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$(N-1)$ [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]. $\bar{}_{18}$ [YLT+19]. 0/+ [GTT10]. 0/+ [TN12]. 1
[Ben17, KSK11, LGW12, LX11, LWD13, PTK11, Pie14]. 11 [HJ13]. 129 [SKMS13]. 13 [Ben17, GMSV14, HJ13, OPR16, PTK11, Pie14, VAMS14]. 15 [RDT14]. $^{15}_{2}$ [RDT14]. 19 [DKE+17]. $^{1}\Delta_g$ [WLF19]. $^{1}\Sigma$ [LWD13]. $^{1}\Sigma^{+}$ [Kop15b]. $^{1}\Sigma^{+}_{g}$ [ZZZ+19]. 2 [GTK10, LGW12, LWD13, OZLSBH12]. 2+ [BHB+17, BHB19, BMFG16, DAdGR15, LBC+19, LPE+10, LWXC16, MG11, PGY15, RRF11, RHT+15, TLY+12, WRG+17, vSGP10]. $^{2}_{18}$− [YLT+19]. 29 [HAI+16]. 2•− [LGW12]. 2Π [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]. $^{+}_{13}$ [OPR16]. $^{+}_{15}$ [OPR16]. 16 [WZH+18]. 18 [DM15, TFQ+10, VIT+15]. 19 [DM15, VIT+15]. $\bar{}_{19}$ [YLZ+19]. 2
[AS15a, AR10, BE14, BPE16, BŁF14, BCNH+11, BPLL12, BLG10, BWKW10a, BWKW10b, BS10b, BS16b, CK10, CCJ+11, CCM15, CKL+11, CXS10, CSNCS+18, DSB+19, DOM+11, DLSD13, DT19, DLW12, DHE+12, DSHLM18, EVR18, EP15, EBPK17b, EB18, FMNC11, GLZ17, GK10, GWJR18, GNI18, GY12, GWJJ12, HSJ18, HYL+11, HZ11, HSY+11, HFSO12, HBL12, HYD10, HRL11, HVS16, Ibr17, JCG+10, JLS+10, JLH+14, KBC12, KIOY19, KMS+19, KKR+13, Kop16, Kop18, Kop19b, KCL+14, LZTV10, LWW12, LYC+13, LAHS16, LBTV12, LLSW14, LWXC16, LLLW19, LPLB16, LCWW10, LWD13, LJG+11, LLL+12, MLQ+12, MLGB16, MP19a, MG15, MKH15, MCUJ15, MLCD11, MS15, MCAY15, NGAS17, NC14, NMLD13, NKD18, OKY18, PVL+13, PLFS18, PBE16, RHNN10, RAGLL11, RDT14, RRC+15, RVdMB16, RHT+15, RSKG14, RSK+15, SSC+19, ŠBD+17, SC17, STS+10]. 2 [SSX+14, SLY+19, TLdG+12, TNY18, Tak11, TSJ+10, TSZQ12, Tsi17, UvSvdWK19, VP19, VT14, VV14, WKC10a, WHL+10, WGL+11, WMW11, WLHZ12, WC13, WWKS16, WLF19, WRM+12, WGN+16, WGLG+16, WYGW12, XFX+16, XCLZ19, YR13, YHX19, YLL11, Yu12a, YZ15b, YXZZ17, ZRCC11, ZRCC12, ZZ10, ZZL+10b, ZSWL12, ZLLL12, ZYG+14, ZLY+16, ZZZ+19, ZZL19, dSDdAR10]. 20 [GBGR16, JCG+11, LdSRR16, MCK17b]. $\bar{}_{20}$ [YLZ+19]. 24 [GBGR16, YW12]. 26 [LAHS16]. 28 [MCK17a]. $^{+}_{2}$ [CG12, EVR18, MH11]. $\bar{}_{2}$ [MN19, Sak18]. 2*h* [ZLY+16]. 3 [Alg17, AR10, ATP18, ASS+17, ABB+12, ABB+13, BE12, CK10, CCJ+11, CXW14, EB12, EBK13, FD16, FHG+19, GSMZ19, HSJ18, HDM+19, Ibr17, JCG+10, KT19, KKR+13, LLBO12, LLLM11, LLB+12,

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

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

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

[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** [BŁS10]. **-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-benzyne** [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** [SFCCK+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, ŚSB+16, SYZ+17, TH13, VSP19, WL14, YB16, ZWLX11,

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

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]. **Al** [LCWW10, Pon10, UT15, YR13, CC18c, GWJJ12, KKR+13, SH14]. **Al-hydroxylated** [SH14]. **Ala** [SZBM13]. **alanine** [IO13b, LL19a, MAMF19, MVKS10, SEM12]. **AlB** [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, dlRL11, 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, ZSTI14]. **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]. **AlN** [wZbZ11]. **AlO** [GWPJ11]. **along** [ABDGN12, AC11b, CM13a, CX10]. **Alpha** [MH10, MKB+13, SPZP18b, XTY+14]. **alphabets** [PHDH13]. **AlPO** [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, JZZM14, 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, ŁBGS16, 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, RKGN10, RB12, RVP+11, SLT14, SZdB19, SEF+16, SH11b, SY16a, Sti15, SLLL13, SGH+16, SM17, TO19, TAG16, TSR+16, VVLG17, WFS19, XZ11, YKO+11, ZSLL17, ZLW10, AIM+18, GFG11, ACD+13a]. **approaches** [BP18, BH13, CME11, DBM+17, ECZWD17, HBI+17, IT19, LSH+11, RLDJ17, RŠRR15, VLB+10, YJ11, ZDT18]. **Appropriate** [LZLC13]. **Approximate** [Gav12, KV12, KV13, RP15, RZ16, SM14a, HH16a]. **approximation** [AO10, Boz18, Cas13, HH17, Kid19, Sch12, WHM10, WDKT19, YD17, YN15].

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** [MJBM12, 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]. **asparaginyl** [LBS10]. **asparaginyl-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, PBLS19, 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, LRVM18, 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, LHSH12, 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, SZZS16, 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** [BŁF14, BRLS08, BRLS12, PHK14, SN16b, TKN13, ACD+13a, ACD+13b, BŁFZ13, BŁŁ13, BŁBG+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, CSAdOM17, FCD10, FTR15, KRTB10, LZY+12a, PD11, TLdG+12]. **belief** [GFPSD17]. **Benchmark** [CXD+19, WSZW15, AF14, ANH+11, CSXZ17, cCVG+14, DGSVGVM19, GAI14, KG15, NH19, RS13, ZWGO16, IKN13]. **benchmarked** [XYW+14]. **Benchmarking** [Ben17, GAJ+17, Hug12, LCM+14, GP11b, HRJ+14, HRJ+15, HZ13, IY18, JRSHP14, 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, BRLS08, BRLS12, 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, MSÅK12, MAP18, MFR+17, MNNK10a, NST14, NHN16, NWW17, NZM18, NFG+13, NF17, NN18, NO16, NNK+16, OBW12, Oht16, OHNK11, OSR16, OCLM14, OOT15, PGCT+12, PBLdS12, PGS+15, Pla11, RLDJ17, RCR+16, RDDS10, RAR+11, RO14b, RZ16, RF15, Rez19]. **binding** [SPS+12, SRA17, SOD+11, STM+15, TYZ+16, TJR19, TS15a, UNT16, VVG13, Vor10, VM11, VHS+19, WS10, WNP+16, WLLH18, WWW19, WL14, XHLH16, YZ15a, YZZ16, YJXZ13, YHH+13, ZZ14, ZJZM13, ZYvIZ14, ZLX+13, dRBO13]. **binding-based** [MAP18]. **binding-site** [ISP+10]. **binds** [XHLH16]. **BINOL** [HPT16a]. **BINOL-phosphoric** [HPT16a]. **Binor** [WJX+10]. **Binor-S** [WJX+10]. **binuclear** [KMS+19, LZTV10]. **bio** [MSvG12, RZ16]. **biochemical** [DGSVGVM19, RB12]. **biofuels** [LGC19]. **bioisosterism** [EdOdS18]. **BioLayer** [JAH+17]. **biological** [BHB12, Ben17, CLK11, DLL+10, DMN15, GREA11, GFPSD17, GLM+17,

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** [VVY17]. **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, MPSG11, MLGB16, MS11, MvBD18, NHF+10, Niz13, PKK17, QZM11, RHRCH16, RvL11, RS17b, Rob13, RRK16, 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** [BŁFZ13, 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, LZY12b, LDG+15, OOK11, PGI19, Rob13, SM16a, SK13, SJ16, TDT19, WS19, XMA+19, YLT+19, YLL11, YKH15, YJ17, ZLY+16, Jab18b, YLZ+19]. **BonnMag** [BBG+18b]. **Book** [CD19, Sch10, Spr10]. **Boolean** [CDC19]. **boost** [KV15a]. **BOP** [SH19a]. **borafluorenes** [ZQ14]. **borane** [BEPM14, Kop15b, LC10, SJZ+15]. **borane-cyclic** [LC10]. **borate** [OSA19]. **borates** [GWJJ12]. **border** [SK12, SK17]. **borides** [ZWMW10]. **born** [AB16b, BLZ+13, DSF17, FCE15, HWLW11, KCPMG12, LL10a, LCH10, MT19b, PS13, RSB+13, SZTSM10, SSBW14, VMPS17, WWKS11]. **boron** [BEPM14, Gra18, GAMAC+14, LT14, Oht16, PGC12, VS14]. **boron-** [BEPM14]. **boron-doped** [VS14]. **boron-nitride** [LT14]. **boronate** [HLI+19]. **boryl** [LC10]. **BOSS** [VKTRJ15]. **BOSS-Gaussian** [VKTRJ15]. **Bosutinib** [GMASBF16]. **both** [AST+16, FNSF+11, LX11, TH13, WZ19, WS19]. **bottleneck** [SRR16]. **bound** [FLM11, GPK+16, LFM12, MAK+14, PMG+16, PZA15, XWSW13]. **Boundary** [Coo19, KB14a, Lun12, MTvG12, NO16, PL14, PS13, SSP19a, Sie15, VECT12, YAO18]. **Boundary-Integral** [Coo19]. **bounded** [LL19b, Pol13, SL10]. **bowls** [WL14]. **box** [Pla11, WS13]. **boxB** [XHLH16]. **Boys** [WO15]. **bptz** [CWT+12]. **bpy** [LWXC16]. **Br** [ATP18, ASS+17, EPH+15, GPK+16, LDJ+10, LLL+11, LZJ+11, PMG+16, YS13, ZLLL12, LZL+15b, MKH15, MSPC19, XhD15, ZWY+10b]. **Branch** [Ish10]. **branching** [BEL+11, OZLSBH12, STM17]. **BrBr** [LGW12]. **Breaking** [HRID16, SRR16, WWWW18, Man19b]. **bridge** [CVG14, PH15, ZSTRS+18, dLvNC18a]. **bridged** [HLI+19, KGR+16, ZLZ14, ZLY+16, ZB18, ZZWX11]. **bridges** [MLY+13, PH15]. **Bridging** [YLL11, dCDP15, LJL+11, MIS+15, BPC13]. **Brillouin** [QS19]. **Bringing** [RR11]. **broad** [MP19c, TZ12]. **broken** [XKW18]. **broken-symmetry** [XKW18]. **bromide** [MG15, OC19]. **bromination** [SGS+16]. **Bromine** [LWL+16]. **BROMOC** [DMN15]. **Bromosuccinimide** [QQY+18]. **Brooker** [TYN15, TKYN17]. **Brooks** [HIS17]. **Brownian** [DMN15, DZT11, LJR+12]. **brushes** [DQ16]. **BSSE** [OLPB19]. **BSSE-correction** [OLPB19]. **btmgp** [RHT+15]. **BtuF** [WWW19]. **buck** [KPF+15, KPF+19]. **Buckybowls** [HVS16, CCCLRO14]. **buffered** [MJG+15, MEH18]. **build** [APK14]. **builder**

[KOY+12, GS12, QLKI19, WCJ+14]. **Building** [MB14, BHI19, CBP14, GS12, KSW16, MJBM12, RLG14, Tak11, TJB12, VVY17]. **building-up** [Tak11]. **buildup** [SS13a]. **built** [FCPJM14, KOP+14]. **bulk** [BC13, KHLM19, 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**$\cdots$ [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, BŁŁ13, BS10a, BTMS12, BH15, Bou14, BS18, BG12, BLZ+13, CR14, CCJC10, CS17, CKKK16, CBDS19, CMvG10, CXS10, CHKR10, CKG18, DGH+11, DSV+19, DGSVGVM19, 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, LEdOLdlV17, LRVM18, LOB18, LMZ11a, LCH10, LYC+13, LCA17, LvG13b, LCK+18, LCM+14, Lun12, MK17, MK19, MUGNVJ+18, MLN+18, MCLD10, MEH18, MCK17a, MCK17b, NWW17, NZM18, NLL19, NCT18, NN18, OHNK11, OLPB19]. **calculations** [OLA15, OOT15, OZLSBH12, PBLdS12, PTK11, PHK14, POB13, PBBP11, PDG+16, PN13, PGW+17, RAR+11, RLZ+18, RHT+15, RLD12, RR11, REV+17, RI10, RK15, SH15, SRSLO15, SP13, SPHF+18, SS16b, SCW11, SWPR11, SRS14, SMP17b, SDMS13, SHB17, SKTT11, SPZP18b, SPZP19, TLdG+12, TNY18, TS10a, TNI19b, UHH+11, VLB+10, VKAM12, VKNT16, VHR16, VFRAR16, VMPS17, VI17, WC13, WSZW15, WHK+12, WTH+16, WGA18, WXY14, XYW+14, YWJ+16, YD17, YN15, YJ19, ZRCC11, ZLT13, ZLZ14, ZWMW10, ZH12, MSPC19, NQB19]. **calculator** [dCLFGL13]. **calibrate** [VVLG17]. **Calibration** [CBP14, DDM+15]. **calix** [GMASBF16, PRRT+10, YCGA10, ZWY+10a, ZWS+10, GMASBF16]. **Call** [ZPF14]. **CAMERRA** [JLS18]. **Can** [ASMS10, IMSR18, KV15b, LZW+11, NH19, PŁAG11, SHL+13, SPZP18a, CIKT13, LCB10, TCPPC14, Zha12b]. **CANADA** [Fel10]. **cancer** [NS10, WC11]. **Canepa** [LHMM11]. **cannabinoid** [ILKR11]. **Canonical** [CPN+17, RHNN10, BW11a, HRK+10, HHNK19, KCK+17, PHH+12]. **Canterakis** [UCRL18]. **CaO** [BL12]. **CAP** [EFS16]. **CAP/SAC** [EFS16]. **CAP/SAC-CI** [EFS16]. **capabilities** [AAC+16]. **capability** [LC10]. **capacity** [KOP+14, PGC12, WKC10a, WKLC12]. **capillary** [NFPD13]. **caps** [WDS+19]. **capture** [GLZ17, SMD18]. **Car** [DL19, KCK+15]. **CARB1/TIP3P** [SA10]. **carbazole** [JYS+12, SLC+17, YJN+11]. **carbazole-based** [SLC+17]. **carbazole-fluorene** [YJN+11]. **CarbBuilder** [KSW16]. **carbene** [CWT+12, LXZ+10, TCPPC14, WS11, WS12, YJ19, dSdLBNB17]. **carbenes** [BAD+19, BSDP16, KYKR15, RF15]. **carbocation** [ONTTL16]. **carbocations** [OPR16]. **carbocyclic** [BAD+19]. **Carbohydrate** [ZYvIZ14, NMF+14]. **Carbohydrate-binding** [ZYvIZ14]. **carbohydrates** [CP15, HH11, JSD+11, PLH16]. **Carbon** [JLLW19, SC17, AJA+19, AS15a, AAMR18, ASL+11, BPE16, CME11, DI11, Den12, DC13, Fom13, FTR15, GSMM15, GPK+16, GBS+17, GZZ12, JWO15, KGHK12, KV14, KPH+19, KHE+19, KGJZ19, LPLS16, LL10c, LT14, LK16b, MSY19, OCW+15, RHNN10, RRK16, Sie18, TSR+16, VS14, WYL+15, WDZN16, YZN13, YZZ+17, ZYW+16, ZLY+16, ZWF15, OSI+19]. **carbon-beryllium** [CME11]. **carbon-carbon** [KGJZ19]. **carbon-germanium** [GSMM15]. **carbonate** [ZSWL12]. **Carbondioxide** [Sea10]. **carbonic** [SSP+13]. **carbons** [MKB+13, RVB+12]. **carbonyl** [BH19, CZH12, CROB16, TS10b, ZBMZH15]. **carbonylation** [MRC+18].

carbonyls [SSX+14]. **carboranes** [HJ13]. **carboxybetaine** [DQ16]. **carboxylates** [AARP17, RVM19]. **carboxylation** [CKG18, DGSVGVM19]. **carboxylic** [LPMT17, RB12, dSH19]. **card** [SR11]. **Carlo** [LHMM11, NQB19, 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, 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, ŠBD+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]. **CFCl** [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, MJBM12, 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$^+$15, RSSG18, RO14b, Rez19, Ric16, REL17, SPS$^+$12, SFM$^+$18, SSGS15, SMiN$^+$19, SMP17a, SFLG$^+$17, SLC$^+$17, TN10, TKNN10, UT15, UGK18, VPR10, VAR12, VL17b, WCT$^+$11, WWCL15, YKO$^+$11, YWZ14, YLZ$^+$10, YJ17, YFH$^+$19, ZDZM13, ZZL19, dSH19, dLC17]. **charge-assisted** [SSGS15]. **charge-inverted** [UT15, YJ17]. **Charge-transfer** [JM11, ANH$^+$11, EFAC13, YLZ$^+$10]. **charge-transport** [HLWD15]. **charged** [BK13, KD10, MRO17, NPP13, RJS17, Tsi14]. **Charges** [WFZ$^+$18, CCB15, IM17, JMLL13, LRVM18, RB13a, SN15, TBSM12, VSA11, Yan14, ZBG11]. **Charles** [HIS17]. **CHARMM** [MSK$^+$12, AKMYB18, BF17, BAF18, DPNM11, GLB16, GZM11, HBJ$^+$17, HC14, JCL$^+$17, KLJ$^+$17, KYB13, LZdlL$^+$10, MSK$^+$10, MMZW14, QLKI19, RR14, VHA$^+$10, WCJ$^+$14, XVA$^+$16, YHVM12]. **CHARMM-based** [MMZW14]. **CHARMM-compatible** [KYB13]. **CHARMM-GUI** [HBJ$^+$17, KLJ$^+$17, QLKI19]. **CHARMM27** [ST11]. **CHARMM36** [HM13]. **CHARMMing** [WPM$^+$15]. **Charts** [SJL18]. **Chatt** [Bac12]. **CHClCH** [WLHZ12]. **CH**$\cdots$ [MVKS10]. **cheapest** [SA13]. **cheapest-path** [SA13]. **checkpoint** [DXL$^+$10, DSX$^+$11]. **chelation** [KYCL11]. **Chem** [ABB$^+$13, CHR$^+$12b, HNWF12, HLXH18, ICS$^+$13, Kne11b, MT20, MSK$^+$12, RK16a, SFCCK$^+$15, SMM15a, GCC14, GKV$^+$13]. **Chemical** [BLG10, BCP$^+$10, BGS$^+$19, JCGVPHT17, OSI$^+$19, OM12, SLLL13, VGTL16, ALK$^+$15, ASS$^+$17, AAC$^+$16, APA$^+$14, Bac12, BPC19, Ben17, Bou14, Cam15, CKG18, CHP11, DKE$^+$17, DDP$^+$18, DS12a, DI11, DB12, Dra19, EOA$^+$11, FB10, FVB10, GH10, GLW19, GGM$^+$12, GPGSM11, GPGSM12, HPT$^+$16b, HHDC16, HJ13, Ihl12, JKS$^+$16, KV12, KASH14, KP11, LK11, LZH$^+$11, Li14a, Li14b, MDTD13, MDTD16, Man19b, MN15, MTS$^+$19, MAPB10, MSvG12, MSSP17, MFR$^+$11, MMJ10, MH10, NCV10, NC13, NC14, OKIS17, OKY18, OSHG17, ONTTL16, OC14, PTK11, PGdO$^+$16, Pie14, PBG17, RRFV$^+$18, RK15, RSKG14, SRA17, SLT14, SFM$^+$18, SCOJ13, SEF$^+$16, SKMS13, SHB17, TLA10, TG12b, TEDT18, TR12, UD12, VBD11, VBMA13, WBT10, WCT$^+$11, WF16, Wei12b, WL14, Wu10, WDP$^+$12, YZ15a, YB16, ZY14, ZBB16, ZT14]. **chemical** [dCDP15, Chu10]. **chemical-bonding** [MDTD13]. **Chemically** [EFAC13, ZZ12, JAHS$^+$19, Zim13]. **chemist** [DHE$^+$12]. **chemistries** [BS10b]. **Chemistry** [Ano10b, Ano15-59, Cam19, HJG09, KKGW19, Spr10, ZLX$^+$19, All11, BRP$^+$12, BGR13, CBH14, CD19, DDM$^+$15, FLM11, GHV17, HSN$^+$18, IGK16, JBB$^+$11, KTNN10, LBC$^+$19, LK16a, MP19c, OZLSBH12, PNW$^+$16, PPUBGD10, RZG$^+$13, Řez16, REL$^+$14, TKNN10, TF15, UDK$^+$18, VVP12, VV14, WDY13, ZVY$^+$15, GS16, MFEM16, XFG$^+$16]. **ChemNetworks** [OC14]. **chemoselectivity** [WWTL19]. **chemosensing** [LZHH11]. **chemosensor** [LZL$^+$10]. **CheY** [Pet11]. **CHFCF** [NMLD13]. **chi** [EJ13]. **chignolin** [HTS15]. **Chiral** [KHE$^+$19, KSO$^+$19, LG14, PC14, ZPP$^+$16]. **Chiral-selective** [KHE$^+$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]. **Cl** [ATP18, ASS+17, CXS10, EPH+15, GPK+16, KKR+13, LDJ+10, LLL+11, LZJ+11, LGW12, PMG+16, Rab12, RVdMB16, Sak18, TFQ+10, TFQ+11, Tsi19, TDT19, WGN+16, WGLG+16, YS13, ZCK+16, ZLLL12, CSNCS+18, JCG+10, JLS+10, JLH+14, LZL+15b, MSPC19, WLHZ12, WLF19, ZWY+10b]. **Clar** [KDS17]. **Clarifying** [RML+15]. **class** [DWL11, HHWL17, LD18, ZLW10]. **classical** [Aki16, BEM14, DHF+11, GA19, HS14a, HLvdV13, LRvdSM15, LM18a, LPE+10, LM18b, MS15, PVAM16, Ras17, RTS+13, RO14b, SM14b, SKA19, WKC+10b, WG14, Yu12a, ZM10]. **classification** [EP15, UT15]. **classifier** [YHH+13]. **classifying** [TO19]. **Clay** [BHB19, BHB+17]. **ClC** [KJ10]. **ClCH** [RVdMB16]. **ClCHO** [SS19]. **ClCl** [LGW12]. **clean** [CCJ+11]. **cleaning** [YR13]. **cleavage** [HEM+17, MS11]. **click** [TKXT13]. **CLL** [dACP12]. **ClNH** [VVMY18]. **close** [BLZ+13, MK17, RS13]. **Closed** [CYI+10, MA16, MS12, WWD14]. **closed-shell** [MA16, WWD14]. **Closo** [HJ13]. **Closo-carboranes** [HJ13]. **closure** [ABDGN12, NR11]. **cloud** [TF15]. **cluspro** [XML+15]. **Cluster** [AST+16, Hes19, MPNS13, SL17, ACD+13a, ACD+13b, AC11b, Avd18, BBG+18a, BYE+16, Cas14, CC18c, DI11, DM15, FF11, GNGCA10, GMG+10, GA18, GS11, HAGK10, HSB+19, HSH15, Höf14, HGCCGR+16, HBI+17, Les19, MC12, MG14, NLL19, Oht16, PGS+15, PB14, PMT16, RS14, RLZ+18, SB11, SLLL13, SM17, TLdG+12, TNY18, TTn19, VIT+15, VV14, WC13, XTn18]. **Cluster-based** [MPNS13]. **cluster-continuum** [WC13]. **cluster-expansion** [HAGK10]. **cluster-in-molecule** [NLL19]. **cluster/configuration** [FF11]. **cluster/Kohn** [VV14]. **clustering** [BSZ+12, LZS+17, PL19, YZ15a, ZSS+13]. **Clusters** [NSN19, SC17, TT18, AFPI13, ATIP18, AF14, Ano11, ASS10, AC12, BPM15, BACSCJ+10, CJL+13, CZZL19, DAG19, DH11, FCW+14, GTT10, GC18, GRD+10, GAMAC+14, GZZ12, GBGR16, GBG+19, HS14a, HS16b, HDM+19, Hsu14, JM11, JCP14, JHMB+09, JHMB+11, JCG+11, KD10, KKPT11, KOP+14, KSNT19, KDB13, LZTV10, LK13, LZZ+11, LCH+15, LCWW10, MCS11, Man19b, MPA10, MPA12, MP13, MBFG15, MBRC16, MCAY15, NC13, NC14, OKY18, PM18b, QZ10b, Rab12, RGVC+19, RSB+13,

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

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

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, SFCCK+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, BŁBG+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** [II10]. **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, ETLS17, 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, BŁBG+13, HDHL15a, HDHL15b, HDHL15c, JYS+12, RSSG18, YJN+11, JCHT18]. **conjugating** [JDW+19]. **conjunction** [CGA19, LBH+11, NC13, RKGN10]. **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, PŁV+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, ŁBGS16]. **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]. **Copyright** [Ano16-89, Ano16-94, Ano16-95, Ano16-96, Ano16-97, Ano16-98, Ano16-99, Ano16-100, Ano16-101, Ano16-102, Ano16-90, Ano16-91, Ano16-92, Ano16-93]. **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, BŁBG+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, MŘ17, OZS+13, RS13, SFA17]. **CovalentDock** [OZS+13]. **covalently** [CZNA11]. **Cover** [Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g, Ano12h, Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n, Ano12o, Ano12p, Ano12q, Ano12r, Ano12s, Ano12t, Ano13a, Ano13l, Ano13t, Ano13u, Ano13v, Ano13x, Ano13y, Ano13w, Ano13z, Ano13-27, Ano13-28, Ano13-29, Ano13-30, Ano13-31, Ano13b, Ano13c, Ano13d, Ano13e, Ano13f, Ano13g, Ano13h, Ano13i, Ano13j, Ano13k, Ano13m, Ano13n, Ano13o, Ano13p, Ano13q, Ano13r, Ano13s, Ano13-32, Ano13-43, Ano13-51, Ano13-52, Ano13-53, Ano13-55, Ano13-56, Ano13-57, Ano13-58, Ano13-54, Ano13-59, Ano13-60, Ano13-61, Ano13-62, Ano13-63, Ano13-64, Ano13-33, Ano13-34, Ano13-35, Ano13-36, Ano13-37, Ano13-38, Ano13-39, Ano13-40, Ano13-41, Ano13-42, Ano13-44, Ano13-45, Ano13-46, Ano13-47, Ano13-48, Ano13-49]. **Cover** [Ano13-50, Ano14a, Ano14b, Ano14c, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14n, Ano14o, Ano14p, Ano14q, Ano14r, Ano14s, Ano14t, Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14-28, Ano14-29, Ano14-30, Ano14-31, Ano14-32, Ano14-33, Ano14-34, Ano14z, Ano14-35, Ano14-36, Ano14-37, Ano14-38, Ano14-39, Ano14-40, Ano14-41, Ano14-42, Ano14-43, Ano14-44, Ano14-45, Ano14-46, Ano14-47, Ano14-50, Ano14-51, Ano14-52, Ano14-53, Ano14-54, Ano14-55, Ano14-27, Ano14-48, Ano14-49, Ano14-56, Ano14-57, Ano14-58, Ano14-59, Ano14-60, Ano14-61, Ano14-62, Ano14-63, Ano14-64, Ano14-65, Ano14-66, Ano14-67, Ano14-68, Ano14-69, Ano14-70, Ano14-71, Ano14-72, Ano14d, Ano14e, Ano14f, Ano15a, Ano15b, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n, Ano15o]. **Cover** [Ano15p, Ano15q, Ano15r, Ano15s, Ano15t, Ano15u, Ano15y, Ano15z, Ano15-27, Ano15-28, Ano15-29, Ano15-30, Ano15-31, Ano15-32, Ano15-33, Ano15-34, Ano15-35, Ano15-36, Ano15-39, Ano15v, Ano15-40, Ano15-41, Ano15-42, Ano15-43, Ano15-44, Ano15w, Ano15x, Ano15-37, Ano15-38, Ano15-45, Ano15-46, Ano15-47, Ano15-48, Ano15-49, Ano15-50, Ano15-51, Ano15-52, Ano15-53, Ano15-54, Ano15-55, Ano15-56, Ano15-57, Ano15c, Ano15d, Ano15e, Ano15f, Ano15g, Ano15h, Ano16a, Ano16b, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m, Ano16n, Ano16o, Ano16p, Ano16q, Ano16r, Ano16u, Ano16v, Ano16w, Ano16x, Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16-29, Ano16-30, Ano16-31, Ano16-32, Ano16-33, Ano16-34, Ano16-35, Ano16-36, Ano16c, Ano16-39, Ano16-40, Ano16-41, Ano16s, Ano16t]. **Cover** [Ano16-37, Ano16-38, Ano16-42, Ano16-43, Ano16-44, Ano16-45, Ano16-46, Ano16-47, Ano16-48, Ano16-49, Ano16-50, Ano16-51, Ano16-52, Ano16-53, Ano16-54, Ano16-55, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h, Ano17a, Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x, Ano17z, Ano17-27,

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]. **CRYSPLOT** [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** [PŁAG11, 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** [LZdlL+10]. **deMon2k** [BTT10]. **Demystifying** [KKGW19]. **Denaturation** [IPAA11, FMG12]. **Dendrimer** [MJBM12]. **dendrimers** [CAD16, HDHL15a, HDHL15b, HDHL15c]. **Deng** [Ano12u]. **dense** [ASK18]. **Densities** [ATM18, ATIP18, HGCCGR+16, LP11c, MA16, REL17, UCRL18, dLC17]. **Density** [AMK11, BS19, BHB19, CD13, CWHH11, CKH19, FPV13, FD16, GMBM18, GNGCA10, GWPJ11, INT18, JYS+12, KKPT11, ŁBGS16, 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, BŁBG+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, LRVM18, 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, SZZS16, STS15, SK11, TLdG+12, TN10, VGV+11]. **density** [VAR12, VECT12, VV14, Vik11, VL17a, VI17, VED10, VHS+19, Vyb16, WKC10a, WHL+10, WGL+11, WCWW11, WWU12, WWCL15, WHX+10, WL14, WTH+16, XYW+14, YLZ+10, YS13, Yu12b, ZTH+15, ZXS+10, ZSWL12, ZKE+17, ZDX11, ZLHH14, ZCWX18, ZGS+10, dSdS12b, dSdLBNB17, dLC17, dLvNC18a, CDM10, FAS+18, VV19]. **density-based** [LZS+17]. **density-density** [DSAS19, SS16a]. **density-fitting** [Boz18, Hil13]. **Density-Functional** [YKNN19, Oht16, CHG+16, HNWF07, HNWF12, IM17, JCP14, KZZ+16, MFR+17, NF17, NN18, NO16, NNK+16, Rez19, RHPWS13, SPS+12, VED10]. **density-peaks** [LZS+17]. **deoxy** [VM11]. **deoxyribonucleoside** [XVN17]. **deoxyribonucleosides** [RJWW12]. **dependant** [PNG10]. **Dependence** [CFM+19, BRLS08, BRLS12, ELP19, FE14, GZZ12, KKO+16, KGM12, Lar12, LPE+10, LLTC12, MP17b, PZA15, PBE16, PS10, SGPJS+17, SY16b, AD10, MGWR12]. **Dependences** [NNT+19, SMM+18]. **dependency** [DKT13, PHDH13]. **Dependent** [YKNN19, AALCM11, BS16a, CHG+16, CP15, CKP10, DP15, EPD+10, GTK10, HNWF07, HNWF12, HG10, HYUS11, JYS+12, KS18, KCPMG12, LPLS16, LZ12, LZGS11, Mat10, NS10, PAK17, PPJ14, PVJ10, RHPWS13, REL17, SY16a, SFBT17, Vik11, WHL+10, WHX+10, YLZ+10, ZXS+10, ZDX11]. **depending** [Lin18]. **depolarized** [KKK+19]. **deposition** [SE14]. **depth** [DDP+18]. **derivates** [UGK18]. **derivation** [SCMA+17, VVV+15b]. **derivative** [MY17b, TPL+10]. **Derivatives** [KTSW11, CWHH11, CZH12, CBTZ16, CROB16, GRN19, HSZ+11, JS17a, JYS+12, KG11, KPL15, LWGZ15, LWWG12, MFR+11, MIS+15, NS10, NF18, PC14, RVB+12, RFN15, REH13, SBR13, SZX13a, SZX13b, VVJ15, VVY18, VSD10, WGL+11, WRG+17, WDP+12, ZsA10, ZWZ11, ZZ12, ZZWX11]. **derive** [RVP+11]. **derived** [CIKT13, GMMH+16, KSR+16, LRVM18, LZGS11, MUGNVJ+18, MCLD10, OSS10, PLZ17, REL17, SOYC12, SE14, TBSM12]. **Deriving** [CCYL11]. **descent** [MS16]. **describe** [LCK+18, RHRCH16, RS13]. **described** [BM12, CCB15, KDS17]. **Describing** [MKGA10, CGA19, DAP+18, JCP14, JBSQG11, MY17b, VBD11]. **Description** [FD16, MŘ17, Rez19, SWW+19, BBG+18a, BD12, BE16, Cam15, CRZ+18, LAM19, LZLC13, MFR+11, PM13, PLH16, PVAM16, RVM19, SRF+17, SSA+17, TKNN10, WvRSM14, WL14]. **descriptor** [DFF+15, MA16, PRYI+17, TMJ15, WMW+10, Yap11]. **descriptor-based** [DFF+15]. **Descriptors** [ELKE19, STF+19, CBDS19, FCL+10, FZL+15, GJMPAM+14, MdOdQ18, MCF+18, MH10, NKJ16, PKIC11, RB13b, SIT18, TTB+10, Wei12b, YLCX10, Yap11, YDX16, ZWX16]. **Design** [LI19, LLX+19, LCM16, Spr18, SCSM19, Tak14, TZ12, VBD11, AM10, AFBR17, BAMR13, BEPM14, BPC13, CBP14, DPB+12, DPOS16, DGL+13,

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

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, RSLS13, 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, SZZS16, 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, BŁBG+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]. **ditetrazoles** [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, SZZS16, 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, PŁAG11, PŁV+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, VLGK+17, WDLG12, ZJZM13, ZLL+10, BLG10, CC11, IYK11].
Effective [GKV+13, IM17, YZ16, AASP18, CVG14, DR11, DMN14, DMN15, GA12, HKNH18, KS13a, KS15, LCM+14, PHC13, PRYI+17, PS13, RLD12, ŚSB+16, UCFR16, WXS+12, YZZ16, YZ15b, ZKH+10]. **Effects** [CS14, GBG+19, HTY19, JAH+17, JLLW19, LGOM+15, LCH+15, Mor15, NNT+19, SEM12, Tac17, WWTL19, YCK16, dCRN18, AS15a, ATIP18, AS18, AK10, ASK18, BBI+11, DMD+18, EPH+13, FAA15, FD16, GNC+18, GMG+10, HS16b, HDM+19, HLBLCCG15, INT18, IN19, JMX+16, KIOY19, KG11, KYCL11, KHE+19, KKA+18, LGVA14, LHT15, LWD13, LKZM18, MUN+19, MKGA10, MBC11, MRK11, MLY+13, MCUJ15, MGS+16, MKK+19, NASH15, ORZ11, OSHG17, OCW+15, PLFS18, PDMT10, PP19, PC14, RMGB11, RRK16, SSWX14, SMP17a, SFLG+17, TM16, TYN15, TY10, UT14, VP19, VKAM12, WXY14, YNH+17, YJ11, ZPP+16, Zha11, ALW+10, THP+15]. **Efficacy** [LC17a]. **efficiencies** [RO14a]. **Efficiency** [AC11b, BB11b, BB11c, FE14, GBSE11, XFG+16, AC12, FSSW19, GSHM10,

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

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

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

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

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

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

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, ŁBGS16, MDT10, MS12, MPBJ11, OV14, dlRL11, 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**$\cdots$ [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, MHRR11, 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, ŁBGS16, 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, LHSH12, 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, DBGO+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** [COHI19, DMAH15, LLvG10, MBC11, WTH+16, ZL11]. **force-fields** [CCLP12]. **force-matched** [KSR+16]. **forcefield** [LDB+17, MMZW14]. **forcefields** [CBP14]. **ForceFit** [WKC+10b]. **forces** [EPD+10, Elk16, Has14, HNWF07, HNWF12, IO13a, RN17, SDB+16]. **ForConX** [LDB+17]. **forest** [WZ17]. **Foreword** [Mor19]. **form** [GKB+19, GWX+12, LZSM19, YZ15b]. **formaldehyde** [CYY+17, GNGCA10, OKY18, YPvD13]. **formaldehydes** [TKCN19]. **Formalism** [MKGA10, SFCCK+14, SFCCK+15, SMP17a]. **formamides** [JSW10]. **format** [LAS+14]. **formate** [CJZS10]. **formate-lyase** [CJZS10]. **Formation** [BPPS19, DWZ+17, BPPS17, CD11, ED15, GRCL12, KSM16, KAR12, KK19, LLH11, LWL+10, MCK17b, NMH19, Oht16, RVP+11, SHL+18, TDP+12, UCFR16, WNM17, WKC11, WDW12, YPC+10, ZSWL12, ZWX19, ZWX16, ZYL+12, MSPC19]. **formations** [HTS17]. **formats** [REL+14]. **formed** [RVB+12]. **formic** [TKCN19, TL16]. **forming** [Car14, ONTTL16]. **FORMS** [RMPAM15, FD14, KG11, PS14]. **formula** [BB11b, Ish12, MA16]. **formulas** [KTSW11]. **Formulation** [BD12, SSSM15, CSKH16, DLMH12, KCL+14, MBA11, SMM15a, SMM15b, WRHF10, ZKE+17]. **formyl** [LZHH11]. **förster** [RCM+13a, Kos16, RML+15]. **forsterite** [DOM+11, DBM+15]. **forth** [PNW+16]. **forward** [KZP+18a]. **Four** [PRJ+17, RK15, BHI19, EB12, HKR+14, JKS+16, LLC+10, LWGZ15, WS11, WS12, ZWZ11, OSI+19]. **Four-component** [RK15, HKR+14, JKS+16]. **four-membered** [WS11, WS12, OSI+19]. **Fourier** [IY18, NZM18, YWJ+16, Ish12, LL13a, SZTSM10]. **fpmb** [CWT+12]. **fraction** [Gil11]. **fractionations** [NASH15]. **fracture** [FPH+19]. **Fragment** [GK15b, IIF+10, LSL+19, WLLH18, CIKT13, DR11, FMG12, GWF11, GKV+13, HB14, ISM18, KS13a, KS15, LMZ11a, LFN+10, MFR+17, NF18, NMH19, NF17, OOT15, OOK11, RKGN10, SZdB19, VBV13b, WCT+11, dLC17]. **Fragment-based** [GK15b, WLLH18, FMG12, HB14, LMZ11a, SZdB19]. **fragment-separation** [NMH19]. **fragmentation** [EFB16, SS19]. **fragmented** [JSXH16]. **fragments** [CM16, Kos16, KSR17, ODB18, Sax12]. **fragments-rooted** [CM16]. **Frame** [AlQ19]. **framework** [BFH+13, EH13, GRN19, GP11a, HPT17, JBB+11, KTNN10, MKGA10, OM12, PHT17, RCM+13a, RML+15, Řez16, SK15b, SWB+12, WDY13]. **frameworks** [LSD+10, PLZ17, RNS19, VVV+15b, VVW+18]. **francium** [TH13]. **Franck** [CHC+13, MCLD10, MLCD11]. **Free** [Bou14, CBG16, GS16, GO13, GMO16, Jia19, MCvdV13, MUGNVJ+18, MYKO18, OCW+15, PK19, PZCL16, SISK10, SC18b, ZQH19, AC11a, Ano10a, AK10, ABS+19, AKN16, BKŠ+11, BSL11, BH15, BS16a, BD11, BB11b, BB11c, BG12, CY09, CX10, CZY11, CY13, Che17, CF18, CZZL19, CS17, CHR+12b, CHR+12a, CMvG10, DSB+19, DMJ17, DGH+11, DHF+11, DPOS16, Fer17, FHZA+18, FBvdB18, GS15, GHK12, GJMPAM+14, Gri13,

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

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

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

[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, RDDS10, 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** [DFF+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, KCPMG12, 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, ŁBGS16, 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]. **HȮ** [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, ŘRH12, 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**$\cdots$ [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, RSLS13, 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, RSLS13, 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, RDRC16, 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, BŁFZ13, BK17a, BLDK+13, CK10, CSAdOM17, 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** [BŁFZ13, 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, BŁBG+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]. **hyperpolarizabilty** [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]. **ICl** [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, KTNN10, 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,

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]. **Image** [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, Cor17, LCM16, SFLG+17, YHH+13]. **images** [LLJ12, MBFP15]. **imaging** [SCF+19]. **imatinib** [AS10]. **imidazo** [QQY+18, YLZ+10, FDCJG18]. **Imidazo-Pyridine** [FDCJG18]. **Imidazole** [FD16, LWGZ15, NS10, YKH+10]. **imidazolinone** [CSC+18]. **Imidazolium** [MG15]. **imidogen** [Kop15a]. **Imine** [DK19, AS11, GG10, HDB15]. **imines** [ZX19]. **imines-external** [ZX19]. **imino** [GRCL12, YMY+19]. **immediate** [HTS17]. **immersive** [SFM+18]. **Impact** [ABM+15, DPNM11, MCS11, MKK+19, VCL18, vADC+14, JMLL13, NW17]. **impacts** [SSNT19]. **Implementation** [AMGB10, BMR11, FBKD19, Hes19, HKR+14, HLEM18, ITIN15, KB14b, KK17b, LRvdSM15, LPLA13, LBB+15, MHT+18, RJPB12, RSG14, SN16a, ZMMM12, AB16a, Boz18, BTB+11, CHG+16, Cas13, CEBO15, CSSB11, EWK+13, GRN19, KS13a, KNHN16, KMLS10, KWG15, LL10a, LLZA12, LMR14, MKGA10, MBR+15, MYT+14, NYH+17, NLL19, NN18, OYK+11, QS19, RSR+12, REV+17, SSP19a, SZX13a, SZX13b, TKT11, WPM+15]. **implementations** [LSD+10]. **implemented** [BVHI17, DLSA14, SR10, VBV13b]. **Implementing** [Nav18, SCOJ13]. **Implications** [CV12, VVY17, CBG16, LP11b, LTP11, RB12]. **Implicit** [BEM14, CAD16, Has14, ALRM18, CBG16, EK15, FBEM11, KJDB12, KB11a, KB11b, LC17b, ML14, SSBW14, SLX+15, SCMA+17, TCC+13, WWKS11, YL13]. **implicit-solvent** [WWKS11]. **Implicitly** [Jia19]. **Importance** [APA+14, CPK12, ENKK+17, NMF+14, OOK11, ESM+12, Ham11, KTNN10, PBDW11, SDZ17, TNSS17, TKNN10]. **important** [AST+16, BZH14, MG11]. **importing** [FN12]. **impregnated** [GLZ17]. **improve** [CIKT13, DLL+10, DPSL16, Gon12, LLL+10, Min18, VLB+10]. **Improved** [BS16a, KPF+19, LRER13, CCM15, DPB+12, DSF17, GCCM15, KSR+16, MP11, OHPR18, PBLS19, RTP+13, RDRC16, SSBW14, VVW+18, XMA+19, YS10]. **improvement** [GSHM10, NLP+16]. **Improvements** [JCX10, ZFOS19, AB16b, LRBB12, BB11c]. **improves** [BBOB16]. **Improving** [AIM+18, DWL11, FSSW19, GS16, LN15, PLH16, RVM19, SB14, SACdG14, SA11, WZ17, ZWX16, ZYS+10, GS15, GFPSD17, GZ14, FZY+12, TO10].

impurities [SBC+11]. **IMSPeptider** [dCLFGL13]. **in-depth** [DDP+18]. **In/Si** [LGKS17]. **inactive** [CV12]. **include** [PZA15]. **includes** [HBKL10]. **Including**
[KL14, SFLG+17, BL12, FAA15, FD16, LH14a, SPH11, TG12a, WC14, YB11]. **inclusion** [CGR16, LZ11]. **Incorporating**
[LHO17, Yan14, CSKH16, GCCM15, ZBP11]. **Incorporation**
[BTT10, DDP16]. **increased** [SPZP18a]. **Incremental**
[ER18, RR19, DCŠ15, LTA+11, SR18]. **increments** [MS15]. **independence** [LC17a]. **Independent**
[LLH+19, BVY+12, FVB10, GR11, yOTn16, ŠB15, ZBB16]. **index**
[CMF+17, OXBW16, RRC+15, TS14]. **indexes** [MGCC19]. **Indexing**
[GPGSM11, GPGSM12, Ihl12, JZL+17]. **indicate** [Jab18a]. **indicator**
[BLG11]. **indicators** [Bar14, BWKW10a, BWKW10b]. **indices**
[BK11, BMPML+13, BVC13, EFAC13, FVB10, GSHM10, HSB+11, MMS16, PRSG13, Pon11, SBR13, SB18, YB16, dLC18a]. **indirect** [SPHF+18]. **indispensable** [BF15]. **individual** [LZY12b, WS10]. **indol** [YZLZ18]. **indole** [AARP17, YHCS11]. **indole-** [AARP17]. **induce** [ASK18]. **Induced**
[ATM18, AB10, AARP17, AKK+16, ATIP18, AS15b, BHNS14, BŁFZ13, BCG10, CC18a, CPN+17, DH11, DLZ15, GDV17, GBS+17, HLBLCCG15, HB15, IMK+16, KL14, LCB10, MTM14, MHT+18, PD12, Tru18, UGK18, WDP+12, YB13, YLZ+10]. **induced-fit** [BHNS14]. **induction**
[BCNH+11, DWR17]. **industry** [RD18]. **industry-standard** [RD18]. **inefficient** [GMO16]. **Inequivalence** [MPSG11]. **inexpensive** [AC12]. **infantum** [VSD10]. **inference** [BFH+13, VZ14]. **Infinite** [CC11, GK15b]. **Influence** [BSL+16, CSS17, CSKH16, HLH+12, KCPMG12, LvG13a, AKK+16, HGHP14, LdSRR16, OSHG17, PLFS18, PG18, ŠBD+17, SRL+15, SPZP18b, HRK+10, HKRS11, HS11]. **influence/trans** [Tsi19]. **influenced** [JXSW15, LLT12]. **Informatics** [SN16b, KSD+12]. **Informatics-Based** [SN16b]. **Information**
[ATM18, 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, Ano16-64, Ano16-65, Ano16-66, Ano16-67, Ano16-68, Ano16-69, Ano16-70, Ano16-71, Ano16-72, Ano16-73, Ano16-74, Ano17-36, Ano17-37, Ano17-62, Ano17-63, Ano17-64, Ano17-65, Ano17-66, Ano17-67, Ano17-38, Ano17-39]. **Information** [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, 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, 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, BMPML+13, CRZ+18]. **information** [CDS16, CCYL11, DWL11, GBVA11, ISN13, RSL16, ZLW10]. **information-theoretic** [CRZ+18, ZLW10]. **informed** [LZL+13]. **Infrared** [EB18, dSH19, DPAB16, HDM+19, HRH+17, KB16, LBC+12, NHF+10, NPG+18]. **ingredients** [CMvG10]. **Inherent** [LLFH16, Rao11]. **inhibition** [BM12, GWZ15, LD18, SSP+13]. **inhibitor** [ETLS17, FMG12, LJL+11, NFG+13, XLY12]. **inhibitors** [AKMT11, ALW+10, AC11a, BM12, DXL+10, DSX+11, MPNS13, NS10, PBLdS12, RZG+13, RAR+11, SOD+11, SJ16, TTB+10, VLB+10, XDL+10, YLCX10]. **inhibitory** [PP19]. **Initial** [GA18, YLS19]. **initial-value** [YLS19]. **initialization** [GR11]. **initiate** [HTS17]. **Initio** [DHOG13, Kop15b, Kop19a, LI19, MSPC19, PAK15, RSR+12, AR10, AG12, BEM14, BLG10, BIL10, BDdS13, BL12, CPRS18, CG15, CLC11, DCOD13, DHF+11, DLSD13, DJ13, EP12, EFOD13, FAA15, FCD10, GK10, GWZ15, GZZ12, HYD10, KT19, KOP+14, KCC+18, KTO11, Kop15a, Kop16, Kop17a, Kop17b, Kop18, Kop19b, KSR+16, Kow11, KVR10, LLH14, LPK16, LDJ+10, LZJ+11, LPE+10, LX11, LJW+11b, LLTC12, LTP11, LCK+18, MK13b, MCLD10, MS12, NASH15, NMLD13, NDD+10, OHNK11, OYK+11, ON14, OPR16, OT12, OZLSBH12, OOK11, PVL+13, PBLS19, RB13a, RFN15, SLT+15, SS13b, SS19, SSNT19, SLIB12, SJZ+15, SLLL13, TLdG+12, TG12b, US11, VVV+15b, VPR10, WLC12, WLF19, WXY14, WDHZ13, XZ11, XYZ18, XCLZ19, YJ19, Yu12b, Yu12a, ZZL+12, ZZ10, ZMMM12, ZLT13, ZLZ14, HEM+17, LL13a, WDKT19]. **initio-based** [XCLZ19]. **inito** [JWST10]. **Inner** [KT12, Avd18, HS16b, VVY17]. **Inner-** [KT12]. **inorganic** [DGSVGVM19, FNSF+11, IGK16, OCW+15, PG18, SGH+16, VVY17]. **input** [VVV+15b]. **insect** [FCL+10]. **insect-growth** [FCL+10]. **insertion** [BB11a, LPK16, MG15, OLY17, WNM17, WHAS+10, WHAS+16]. **Insight** [CSM16, WC13, ZLHH14, ZZZ+19, CHKR10, DM15, GA18, LWGZ15, LGC19, LZL+16, PM13, VIT+15, VBMA13, YXZZ17, YZLZ18, KKL+13]. **Insights** [EK15, FVP14, HRJ+14, HGHP14, HRJ+15, JRSHP14, KPH+19, RLZ+18, RSB+13, SIT18, ZWGO16, Alg17, AWF+18, GNDA+12, HRMAL+13, HVS16, KP11, LD18, NDG14, OAN15b, PKK17, PSP15, QQY+18, RTS+13, SM16a, TN12, VVJ15, WMW11, WDP+12, YZ17, BTMS12, LJL+11].

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, dlRL11, 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, BŁFZ13, BŁF14, 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, KTNN10, LL10a, LMZ11a, LPS+13, Li14a, Li14b, LHHW14, LZL+15b, LPLB16, LCWW10, Min18, MSÅK12, 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** [BŁFZ13]. **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, MŘ17, MJM+15, MVKS10, MG14, MFR+17, MPBJ11, OHNK11, PPJ14, PŁV+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** [SJL18, All11, BDTP11, CSSB11, GRP+12, GCW14, HL14, JJW+14, KG13, LJR+12, LZdlL+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, BŁF14, BLDK+13, CCLP12, KSNT19, KCL+14, LZY12b, LZLC13, ŘRH12, SN10, TY10, TNG+10, VVP12, VMV19, WGD+16, ZZL+12, ZLT13]. **Internal** [AlQ19, LL15, REH13, LWK+14, NCV10, PH10a, TNG+10, VLGK+17, VBV13b, WBN+13]. **Internal-to-Cartesian** [REH13]. **internally** [SMP17b]. **Internucleotide** [LZH+11]. **interoperability** [REL+14]. **interphase** [BVY+12]. **Interplay** [FC16, LLL+11, YKH15, BSF18, CCCLCGRO14]. **interpolated** [MK19]. **interpolation** [Min18]. **Interpretation** [STF+19, ZDW18, DCOD13, TLA10, WXL17, XFX+16]. **Interpreting** [AVHB18, CLA16]. **interprotein** [JZ12]. **intersection** [Mat18]. **intersite** [LLLM11]. **interstitial** [GM17]. **intersystem** [AMQ+14, QCR12]. **intervalence** [DAdGR15]. **intervals** [LL11]. **intra** [LZY12b]. **intra-** [LZY12b]. **intraminimum** [ABD11]. **Intramolecular** [DBG11, GWF11, KP10, MH17, Spr18, CROB16, HB15, KFY+13, KV14, LWGZ15, LTP11, MTM14, MPSG11, SSB11, SSB13, VVJ15, YK13, YLZ+10, dALdS+15, dLC17]. **intraphase** [BVY+12]. **intrinsic** [AMGB10, OVPK15]. **intrinsically** [LC16]. **Introducing** [DJD12]. **Introduction** [HIS17, LL19b, Sie15, SJ17]. **intuitive** [EFAC13]. **invariant** [CWZB10, MK19]. **Inverse** [KTT16, GD10, JMS13, SKGP19, WHK+12]. **inversion** [HLI+19, Hei18, SP13, SM18, GG10]. **invert** [KZZ+16]. **inverted** [UT15, YJ17]. **investigate** [dSAdSL13]. **investigated** [SLY+10, SCW11, YS13]. **Investigating** [KGJZ19]. **Investigation** [ALW+10, CAP17, GY10, PH10b, WS10, YZLZ19, ZY14, AvKSP16, AMK11, ABB+12, ABB+13, BAD+19, CWT+12, CYY+17, CR19, CZH12, CH10, GDV17, HXM+16, KCB+12, KV15b, LLLM11, LLB+12, LZY+12a, LLD17, LXZ+10, MLQ+12, MP13, OAN15b, PZA15, PVS12, QCR12, RDT14, RRC+15, SBGP18, SH14, Tak11, TPL+10, TS10b, TR12, VVP12, VM19, YS18, YJN+11, Yu12a, ZZ10, ZSWL12, ZBMZH15]. **Investigations** [DL19, NSN19, GZL+12, HDM+19, KSO+19, KAR12, LWWG12, TSJ+10, Tsu19, WS12, YPvD13]. **Invisible** [SDM+16]. **involving** [ARLP13, CC18c, GNDA+12, LEdOLdlV17, LRER13, MEH18, NFG+13, OSHG17, SLT14, SLT+15, SWW+19, YZZ+17]. **iodanes** [SLT14]. **iodate** [SC18a]. **iodine** [ACS12, SLT14, SLT+15, KLN12]. **iodothyronine** [CFM+19]. **Ion** [Fra15, Fra16, LZTV10, BP18, DMN14, DMN15, EK15, JAH+17, JLCA17, KTK17, KJ10, LEdOLdlV17, LJR+12, LPE+10, MMB+17, MH11, NSK18, NC13, PGY15, PL14, RTS+13, SSGS15, SC18a, SMiN+19, SV11, TO19, TNY18, TJR19, Tru18, TCX+13, VPR10, Vik11, WC14, YZLZ19, ZZ10]. **ion-associated** [ZZ10]. **Ion-exchanged** [LZTV10]. **ion-pair** [TNY18].

ion-pairing [KTK17]. **ion/water** [SV11]. **Ionic** [FDCJG18, JXSW15, AFPI13, APY+16, CG15, CFC15, EK15, GC11, IN19, IM17, LEdOLdlV17, 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, ŚSB+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, DBGO+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, SFCCK+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, ŚSB+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** [RSLS13, 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, PŁV+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, MSÅK12, 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, NTNY15, RJS17, SBvG14, SAvG15, WCWV15, ZSTI14]. **liquid/lithium** [EK15]. **liquids** [AFPI13, CG15, CFC15, CVG14, DASA15, LEdOLdlV17, 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, BŁBG+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** [BŁBG+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** [BŁBG+13]. **LPol-** [BŁBG+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]. **magnetoresponsive** [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, JRSHP14, KNHN16, LYC+13, RHPWS13, VMPS17, WCWV15]. **Many-body** [CGPP11, HRJ+14, HRJ+15, JRSHP14, 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, RSLS13]. **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, ŁBGS16, LPK16, LCH10, LL11, LLZA12, LWZ+19, LN15, LLSW14, LL19a, MK13a, MTM14, MHT+18, MC12, MKGA10, MPA12, MN15, Mat10, MDT10]. **method** [MRK11, MA17, MJG+15, MFR+17, MS15, MNNK10b, MH10, NF18, NR11, NFPD13, NF17, NO16, OLA15, OK16, OOT15, PSS14, Pet11, PSC11, PKIC11, PPJ14, PŁV+11, PM18b, Pon10, QLQ11, QB10, QB11, RHRCH16, RKGN10, RSLS13, RGVC+19, Rod13, RKB+14, RFHG10, SSO19, SF18, SS13a, SCM+15, SBB10, SSWX14, SBN13a, SBN13b, ŠB15, STM17, SG13, SSAS10, Tak14, TKNN10, Tak10, Tak18, TSZQ12, TSNC+17, US11, UIW+10, VLB+10, VDVR14, Vor10, WXS+12, WJG+13, WLQ19, WHM10, WTH+16, YO19, YWJ+16, Yon16, YAO18, YN15, YHH+13, ZDZM13, ZMMM12, Zha12b, Zha12a, ZLM+15, ZGZC19, ZZMW19, ZW17, ZFS18, ZH12, ZA15, ZZZ+19, Zim15, CKH19, JCHT18]. **method-based** [GKJ+19]. **Methodological** [VKNT16]. **methodologies** [Rob13]. **Methodology** [CPK19, Aki16, FF11, GAI13, GMASBF16, HPT17, OHPR17, OHPR18, RJWW12, HCD+10]. **Methods** [SGP18, Ano12u, Ano15-59, ASMS10, BG13, CLFRO18, CSGOA17, CXS10, CNK97, DKE+17, DCOD13, DBM+15, EWK+13, ESM+12, EV14, Fer13b, Fer13a, FB10, FSSW17, FSSW19, GAI14, GFPSD17, GD10, GSS13, GMO16, HCB11, HSB+11, Höf14, HWLW11, JJH+13, KSM17, KB13, KHWB17, LEdOLdlV17, LZLC13, LLSW14, MS13, MY17b, MHO18, MŘ17, MVKS10, MOS12, NYH+17, NASH15, NC13, NC14, NTNY15, OSHG17, PN13, PVAM16, RZG+13, ŘRH12, Rez19, SRF+17, ŚSB+16, SACdG14, STM+15, SWW+19, SGWA17, TG12b, TS15b, Tsi17, WBT10, WX12, YLCX10, YAS13, YJ17, ZGS+10, dSdLBNB17]. **methoxy** [PNE18]. **methoxybenzyl** [YZLZ18]. **methyl** [AARP17, BIL10, CPLL11, GZL+12, GMG+10, LK11, LZL+16, MG15, MSBF16, VKTRJ15, YYT12]. **methyl-methyl** [LK11]. **methylacetamide** [HLH+12, KSK11]. **methylacetylene** [WCWW11]. **methylated** [LRVM18]. **Methylation** [SCW11, KYCL11, QZM11, dALdS+15]. **methylbenzyl** [NDG14]. **methylcobalamin** [KKL+13]. **methylformamides** [JSW10]. **methyllysine** [GHK12]. **methyltransferase** [CPLL11, GH10, PBLdS12]. **Methyluracil** [HvM17, HvM16]. **MetREx** [Sti15]. **metric** [CXS10, LLFH16, PKIC11, SOJ14, ZT14]. **metrics** [Hug14, PBBP11, RCM+13b]. **Metropolis** [MO15, Pon10]. **Mezey** [HJJ13]. **MF** [YKH15]. **Mg** [HDM+19, LDJ+10, LLX+19, BMFG16, DOM+11,

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** [RSLS13]. **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** [BŁF14, 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, BŁS10, HM16, Jia19, MT20, Pog10, AASP18, AOW11, AS10, ALRM18, ATP18, AS15b, APA+14, AB16b, Bac12, BK17a, BH19, BEEL14, BS10b, BBG+18b, Cam15, Can10, Can11, CGP12, CGA19, CBTZ16, CFC15, CAD16, CG12, CMS13, CJZS10, DLL+10, DSF17, FCE15, FNSF+11, GRN19, GRS15, GM17, Gil11, GKR13, HLS12, HAL14, HLH+12, HOK17, HZSS17, Hug12, HRH+17, ISO+13, IN13, II18, JSXH16, Jor17, KFY+13, KCK+17, KMS+19, KR12, KOY+12, KD18, KCPMG12, KB14b, KDS17, LSL+19, LTT16, LY10, LRvdSM15, LFN+10, LPS+13, LHHW14, LZL+15a, LDG+15, LCK+18, LHMM11, MSLS10, MT19a, MPJ+19, MBC11, MBC13, MMB+17, MHO18, NJX+10, NTNY15, OPBR17, PB14, PCLL11, Pla11, Pon11, Ray13, RTS+13, Ric16, RMRBH+19, REL+14, RKG11, SM14b, SDF+17, SHF11, SSBW14, SK12]. **model** [SK17, SLX+15, SDZ17, SZBM13, SB11, TYN15, TCC+13, Tia12, TLA10, TTn19, UIW+10, VV14, VHS+19, WWKS11, WXL+12, WC13, WWW19, WNM17, WRHF10, WKC11, WCAH10, XZ11, XTY+14, XP13, YS18, YOMT14, YB13, YSG12, ZSTI14, ZKH+10, ZM10, dSDdAR10, dSH19, CCR18, FAS+18, MJBM12]. **model-tuned** [HZSS17]. **modeled** [MPA12]. **modeler** [BHI19, KLJ+17]. **Modeling** [ASW19, CB11a, DLSA14, FD13, FTW12, GMG+10, GBS+17, HPL13, JW16, KDR+18, Mat14, NS10, NDLW13, PLP+16, SZdB19, SK11, Tia12, Vyb15, AKMT11, Aou16, BEM14, BPC13, Bow16, BS10c, ĆMD13, CLA16, CZNA11, DAG19, DWR17, DSX+11, DLMH12, EBPK17a, FXC+13, GH10, GP12, GMZ12, GWJR18, GR10b, GWZX12, HLvdV13, HBJ+17, JC16, JCL+17, KSD+12, LABSG17, LLH14, LZGS11, LT13, LN15, MBA11, MJLV14b, MA17, MBA14, MPBJ11, NSO+14, NW17, PHC13, PSS14, PSG+17, PMT16, QLKI19, RJS17, SN16a, SKGP19, TTR+12, VKNT15, VÅA14, VCM15, WXL17, WPM+15, WLO+17, XDL+10, XLY12, YMY+19, YJ11, ZX11, DHE+12]. **modelling** [DBM+15]. **Models** [Hes19, NNT+19, ND19, BEM14, BLKP12, BPB11, CD11, Cor17, CBG16, CK17, DDP16, DSM+11, DI11, DGC14, DLC18b, EK15, EPD+10, GMPB12, GMMH+16, GMG+10, GKR13, GCP+13, GCC14, GAJ+17, HS16b, HGY15, JCP14, JGS+17, KJDB12, KKO+16, KB11b, KSR+16, KSW16, LTT16, LKL10, LZ12, LLSW14, LM18b, MPSA17, MSÅK12, MCUJ15, MKB+13, NNS15, OL13, PHC13, PGY15, PL18, Ray13, RTP+13, RKG11, SPHF+18, SCMA+17, SFLG+17, SAvG15, TH13, TTB+11, TTL+12, VKC10, VMPS17, VZ14, WS10, WXY14, WSWD19, XTn18, YJ11, YL13, ZsA10, ZDW18, dSdLBNB17]. **modern** [AB16a, AB16b, DH17, Fom11, LMR14, SF18, SDM+16]. **modes** [CBP+15, EB18, GMPB12, KKH18, LLTC12, MS17, dSH19, dSAdSL13]. **modification** [Ano12u, MIS+15]. **modified** [BD12, CH16, DPSL16, DJX+11b, GSD10, MRO17, Mit13, SMM15a, SMM15b, SMM+18, XYX17, XVA+16, ZZ12]. **modify** [ZX19]. **Modifying**

[CYG+15, LBS10]. **modular**
[HPT+16b, JP15, LWK+14, MBR+15, PSG+17]. **modulate** [WC13].
Modulating [LTR18]. **modulation** [PE11, RS17a]. **modulator** [ILKR11].
modulators [SRA17]. **module** [PHH+12, VBV13b]. **MOFs** [LPK16].
moieties [SPL+18]. **MOLCAS** [ADF+10, VBV13b, AAC+16]. **Moldyn**
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[CH16, CCOH14, CBDS19, CVG14, CCW+10, CHKR10, CJPTC18, CB11b, CB11c, CM16, DMJ17, DSD+11, DJX+11b, DJX+11a, DJS+18, DLZ15, DDM+15, DN19, DL19, DL16, EP10, EK15, EJ13, EPH+13, EPH+15, ENKK+17, EPD+11, Fer13b, Fer13a, FBvdB18, FBEM11, FDH19, FSC+14, FPH+19, GBL+11, GDV17, Gar12, GJMPAM+14, GSHM10, GR11, GMZ12, GPM17, GMMH+16, GFGS18, GY10, GWZ15, GCW14, GGM+12, GBW+14, GEP+14, GPdC+16, GP11b, GR10b, GPK12, HS17b, HHNK19, HSW+19, HB14, HS12, HCD+10, HDM+15, HPSK12, HH16b, HWLW11, HJ10, HXM+16, HHWL17, HRID16, HC14, IUK+11, IIF+10, IN19, ISM18, IM17, II10, JIS13, JBSQG11, JAH+17, JSXH16, JWST10, JGS+17, Jor17, JMS14, JS17b, JND+19, JP15, KT19, KCK+17, KCK+15, KVQC+11, KGHK12, KSNT19, KGHC15, KCC+18, KLN12, KJDB12, KDB13, KERY+16].
molecular [KTSW11, KLOS10, KJM+17, KC14, KKK+19, Kos16, KSR+16, KG13, Kow11, KTNN10, KZP+18a, KV15a, KVR10, KSW16, LPAS11, LL15, LRVM18, Lar12, LWK+14, LBGS16, LH11, LL13a, LZ12, LFN+10, LLC+10, LL11, LZY+12a, LMI+14, LAHS16, LPE+10, LLTC12, LCB10, LZW+11, LTP11, LZL+13, LWXC16, LZS+17, LJL+11, LP11c, LAS+14, MSY19, MRB14, Man19b, MKS+12, MSC+10, MJC14, MCRL17, Mat10, Mat14, MSvG12, MLN+18, MWJ+11, MFEM15, MADWB11, Min18, MPNS13, MKM+17, MBA14, MHRR11, MCC12, MFR+17, MO17, MS12, NPTS16, NF18, NSO+14, NPG+18, NLP+16, NST14, NPG17, NFPD13, NFG+13, NF17, NNK+16, NHK+13, NS17, NTNY15, ODB18, Oht16, OHNK11, ON14, OGL10, OHPR17, OHPR18, OCL11, OLY17, OT12, OME16, OVPK15, OOT15, OCW+15, OZS+13, OOK11, PMC+17, PSS14, PAK15, PAK17, PH17, PSG+17, PL19]. **molecular**
[PM13, PGW+17, PVZ13, PJ13, PBG17, PS10, PVAM16, PLP+16, Pro16,

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

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, ŁBGS16, 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, WDZN16]. **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, BŁF14, 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]. **nanostructures** [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** [AlQ19, 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, IIHY15, 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, 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, LHSH12, Leh15, LRvdSM15, LRvE17, LDB+17, LLZA12, LBB+15, LWZ+17, LC12, LAS+14, MHT+18, MDTD16, MBR+15, MYT18, MSSP17, MB14, MB16, NKJ16, OV14, 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, 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, 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**$\cdots$ [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]. **nitrilotri** [CM16]. **nitrilotri-** [CM16]. **nitrilotriacetic** [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, MŘ17, NHN16, PHC13, RS13, VCL18, YWJ+16]. **Non-Boltzmann** [KB11c]. **non-bonded** [BSD18]. **Non-Born** [LCH10]. **non-classical** [GA19]. **non-covalent** [MŘ17, 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, ŘRH12, 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, WWWW18]. **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, LLLC11, 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**$\cdots$ [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** [ŚSB+16]. **opsin** [RLG11]. **Optical** [LLX+19, WGLG+16, ARLP13, BŁŁ13, BŁS10, 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, SZZS16]. **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, ŚSB+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, ŚSB+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** [BLŁ13]. **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]. **OSPREY** [HMO+18]. **other** [AFBR17, SK12]. **out-of-plane** [Gav12]. **outcome** [WCDM11]. **Outer** [TEDT18, BHI19, HS16b, KT12]. **outer-sphere** [KT12]. **outlier** [CLX+10, HNS16, HYNS19, 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, SOvG12, 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, LHSH12, MLN+18, SKA19, SWA13, SHFJ18, SMRM+17, SJ17, SJ16, UU12, VBV13b, WSGN11, ZCS+15]. **packages** [MSvG12, MJG+15]. **packet** [LWD13]. **packing** [MCAG+16, MP17b, NS11]. **PaDEL** [HLS+13, Yap11]. **PaDEL-DDPredictor** [HLS+13]. **PaDEL-descriptor** [Yap11]. **PAEM** [ZY14]. **PAEM-MO** [ZY14]. **paint** [BEFS13]. **pair** [BSF18, BH13, CYG+15, CVG14, Hei18, KS18, MPA12, OM12, Sch12, SSGS15, SB14, TNY18, WCY+11, WWU12]. **Paired** [ZR10, WAB17]. **pairing** [KTK17, ZLL+10, ZM11]. **pairs** [BSG18a, DKT13, ENKK+17, LEdOLdlV17, LZH+11, MPSG11, Mau14, PL19, GMBM18]. **Pairwise** [GS14, Gon12, RVM19, VMPS17, XTY+14]. **pairwise-additive** [VMPS17]. **palladium** [MRC+18, WCWW11, YHG+11, dCDP15]. **palladium-catalyzed** [dCDP15]. **palladium-phenanthroline** [MRC+18]. **paper** [GPGSM12, Ihl12, JW12, WM12, HP10a]. **para** [KYCL11]. **para-substituted** [KYCL11]. **paracyclophane** [KGR+16]. **paracyclophane-bridged** [KGR+16]. **Paradoxical** [UT14]. **Parallel** [BTB+11, FBKD19, KDB13, NN18, UIW+10, WWKS16, BW11a, BTT10, CEBO15, CSSB11, GJMPAM+14, GRARO+14, GC18, HP10a, HS17b, HPSK12, KS13a, KNHN16, KN17, KZZ+16, KCC+18, KJM+17, KDT+12, LL10a, LPLA13, MBR+15, MCRL17, MYT+14, MJM+15, NNK+16, OPB+12, RFN15, SHMO11, TCX+13, TJB12, WHK+12, Yes15, ZWL13, ZSS+13, CJL+13, KDT+12, LMR14]. **parallel-generalized** [LL10a]. **Parallel-ProBiS** [KDT+12]. **parallelism** [FRN15, Gon12]. **Parallelization** [AB16b, RC18, VDL+13, BWMSM10, IUK+11, JMS14, KS15, KKNN11, LLZA12, RŠRR15, SHL19, vW11, ZDKM12]. **parallelize** [vW11]. **Parallelized** [AlQ19, DBDP16]. **parallelizing** [BMBJ11]. **parameter** [NB19, PFVL14, SH19a, VCL18, VVLG17, WDHZ13, LL11]. **Parameterization** [HK18, HJLV16, ILKR11, IHJ+13, MPSA17, PRRT+10, TCC+13, BAS14, CCLP12, DLMH12, KYB13, LTP11, LCL+18, MSS+13, VLB+10, VBD11, VHS+19]. **parameterizations** [SH15]. **parameterized** [OZS+13]. **Parameters** [CTR13, AG11, AKMYB18, BCSCJ+13, BCJC+14, BSD18, BW15, BC13, CYG+15, DPSL16, DMAH15, FHT+15, GSD10, HLS12, HM16, HBI+17, HLH+12, KvdV14, KGHK12, KGJZ19, LvDH13, LPS+13, LLvG10, LSH+11, MRO17, MP11, PBLS19, Pog10, RKB+14, SOYC12, SZBM13, SPR+13, SPZP18b, VYM15, VLGK+17, WAM17, WOH16, WOH18, WC14, YWZ14, ZRL+15]. **Parametric** [LM18b]. **Parametrization** [PG15, COHI19, DGPM14, GCWS15, SPS+12]. **Paramfit** [BW15]. **parasite** [FZL+15]. **paratropic** [CPN+17]. **Parrinello** [DL19, KCK+15]. **Part** [HRJ+15, CDBM11, CD13, HRJ+14, Fer13b, SK13]. **Partial** [HTS17, JMLL13, SMP17b, WOH16, GVP+10, MPBJ11, PL14]. **Partially** [XTn18, UT14]. **participating** [GSMZ19]. **particle** [AG11, BSD18, BK13, Cas13, ER18, Hei18, NO16, PH17, RJBH18, SCK18, ZDKM12]. **particle-field** [ZDKM12]. **particle-mesh** [AG11]. **Partition**

[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** [JJH+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, BŁBG+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, ŘRH12, RSLS13, 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, ŁBGS16, 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, KKNN11, 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, ZWMW10, 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]. **phenoxyl** [IYK11]. **phenoxyl/phenol** [IYK11].

phenyl [GZL+12, ZWY+10a]. **phenylacetylene** [ZZL+12]. **phenylacetylene-containing** [ZZL+12]. **phenylalanine** [GWF11, PVS12]. **phenylaziridines** [KYCL11]. **phenylene** [CH10]. **phenylhydrazone** [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** [BŁS10]. **pincer** [ED15, JJAB16]. **pincers** [KJDB12]. **pinene** [BŁS10]. **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, VMRSH+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]. **pnicogen** [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** [WWWW18]. **polarizabilities** [BŁBG+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, BŁBG+13, DLZ15, JZZM14, 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]. **Polyethylenimine** [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, ŘRH12]. **post-Hartree** [CB11d, ŘRH12]. **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, BŁF14, 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, ŚSB+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, PŁV+11, RCR+16, RMRBH+19, RKB+14, SM11,
SYH12, SSD19, TYZ+16, VKC10, WLF11, WH11, WXS+12, WXL+12,
WWWW18, 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, LHSH12, 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, PŁAG11, 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, BŁFZ13, 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, LHSH12, 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, SFCCK+15]. **property** [CD13, GPS10, GBS+17, GWX+12, PH15, VÅA14, 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, IIHY15, 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, PŁV+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, VMRSH+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]. **protofibrilation** [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, LZdlL+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, dlRL11, Rod13, RSKG14, VVJ15, Wei12b, WvRSM14, XFX+16, ZZL+12, ZCWX18, 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, VÅA14, 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, BŁBG+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]. **rationale** [AARP17]. **Rationalization** [TLdG+12, SLC+17]. **ratios** [OZLSBH12]. **Raton** [CD19]. **rats** [TTB+11]. **Ray**
[CPR18, FLM11, LLBO12, LHSH12, 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, RSLS13, 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** [RSLS13]. **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, BŁBG+13, SWM10, SRR16, SLC+17, VI17, WRG+17]. **Reduced-cost** [BYE+16]. **reduced-size** [BŁBG+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, MNNK10a]. **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, LEdOLdlV17, 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, PŁAG11, 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, RKGN10]. **RI-MP2** [BK17c, KNHN16, TKN13, RKGN10]. **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, LJL+11, MCK17a, VL19, ZLX+19, ZT14, AALCM11, CFM+19, EJ13, GLF16, GFPSD17, HLBLCCG15, LEdOLdlV17, 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, BŁŁ13, BŁS10, 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, ŚSB+16]. **scaled-opposite-spin** [ŚSB+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, ŚSB+16, TAG16, WYT17, WLQ19, XKW18]. **Second-** [TKN13]. **Second-order** [MCC11, DCHL12, FSSW19, Hil13, KKNN11, KN17, LCL+10, MLQ+12, yOTn16, ŚSB+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, SZZS16, 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** [PBLS19, PZA15, SPM+19, XML+15, XYX17, XYZ18, dVAG16]. **servers** [UHH+11]. **services** [LP11a, UHH+11]. **Set**

[SN16b, BŁŁ13, 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, BŁFZ13, BŁBG+13, BŁF14, 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** [PŁAG11]. **sextet** [KDS17]. **SG** [DH17]. **SG-2** [DH17]. **SG-3** [DH17]. **SH** [XCLZ19]. **SH2** [AC11a]. **Sham** [BWMSM10, ŚSB+16, VV14]. **Shao** [Ano12u]. **Shape** [KC14, Zha11, GPS10, HCB11, Hsu14, MNNK10a, 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, BŁS10]. **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]. **sila** [DM15, VIT+15]. **sila-bi** [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, PRYI+17, RHRCH16, RGVC+19, SEF+16, SS13c, YS18, dSAdSL13, KTSW11]. **simplified** [KOY+12]. **simplify** [BLZ+13]. **Simplifying** [BL19]. **SIMPRE** [BCSCJ+13, BCJC+14, KR14]. **SIMPRE1.2** [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, QLKI19, RHNN10, RAR+11, RO14a, RO14b, RSR+12, RSLS13, 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, BŁBG+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]. **smeared** [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, LHSH12, Leh15, LRvdSM15, LRvE17, LDB+17, LLZA12, LBB+15, LWZ+17, LC12, LAS+14, MHT+18, MDTD16, MBR+15, MYT18, MSSP17, MB14, MB16, NKJ16, OV14].

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

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

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

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

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

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

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

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, JZZM14, 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** [BŁF14, 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, CSAdOM17, 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** [BJSI12]. **Steric** [RMGB11, MJLV14b, MP17a, YNH+17]. **sterically** [MH17]. **Stern** [MBA11]. **steroelectronic** [HLBLCCG15]. **Stevens** [BCJC+14]. **sticks** [CVT+11]. **stilbene** [BW11b]. **stk** [TBJ18]. **Stochastic** [AFPI13, CGP12, ITY+19, AC12, ESD18, KV12, KV13, MS16, MCP18, NC13, PH17, RSLS13, 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, KTNN10, 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, CYI+10, DWL11, DH11, GWT+17, GNI18, HS17b, HVS16, KKPT11, KG11, KNE11a, KDT+12, LK13, LL13a, MCF10, OSA19, PHC13, PGY15, PNG10, RRF11, RKB+14, RSL16, SFA17, SS13c, TYX+18, VVW+18, WC11, XMSZ16, YVEI+17, ZYvIZ14, ZLW10, FAS+18, VPR10]. **structurally** [TZCK18]. **Structure** [BPPS19, BJP15, CGBK13, DXL+10, GPK+16, GWJJ12, GBGR16, HLB15, JLLW19, LAHS16, MM19, MHRR11, NC12, NC13, PMG+16, Rab12, SGH+16, VDVR14, WZK+13, AFPI13, AR15, AM19a, AM19b, AJR16, AC12, BPPS17, BFH+13, BDdS13, CPRS18, CD13, CvM19, CM13b, Clo15, DKE+17, DKT13, DSB+19, DDP16, DVVP14, DGSVGVM19, DLW12, EH13, EWK+13, EFOD13, FZY+12, FDH19, FSC+14, GLB16, GMSdG15, GRARO+14, GP12, GK10, GRD+10, GPdC+16, GBG+19, HASR+12, HNHR13, HSB+19, HNyH19, HS14a, HRB+17, HH15, HYMZ16, HZ13, HLWD15, Hua16, Ibr17, KYT+17, KKH19, KSM17, KT10, KS12, Kop19b, KKL+13, KLS10, KMLS10, LLBO12, LFB14, LKL10, LZJ+11, LMI+14, LYL16, LPE+10, LGL11, LHG11, LWWG12, LLFH16, Mat10, MDT10, Mau14, MAPB10, MV17, NGAS17, NCT18, OCL11, OL13, OLA15, PSS14, PdSC18, PML+12]. **structure** [PN13, RLG14, RCM+13b, RR11, SHMO11, SB10, SM11, SLP+12, SB19, SLIB12, SRS14, SYN+12, SKGB13, SPZP18a, SPZP18b, Tac19, TN12, TTB+11, TG12b, UNT16, VVP12, VHR16, VVBL17, VÅA14, VBMA13, VKC10, VI17, VLGK+17, WO15, WRM+12, WSGN11, YW12, YZZ16, ZRCC11, ZHHX11, CPR18, FDCJG18, OSF12, SA10]. **structure-** [HH15]. **structure-activity** [DXL+10]. **Structure-based** [CGBK13, DXL+10, DVVP14, GLB16, VKC10, YZZ16]. **structured** [GEP+14]. **Structures** [DLT17, HDM+19, NSN19, SNS16, SZL19, ZLX+19, AHK+19, BHNS14, BPM15, Ber17, CL16, CCOH14, CBDS19, CV12, DVVP14, DH14, DLC18b, DT19, DZA11, GS12, GSS13, HSY+11, HTS17, HPL+18, HS12, Hua16, IYK11, KNE11a, KOY+12, KTO11, KTO13, KDT+12, KSW16, LABSG17, uLhY11, LXZ+10, LLSW14, LL19b, Lüc14, MCS11, MTM14, MPA10, MPA12, MP13, Mau14, MN19, MH10, MCAY15, MP17b, NS18, PRP15, PNW+16, QZM11, RHRCH16, Rao11, RCR+16, RvL11, RHJ11, RVVK13, RSG+10, Sak18, SWA13, SFR+11, SJD11, SIT18, SPM+19, SKY+11, TN10, Tak11, TFQ+10, TFQ+11, Tsu19, UCFR16, WKC11, WD10, YNH+17, ZSL+11, ZLY+16, ZP13, ĆMD13, OSI+19, PGCT+12]. **studied** [Ish10, KRTB10, OLY17, RHPWS13, RI10, TS15b]. **Studies** [JW12, AALCM11, BŁS10, BRGN12, BLG10, BIL10, DMN15, DXL+10, FWS+18, GZZM16, GEP+14, JLS+10, KG15, KP11, LXFC17, LCWW10, LJL+11, LWD13, RCM+13b, SB10, SFA17, SLHW09, SZZ+18, TNI+19a,

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

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]. **substitutionally** [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** [PBLS19, 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, ŁBGS16, 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** [SFCCK+15, CMF+17, LRBB12, MS11, QCR12, SFCCK+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, NIIT15, 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, ŘRH12]. **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, LZY+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, SZZS16, 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, BŁS10, BAD+19, BE16, CZH12, CKL+11, CBTZ16, EV14, GG10, HDB15, HGHP14, LWW12, LLD17, LZW+11, LCL+18, MRC+18, MPSG11, 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, BŁBG+13, BS19, BMD19, BZB+13, BG13, CHG+16, CRZ+18, CSAdOM17, 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, ŁBGS16, 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, SZZS16, 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** [CGVBAI19]. **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, IGK16, MJBM12, 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, BŁS10]. **Trans-** [MSBF16]. **Trans-2-Butene** [CSM16]. **trans-effect** [Tsi19]. **trans-influence** [Tsi19]. **trans-influence/trans-effect** [Tsi19]. **Trans-philicity** [Tsi19]. **trans}-pinane** [BŁS10]. **transcription** [XMSZ16]. **transfer** [Alg17, AK10, ANH+11, BHB12, CMF+17, CSAdOM17, 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, SZZS16]. **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]. **typing** [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, LHSH12, Leh15, LRvdSM15, LRvE17, LDB+17, LLZA12, LBB+15, LWZ+17, LC12, LAS+14, MHT+18, MDTD16, MBR+15, MYT18, MSSP17, MB14, MB16, NKJ16, OV14, OPB+12, OZS+13, OC14]. **Updates** [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, 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, 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, PŁAG11, 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, SZZS16, STS15, TYZ+16, TYX+18, Tak14, TKNN10, Tsi17, TTn19, TJB12, UTM11, VKAM12, VECT12, VI17, WKLC12, WdVN12, WLC12, WZ17, WJX+10, WDHZ13, XTY+14, XYX17, XWW+11, YWJ+16, Yon16, YN15, YDX16, YFH+19, ZWLX11, ZL11, ZLT13, ZWX19, ZWS+10, ZP13, ZH12, ZZZ+19, ZHHX11, dLC17, AIM+18, JCHT18, LHL+10]. **utility** [YHVM12]. **utilizing** [BVY+12, BP18]. **UV** [GGM+12, KASH14, RDF+11, RVdMB16]. **UV-photoexcitation** [RVdMB16]. **UV/Vis** [GGM+12].

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

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, 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]. **Volume**

[Ano13-50, Ano14a, Ano14b, Ano14c, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14n, Ano14o, Ano14p, Ano14q, Ano14r, Ano14s, Ano14t, Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14-28, Ano14-29, Ano14-30, Ano14-31, Ano14-32, Ano14-33, Ano14-34, Ano14z, Ano14-35, Ano14-36, Ano14-37, Ano14-38, Ano14-39, Ano14-40, Ano14-41, Ano14-42, Ano14-43, Ano14-44, Ano14-45, Ano14-46, Ano14-47, Ano14-50, Ano14-51, Ano14-52, Ano14-53, Ano14-54, Ano14-55, Ano14-27, Ano14-48, Ano14-49, Ano14-56, Ano14-57, Ano14-58, Ano14-59, Ano14-60, Ano14-61, Ano14-62, Ano14-63, Ano14-64, Ano14-65, Ano14-66, Ano14-67, Ano14-68, Ano14-69, Ano14-70, Ano14-71, Ano14-72, Ano14d, Ano14e, Ano14f, Ano15a, Ano15b, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n, Ano15o].
Volume
[Ano15p, Ano15q, Ano15r, Ano15s, Ano15t, Ano15u, Ano15y, Ano15z, Ano15-27, Ano15-28, Ano15-29, Ano15-30, Ano15-31, Ano15-32, Ano15-33, Ano15-34, Ano15-35, Ano15-36, Ano15-39, Ano15v, Ano15-40, Ano15-41, Ano15-42, Ano15-43, Ano15-44, Ano15w, Ano15x, Ano15-37, Ano15-38, Ano15-45, Ano15-46, Ano15-47, Ano15-48, Ano15-49, Ano15-50, Ano15-51, Ano15-52, Ano15-53, Ano15-54, Ano15-55, Ano15-56, Ano15-57, Ano15c, Ano15d, Ano15e, Ano15f, Ano15g, Ano15h, Ano16a, Ano16b, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m, Ano16n, Ano16o, Ano16p, Ano16q, Ano16r, Ano16u, Ano16v, Ano16w, Ano16x, Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16-29, Ano16-30, Ano16-31, Ano16-32, Ano16-33, Ano16-34, Ano16-35, Ano16-36, Ano16c, Ano16-39, Ano16-40, Ano16-41, Ano16s, Ano16t].
Volume [Ano16-37, Ano16-38, Ano16-42, Ano16-43, Ano16-44, Ano16-45, Ano16-46, Ano16-47, Ano16-48, Ano16-49, Ano16-50, Ano16-51, Ano16-52, Ano16-53, Ano16-54, Ano16-55, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h, Ano16-75, Ano16-89, Ano16-80, Ano16-94, Ano16-81, Ano16-95, Ano16-82, Ano16-96, Ano16-83, Ano16-97, Ano16-84, Ano16-98, Ano16-85, Ano16-99, Ano16-86, Ano16-100, Ano16-87, Ano16-101, Ano16-88, Ano16-102, Ano16-76, Ano16-90, Ano16-77, Ano16-91, Ano16-78, Ano16-92, Ano16-79, Ano16-93, Ano16-129, Ano16-108, Ano16-109, Ano16-110, Ano16-130, Ano16-111, Ano16-112, Ano16-113, Ano16-114, Ano16-103, Ano16-104, Ano16-105, Ano16-106, Ano16-107, Ano16-115, Ano16-121, Ano16-122, Ano16-123, Ano16-124, Ano16-125, Ano16-126, Ano16-127, Ano16-128, Ano16-116, Ano16-117, Ano16-118, Ano16-119, Ano16-120, Ano17a, Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x]. **Volume**
[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** [PŁV+11].

W4 [KSM17]. **W4-17** [KSM17]. **Waals** [BŁF14, 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**

[WPM+15]. **WEGA** [YLGX14]. **Weighted** [HGW18, Fer17, HNS16, HHWL17, LMZ+11b, PRYI+17, RHJ11, ZH12, Hil13]. **weighting** [WDHZ13]. **weightings** [GWW19]. **Weinheim** [Spr10]. **well** [CME11, LRvE17]. **well-done** [LRvE17]. **wells** [GKSS14]. **Wentzel** [QS19]. **were** [GS16, MFEM16, XFG+16]. **wettability** [SBC+11]. **wheat** [NMF+14]. **where** [AST+16]. **Which** [RS13, SH11a]. **white** [ZP13]. **whole** [HPL+18, RZ16]. **whole-sequence** [HPL+18]. **whose** [KYT+17]. **Wiberg** [SB18]. **Widom** [LPK16]. **Wiley** [Spr10]. **Wiley-VCH** [Spr10]. **windmill** [LZSM19]. **Window** [DAB16]. **Window-Exchange** [DAB16]. **wires** [LZY+12a, NS17]. **wise** [KSR17]. **withdrawing** [CWHH11]. **within** [AIGP15, BBG+18b, CKL+11, DVVP14, GLB16, GRN19, HKR+14, IIHY15, Lar12, MKH+13, MLN+18, RCM+13a, RML+15, RHPWS13, SFCCK+14, SFCCK+15, SFG+17, Sch12, SJZ+15, WC11, WPM+15, dLC18a]. **Without** [SMB18, FSD+18, GA14, KJ10, TH13, UvSvdWK19, dLC17]. **WKB** [QS19]. **Wolf** [GPGSM12]. **Wordom** [SFR+11]. **work** [Bou14, CME11, KHWB17, NHN16, SPZP19]. **Workbook** [HJG09, Spr10]. **workflow** [HG13]. **wrong** [SJWE10]. **WS** [EBPK17b]. **Wu** [Ano12u].

X [ATP18, ASS+17, CPR18, CXS10, EPH+15, GPK+16, LDJ+10, LLL+11, LZJ+11, Li14a, Li14b, LGW12, LCWW10, LWD13, PMG+16, SPS+12, SZBM13, SLIB12, TFQ+11, YS13, ZYLL12, ZLLL12, ZLX+19, BSF18, FZY+12, FLM11, JJJ16, Kop15b, LLBO12, LHSH12, LZL+15b, LCWW10, MKK+19, PDG+16, SKY+11, WWD14, XML+15, XhD15, ZLLL12, LX11]. **X-** [SKY+11]. **X-Ray** [CPR18, FLM11, LLBO12, LHSH12, MKK+19, PDG+16, WWD14, XML+15]. **X10** [LMR14]. **X=O** [AM19b]. **Xa** [WLF11]. **xanthine** [FF11]. **xanthophylls** [LLH11]. **XCCH** [LLL+11]. **Xe** [SKMS13, BBI+11, MLGB16, SKMS13]. **XF** [ASS+17]. **XH** [CCCLCGRO14]. **Xiaobo** [Ano12u]. **Xiaojian** [Ano12u]. **Xinli** [JW12]. **XML** [LDB+17]. **XO** [GWZX12]. **XPS** [IN13]. **XQDPT2** [KKL+13]. **xx** [CD19]. **XY** [CXS10]. **XYG3** [CSXZ17, SZX13a, SZX13b, ZWLX11, ZWX19].

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].

Z [JJJ16, FCOGM12, FZL+19, JJJ16]. **Z-Scheme** [FZL+19]. **zebularine** [SCW11]. **zeolite** [SN16a]. **zeolites** [DAP+18, LZTV10, Lar11, SN15, SDB+16]. **Zernike** [Hei18, UCRL18]. **zero** [AA18, Pol13, RLA18, SF18, Tac17, VED10, NQB19]. **zero-flux** [AA18, Pol13, RLA18]. **zero-multipole** [SF18]. **Zero-Point** [NQB19]. **zeroth** [VFRAR16, WGA18]. **zeroth-order** [VFRAR16, WGA18]. **zeta** [LOB18, OLPB19, POB13]. **Zif268** [YZWC11]. **zigzag** [DWZ+17, VS14, WDZN16]. **Zinc** [AALCM11, GWZ15, SPS+12, YSSB12]. **Zintl** [RDT14].

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:CIIe

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

Anonymous:2012:CIIf

[Ano12f] Anonymous. Cover image: Inside cover, volume 33, issue 28. *Journal of Computational Chemistry*, 33(28):iii–iv, October 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIIg

[Ano12g] Anonymous. Cover image: Inside cover, volume 33, issue 29. *Journal of Computational Chemistry*, 33(29):iii–iv, November 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIIh

[Ano12h] Anonymous. Cover image: Inside cover, volume 33, issue 30. *Journal of Computational Chemistry*, 33(30):iii–iv, November 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIIi

[Ano12i] Anonymous. Cover image: Inside cover, volume 33, issue 31. *Journal of Computational Chemistry*, 33(31):iii–iv, December 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIIj

[Ano12j] Anonymous. Cover image: Inside cover, volume 33, issue 32. *Journal of Computational Chemistry*, 33(32):iii–iv, December 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVa

[Ano12k] Anonymous. Cover image, volume 33, issue 23. *Journal of Computational Chemistry*, 33(23):i–ii, September 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVb

[Ano12l] Anonymous. Cover image, volume 33, issue 24. *Journal of Computational Chemistry*, 33(24):i–ii, September 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVc

[Ano12m] Anonymous. Cover image, volume 33, issue 25. *Journal of Computational Chemistry*, 33(25):i–ii, September 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVd

[Ano12n] Anonymous. Cover image, volume 33, issue 26. *Journal of Computational Chemistry*, 33(26):i–ii, October 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVe

[Ano12o] Anonymous. Cover image, volume 33, issue 27. *Journal of Computational Chemistry*, 33(27):i–ii, October 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVf

[Ano12p] Anonymous. Cover image, volume 33, issue 28. *Journal of Computational Chemistry*, 33(28):i–ii, October 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVg

[Ano12q] Anonymous. Cover image, volume 33, issue 29. *Journal of Computational Chemistry*, 33(29):i–ii, November 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVh

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

Anonymous:2012:CIVi

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Anonymous:2012:CIVj

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Anonymous:2012:RPP

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

Anonymous:2013:CIIa

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

Anonymous:2013:CIIj

[Ano13b] Anonymous. Cover image: Inside cover, volume 34, issue 10. *Journal of Computational Chemistry*, 34(10):iii–iv, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIk

[Ano13c] Anonymous. Cover image: Inside cover, volume 34, issue 11. *Journal of Computational Chemistry*, 34(11):iii–iv, April 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIl

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

Anonymous:2013:CIIm

[Ano13e] Anonymous. Cover image: Inside cover, volume 34, issue 13. *Journal of Computational Chemistry*, 34(13):iii–iv, May 15,

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Anonymous:2013:CIIn

[Ano13f] Anonymous. Cover image: Inside cover, volume 34, issue 14. *Journal of Computational Chemistry*, 34(14):iii–iv, May 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIo

[Ano13g] Anonymous. Cover image: Inside cover, volume 34, issue 15. *Journal of Computational Chemistry*, 34(15):iii–iv, June 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIp

[Ano13h] Anonymous. Cover image: Inside cover, volume 34, issue 16. *Journal of Computational Chemistry*, 34(16):iii–iv, June 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIq

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

Anonymous:2013:CIIr

[Ano13j] Anonymous. Cover image: Inside cover, volume 34, issue 18. *Journal of Computational Chemistry*, 34(18):iii–iv, July 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIs

[Ano13k] Anonymous. Cover image: Inside cover, volume 34, issue 19. *Journal of Computational Chemistry*, 34(19):iii–iv, July 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIb

[Ano13l] Anonymous. Cover image: Inside cover, volume 34, issue 2. *Journal of Computational Chemistry*, 34(2):iii–iv, January 15,

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Anonymous:2013:CIIt

[Ano13m] Anonymous. Cover image: Inside cover, volume 34, issue 20. *Journal of Computational Chemistry*, 34(20):iii–iv, July 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIu

[Ano13n] Anonymous. Cover image: Inside cover, volume 34, issue 21. *Journal of Computational Chemistry*, 34(21):iii–iv, August 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIv

[Ano13o] Anonymous. Cover image: Inside cover, volume 34, issue 22. *Journal of Computational Chemistry*, 34(22):iii–iv, August 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIw

[Ano13p] Anonymous. Cover image: Inside cover, volume 34, issue 23. *Journal of Computational Chemistry*, 34(23):iii–iv, September 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIx

[Ano13q] Anonymous. Cover image: Inside cover, volume 34, issue 24. *Journal of Computational Chemistry*, 34(24):iii–iv, September 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIy

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

Anonymous:2013:CIIz

[Ano13s] Anonymous. Cover image: Inside cover, volume 34, issue 26. *Journal of Computational Chemistry*, 34(26):iii–iv, October 5,

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Anonymous:2013:CIIba

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

Anonymous:2013:CIIbb

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

Anonymous:2013:CIIbc

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

Anonymous:2013:CIIc

[Ano13w] Anonymous. Cover image: Inside cover, volume 34, issue 3. *Journal of Computational Chemistry*, 34(3):iii–iv, January 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIbd

[Ano13x] Anonymous. Cover image: Inside cover, volume 34, issue 31. *Journal of Computational Chemistry*, 34(31):iii–iv, December 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIbe

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

Anonymous:2013:CIId

[Ano13z] Anonymous. Cover image: Inside cover, volume 34, issue 4. *Journal of Computational Chemistry*, 34(4):iii–iv, February 5,

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Anonymous:2013:CIIe

[Ano13-27] Anonymous. Cover image: Inside cover, volume 34, issue 5. *Journal of Computational Chemistry*, 34(5):iii–iv, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIf

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

Anonymous:2013:CIIg

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

Anonymous:2013:CIIh

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

Anonymous:2013:CIIi

[Ano13-31] Anonymous. Cover image: Inside cover, volume 34, issue 9. *Journal of Computational Chemistry*, 34(9):iii–iv, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVa

[Ano13-32] Anonymous. Cover image, volume 34, issue 1. *Journal of Computational Chemistry*, 34(1):i–ii, January 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVj

[Ano13-33] Anonymous. Cover image, volume 34, issue 10. *Journal of Computational Chemistry*, 34(10):i–ii, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVk

[Ano13-34] Anonymous. Cover image, volume 34, issue 11. *Journal of Computational Chemistry*, 34(11):i–ii, April 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVl

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

Anonymous:2013:CIVm

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

Anonymous:2013:CIVn

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

Anonymous:2013:CIVo

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

Anonymous:2013:CIVp

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

Anonymous:2013:CIVq

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

Anonymous:2013:CIVr

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

Anonymous:2013:CIVs

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

Anonymous:2013:CIVb

[Ano13-43] Anonymous. Cover image, volume 34, issue 2. *Journal of Computational Chemistry*, 34(2):i–ii, January 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVt

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

Anonymous:2013:CIVu

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

Anonymous:2013:CIVv

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

Anonymous:2013:CIVw

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

Anonymous:2013:CIVx

[Ano13-48] Anonymous. Cover image, volume 34, issue 24. *Journal of Computational Chemistry*, 34(24):i–ii, September 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVy

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

Anonymous:2013:CIVz

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

Anonymous:2013:CIVba

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

Anonymous:2013:CIVbb

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

Anonymous:2013:CIVbc

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

Anonymous:2013:CIVc

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

Anonymous:2013:CIVbd

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

Anonymous:2013:CIVbe

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

Anonymous:2013:CIVbf

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

Anonymous:2013:CIVbg

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

Anonymous:2013:CIVd

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

Anonymous:2013:CIVe

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

Anonymous:2013:CIVf

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

Anonymous:2013:CIVg

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

Anonymous:2013:CIVh

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

Anonymous:2013:CIVi

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

Anonymous:2014:CII

[Ano14a] Anonymous. Cover image: Inside cover, volume 35, issue 14. *Journal of Computational Chemistry*, 35(14):iii–iv, May 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVa

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

Anonymous:2014:CIVb

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

Anonymous:2014:CIVx

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

Anonymous:2014:CIVy

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

Anonymous:2014:CIVz

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

Anonymous:2014:CIVba

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

Anonymous:2014:CIVbb

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

Anonymous:2014:CIVbc

[Ano14i] Anonymous. Cover image, volume 35, issue 11. *Journal of Computational Chemistry*, 35(11):v–vi, April 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbd

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

Anonymous:2014:CIVbe

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

Anonymous:2014:CIVbf

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

Anonymous:2014:CIVbg

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

Anonymous:2014:CIVbh

[Ano14n] Anonymous. Cover image, volume 35, issue 13. *Journal of Computational Chemistry*, 35(13):iii–iv, May 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbi

[Ano14o] Anonymous. Cover image, volume 35, issue 14. *Journal of Computational Chemistry*, 35(14):i–ii, May 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbj

[Ano14p] Anonymous. Cover image, volume 35, issue 15. *Journal of Computational Chemistry*, 35(15):i–ii, June 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbk

[Ano14q] Anonymous. Cover image, volume 35, issue 15. *Journal of Computational Chemistry*, 35(15):iii–iv, June 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbl

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

Anonymous:2014:CIVbm

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

Anonymous:2014:CIVbn

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

Anonymous:2014:CIVbo

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

Anonymous:2014:CIVbp

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

Anonymous:2014:CIVbq

[Ano14w] Anonymous. Cover image, volume 35, issue 18. *Journal of Computational Chemistry*, 35(18):iii–iv, July 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbr

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

Anonymous:2014:CIVbs

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Anonymous:2014:CIVc

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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

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Anonymous:2014:CIVcc

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Anonymous:2014:CIVcd

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Anonymous:2014:CIVce

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Anonymous:2014:CIVcf

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Anonymous:2014:CIVcg

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Anonymous:2014:CIVch

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Anonymous:2014:CIVci

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Anonymous:2014:CIVcj

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Anonymous:2014:CIVck

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Anonymous:2014:CIVcl

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Anonymous:2014:CIVcm

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Anonymous:2014:CIVe

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Anonymous:2014:CIVf

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Anonymous:2014:CIVcn

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Anonymous:2014:CIVco

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Anonymous:2014:CIVcp

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Anonymous:2014:CIVcq

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Anonymous:2014:CIVcr

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Anonymous:2014:CIVcs

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Anonymous:2014:CIVg

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Anonymous:2014:CIVh

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Anonymous:2014:CIVi

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Anonymous:2014:CIVj

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Anonymous:2014:CIVk

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Anonymous:2014:CIVl

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Anonymous:2014:CIVm

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Anonymous:2014:CIVn

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Anonymous:2014:CIVo

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Anonymous:2014:CIVp

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Anonymous:2014:CIVq

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Anonymous:2014:CIVr

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Anonymous:2014:CIVs

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Anonymous:2014:CIVt

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Anonymous:2014:CIVu

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Anonymous:2014:CIVv

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Anonymous:2014:CIVw

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Anonymous:2015:CIVa

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Anonymous:2015:CIVb

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Anonymous:2015:CIVu

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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

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Anonymous:2015:CIVz

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Anonymous:2015:CIVba

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Anonymous:2015:CIVbb

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Anonymous:2015:CIVbc

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Anonymous:2015:CIVbd

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Anonymous:2015:CIVbe

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Anonymous:2015:CIVbf

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Anonymous:2015:CIVbg

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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:CIVbk

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Anonymous:2015:CIVbl

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Anonymous:2015:CIVbm

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

Anonymous:2015:CIVc

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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:CIVbs

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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:CIVca

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Anonymous:2015:CIVcb

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Anonymous:2015:CIVcc

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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:CIVm

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Anonymous:2015:CIVn

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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:2015:ECS

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

Anonymous:2015:ECG

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Anonymous:2015:OPS

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Anonymous:2016:CIVa

[Ano16a] Anonymous. Cover image, volume 37, issue 1. *Journal of Computational Chemistry*, 37(1):i, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVb

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

Anonymous:2016:CIVc

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

Anonymous:2016:CIVv

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

Anonymous:2016:CIVw

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

Anonymous:2016:CIVx

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

Anonymous:2016:CIVy

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

Anonymous:2016:CIVz

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

Anonymous:2016:CIVba

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

Anonymous:2016:CIVbb

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

Anonymous:2016:CIVbc

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

Anonymous:2016:CIVbd

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

Anonymous:2016:CIVbe

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

Anonymous:2016:CIVbf

[Ano16n] Anonymous. Cover image, volume 37, issue 15. *Journal of Computational Chemistry*, 37(15):ii, June 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbg

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

Anonymous:2016:CIVbh

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

Anonymous:2016:CIVbi

[Ano16q] Anonymous. Cover image, volume 37, issue 18. *Journal of Computational Chemistry*, 37(18):i, July 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbj

[Ano16r] Anonymous. Cover image, volume 37, issue 19. *Journal of Computational Chemistry*, 37(19):i, July 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVd

[Ano16s] Anonymous. Cover image, volume 37, issue 2. *Journal of Computational Chemistry*, 37(2):i, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVe

[Ano16t] Anonymous. Cover image, volume 37, issue 2. *Journal of Computational Chemistry*, 37(2):ii, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbk

[Ano16u] Anonymous. Cover image, volume 37, issue 20. *Journal of Computational Chemistry*, 37(20):i, July 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbl

[Ano16v] Anonymous. Cover image, volume 37, issue 21. *Journal of Computational Chemistry*, 37(21):i, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbm

[Ano16w] Anonymous. Cover image, volume 37, issue 21. *Journal of Computational Chemistry*, 37(21):ii, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbn

[Ano16x] Anonymous. Cover image, volume 37, issue 22. *Journal of Computational Chemistry*, 37(22):i, August 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbo

[Ano16y] Anonymous. Cover image, volume 37, issue 23. *Journal of Computational Chemistry*, 37(23):i, September 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbp

[Ano16z] Anonymous. Cover image, volume 37, issue 23. *Journal of Computational Chemistry*, 37(23):ii, September 5, 2016. CO-

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Anonymous:2016:CIVbq

[Ano16-27] Anonymous. Cover image, volume 37, issue 23. *Journal of Computational Chemistry*, 37(23):iii, September 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbr

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

Anonymous:2016:CIVbs

[Ano16-29] Anonymous. Cover image, volume 37, issue 24. *Journal of Computational Chemistry*, 37(24):ii, September 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbt

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

Anonymous:2016:CIVbu

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

Anonymous:2016:CIVbv

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

Anonymous:2016:CIVbw

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

Anonymous:2016:CIVbx

[Ano16-34] Anonymous. Cover image, volume 37, issue 27. *Journal of Computational Chemistry*, 37(27):i, October 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVby

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

Anonymous:2016:CIVbz

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

Anonymous:2016:CIVf

[Ano16-37] Anonymous. Cover image, volume 37, issue 3. *Journal of Computational Chemistry*, 37(3):i, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVg

[Ano16-38] Anonymous. Cover image, volume 37, issue 3. *Journal of Computational Chemistry*, 37(3):ii, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVca

[Ano16-39] Anonymous. Cover image, volume 37, issue 30. *Journal of Computational Chemistry*, 37(30):i, November 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVcb

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

Anonymous:2016:CIVcc

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

Anonymous:2016:CIVh

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

Anonymous:2016:CIVi

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

Anonymous:2016:CIVj

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

Anonymous:2016:CIVk

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

Anonymous:2016:CIVl

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

Anonymous:2016:CIVm

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

Anonymous:2016:CIVn

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

Anonymous:2016:CIVo

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

Anonymous:2016:CIVp

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

Anonymous:2016:CIVq

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

Anonymous:2016:CIVr

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

Anonymous:2016:CIVs

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

Anonymous:2016:CIVt

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

Anonymous:2016:CIVu

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

Anonymous:2016:EPR

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Anonymous:2016:IIa

[Ano16-57] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(15):1329–1333, June 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIb

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

Anonymous:2016:IId

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

Anonymous:2016:IIf

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

Anonymous:2016:IIg

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

Anonymous:2016:IIh

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

Anonymous:2016:IIi

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

Anonymous:2016:IIj

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

Anonymous:2016:IIk

[Ano16-65] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(23):2119–2123, September 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIl

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

Anonymous:2016:IIm

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

Anonymous:2016:IIn

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

Anonymous:2016:IIo

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

Anonymous:2016:IIp

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

Anonymous:2016:IIq

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

Anonymous:2016:IIr

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

Anonymous:2016:IIs

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

Anonymous:2016:IIu

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

Anonymous:2016:IICa

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

Anonymous:2016:IICs

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

Anonymous:2016:IICu

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

Anonymous:2016:IICw

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

Anonymous:2016:IICy

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

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

Anonymous:2016:IICba

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

Anonymous:2016:IICc

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

Anonymous:2016:IICe

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

Anonymous:2016:IICg

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

Anonymous:2016:IICi

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

Anonymous:2016:IICk

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

Anonymous:2016:IICm

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

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:IICh

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

Anonymous:2016:IICj

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

Anonymous:2016:IICl

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

Anonymous:2016:IICn

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

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:IIEa

[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:IIEe

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

Anonymous:2017:CIVa

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Anonymous:2017:CIVj

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Anonymous:2017:CIVk

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Anonymous:2017:CIVl

[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:CIVm

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Anonymous:2017:CIVn

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Anonymous:2017:CIVo

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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

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Anonymous:2017:CIVr

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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

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Anonymous:2017:CIVb

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Anonymous:2017:CIVv

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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

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Anonymous:2017:CIVz

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Anonymous:2017:CIVba

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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).

Anonymous:2017:IIb

[Ano17-37] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(2):59–63, January 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIc

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

Anonymous:2017:IId

[Ano17-39] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(4):189–193, February 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIe

[Ano17-40] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(5):251–255, February 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIf

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

Anonymous:2017:IIg

[Ano17-42] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(7):395–399, March 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIh

[Ano17-43] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(8):475–479, March 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIi

[Ano17-44] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(9):563–567, April 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIj

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

Anonymous:2017:IIk

[Ano17-46] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(11):767–771, April 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIl

[Ano17-47] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(12):855–859, May 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIm

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

Anonymous:2017:IIn

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

Anonymous:2017:IIo

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

Anonymous:2017:IIp

[Ano17-51] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(16):1283–1290, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIq

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

Anonymous:2017:IIr

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

Anonymous:2017:IIs

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

Anonymous:2017:IIt

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

Anonymous:2017:IIu

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

Anonymous:2017:IIv

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

Anonymous:2017:IIw

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

Anonymous:2017:IIx

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

Anonymous:2017:IIy

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

Anonymous:2017:IIz

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

Anonymous:2017:IIba

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

Anonymous:2017:IIbb

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

Anonymous:2017:IIbc

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

Anonymous:2017:IIbd

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

Anonymous:2017:IIbe

[Ano17-66] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(31):2665–2670, December 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIbf

[Ano17-67] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(32):2747–2751, December 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVa

[Ano18a] Anonymous. Cover image, volume 39, issue 1. *Journal of Computational Chemistry*, 39(1):i, January 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVb

[Ano18b] Anonymous. Cover image, volume 39, issue 1. *Journal of Computational Chemistry*, 39(1):ii, January 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVk

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

Anonymous:2018:CIVl

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

Anonymous:2018:CIVm

[Ano18e] Anonymous. Cover image, volume 39, issue 11. *Journal of Computational Chemistry*, 39(11):i, April 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVn

[Ano18f] Anonymous. Cover image, volume 39, issue 12. *Journal of Computational Chemistry*, 39(12):i, May 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVo

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

Anonymous:2018:CIVp

[Ano18h] Anonymous. Cover image, volume 39, issue 14. *Journal of Computational Chemistry*, 39(14):i, May 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVq

[Ano18i] Anonymous. Cover image, volume 39, issue 15. *Journal of Computational Chemistry*, 39(15):i, June 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVr

[Ano18j] Anonymous. Cover image, volume 39, issue 16. *Journal of Computational Chemistry*, 39(16):i, June 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVs

[Ano18k] Anonymous. Cover image, volume 39, issue 17. *Journal of Computational Chemistry*, 39(17):i, June 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVt

[Ano18l] Anonymous. Cover image, volume 39, issue 18. *Journal of Computational Chemistry*, 39(18):i, July 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVu

[Ano18m] Anonymous. Cover image, volume 39, issue 19. *Journal of Computational Chemistry*, 39(19):i, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVc

[Ano18n] Anonymous. Cover image, volume 39, issue 2. *Journal of Computational Chemistry*, 39(2):i, January 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVv

[Ano18o] Anonymous. Cover image, volume 39, issue 20. *Journal of Computational Chemistry*, 39(20):1, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVw

[Ano18p] Anonymous. Cover image, volume 39, issue 20. *Journal of Computational Chemistry*, 39(20):1, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVx

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

Anonymous:2018:CIVy

[Ano18r] Anonymous. Cover image, volume 39, issue 21. *Journal of Computational Chemistry*, 39(21):C2, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVz

[Ano18s] Anonymous. Cover image, volume 39, issue 22. *Journal of Computational Chemistry*, 39(22):C1, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVba

[Ano18t] Anonymous. Cover image, volume 39, issue 22. *Journal of Computational Chemistry*, 39(22):C2, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbb

[Ano18u] Anonymous. Cover image, volume 39, issue 23. *Journal of Computational Chemistry*, 39(23):C1, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbc

[Ano18v] Anonymous. Cover image, volume 39, issue 23. *Journal of Computational Chemistry*, 39(23):C2, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbd

[Ano18w] Anonymous. Cover image, volume 39, issue 24. *Journal of Computational Chemistry*, 39(24):C1, September 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbe

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Anonymous:2018:CIVbf

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Anonymous:2018:CIVj

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Anonymous:2018:IIb

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Anonymous:2018:IIc

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Anonymous:2018:IId

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Anonymous:2018:IIe

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Anonymous:2018:IIg

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Anonymous:2018:IIh

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Anonymous:2018:IIi

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Anonymous:2018:IIn

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Anonymous:2018:IIo

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Anonymous:2019:CIVk

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Anonymous:2019:CIVw

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Anonymous:2019:CIVx

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Anonymous:2019:CIVy

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Anonymous:2019:CIVz

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Anonymous:2019:CIVbb

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Anonymous:2019:CIVbc

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Anonymous:2019:CIVc

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Anonymous:2019:CIVbd

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Anonymous:2019:CIVbe

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Anonymous:2019:CIVbf

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Anonymous:2019:CIVe

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Anonymous:2019:CIVg

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Anonymous:2019:CIVi

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Anonymous:2019:IIa

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Anonymous:2019:IIb

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Anonymous:2019:IIf

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