA12, GTK10, HDHL15a, HDHL15b, HDHL15c, JCGVPHT17, KKH19, KT19, KKA⁺18, KPG18, KB14b, LLBO12, LLW12, LWW12, LGC19, LX11, LS11b, LYSS11, LCK⁺18, MS10, MN15, MGCC19, MH11, MEH18, PBDW11, RHRCH16, SRF⁺17, SSC⁺19, SOYC12, SMiN⁺19, ŠB13, ŠB15, SZZS16, TN10, Tia12, TSN17, VVV⁺15a, XWSW13, YZGS14b, YK13, YLZ⁺10, YB11, ZXS⁺10, ZBB16, ZDT18, dLC17]. **Static** [KBC12, BS10a, KZK⁺12, Lu11, PC14, PNW⁺16, PM13, WYT17]. **Statics** [Pon10]. **stationary** [BHR15, Can10, Can11, LHMM11, SLT14]. **stationary-point** [BHR15]. **stationary-wave** [Can10, Can11, LHMM11]. **Statistical** [JHH⁺13, PZA15, PTB⁺15, FL15, GZ14, HYMZ16, ICS⁺12, ICS⁺13, Kan15, KMLS10, PTK11, RB13a]. **statistically** [GR10a, GR11]. **statistics** [QZ10c]. **steepest** [MS16]. **steepest-descent** [MS16]. **Steered** [Won18, FBEM11, KERY⁺16, MJC14, NFG⁺13, SJ17, WTD⁺19]. **step** [AYYO17, DS12b, DGC14, GRCL12, JWO15, JS17b, KvdV14, LLvG10, LGL11, LvG13b, LvG13a, LL10c, RLDJ17, RS12, SJC11, TCPPC14]. **steps** [REH13, Zim13]. **Stepwise** [DLP11, LZ18, GRCL12, ZL11]. **stereochemical** [WCDM11]. **stereochemistry** [PPJ14]. **stereochemistry-dependent** [PPJ14]. **stereodynamics** [Chu10, CSNCS⁺18, LWD13]. **stereoelectronic** [AS11]. **Stereoselection** [BJS12]. **Steric** [RMGB11, MJLV14b, MP17a, YNH⁺17]. **sterically** [MH17]. **Stern** [MBA11]. **stereoelectronic** [HLBLCCG15]. **Stevens** [BCJC⁺14]. **sticks** [CVT⁺11]. **stilbene** [BW11b]. **stk** [TBJ18]. **Stochastic** [AFPI13, CGP12, ITY⁺19, AC12, ESD18, KV12, KV13, MS16, MCP18, NC13, PH17, RSL13, SWB⁺12, VBD11]. **STOCK** [BJP15]. **stockholder** [FHZA⁺18]. **stoichiometric** [VI17]. **stoichiometry** [FSD⁺18]. **Stone** [DWZ⁺17, YZN13]. **stool** [FPB12, FB14b, ZCK⁺16]. **storage** [BEM14, BEPM14, DLT17, WKLC12]. **Story** [Sce07, Sch10]. **Strain** [DM15, FB12, FC16, FLM11, JWO15, LSL⁺19, PBE16, She12, SHL⁺13, SH19b, VIT⁺15]. **strand** [XLY12]. **stranded** [HLI⁺19]. **strands** [SPM⁺19]. **strategies** [AFBR17, BSDP16, cCVG⁺14, DSX⁺11, LTT16, Rao11, SCOJ13]. **Strategy** [Jia19, CLX⁺10, CZNA11, HJKJ13, KTTN10, KKH18, LLL⁺10, PHC13, PH17, RVVK13, SHL19, TKNN10, WO15, XHLH16, YDGZ15, ZGZC19, SMD18]. **StreaMD** [DJS⁺18]. **Strength** [ELKE19, JLLW19, Fra15, Fra16, KSC16, LGKS17, MPSG11, YJ17, YHW17]. **strengthening** [MS11, LYSS11]. **strengths** [CKL⁺11, MLC13]. **streptavidin** [MLZZ12, ZJZM13]. **streptavidin-biotin** [MLZZ12]. **streptocyanines** [WYT17, XKW18]. **Stress** [BS19, GMBX⁺16, HXM⁺16, JMX⁺16, NIIT15, NFI⁺16, XFX⁺16]. **stretch** [CK10, RS17b]. **stretching** [KLS10, KMLS10, TKCN19, dSH19]. **string**

[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, CYT⁺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, MHR11, 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, VLK⁺17, WO15, WRM⁺12, WSGN11, YW12, YZZ16, ZRCC11, ZHHX11, CPR18, FDCJG18, OSF12, SA10]. **structure-activity** [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, ČMD13, OSI⁺19, PGCT⁺12]. **studied** [Ish10, KRTB10, OLY17, RHPWS13, RI10, TS15b]. **Studies** [JW12, AALCM11, BLS10, 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, SZS16, 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].

substituents [CBTZ16]. **substituted** [AARP17, BEPM14, CCCLRO14, CZH12, DCHL12, KYCL11, KV15b, LZH16, LWL⁺¹¹, LTP11, Lu11, OSF12, PRRT⁺¹⁰, QCR12, SSP⁺¹³, SK12, SKGB13, UT14, WGL12, YPC⁺¹⁰, ZZWT12]. **Substitution** [MUN⁺¹⁹, CFM⁺¹⁹, ITY⁺¹⁹, LGW12, MPSG11, TZ12]. **stitutionally** [VS14]. **substrate** [AALCM11, BHNS14, BEL⁺¹¹, JDW⁺¹⁹, LZL⁺¹⁶, VCM15, WWW19, YZLZ18]. **substrate-binding** [WWW19]. **substrate-enzyme** [BHNS14]. **substrates** [QQY⁺¹⁸, Tsi17]. **substructural** [PSdPE⁺¹⁰]. **subsystem** [SFG⁺¹⁷, UDK⁺¹⁸]. **subsystems** [DK11, PL14]. **subtilis}** [CPK12]. **Subtraction** [Hes19]. **sugar** [JSD⁺¹¹]. **suggested** [GZL⁺¹²]. **Suitability** [BVHI17]. **suitable** [TZ12]. **suite** [DMN15, PGL⁺¹⁵, FPV13, LJC⁺¹⁹]. **suited** [EK17]. **sulfate** [CHKR10, PP19, TFYO19, YZGS14a]. **sulfide** [LAW⁺¹⁶, ZYG⁺¹⁴]. **sulfides** [OSF12]. **sulfonyl** [YHVM12]. **sulfonyl-containing** [YHVM12]. **sulfoxide** [GC11, KPH⁺¹⁹]. **sulfur** [CTR13, DT19, HSB⁺¹⁹, HS14a, HS16b, Kop17b, OSF12, WGL12, WZC⁺¹⁹, YB11, ZM10]. **sulfur-containing** [DT19, ZM10]. **sulfurization** [TR12]. **sum** [ŠB13, ŠB15, Tak14, Tia12]. **sum-over-states** [ŠB13, Tia12]. **sumanene** [CLFRO18, CBTZ16]. **summation** [GBFD12, SF18]. **summations** [ŠB13]. **super** [CSSB11, KSHP⁺¹⁹]. **super-CI** [KSHP⁺¹⁹]. **super-computers** [CSSB11]. **Superacid** [KS19]. **superacids** [EHSPT16]. **superalkali** [LLD17]. **superatom** [LYL16]. **supercharger** [FRN15, RFN15]. **Supercluster** [Hes19]. **supercomputers** [KNHN16, KN17]. **Superhalogen** [KS19]. **superlattices** [KC13b]. **supermolecule** [XZ11]. **superoxide** [GEP⁺¹⁴, CPR18]. **superoxo** [ZRCC12]. **superposition** [CDBM11, HS12, PD11, YLGX14]. **superpositions** [Kne11b, LAT10, LAT11]. **Supersecondary** [ZHHX11]. **Supersites** [Hes19]. **supertetrahedral** [GKB⁺¹⁹]. **supervised** [DGPM14]. **support** [GTZ⁺¹⁸, HJ13, RLL⁺¹⁰, RMRBH⁺¹⁹, Sie18, TYZ⁺¹⁶]. **supported** [CZZL19, SN16a]. **supramolecular** [CSGOA17, HLB15, OAN15b, SMDP18, TBJ18]. **Surface** [Hes19, LLLW19, LK16a, SRS14, Ano15-58, BPM15, BH14, CM13a, CR14, Che17, CZZL19, DBM⁺¹⁵, DS12b, FZY⁺¹², FMNC11, FVP14, FDH19, GCWS15, GY10, HLvdV13, HTY19, HWLW11, HYD10, IN19, JZ17, JCX10, KT19, KKR⁺¹³, KTSW11, Kop16, Kop17a, Kop17b, Kop18, LLH14, LL13a, LYC⁺¹³, LWZ⁺¹⁷, MK13b, MAK⁺¹⁴, MB14, MOS12, NW17, OKIS17, OHPR17, OHPR18, PZA15, SRSLO15, SKA19, SH14, SBC⁺¹¹, SLG15, SLLL13, SIG⁺¹⁵, TSR⁺¹⁶, WXL⁺¹², WXL17, WBF17, XFX⁺¹⁶, XCLZ19, YPvd13, Yan14, ZLT13, ZKE⁺¹⁷, MK11]. **surface-enhanced** [SLLL13]. **surface-supported** [CZZL19]. **Surfaces** [BHB19, ZQH19, AKN16, BPC19, BHB⁺¹⁷, BS16b, CCJ⁺¹¹, CSXZ17, CZNA11, GFG11, Hei10, HRL11, IN13, KIOY19, KLS10, KMLS10, LX11, LAW⁺¹⁶, MCC11, MSC⁺¹⁰, MCF10, MK19, NPP13, OHPR18, Pol13, RNSF⁺¹⁶, RRC⁺¹⁵, RBOH11, RLA18, SRF⁺¹⁷, SFR⁺¹¹, SC15, SFLG⁺¹⁷, TG12a, VT14, VVY18, WKC^{+10b}, YZ15a, YR13, OSI⁺¹⁹]. **surfactant**

[WWKS11]. **SurfKin** [LLH14]. **Surprisingly** [KG15]. **surrounding** [BSL⁺16]. **survey** [GRARO⁺14, SJD11]. **Surveying** [KB11b]. **Sust** [Ihl12]. **Suwa** [MO15]. **SVM** [XWW⁺11]. **swarm** [BSD18, LZL⁺13]. **SwissParam** [ZCGM11]. **switch** [LCB10, MWJ⁺11, MB16, XMA⁺19]. **switchable** [MLQ⁺12, RJBH18]. **Switching** [GA19, AB16b, KOP⁺14, LCH10]. **Symmetric** [PBL19, HOM⁺16, KZK⁺12, LPS12, RSSG18]. **symmetries** [GR10b]. **Symmetrization** [MSK⁺10, MSK⁺12]. **Symmetrizer** [LPS12]. **Symmetry** [CAA10, CW19, ELKE19, EP15, EB18, VVV⁺15a, BV14, CWZB10, DZA11, Dry14, FF11, HB14, KTT16, KC13b, NDD⁺10, PZBA13, Sch13, TTn19, VGTL16, XKW18, YKH15, vS18]. **Symmetry-Adapted** [ELKE19, FF11, YKH15]. **symmetry-invariant** [CWZB10]. **synchronicity** [dSVdM⁺16]. **synthase** [AALCM11, EvRC⁺18, SYH12, XLYZ10, vRET19]. **synthase-catalyzed** [XLYZ10]. **synthesis** [QQY⁺18, YZLZ18, ZZWT12]. **synthesized** [CBDS19]. **synthetase** [LBS10]. **synthetic** [SBGP18]. **synthons** [LZSM19]. **syringe** [ZWS⁺10]. **System** [NN19, BEEL14, BTT10, BCCO10, CS14, CJZS10, GRS15, HSY⁺11, HKNH18, HHNK19, HDM⁺15, IMSR18, KNR⁺18, LL11, LYL16, LZY12b, MHO18, MLZZ12, NTNY15, NSP15, RHT⁺15, SZBM13, SWW⁺19, TL16, VBDS⁺11, WLF11, XCLZ19]. **Systematic** [GP11b, KT18, ML14, SDIP18, SA13, SCMA⁺17, UT15, VLGK⁺17, AIGP15, BEL⁺11, FM10, IY18, Ish12, LG11, MAMF19, Pet11, STS15, VVLG17, WG12, RFHG10]. **Systems** [RMM16, SZL19, VL19, AST⁺16, APK14, BS19, BV14, BGL⁺18, BVY⁺12, BK13, BBG⁺18b, BG13, CCR18, CSS17, CEBO15, CKL⁺11, CLK11, CAP17, EP12, GG10, Gar12, GP12, GA19, GBW⁺14, GR10b, GWZX12, HS11, HCD⁺10, HH18, HvM16, ITIN15, JSXH16, JS17b, KV12, KZP⁺18b, KGM12, KKH18, LBG16, LCPS13, LPLA13, MP19a, MSC⁺10, MG14, MOS12, MS12, NYN17, NCV10, NLL19, NFG⁺13, NO16, NNK⁺16, NS17, ODB18, OPB⁺12, OC14, PAK17, PAT⁺10, PBBP11, PD12, QLKI19, RJPB12, RVCFF13, SSO19, SCOJ13, Sch12, Sea10, SKGP19, SEJ⁺18, SH18b, SWB⁺12, SG13, SMM17, TSN16, TCX⁺13, UT15, WCY⁺11, WWU12, WS11, YCK16, ZSB⁺11, ZFS18, ZT14, HvM17].

T [BBI⁺11, CSGOA17, Gil11, MSPC19, MLCD11, OPR16, SRR16, XKW18, YJ17, BBG⁺11, BH13, CGBK13, HLS⁺13, Sch13]. **T-cell** [CGBK13]. **Table** [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, Sce07, Sch10, AAC⁺16, CDC19, Fom11, JMS13, MGS⁺16]. **tables** [BDdS13, LZ12]. **TaBoo** [HTS15]. **tabu** [GBSE11]. **tabu-search-based** [GBSE11]. **tabulated** [LL10a]. **TacoxDNA** [SPM⁺19]. **tail** [MBC13]. **tailoring** [KKK⁺19, RKGN10]. **tails** [GSD10]. **Taming** [CCM15]. **Tamm** [HH17]. **TANGO** [GKJ⁺19]. **tar** [HCD⁺10]. **tar-MD** [HCD⁺10]. **target** [FMG12]. **TargetATPsite** [YHH⁺13]. **targets** [AFBR17, BK13, MPBJ11]. **Task** [CSSB11, HPSK12, KG13, WZWW18]. **task-oriented** [KG13]. **Task-parallel** [CSSB11]. **TATA** [YZWC11].

Taurine [YW13]. **tautomer** [WHJH13]. **tautomeric** [SJWE10].
tautomerism [BMB13, LGOM⁺15, SC18b]. **tautomerization**
 [BH13, BZH14]. **tautomers** [BZH14, dALdS⁺15]. **taxadiene**
 [EvRC⁺18, vRET19]. **Tb** [SRL⁺15]. **TD** [HL19, TS15b, CCB15, CH10,
 DSB⁺19, EFAC13, HRJ⁺14, HRJ⁺15, HL19, JRSHP14, KKL⁺13, KP10,
 LZL⁺10, LZHH11, LSH⁺11, LYSS11, RDF⁺11, SRF⁺17, SCF⁺19]. **TD-DFT**
 [CCB15, CH10, DSB⁺19, EFAC13, HRJ⁺15, HL19, JRSHP14, KKL⁺13,
 KP10, LZHH11, LXZ⁺10, LYSS11, RDF⁺11, SRF⁺17, SCF⁺19]. **TD-DFT-**
[LSH⁺11]. TD-HF-based [LSH⁺11]. TDDFT
 [SFCKK⁺15, CMF⁺17, LRBB12, MS11, QCR12, SFCKK⁺14]. **Te**
 [AM19a, AM19b, PLFS18, SPS⁺12, HSJ18]. **technique**
 [AMGB10, BG17, LZL⁺13, SMM17, TSR⁺16, TTn19]. **techniques** [BCP⁺10,
 BCG10, GVP⁺10, MCP18, RD18, SDF⁺17, SPL⁺18, SY11, WBN⁺13].
Teller [BMD19]. **tellurium** [RRK16, ZWGO16]. **Temperature**
 [HS17b, HYNS19, KKO⁺16, LPE⁺10, LLTC12, PBE16, SY16b, SMM⁺18,
 ZQH19, CH16, DKT13, DLSD13, HDM⁺19, KCK⁺17, LL11, MK17, MKK⁺19,
 OGL10, TLdG⁺12, TM16, VED10, WMW11, WWTL19, YW12, OCW⁺15].
Temperature-pressure [HYNS19]. **Temperature-shuffled** [HS17b].
temperature/Hamiltonian [KCK⁺17]. **temperatures**
 [NMLD13, RHNN10]. **tempering**
 [GC18, LAW⁺16, MO15, MO17, NPTS16, TKT11]. **Template**
 [LI19, Mau14, GLF16, KCK⁺17, ME10, YHH⁺13]. **Template-Based** [LI19].
Template-free [Mau14, YHH⁺13]. **template-restrained** [KCK⁺17].
tension [NFPD13]. **tensor**
 [BS19, CPZ19, Elk16, EWK⁺13, GMBX⁺16, HXM⁺16, JMX⁺16, KK17a,
 NFPD13, NIT15, NFI⁺16, TKC⁺11, XFX⁺16, YAO18]. **tensors**
 [EPD⁺11, PHK14]. **tepidum** [KPG18]. **terahertz** [KB16]. **term**
 [DSF17, JBSQG11]. **terminal** [IMK⁺16, YXZZ17]. **terminally**
 [KLS10, KMLS10]. **terminally-blocked** [KLS10, KMLS10]. **Terminated**
 [BHP19]. **terms** [BAS14, CZY11, CWZB10, ĤRH12]. **ternary** [RDT14].
tertiary [OPR16, SM11]. **tessellation** [MOS12]. **Test**
 [PHC13, BS10b, DSB⁺19, DPOS16, Won18]. **tested** [HMM10]. **Testing**
 [Gil11, II18, MPSA17, RLD12, JGS⁺17]. **tests**
 [Ano15-59, CNK97, ENKK⁺17]. **tether** [FDH19]. **tethered** [CZNA11].
Tetra [BHP19, WDLG12]. **Tetra-Anionic** [BHP19]. **tetraamines** [SB10].
tetracarboxylates [CRC13]. **tetracoordinate** [XhD15, ZYW⁺16, ZLY⁺16].
tetraene [ABDGN12]. **tetragonal** [LKZM18]. **Tetrahedral** [LBC⁺19].
tetramer [Ish10]. **tetramers** [LYL16, SZZS16]. **Tetraoxide**
 [JW12, SLHW09]. **tetraprotonated** [ZWY⁺10b]. **tetraradical**
 [Cas14, YSSB12]. **tetrasaccharide** [NPG17]. **tetrathiafulvalene** [MCF10].
Tetrazine [JW12, MCAG⁺16, SLHW09]. **Tetrazino** [JW12, SLHW09].
Tetrazino-Tetrazine-Tetraoxide [JW12, SLHW09]. **tetrel** [YKH15].
tetroxide [MCAG⁺16]. **text** [HKRS11, HS11]. **text-based** [HKRS11, HS11].
TF [XMSZ16]. **TGMin** [CZZL19]. **Th** [MCK17a]. **ThCl** [LCL⁺18]. **their**

[ARRC15, Ano11, AM19a, BSG18a, CC12a, CBTZ16, CFC15, CB11a, DLT17, DSM⁺¹¹, GPM17, HJ13, JMLL13, JHMB⁺⁰⁹, JHMB⁺¹¹, KG15, KNE11a, KRSC12, NYH⁺¹⁷, SBR13, TN12, Tak11, TY10, TS11, VVJ15, VVY17, VVBL17, XDL⁺¹⁰, ZWY^{+10a}, GMBM18]. **them** [WCWV15]. **theorem** [CDB10, KSH13, YB16, ZM11]. **theoretic** [CRZ⁺¹⁸, MCC12, ZLW10].

Theoretical

[AvKSP16, AMAA⁺¹¹, AWF⁺¹⁸, AHK⁺¹⁹, BHB⁺¹⁷, BSDP16, CWT⁺¹², DBM⁺¹⁷, DGL⁺¹³, FF11, FWS⁺¹⁸, GYX⁺¹⁰, GLZ17, GLM⁺¹⁷, HW19, HDHL15c, JW12, KCB⁺¹², KSO⁺¹⁹, KMT⁺¹⁹, KS13b, LCL⁺¹⁰, LWL⁺¹¹, LLW12, LZ^{+12a}, Lin18, LWWG12, LWXC16, LXFC17, LD18, LJG⁺¹¹, MLQ⁺¹², MSV16, NSN19, NFI⁺¹⁶, OSS10, OAN15b, PKK17, PM13, PE11, RS17b, SB10, SMiN⁺¹⁹, SSD19, SKY⁺¹¹, STS⁺¹⁰, SZS16, SLC⁺¹⁷, SGHL13, TPL⁺¹⁰, Tsu19, WMW11, WHDL11, WCL⁺¹¹, WS12, XBSS19, YJN⁺¹¹, YPC⁺¹⁰, YHG⁺¹¹, YCGA10, YYT12, YDGZ15, ZZL^{+10b}, ZZL^{+10a}, ZYLL12, ZLLL12, ZSZ⁺¹⁴, ZYG⁺¹⁵, ZGZ19, ZBMZH15, dSdLBNB17, BLS10, BAD⁺¹⁹, BE16, CZH12, CKL⁺¹¹, CBTZ16, EV14, GG10, HDB15, HGHP14, LWW12, LLD17, LZW⁺¹¹, LCL⁺¹⁸, MRC⁺¹⁸, MSPG11, MP19a, MKK⁺¹⁹, NHF⁺¹⁰, NJX⁺¹⁰, PH12, PdSC18, PSdPE⁺¹⁰, Pog10, PH10b, RZG⁺¹³, RVCFF13, RVP⁺¹¹, SSP⁺¹³, SSC⁺¹⁹, SJD11, SLHW09].

theoretical [SKTT11, SGH⁺¹⁶, Tak11, TL16, UCRL18, WSH10, WZQW10, YK13, YZWC11, YZN13, YB11, Zha12b, dSAdSL13, HDHL15a, HDHL15b, KZK⁺¹², TDP⁺¹²]. **Theoretically** [LLX⁺¹⁹]. **theories** [OM12, WCWV15].

Theory [BHB19, CKH19, EVR18, ELKE19, GNC⁺¹⁸, IUK⁺¹¹, LLX⁺¹⁹, MP19b, Sah18, SZX13a, SZX13b, WBKS19, WM12, AMK11, ALK⁺¹⁵, AR10, Ali18, ARAG17, ABDGN12, ASW19, AG12, ASS10, BY11, BLBG⁺¹³, BS19, BMD19, BZB⁺¹³, BG13, CHG⁺¹⁶, CRZ⁺¹⁸, CSAAdOM17, CWHH11, CKH17, CCM15, CF14, CC11, DAP⁺¹⁸, DCHL12, FRSA14, FD16, GHL17, GZL⁺¹², GCCM15, GWW19, GLW19, GY10, GNGCA10, GNDA⁺¹², GA18, GEG11, GPK12, Han11, HPT17, Hil13, HNN⁺¹⁷, HRJ⁺¹⁴, HRJ⁺¹⁵, HG10, ISN13, IKN13, IM17, JRSHP14, JLH⁺¹⁴, JW16, JYS⁺¹², KHWB17, KLN12, KM13, LCW12, LBGs16, LCL⁺¹⁰, LLH17, LPMT17, MCC11, MMH19, MAK⁺¹⁴, MWJ⁺¹¹, ME10, NPG⁺¹⁸, NMLD13, NO16, Niz13, ORZ11, OZLSBH12, PAK17, PML⁺¹², PPH⁺¹⁴, Pie14, Pyy13, QZ10b, QZ10c, QB16, RAGLL11, RJPB12, RCM^{+13a}, RML⁺¹⁵, RB12, RSLML12]. **theory**

[RHPWS13, RNS19, RR19, Rui11, SM14a, SFG⁺¹⁷, SHL⁺¹⁸, SCW11, SSSM15, SHF11, SEF⁺¹⁶, SE14, SH14, ST13, SHL⁺¹³, SSMW09, SB14, SMM⁺¹⁸, SKTT11, SZS16, STS15, TLdG⁺¹², TAG16, UvSvdWK19, VDL⁺¹³, VVP12, VV14, VL17a, VAMS14, WHL⁺¹⁰, WDLG12, WHX⁺¹⁰, WO15, WL14, WGN⁺¹⁶, XTY⁺¹⁴, XYW⁺¹⁴, YJ11, YLZ⁺¹⁰, YS13, YKH15, ZXS⁺¹⁰, ZSWL12, ZLZ14, ZDX11, ZYG⁺¹⁴, ZWY^{+10b}, ZWY^{+10a}, ZLHH14, dSdS12a, dSdS12b, vLBBR12, FAS⁺¹⁸]. **theory-based** [YJ11].

theory/configuration [HPT17]. **theory/time** [JYS⁺¹²].

theory/time-dependent [JYS⁺¹²]. **therapeutic** [AFBR17]. **therapy** [ZZ12]. **there** [MLGB16, Sie18]. **Thermal**

[LL10c, SJSS19, ASL⁺¹¹, BIL10, NGAS17, OZLSBH12, VVW⁺¹⁸].
thermally [FWS⁺¹⁸, IIHY15, ZGZ19]. **thermocalc** [HDH12].
Thermochemical [TFQ⁺¹¹, KSM16, TN12, WDW12]. **thermochemistry** [HDH12, Sán17, SB14, TCGNT18, VRKT19]. **Thermochromatium** [KPG18]. **Thermodynamic** [EOO⁺¹⁶, NSK18, PAT⁺¹⁰, BE12, BPE16, BB11b, BB11c, CBH14, CC18a, EBPK17b, HDL⁺¹⁷, Hug12, MMB⁺¹⁷, PGY15, PBE16, RNSF⁺¹⁶, RRF11, RKB⁺¹⁴, SS13c, SJC11, SJ16, WC11, dRBO13]. **Thermodynamics** [DS12a, RS12, BRE16, DMJ17, EHSPT16, HRC13, Kan15, WRM⁺¹², ZYL⁺¹²].
thermoelectric [KLZ⁺¹⁸, NGAS17, YW12]. **thermolysin** [DHF⁺¹¹].
thermometer [SPZP19]. **thermophilus** [TNI19b]. **thermostabilizing** [KYT⁺¹⁷]. **thermostat** [JWO15]. **thermostatization** [PH17]. **Thermus** [TNI19b]. **thia** [GMASBF16]. **thia-calix** [GMASBF16]. **thiaphosphiranes** [TR12]. **thiazol** [BMB13]. **thiazol-2-amine** [BMB13]. **thienylenevinylene** [TZ12]. **thin** [MBA11]. **thin-shell** [MBA11]. **thioacetamide** [LCB10].
thioamide [KG11]. **thioformaldehydes** [TKCN19]. **Thiol** [GWZ15].
thiolate [EH13]. **thiolate-ligated** [EH13]. **thiolates** [FHT⁺¹⁵]. **thiophene** [PH10b, PRRT⁺¹⁰, YHCS11, ZSTRS⁺¹⁸, ZSLL17]. **thiophene-based** [ZSLL17]. **thiophenes** [Su10]. **thiophenic** [NHF⁺¹⁰]. **thiophenol** [AMAA⁺¹¹]. **Thiophenols** [CGVBAl19]. **thiotropolone** [DL19]. **thiourea** [Kow11]. **thiourea-** [Kow11]. **Third** [BF19a, TKN13, HKRS11]. **Third-Row** [TKN13]. **Thole** [AS15b]. **Thomas** [Spr10]. **thorium** [KKH19]. **those** [SIG⁺¹⁵]. **ThQs** [ZZL19]. **ThQs-C** [ZZL19]. **threading** [Mau14]. **Three** [CKH19, NR11, NF17, NNK⁺¹⁶, TYN15, TKC⁺¹¹, CXD⁺¹⁹, HJKJ13, KYT⁺¹⁷, KRSC12, LYSS11, LK16b, MBT14, MS16, RVM19, SLT⁺¹⁵, TDKT10, TCX⁺¹³, UT15, WC14, YLL11, ZZL⁺¹², ZWX16]. **Three-body** [NF17, RVM19]. **three-center** [CXD⁺¹⁹, YLL11]. **Three-dimensional** [TYN15, TKC⁺¹¹, KYT⁺¹⁷, KRSC12, TCX⁺¹³, ZWX16]. **three-domain** [MBT14]. **three-level** [HJKJ13]. **three-membered** [TDKT10].
Three-Range [CKH19]. **Three-residue** [NR11]. **threshold** [LCM16].
through-put [GKJ⁺¹⁹]. **throughput** [ESB13, JBAM11, PVJ10, RNS19].
thymine [HvM12, LJW11a, ŠBD⁺¹⁷]. **thymine/thymine** [HvM12]. **Ti** [MP19b, WWKS16, WZH⁺¹⁸, YW12, BH15, SDB⁺¹⁶]. **Tian** [Ano12u]. **Tide** [RB12]. **Tight** [Lar12, NN19, YKNN19, GAJ⁺¹⁷, HNWF07, HNWF12, JCP14, KZZ⁺¹⁶, MSY19, MAP18, MFR⁺¹⁷, NF17, NN18, NO16, NNK⁺¹⁶, Oht16, Rez19, SPS⁺¹², VHS⁺¹⁹]. **Tight-Binding** [NN19, YKNN19, Lar12, HNWF07, HNWF12, JCP14, KZZ⁺¹⁶, MFR⁺¹⁷, NF17, NN18, NO16, NNK⁺¹⁶, Oht16, Rez19, SPS⁺¹²]. **tightly** [PGI19].
Time [GTK10, KS18, PAK17, WHL⁺¹⁰, WHX⁺¹⁰, YLZ⁺¹⁰, YKNN19, ZDX11, AYYO17, CHG⁺¹⁶, DGC14, Fom11, FSSW17, HCD⁺¹⁰, HNWF07, HNWF12, HG10, JWO15, JS17b, KNR⁺¹⁸, LL13a, PNG10, RS12, RHPWS13, REL17, VHR16, Vik11, ZXS⁺¹⁰]. **time-averaged** [HCD⁺¹⁰].
Time-Dependent [YKNN19, GTK10, KS18, PAK17, WHL⁺¹⁰, WHX⁺¹⁰, YLZ⁺¹⁰, ZDX11,

CHG⁺¹⁶, HNWF07, HNWF12, HG10, JYS⁺¹², RHPWS13, Vik11, ZXS⁺¹⁰.
time-resolved [KNR⁺¹⁸]. **time-step** [AYYO17]. **times** [VBDS⁺¹¹].
timescales [MCRL17]. **tin** [ASS10]. **Tinker** [HLW⁺¹⁷]. **TiO**
 [NC14, TSZQ12, CCJ⁺¹¹, DSB⁺¹⁹, EP15, HRL11, MP19a]. **TIP3P** [SA10].
TiS [BE14, RSKG14]. **Titan** [OZLSBH12]. **titanium** [QZ10b]. **titration**
 [HS14b]. **TMBiimH** [LWXC16]. **TmoleX** [STH⁺¹⁰]. **TMS** [YXZZ17].
TMS-N [YXZZ17]. **tobermorite** [TZ11]. **Todo** [MO15]. **toluene**
 [AAMD⁺¹¹]. **Tool** [LLH⁺¹⁹, BPC19, GKJ⁺¹⁹, HRK⁺¹⁰, HKRS11, HS11,
 HG13, JLS18, KDB13, LP11a, LK11, LDB⁺¹⁷, LCA17, LBB⁺¹⁵, LG11,
 LP11c, MDTD16, MCC12, NHK⁺¹³, OV14, OVPK15, OC14, PNW⁺¹⁶,
 SDMS13, SH19b, WCDM11, ZCGM11, dVAG16, JCGM18]. **toolbox**
 [HPT^{+16b}]. **toolchain** [KSH⁺¹⁷]. **toolkit** [FSC⁺¹⁴, GS12, IKG16, MJB12,
 MSS⁺¹³, MADWB11, NKJ16, PG15, PPM15, TS10a, TBJ18, ZLL⁺¹³].
Tools [RLG14, ZFOS19, GMZ12, SLG15]. **toolset** [YPKB12]. **Top**
 [WZWW18]. **Topo** [BGL⁺¹⁸]. **topographical** [KYG⁺¹⁵]. **Topography**
 [PK19]. **Topological** [Jan16, AR15, BGL⁺¹⁸, PRYI⁺¹⁷, Pop18, SB11,
 TSZQ12, Tan19, VAR12, VBMA13, Wei12b, vSGP10]. **topologies**
 [Gar12, TSNC⁺¹⁷]. **topology** [AD10, ASS⁺¹⁷, Dil15, FED17, GMSdG15,
 KP11, MSSP17, yOaCG10, Rod13, dCDP15, BLG10]. **topomerization**
 [GG10]. **toroidal** [SS13b]. **Torque** [Elk16]. **torquoselectivity** [GMBX⁺¹⁶].
torsion [DPSL16, FZY⁺¹², HP10b, HXM⁺¹⁶, JMX⁺¹⁶, YZ16]. **Torsional**
 [VL19, BAS14, PRRT⁺¹⁰]. **torture** [RHT⁺¹⁵, ENKK⁺¹⁷]. **torus**
 [WRG⁺¹⁷]. **total** [BEEL14, IKN13, MA16, SM16a, WX12]. **toxicity**
 [TTB⁺¹¹, TTL⁺¹²]. **TQ1** [VL17b]. **TQ1/PC** [VL17b]. **track**
 [ENKK⁺¹⁷, RHT⁺¹⁵]. **tracking** [BHR15, GBPCC19]. **tractability**
 [KFY⁺¹³]. **training** [DBDP16]. **trajectories** [AST⁺¹⁶, HRID16, JZL⁺¹⁷,
 KG13, LZS⁺¹⁷, PSP15, RN17, SKA19, SFR⁺¹¹, ZSS⁺¹³, dSVdM⁺¹⁶].
trajectory [IUK⁺¹¹, JJW⁺¹⁴, LWD13, LAS⁺¹⁴, MKS⁺¹², PVZ13, RC18,
 ŠBD⁺¹⁷, Yu12a]. **Trans** [CSM16, MSBF16, Tsi19, WS19, BLS10]. **Trans-**
 [MSBF16]. **Trans-2-Butene** [CSM16]. **trans-effect** [Tsi19].
trans-influence [Tsi19]. **trans-influence/trans-effect** [Tsi19].
Trans-philocity [Tsi19]. **trans}-pinane** [BLS10]. **transcription** [XMSZ16].
transfer [Alg17, AK10, ANH⁺¹¹, BHB12, CMF⁺¹⁷, CSAAdOM17, CPLL11,
 DWR17, DAdGR15, EFAC13, ENKK⁺¹⁷, FC16, HSH15, HAP⁺¹², HDHL15a,
 HDHL15b, HDHL15c, IYK11, JM11, JCGVPHT17, KGR⁺¹⁶, KDR⁺¹⁸,
 LZL⁺¹⁰, LLLM11, LWGZ15, LPLB16, MPSG11, MRB14, MSV16, MCF⁺¹⁸,
 MT19b, PGCT⁺¹², PG18, PAK17, PL14, PTB⁺¹⁵, Ras17, RCM^{+13a},
 RML⁺¹⁵, Ric16, REL17, RKDM14, SRF⁺¹⁷, ŠBD⁺¹⁷, SMP17a, SZB19,
 SHB17, TM16, Tsi17, VKTRJ15, VMTL10, VL17b, WCT⁺¹¹, WZ19, WG14,
 XBSS19, XLY12, YKH⁺¹⁰, YHX19, YLZ⁺¹⁰, YYT12, YFH⁺¹⁹, ZW17,
 dALdS⁺¹⁵]. **Transferability** [FP17a, ZRL⁺¹⁵, HOK17]. **Transferable**
 [EKH14, VVLG17]. **transfers** [YZGS14a]. **transform**
 [Ano15-58, BH14, Ish12, LL13a, SZTSM10, IY18, NZM18, YWJ⁺¹⁶].
Transformation

[CCOH14, WZC⁺19, APY⁺16, DLW12, KZZ⁺16, REH13, RSK⁺15].
transformations [HDL⁺14, Min18, SJC11]. **Transiting** [CM13a].
Transition [BF19a, BGS⁺19, OZLSBH12, QZ10c, YB13, Alg17, AR10, BS15, CSAdOM17, CMS13, DLSD13, GK15a, GFGS18, GPE13, Hsu14, IYK11, JZ17, JSF19, LYL16, LDZW17, LN15, LZW⁺11, LGKS17, LLL⁺12, MTM14, MS10, MN15, MKK⁺19, NMLD13, PHK14, RAGLL11, RIJ⁺11, SJZ⁺15, VVV⁺15a, VHS⁺19, YZGS14b, YWZ14, ZWW10, Zim15]. **transition-metal** [LDZW17]. **transition-state** [CSAdOM17, RAGLL11]. **transitions** [AKK⁺16, BD11, DH11, HS17b, HB15, KIOY19, MCvdV13, PBDW11, SBT17, SPZP18a]. **translationally** [MRO17, MK19]. **translocation** [MJC14]. **transmembrane** [DSF17, LMI⁺14, LAW⁺16, WXL⁺12]. **transmission** [LLJ12]. **transphosphorylation** [WXY14]. **Transport** [DJX⁺11a, AWF⁺18, CWHH11, CBTZ16, DMN14, DMN15, DJX⁺11b, HLWD15, LHO17, LJR⁺12, NSK18, NS17, PGY15, RJBH18, RSSG18, SLIB12, SY16b, TCX⁺13, ZYG⁺15]. **transportation** [LZY⁺12a].
transporter [HYSF19]. **transporters** [TO19]. **trapped** [DM15, VIT⁺15, WLW⁺10]. **treat** [CJPTC18]. **Treating** [JLCA17, SMP17a].
Treatment [HSH15, CSGOA17, GPK12, Has14, HGHP14, MG14, NS10, Sch12, SSWX14, SJL18]. **tree** [JCPC11]. **treecodes** [BK13]. **trees** [AGR11b, RDRC16]. **Trends** [CXS10, PH15, RLA18, dSdLBNB17]. **tri** [ZP13]. **tri-N-acetyl-** [ZP13]. **triad** [LY10, SM16a]. **triadic** [PPUBGD10]. **triads** [YKH⁺10]. **triaminoguanidinium** [ZYL⁺12]. **triangles** [She12]. **triangular** [TS11]. **triangularly** [LWZK13]. **triangulenes** [GSMM15]. **triarylamine** [KGR⁺16]. **triazenyl** [SB19]. **triazine** [WDLG12]. **triazines** [YPC⁺10]. **triazol** [ZZWT12]. **triazole** [NS10]. **triazoles** [GKR13, Ray13, RKG11]. **trichlorostannate** [PKK17]. **tricyclic** [VSD10]. **Triel** [Jab18b, Gra18, YKH15]. **triene** [ABDGN12]. **triethylgermanium** [WHX⁺10]. **triflate** [SV11]. **triflic** [LBC⁺12, SV11]. **Trifluorides** [MP19b]. **trifluoroethanol** [JA10]. **trifluoroethanol/water** [JA10]. **trifluoromethane** [CLC11]. **trifurcation** [HOM⁺16]. **Trigger** [SB18]. **triggered** [DAdGR15, TTC⁺18]. **triggering** [LLD17]. **trigonal** [Ano11, Gav12, GRD⁺10, JHMB⁺09, JHMB⁺11]. **trihalide** [Gra18]. **trihydride** [PM13]. **triiodide** [VVMY18]. **trimer** [THP⁺15, YCGA10]. **Trimeric** [PMT16, RCM⁺13a, RML⁺15]. **trimetallic** [GLF16]. **trimethylsilyl** [BIL10]. **trinitrotoluene** [SH14]. **tripeptide** [BH15, GMO16, MHO18]. **tripeptide-water** [MHO18]. **triphenyl** [AS18]. **triphenylamine** [MSV16]. **triple** [ACD⁺13a, ACD⁺13b, LOB18, Les19, OLPB19, POB13]. **triple-zeta** [LOB18, OLPB19, POB13]. **triplet** [RS17a, SSC⁺19, THP⁺15, ZZL19]. **triplets** [EK15]. **tripodal** [SB10]. **tripropylamine** [LL10c]. **tris** [KPL15]. **trivial** [IUK⁺11]. **tRNA** [LBS10]. **tropocollagen** [PP10]. **tropolone** [DL19]. **Trotter** [VKAM12]. **Trp** [EJ13]. **Trp-Glu** [EJ13]. **TRREAT** [CM13a]. **truncated** [CME11]. **truncated-CI** [CME11]. **truncation** [ACD⁺13a, ACD⁺13b, CS14, IMSR18, MC12]. **trust** [PLAG11]. **trying**

[BRGN12]. **trypanothione** [VSD10]. **tryptophan** [EOA⁺11, LM18b, PS14, SHB17, VMTL10]. **Tsallis** [QZ10c]. **tsscds2018** [RRFV⁺18]. **TTTO** [JW12, SLHW09]. **tuberculosis** [MPNS13]. **tubes** [TS15b]. **tubular** [uLhY11, ZLY⁺16, YLZ⁺19]. **tularensis** [STM⁺15]. **tumor** [JAH⁺17]. **Tunable** [MPJ⁺19]. **tuned** [Ali18, BK17b, ELP19, HZSS17, LCK⁺18, SZSS16]. **tuned-range** [ELP19]. **tungsten** [TS15a]. **Tuning** [Ano11, JHMB⁺09, JHMB⁺11, BK17b, LWL⁺11, Mor15, RLG11, SLY⁺19, VCL18, WYT17, LZ12]. **tunnel** [KL14]. **tunneling** [CSAdOM17, CSNCS⁺18, HS16a, LZW⁺11, OT12, QS19, dCRN18]. **TUNNEX** [QS19]. **TURBOMOLE** [KK17b, RR14, STH⁺10, vW11, BS18]. **turn** [SZB19]. **tweezers** [MBA14]. **twelve** [Pog10]. **twist** [KTK17]. **twisted** [YLZ⁺10]. **Two** [DS12b, Gra18, KKNN11, KTO13, SPHF⁺18, SC17, CCOH14, CXD⁺19, DPB⁺12, ECZWD17, FRSA14, FZL⁺19, GAMAC⁺14, HSN⁺18, HLH⁺12, LPAS11, LRER13, NASH15, PS17, PW12, SLT14, SS19, SH19a, SJC11, TCPPC14, VT14, YAS13, YZLZ19, YLL11, ZTH⁺15, SM17]. **Two-Body** [SC17]. **two-center** [LRER13]. **two-component** [HSN⁺18, NASH15, PW12]. **Two-dimensional** [KTO13, FZL⁺19, YZLZ19]. **two-electron** [CXD⁺19, PS17, YLL11]. **two-Gaussian** [SH19a]. **Two-level** [KKNN11]. **two-photon** [DPB⁺12, ZTH⁺15]. **two-scale** [FRSA14]. **Two-step** [DS12b, SJC11, TCPPC14]. **type** [BM12, BE16, CYY⁺17, CRC13, CB11c, Dil15, HLWD15, JYC⁺16, Kid19, LH14a, MY17a, MY17b, MKH15, RKB⁺14, SZX13a, SZX13b, SLY⁺19, VED10, WvRSM14, ZWX19, ZX11]. **type-II** [CB11c]. **types** [Lin18, SKY⁺11, UT15]. **typical** [BT18, TZ12]. **tying** [FP17b, YPKB12]. **Tyrosine** [DMD⁺18].

U [MCK17a, PGI19, RKB⁺14]. **U-shaped** [PGI19]. **Ubbelohde** [KTT16]. **ubiquitin** [JDW⁺19, MO17]. **ubiquitin-conjugating** [JDW⁺19]. **UCCSD** [MLCD11]. **UK** [WSGN11]. **ultra** [FBvdB18, VVY17]. **ultra-strong** [VVY17]. **ultrafast** [RVdMB16]. **ultrastability** [DM15]. **Umbrella** [DAB16, FB14b, JL19, AKN16, HH10, HDM⁺15, Ish10, KTO11, LMI⁺14, OL13, ZZ14, MYKO18]. **Un-Doped** [LLLW19]. **unactivated** [YXZZ17]. **unbiased** [ISO⁺13, ZGZC19]. **unbinding** [NJR18]. **uncertainty** [Fer17, Han11, SKGP19]. **unconventional** [LDJ⁺10, WWW19]. **uncoupled** [HH17]. **uncovering** [Won18]. **underdamped** [WZ19]. **undergoing** [GC18]. **underlying** [RN17, SGPJS⁺17]. **underpinning** [MCF⁺18]. **Understanding** [DLZ15, LLLW19, Lun12, RCM⁺13a, THI⁺19, TZ11, dCDP15, BH13, FCOGM12, HTY19, KNE11a, LGVA14, LGKS17, VVJ15, ZX11]. **unexpected** [HYYZ13]. **Unexpectedly** [SDF12]. **Unfavorable** [MP17a, PRP15]. **Unified** [PPUBGD10, CVT⁺11, TNYN16]. **uniform** [TH13, YWJ⁺16]. **unimolecular** [AMAA⁺11, STM17]. **union** [KRSC12, Mat18]. **unique** [GS11, uLhY11]. **unit** [CKKK16, DZA11, DGL⁺13, EP10, Elk16, PMT16, SRL⁺15, WS13, ZSTRS⁺18]. **unit-based** [WS13]. **Unitary** [SSSM15]. **united** [JGS⁺17, Jor17, ST11]. **united-atom** [JGS⁺17, Jor17, ST11]. **units**

[CCCLCGRO14, CYI⁺¹⁰, FCOGM12, GBL⁺¹¹, HASR⁺¹², HEMCZE⁺¹⁴, WSGN11, YWJ⁺¹⁶, YN15, YFH⁺¹⁹, ZKE⁺¹⁷]. **Universal**
 [LLH⁺¹⁹, AH10, AJR16, Gar12, SYN⁺¹²]. **unknown**
 [GPdC⁺¹⁶, KYT⁺¹⁷, MFR10]. **unperturbed** [Gri13]. **unprotonated**
 [Sie18, WGA18]. **unraveling** [HYYZ13]. **UNRES**
 [KMLS10, Sie15, SJ17, SGY⁺¹⁸]. **unrestricted** [BW11a, MMH19]. **Unrolr**
 [ESD18]. **Unsaturated** [HPT16a, Tsi17]. **unsolved** [CD19]. **unsulfated**
 [SA10]. **ununoctium** [TH13]. **unusual** [KYCL11, LZJ⁺¹¹]. **unzipping**
 [SM15, SM16b]. **Update** [CZAF17, MRO17, ER18, SPL⁺¹⁸, DPNM11].
Updated [SvLK18, BCJC⁺¹⁴]. **Updates**
 [AIGP15, Aki16, APK14, AAC⁺¹⁶, BTA⁺¹³, BHB12, BCSCJ⁺¹³, BSZ⁺¹², Ber17, BJP15, BFH⁺¹³, BBG^{+18b}, CBH14, CSEMB⁺¹⁶, CZAF17, CAT⁺¹³, 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, KB16, KDR⁺¹⁸, KLJ⁺¹⁷, KJM⁺¹⁷, KDT⁺¹², Kos16, KG13, KWL⁺¹⁶, KK17b, KWG15, KYG⁺¹⁵, KAG⁺¹², KSW16, KPF⁺¹⁵, LPS12, LJR⁺¹², LSH12, Leh15, LRvdSM15, LRvE17, LDB⁺¹⁷, LLZA12, LBB⁺¹⁵, LWZ⁺¹⁷, LC12, LAS⁺¹⁴, MHT⁺¹⁸, MDTD16, MBR⁺¹⁵, MYT18, MSSP17, MB14, MB16, NKJ16, OV14, OPB⁺¹², OZS⁺¹³, OC14]. **Updates**
 [PSS14, PGL⁺¹⁵, PSG⁺¹⁷, PW12, PPM15, PHH⁺¹², PVZ13, PG14, RLLHL12, RNSF⁺¹⁶, Ras17, Rez16, RR14, RdA12, RSR⁺¹², RCM^{+13b}, SM14a, SFG⁺¹⁷, SK15b, SWA13, SMRM⁺¹⁷, She12, SC15, Sie15, SJ17, SWB⁺¹², SDMS13, TNYN16, TSC⁺¹³, TTR⁺¹², TTL⁺¹², UU12, VMRS⁺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, ZDKM12, ZLL⁺¹³, dVAG16, KKR⁺¹³, SR18].
updating [UM13]. **upgrade** [ZSLL17]. **uptake** [WKC10a]. **uracil**
 [HvM12, LGOM⁺¹⁵, LJW11a]. **uracil/uracil** [HvM12]. **uranium** [OSS10].
uranyl [OSS10]. **URBOMOLE** [BBG⁺¹¹]. **urea** [SMDP18]. **ureas**
 [FCL⁺¹⁰]. **ureido** [SSP⁺¹³]. **ureido-benzenesulfonamide** [SSP⁺¹³].
uridines [DPSL16]. **urokinase** [BM12]. **uroporphyrinogen** [BEL⁺¹¹].
uroporphyrinogen-III [BEL⁺¹¹]. **Use**
 [DCOD13, SJL18, GPM17, HCD⁺¹⁰, KPF⁺¹⁹, MPA12, MMZW14, NPTS16, NC14, NDD⁺¹⁰, QS19, RLD12, WM17, Yes12, BCP⁺¹⁰, CKH19]. **used**
 [PGY15, Pie14, PLAG11, TH13]. **useful** [SMGB11]. **usefulness** [PSP15].
User [SJL18, All11, DBF14, HH16b, JJW⁺¹⁴, LBB⁺¹⁵, PVZ13, SFR⁺¹¹, STH⁺¹⁰, SPM⁺¹⁹, WPM⁺¹⁵]. **user-friendly** [SFR⁺¹¹, SPM⁺¹⁹]. **users**
 [GKV⁺¹³]. **uses** [BCJC⁺¹⁴, FHMB15]. **Using**
 [BS15, Car14, DLL⁺¹⁰, HH10, HPSK12, LLvG10, LG14, MGCC19, MSPC19, MP11, NZM18, ND19, QLQ11, SK17, TNG⁺¹⁰, WF16, AASP18, AJA⁺¹⁹, AG11, AS18, ABS⁺¹⁹, AGM⁺¹³, AC12, BW11b, BMR11, BDTP11, BS19,

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, SZSS16, STS15, TYZ⁺¹⁶, TYX⁺¹⁸, Tak14, TKNN10, Tsi17, TTh19, 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, MJB12, 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].

Verlet [Fom11, Gon12]. **versatile** [KKR⁺13, Pet11, SM14a, SWB⁺12].
version [BCJC⁺14, EVR18, KYG⁺15, OPB⁺12, Pyy13]. **versus**
 [BF19a, BH15, FD16, GMPB12, GWZ15, ITY⁺19, KCPMG12, LLFH16,
 MG11, OSF12, PGS⁺15, RP15, TR12, WCT⁺11, WvRSM14, YSSB12].
vertex [RNP13]. **vertical** [UD12]. **vertices** [LK16b, OV14, RNVP13]. **Very**
 [Ran13, CSSB11, SAGC16, Ran12]. **VESPA** [Ran12]. **VGe** [TT18]. **VI**
 [OSS10]. **via** [AKMT11, ACD⁺13a, ACD⁺13b, BSPP⁺13, BH13, CS17,
 DDP⁺18, DLZ15, DL19, GRCL12, HGCCGR⁺16, KHWB17, KKH18,
 LAW⁺16, NSO⁺14, RO14b, RJWW12, RNS19, SS13b, SISK10, ŠB15, SM17,
 TM18, TZ12, WBVE16, ZWP11, ZLY⁺16]. **viable** [SSX⁺14]. **VIBPACK**
 [CJPTC18]. **Vibration** [Kop19a, GK10, Kop15a, Kop16, Kop17a, Kop17b,
 Kop18, Kop19b, MK13b, Tac17, WZ19, YHX19]. **vibration-rotation**
 [GK10, Kop15a, Kop16, Kop17a, Kop17b, Kop18, Kop19b, MK13b].
vibration-vibration [YHX19]. **Vibrational** [DB12, LCW12, OC19, QZM11,
 ARLP13, BZB⁺13, CJPTC18, DOM⁺11, DHF⁺11, DT19, EB18, HYD10,
 IY18, KKA⁺18, KCPMG12, Kow11, KKH18, LBH⁺11, LLTC12, LBTV12,
 LS11b, MCF10, MAK⁺14, MN19, RLA⁺11, RRK16, SS13a, SSWX14,
 SST⁺18, TZCK18, VVW⁺18, WX12, XSZL11, dSAdSL13, WHK⁺12].
vibrationally [YHX19]. **vibronic** [MCLD10, ZTH⁺15]. **view**
 [BT18, DMJ17, MT19b]. **viewpoint** [PNE18]. **VIII** [LMR14]. **villin**
 [LKL10]. **Vina** [TO10]. **VinaMPI** [ESB13]. **vinylidene** [HSY⁺11].
violating [FL15, GZH10]. **virial** [FED17]. **viridis** [IIF⁺10]. **Virtual**
 [GRP⁺12, HDM⁺15, CCM15, ESB13, GCCM15, HKNH18, HHNK19, HJJ13,
 JBAM11, KC14, KLS10, KMLS10, LBB⁺15, MRB14, MNNK10b, MH10,
 SFM⁺18, VKC10, YZZ16, YD17]. **virtual-bond-stretching**
 [KLS10, KMLS10]. **virtual-system** [HHNK19]. **Virtual-system-coupled**
 [HDM⁺15]. **viruses** [OLY17]. **Vis** [GGM⁺12]. **viscoelastic** [YSG12].
viscosity [BBI⁺11, GM17]. **VISM** [ZCS⁺15]. **vistas** [GLW19].
visualization [CVT⁺11, HH16b, TKC⁺11, TEDT18, You10]. **Visualize**
 [GH16b, BPC19, QLQ11]. **Visualizing** [SOJ14, WM17, RD18]. **vivo** [HW19].
VMD [BHB12, FRC18, KLOS10]. **vmdICE** [KLOS10]. **VMS** [LBB⁺15].
VMS-Draw [LBB⁺15]. **Voids** [CC12a]. **voltage** [ACS12, SFBT17].
voltage-dependent [SFBT17]. **Volume**
 [Ano10b, 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,
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 Ano13i, Ano13j, Ano13k, Ano13m, Ano13n, Ano13o, Ano13p, Ano13q,
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[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].

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[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, Ano18a, Ano18b, Ano18t, Ano18u, Ano18v, Ano18w, Ano18x, Ano18y, 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, Ano18l, Ano18m, Ano18o, Ano18p,

Ano18q, Ano18r, Ano18s, Ano19a, Ano19l, Ano19t, Ano19u, Ano19v, Ano19x, Ano19y, Ano19z, Ano19w, Ano19-27, Ano19-28, Ano19-29, Ano19-30, Ano19-31, Ano19-32, Ano19b, Ano19c, Ano19d]. **Volume** [Ano19e, Ano19f, Ano19g, Ano19h, Ano19i, Ano19j, Ano19k, Ano19m, Ano19n, Ano19o, Ano19p, Ano19q, Ano19r, Ano19s, GY10, KRSC12, KTSW11, MK11, NASH15, NW17, Pop18, SZTSM10, Yan14, ZKE⁺17]. **volumetric** [KC14, MYT⁺14]. **Voronoi** [EFS16, Man19a, MOS12, OV14, REL17]. **Voronoi-based** [Man19a]. **Voronota** [OV14]. **Vorticity** [BL19]. **VoteDock** [PLV⁺11].

W4 [KSM17]. **W4-17** [KSM17]. **Waals** [BLF14, BB11a, BC13, CR14, DS12b, DSF17, FZL⁺19, KBC12, KCK⁺15, KGHK12, KLN12, LCH⁺15, SMGB11, SLIB12, SJZ⁺15, SYZ⁺17, Tan19, VP19, YZZ⁺17, ZY14]. **Wales** [DWZ⁺17, YZN13]. **walk** [CY09, CY13]. **Walker** [JL19]. **Walking** [CH16]. **wall** [BE14, Den12, FTR15, KGJZ19, MSY19, TSR⁺16]. **walled** [AS15a, PBE16, RHNN10, VS14, WYL⁺15, YZN13]. **Wang** [Ano12u, JW12, SA11]. **Water** [BHP19, DBGO⁺17, HvM17, LWL⁺16, MCUJ15, RBOH11, UNT16, ZLX⁺13, AASP18, AIGP15, AOW11, AF14, BSD18, BRLS08, BRLS12, CYY⁺17, CZH12, CXW14, CCOH14, DSB⁺19, DDP16, DAG19, DLC18b, FZL⁺19, GHL17, GM17, HH10, HTY19, HvM16, Hug12, IUK⁺11, JCP14, JIS13, JA10, KUDG12, KGHK12, KGHC15, KB13, KPH⁺19, KJ10, KSR⁺16, LH11, LK13, LPLS16, LP11b, LIRL⁺16, LCM⁺14, LJL⁺11, LAW⁺16, MC10, Man19b, MHO18, MKH15, MJM⁺15, MHRR11, NC12, NC13, OSS10, PAK15, PD11, PM18b, QQY⁺18, RTS⁺13, RZ16, Ric16, RRF11, RSB⁺13, SBGP18, SG10b, SNS16, SC18a, SISK10, SMP17a, SY16b, SV11, SIG⁺15, SM17, Tac17, TM16, TKYN17, TG12a, TL16, US11, VMTL10, Vor12, WC13, WCWV15, WG12, YDR13, YZ17, YZLZ18, ZCK⁺16, Zha12b, SGP18]. **water-fluoride** [NC12]. **water-halide** [NC13]. **Water-Terminated** [BHP19]. **water-vapor** [SISK10]. **water/** [RRF11]. **water/aromatic** [MJM⁺15]. **waters** [GEP⁺14]. **WATsite** [HL14]. **Watson** [BZH14]. **Wave** [HH16a, BVHI17, BP18, BLZ⁺13, BTB⁺11, Can10, Can11, EH13, Fer13b, Fer13a, FFA14, IT19, KSHP⁺19, LHMM11, LWD13, MDTD13, MDTD16, NFPD13, ON14, PHT17, RHRCH16, RvL11, SFM14, SH14]. **Wave-function** [HH16a]. **wave-functions** [Fer13b, Fer13a]. **wavefunction** [FD16, GSS13, HPT⁺16b, KSH⁺17, LC12]. **wavefunction-based** [GSS13]. **wavefunctions** [Bar14, BWKW10a, BWKW10b, DSV⁺19, DN19, LP11c, MDTD13, RGVC⁺19, SAGC16]. **wavelengths** [LM18b]. **Wavelet** [WRHF10, PN13]. **wavelet-based** [PN13]. **WavePacket** [SKA19]. **waves** [TCB16]. **Way** [SvLK18]. **ways** [KV15a]. **WC1LYP** [DOM⁺11]. **weak** [JJJ16, KSSH13]. **weakening** [LYSS11]. **weakly** [WL14]. **weaving** [Che17]. **Web** [CPK19, Che17, MdOdQ18, PBLs19, SPM⁺19, WPM⁺15, Gar12, JJW⁺14, LP11a, LJR⁺12, MdOdQ18, UHH⁺11, XYX17]. **Web-4D-QSAR** [MdOdQ18]. **Web-Based** [CPK19, MdOdQ18, Gar12, JJW⁺14]. **web-user**

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Y-zeolite [SN16a]. **yCD** [ZZY⁺16]. **years** [JCL⁺17]. **yeast** [ZZY⁺16]. **yield** [SHL⁺13, SSX⁺14]. **yields** [RDRC16]. **Yingjie** [Ano12u]. **yl** [BMB13, LXFC17, YZLZ18]. **YMn** [LLB⁺12]. **Yoink** [ZW18]. **Yongcui** [Ano12u]. **Yun** [Ano12u]. **yy** [ZLL⁺10]. **yy-DNA** [ZLL⁺10].

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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:CIIIf

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Anonymous:2012:CIIg

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Anonymous:2012:CIIh

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Anonymous:2012:CIIIi

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Anonymous:2012:CIVa

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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:CIVi

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Anonymous:2012:CIVj

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Anonymous:2013:CIIk

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Anonymous:2013:CIIl

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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

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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

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Anonymous:2013:CIIz

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Anonymous:2013:CIIba

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Anonymous:2013:CIIbb

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Anonymous:2013:CIIbc

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Anonymous:2013:CIIc

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Anonymous:2013:CIIbd

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Anonymous:2013:CIIbe

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Anonymous:2013:CIIId

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Anonymous:2013:CIIe

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Anonymous:2013:CII f

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Anonymous:2013:CII g

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Anonymous:2013:CII h

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Anonymous:2013:CII i

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Anonymous:2013:CIV a

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Anonymous:2013:CIV j

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Anonymous:2013:CIVk

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Anonymous:2013:CIVl

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Anonymous:2013:CIVm

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Anonymous:2013:CIVn

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Anonymous:2013:CIVo

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Anonymous:2013:CIVp

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Anonymous:2013:CIVq

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Anonymous:2013:CIVr

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Anonymous:2013:CIVs

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Anonymous:2013:CIVb

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Anonymous:2013:CIVt

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Anonymous:2013:CIVu

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Anonymous:2013:CIVv

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Anonymous:2013:CIVw

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Anonymous:2013:CIVx

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Anonymous:2013:CIVy

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Anonymous:2013:CIVz

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Anonymous:2013:CIVba

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Anonymous:2013:CIVbb

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Anonymous:2013:CIVbc

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Anonymous:2013:CIVc

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Anonymous:2013:CIVbd

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Anonymous:2013:CIVbe

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Anonymous:2013:CIVbf

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Anonymous:2013:CIVbg

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Anonymous:2013:CIVd

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Anonymous:2013:CIVe

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Anonymous:2013:CIVf

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Anonymous:2013:CIVg

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Anonymous:2013:CIVh

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Anonymous:2013:CIVi

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Anonymous:2014:CII

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Anonymous:2014:CIVa

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Anonymous:2014:CIVb

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Anonymous:2014:CIVx

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Anonymous:2014:CIVy

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Anonymous:2014:CIVz

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Anonymous:2014:CIVba

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Anonymous:2014:CIVbb

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Anonymous:2014:CIVbc

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Anonymous:2014:CIVbd

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Anonymous:2014:CIVbe

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Anonymous:2014:CIVbf

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Anonymous:2014:CIVbg

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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

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Anonymous:2014:CIVbm

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Anonymous:2014:CIVbn

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Anonymous:2014:CIVbo

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Anonymous:2014:CIVbp

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Anonymous:2014:CIVbq

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Anonymous:2014:CIVbr

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Anonymous:2014:CIVbs

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Anonymous:2014:CIVc

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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

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Anonymous:2014:CIVcb

- [Ano14-36] Anonymous. Cover image, volume 35, issue 24. *Journal of Computational Chemistry*, 35(24):i–ii, September 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcc

- [Ano14-37] Anonymous. Cover image, volume 35, issue 24. *Journal of Computational Chemistry*, 35(24):iii–iv, September 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcd

- [Ano14-38] Anonymous. Cover image, volume 35, issue 25. *Journal of Computational Chemistry*, 35(25):i–ii, September 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVce

- [Ano14-39] Anonymous. Cover image, volume 35, issue 25. *Journal of Computational Chemistry*, 35(25):iii–iv, September 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcf

- [Ano14-40] Anonymous. Cover image, volume 35, issue 26. *Journal of Computational Chemistry*, 35(26):i–ii, October 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcg

- [Ano14-41] Anonymous. Cover image, volume 35, issue 26. *Journal of Computational Chemistry*, 35(26):iii–iv, October 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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

- [Ano14-51] Anonymous. Cover image, volume 35, issue 30. *Journal of Computational Chemistry*, 35(30):iii–iv, November 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcp

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Anonymous:2014:CIVcq

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Anonymous:2014:CIVcr

- [Ano14-54] Anonymous. Cover image, volume 35, issue 32. *Journal of Computational Chemistry*, 35(32):i–ii, December 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcs

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Anonymous:2014:CIVg

- [Ano14-56] Anonymous. Cover image, volume 35, issue 4. *Journal of Computational Chemistry*, 35(4):i–ii, February 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVh

- [Ano14-57] Anonymous. Cover image, volume 35, issue 4. *Journal of Computational Chemistry*, 35(4):iii–iv, February 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVi

- [Ano14-58] Anonymous. Cover image, volume 35, issue 5. *Journal of Computational Chemistry*, 35(5):i–ii, February 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVj

- [Ano14-59] Anonymous. Cover image, volume 35, issue 5. *Journal of Computational Chemistry*, 35(5):iii–iv, February 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVk

- [Ano14-60] Anonymous. Cover image, volume 35, issue 5. *Journal of Computational Chemistry*, 35(5):v–vi, February 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVl

- [Ano14-61] Anonymous. Cover image, volume 35, issue 6. *Journal of Computational Chemistry*, 35(6):i–ii, March 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVm

- [Ano14-62] Anonymous. Cover image, volume 35, issue 6. *Journal of Computational Chemistry*, 35(6):iii–iv, March 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVn

- [Ano14-63] Anonymous. Cover image, volume 35, issue 6. *Journal of Computational Chemistry*, 35(6):v–vi, March 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVo

- [Ano14-64] Anonymous. Cover image, volume 35, issue 7. *Journal of Computational Chemistry*, 35(7):i–ii, March 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVp

- [Ano14-65] Anonymous. Cover image, volume 35, issue 7. *Journal of Computational Chemistry*, 35(7):iii–iv, March 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVq

- [Ano14-66] Anonymous. Cover image, volume 35, issue 7. *Journal of Computational Chemistry*, 35(7):iv–v, March 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVr

- [Ano14-67] Anonymous. Cover image, volume 35, issue 8. *Journal of Computational Chemistry*, 35(8):i–ii, March 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVs

- [Ano14-68] Anonymous. Cover image, volume 35, issue 8. *Journal of Computational Chemistry*, 35(8):iii–iv, March 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVt

- [Ano14-69] Anonymous. Cover image, volume 35, issue 8. *Journal of Computational Chemistry*, 35(8):v–vi, March 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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

- [Ano14-72] Anonymous. Cover image, volume 35, issue 9. *Journal of Computational Chemistry*, 35(9):v–vi, April 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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

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Anonymous:2015:CIVbb

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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

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Anonymous:2015:CIVbe

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Anonymous:2015:CIVbf

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Anonymous:2015:CIVbh

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Anonymous:2015:CIVbi

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Anonymous:2015:CIVbj

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Anonymous:2015:CIVbl

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Anonymous:2015:CIVbm

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Anonymous:2015:CIVd

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Anonymous:2015:CIVe

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Anonymous:2015:CIVbn

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Anonymous:2015:CIVbo

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Anonymous:2015:CIVbp

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Anonymous:2015:CIVbq

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Anonymous:2015:CIVbr

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Anonymous:2015:CIVbt

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Anonymous:2015:CIVbu

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Anonymous:2015:CIVbv

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Anonymous:2015:CIVbw

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Anonymous:2015:CIVbx

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Anonymous:2015:CIVby

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Anonymous:2015:CIVf

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Anonymous:2015:CIVg

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Anonymous:2015:CIVbz

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Anonymous:2015:CIVcd

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Anonymous:2015:CIVce

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Anonymous:2015:CIVh

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Anonymous:2015:CIVi

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Anonymous:2015:CIVj

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Anonymous:2015:CIVk

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Anonymous:2015:CIVl

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Anonymous:2015:CIVo

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Anonymous:2015:CIVp

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Anonymous:2015:CIVq

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Anonymous:2015:CIVr

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Anonymous:2015:CIVs

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Anonymous:2015:CIVt

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Anonymous:2016:CIVb

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Anonymous:2016:CIVc

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Anonymous:2016:CIVv

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Anonymous:2016:CIVw

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Anonymous:2016:CIVx

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Anonymous:2016:CIVy

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Anonymous:2016:CIVz

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Anonymous:2016:CIVbb

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Anonymous:2016:CIVbc

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Anonymous:2016:CIVbd

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Anonymous:2016:CIVbe

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Anonymous:2016:CIVbg

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Anonymous:2016:CIVbh

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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

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Anonymous:2016:CIVbs

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Anonymous:2016:CIVbt

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Anonymous:2016:CIVbu

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Anonymous:2016:CIVbv

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Anonymous:2016:CIVbw

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Anonymous:2016:CIVbx

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Anonymous:2016:CIVby

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Anonymous:2016:CIVbz

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Anonymous:2016:CIVf

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Anonymous:2016:CIVg

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Anonymous:2016:CIVca

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Anonymous:2016:CIVcb

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Anonymous:2016:CIVcc

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Anonymous:2016:CIVh

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Anonymous:2016:CIVi

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Anonymous:2016:CIVj

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Anonymous:2016:CIVk

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Anonymous:2016:CIVl

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Anonymous:2016:CIVm

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Anonymous:2016:CIVo

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Anonymous:2016:CIVp

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Anonymous:2016:CIVq

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Anonymous:2016:CIVr

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Anonymous:2016:CIVs

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Anonymous:2016:CIVt

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Anonymous:2016:CIVu

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Anonymous:2016:EPR

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Anonymous:2016:IIb

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Anonymous:2016:IIc

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Anonymous:2016:IIe

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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

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- [Ano16-64] **Anonymous:2016:IIj**
Anonymous. Issue information. *Journal of Computational Chemistry*, 37(22):2039–2043, August 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano16-65] **Anonymous:2016:IIk**
Anonymous. Issue information. *Journal of Computational Chemistry*, 37(23):2119–2123, September 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano16-66] **Anonymous:2016:III**
Anonymous. Issue information. *Journal of Computational Chemistry*, 37(24):2165–2169, September 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano16-67] **Anonymous:2016:IIIm**
Anonymous. Issue information. *Journal of Computational Chemistry*, 37(25):2243–2247, September 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano16-68] **Anonymous:2016:IIIn**
Anonymous. Issue information. *Journal of Computational Chemistry*, 37(26):2335–2339, October 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano16-69] **Anonymous:2016:IIo**
Anonymous. Issue information. *Journal of Computational Chemistry*, 37(27):2403–2407, October 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano16-70] **Anonymous:2016:IIp**
Anonymous. Issue information. *Journal of Computational Chemistry*, 37(28):2479–2483, October 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano16-71] **Anonymous:2016:IIq**
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

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

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

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

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:IICg

- [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,

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

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,

May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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,

April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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):

784–785, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:II Ea

[Ano16-129] Anonymous. Issue information – Editorial Board, volume 37, issue 1. *Journal of Computational Chemistry*, 37(1):3, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:II Ee

[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:CIV a

[Ano17a] Anonymous. Cover image, volume 38, issue 1. *Journal of Computational Chemistry*, 38(1):i, January 05, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIV j

[Ano17b] Anonymous. Cover image, volume 38, issue 10. *Journal of Computational Chemistry*, 38(10):i, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIV k

[Ano17c] Anonymous. Cover image, volume 38, issue 11. *Journal of Computational Chemistry*, 38(11):i, April 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIV l

[Ano17d] Anonymous. Cover image, volume 38, issue 12. *Journal of Computational Chemistry*, 38(12):i, May 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIV m

[Ano17e] Anonymous. Cover image, volume 38, issue 13. *Journal of Computational Chemistry*, 38(13):i, May 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVn

- [Ano17f] Anonymous. Cover image, volume 38, issue 14. *Journal of Computational Chemistry*, 38(14):i, May 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVo

- [Ano17g] Anonymous. Cover image, volume 38, issue 15. *Journal of Computational Chemistry*, 38(15):i, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVp

- [Ano17h] Anonymous. Cover image, volume 38, issue 15. *Journal of Computational Chemistry*, 38(15):ii, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVq

- [Ano17i] Anonymous. Cover image, volume 38, issue 16. *Journal of Computational Chemistry*, 38(16):i, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVr

- [Ano17j] Anonymous. Cover image, volume 38, issue 16. *Journal of Computational Chemistry*, 38(16):ii, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVs

- [Ano17k] Anonymous. Cover image, volume 38, issue 17. *Journal of Computational Chemistry*, 38(17):i, June 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVt

- [Ano17l] Anonymous. Cover image, volume 38, issue 18. *Journal of Computational Chemistry*, 38(18):i, July 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVu

- [Ano17m] Anonymous. Cover image, volume 38, issue 19. *Journal of Computational Chemistry*, 38(19):i, July 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVb

- [Ano17n] Anonymous. Cover image, volume 38, issue 2. *Journal of Computational Chemistry*, 38(2):i, January 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVv

- [Ano17o] Anonymous. Cover image, volume 38, issue 20. *Journal of Computational Chemistry*, 38(20):i, July 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVw

- [Ano17p] Anonymous. Cover image, volume 38, issue 21. *Journal of Computational Chemistry*, 38(21):i, August 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVx

- [Ano17q] Anonymous. Cover image, volume 38, issue 22. *Journal of Computational Chemistry*, 38(22):i, August 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVy

- [Ano17r] Anonymous. Cover image, volume 38, issue 23. *Journal of Computational Chemistry*, 38(23):i, September 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVz

- [Ano17s] Anonymous. Cover image, volume 38, issue 24. *Journal of Computational Chemistry*, 38(24):i, September 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVba

- [Ano17t] Anonymous. Cover image, volume 38, issue 25. *Journal of Computational Chemistry*, 38(25):i, September 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVbb

- [Ano17u] Anonymous. Cover image, volume 38, issue 26. *Journal of Computational Chemistry*, 38(26):i, October 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVbc

- [Ano17v] Anonymous. Cover image, volume 38, issue 27. *Journal of Computational Chemistry*, 38(27):i, October 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVbd

- [Ano17w] Anonymous. Cover image, volume 38, issue 28. *Journal of Computational Chemistry*, 38(28):i, October 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVbe

- [Ano17x] Anonymous. Cover image, volume 38, issue 29. *Journal of Computational Chemistry*, 38(29):i, November 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVc

- [Ano17y] Anonymous. Cover image, volume 38, issue 3. *Journal of Computational Chemistry*, 38(3):i, January 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVbf

- [Ano17z] Anonymous. Cover image, volume 38, issue 30. *Journal of Computational Chemistry*, 38(30):i, November 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVbg

- [Ano17-27] Anonymous. Cover image, volume 38, issue 31. *Journal of Computational Chemistry*, 38(31):i, December 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVbh

- [Ano17-28] Anonymous. Cover image, volume 38, issue 32. *Journal of Computational Chemistry*, 38(32):i, December 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVd

- [Ano17-29] Anonymous. Cover image, volume 38, issue 4. *Journal of Computational Chemistry*, 38(4):i, February 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVe

- [Ano17-30] Anonymous. Cover image, volume 38, issue 5. *Journal of Computational Chemistry*, 38(5):i, February 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVf

- [Ano17-31] Anonymous. Cover image, volume 38, issue 6. *Journal of Computational Chemistry*, 38(6):i, March 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVg

- [Ano17-32] Anonymous. Cover image, volume 38, issue 7. *Journal of Computational Chemistry*, 38(7):i, March 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVh

- [Ano17-33] Anonymous. Cover image, volume 38, issue 8. *Journal of Computational Chemistry*, 38(8):i, March 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVi

- [Ano17-34] Anonymous. Cover image, volume 38, issue 9. *Journal of Computational Chemistry*, 38(9):i, April 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:E

- [Ano17-35] Anonymous. Erratum. *Journal of Computational Chemistry*, 38(13):1015, May 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIa

- [Ano17-36] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(1):1–5, January 05, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

- [Ano17-37] **Anonymous:2017:IIb**
Anonymous. Issue information. *Journal of Computational Chemistry*, 38(2):59–63, January 15, 2017. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano17-38] **Anonymous:2017:IIc**
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- [Ano17-40] **Anonymous:2017:IIe**
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- [Ano17-41] **Anonymous:2017:II f**
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Anonymous. Issue information. *Journal of Computational Chemistry*, 38(8):475–479, March 30, 2017. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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Anonymous. Issue information. *Journal of Computational Chemistry*, 38(9):563–567, April 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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Anonymous. Issue information. *Journal of Computational Chemistry*, 38(10):639–644, April 15, 2017. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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Anonymous. Issue information. *Journal of Computational Chemistry*, 38(13):935–939, May 15, 2017. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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Anonymous. Issue information. *Journal of Computational Chemistry*, 38(15):1103–1110, June 5, 2017. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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Anonymous. Issue information. *Journal of Computational Chemistry*, 38(16):1283–1290, June 15, 2017. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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Anonymous:2017:IIr

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Anonymous:2017:IIs

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Anonymous:2017:IIt

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Anonymous:2017:IIu

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Anonymous:2017:IIv

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Anonymous:2017:IIw

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Anonymous:2017:IIx

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Anonymous:2017:IIy

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Anonymous:2018:CIVb

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Anonymous:2018:CIVk

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Anonymous:2018:CIVl

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Anonymous:2018:CIVm

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Anonymous:2018:CIVn

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Anonymous:2018:CIVo

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Anonymous:2018:CIVp

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Anonymous:2018:CIVq

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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:CIVb1

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Anonymous:2018:CIVe

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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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- [Ano18-44] **Anonymous:2018:II f**
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- [Ano18-45] **Anonymous:2018:II g**
Anonymous. Issue information. *Journal of Computational Chemistry*, 39(7):339–342, March 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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Anonymous. Issue information. *Journal of Computational Chemistry*, 39(8):381–385, March 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano18-47] **Anonymous:2018:II i**
Anonymous. Issue information. *Journal of Computational Chemistry*, 39(9):451–455, April 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

- [Ano18-48] **Anonymous:2018:IIj**
Anonymous. Issue information. *Journal of Computational Chemistry*, 39(10):521–525, April 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano18-49] **Anonymous:2018:IIk**
Anonymous. Issue information. *Journal of Computational Chemistry*, 39(11):615–619, April 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano18-50] **Anonymous:2018:III**
Anonymous. Issue information. *Journal of Computational Chemistry*, 39(12):699–703, May 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano18-51] **Anonymous:2018:IIIm**
Anonymous. Issue information. *Journal of Computational Chemistry*, 39(13):757–761, May 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
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Anonymous. Issue information. *Journal of Computational Chemistry*, 39(14):815–819, May 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano18-53] **Anonymous:2018:IIo**
Anonymous. Issue information. *Journal of Computational Chemistry*, 39(15):869–873, June 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano18-54] **Anonymous:2018:IIp**
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- [Ano18-55] **Anonymous:2018:IIq**
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- [Ano18-60] **Anonymous:2018:IIv**
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- [Ano18-61] **Anonymous:2018:IIw**
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- [Ano18-62] **Anonymous:2018:IIx**
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- [Ano18-63] **Anonymous:2018:IIy**
Anonymous. Issue information. *Journal of Computational Chemistry*, 39(26):2147–2151, October 5, 2018. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

- [Ano18-64] **Anonymous:2018:IIz**
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- [Ano18-67] **Anonymous:2018:IIbc**
Anonymous. Issue information. *Journal of Computational Chemistry*, 39(30):2489–2493, November 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).
- [Ano18-68] **Anonymous:2018:IIbd**
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- [Ano18-69] **Anonymous:2018:IIbe**
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- [Ano19b] **Anonymous:2019:CIVj**
Anonymous. Cover image, volume 40, issue 10. *Journal of Computational Chemistry*, 40(10):C1, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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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