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(001) [dLdOdAD12]. (100) [MFK+12]. ($1 \leq n \leq 6$) [UDVD10]. ($2 \leq n \leq 8$) [BLRdA+10]. ($3 + 2$) [WLS+19]. ($3 + 3$) [LFTL18]. ($A = N, B$) [ASW13]. ($k + l + m = 4$) [KYLC19]. ($m + n = 3$) [UKF+11]. ($m = 5, n = 2$) [MHHPR+17]. ($m = 6, n = 3$) [MHHPR+17]. ($n = 1, 2$) [Men10]. ($n = 1, 2, 3$) [EML+11]. ($n = 1--4$) [LL11]. ($n = 1--7$) [CAZ+11]. ($n = 2, 3$) [DTEMK11]. ($n = 2--10$) [WJL+11]. ($n = 2--34$) [QSLY10]. ($N = 28$) [GD11]. (r, s) [Bib13]. ($\varphi - \psi$) [MAW+18]. + [Buc12a, CdAFS+12, DMAB12, FRNM12, GKT+12, KT12b, LWWZ13, MEEA+13, MPRCEG12, MOH+12, RSN12, SÁBA+12, SD12, WZHZ13, XZL+12, YGL+11, YZ10, ZH12]. 1 [BEM12, DFK16, JW19, PSKV19]. 1/3 [KLZQ15]. 13 [LXD13]. 14 [YD17]. 16 [GAPK+19a]. 18 [YD17, GAPK+19b]. $1^3A''$ [GWZ+14a]. 2 [ABTW14, CPL15, HMA+19, HGB08, IK14, LLZaH14, LD17, NF11, PSKV19, SPD+18, SSdS17, YSW11]. $2(N + 1)^2$ [MC18a]. $2n$ [BBYZ18].

$2n + 2\pi$ [MB13]. $2n = 68, 70, 78,$ [WLZ+12a]. $2p\pi$ [VLFG12]. 3 [ABTW14, BMX+19, GWJ12, KSO19, LQZZ12, LD17, RLW+13, SM14c, VVY18]. 30 [GGD12, SLZ+12]. $3d$ [ALA15, DD17, RZC13]. $3d\sigma$ [VLFG12]. 4 [ABTW14, CD12, GAPK+19b, GB13, GWJ12, HCL13, LKN13, SM14c, WLS+19]. $4d\sigma$ [VLFG12]. $4f\pi$ [VLFG12]. $4f\sigma$ [VLFG12]. 5 [ABTW14, BGMD15, BJdlMAV12, CDSK12, HDQ+13, MPE15, SM14d, SM16]. $5g\sigma$ [VLFG12]. $5 \leq n \leq 7$ [LCZ15]. 6 [CWSZ13, HDQ+13, LdMCdA+12, MPE15, MJ14, MMV+19, Pli18, PAKA15, SS18a, VBO+15]. $6; y = 1, 2$ [BCGC12]. $6i\sigma$ [VLFG12]. $6j$ [RBD+10]. 7 [CHV14, GGJD13, SR13, WCS+13]. $7i\pi$ [KMF+11]. $7j\sigma$ [KMF+11]. 8 [YC13]. 80 [WLZ+12a]. $8jp$ [KMF+11]. $8j\sigma$ [KMF+11]. $8k\sigma$ [KMF+11]. $8 \leq n \leq 14$ [NW12]. 9 [Ali14, SBB16]. $<$ [BTH18]. $=$ [BPG+10, BL10, BDR12, ČFČ11, DIOG12, DPDR11, ESS13, FTB11, GB13, JL12a, KyH13a, LZZ+11, LMZ+11, LLG+12, MLW10, MPRB+10, dMOB12, Qu13, SZZZ11, SYQ+10, SZL+14, TFB11, WCY+10, WSL+11, XZZ+10, XWC11a, XWCY11, YK11, YIY+13, YL11, ZQJW13]. $>$ [BTH18]. $[2 + 2]$ [MBS+18]. $[2 + 4]$ [LLF17]. $[2, 7]$ [WWL+11]. $[2n, 2]$ [LSW19]. $[3 + 2]$ [ZRGE+19]. $[3 + 3]$ [ZQW+17]. $[4 + 2]$ [HZZ+19]. $[4 + 3]$ [XZG+18]. $^{+}$ [ADB10, AGRI+12, BD12, BCK19, BHV+11, Ber13a, BG11c, DWJZ11, DZ11a, DCHC11, FBM+10, GWHH17, GFB12b, GR10, HMI+15, HHCA10, HDC+11, JMPP19, KH12, KMF+11, KHH10, LCL+10a, LP10b, LGP+11, LPG+12, LLC+11, LLZZ10, LdAA+11, Ma14, MT11, MMRRA10, NKWT19, NWQX11, NZLG15, RFEGPP+16, RI19, RRCO11, SLZ+11a, SLS+11, SZZZ11, SLZH12, SSW16, SWS12, TFB11, Vik13, WLG+11, XWCY11, YLW+13, ZQJW13, ZLWL16, ZCG+17]. $^{++}$ [ZPM10]. $^{+}_{5}$ [BN12]. $^{-}$ [ADB10, BCK19, CS17, DZO11, DSZB18, FT15, KMM16, LCL+10b, LIK15, Ma14, MPM15, McC13a, MEEA+13, MMRRA10, RWW+19, RGR12, SSAM13, TFB11, XWCY11, YGLL10]. $^{-\bullet}$ [ZLWZ16]. $^{0,\pm}$ [ZPR10]. ^{1} [DSD18, Kan11, LGW11, MKD19, OD12, RR19, SBMM11, STL12, SZY17, TSL11]. ^{1,3} [DSSM18, ARG11]. ^{13} [TKSK17]. ^{14}N [BJ12]. $^{1}\Sigma^{+}$ [LJSS12, SPO+11, SLZ+11b, SLZ+11c, YLC17]. $^{1}\Sigma^{+}_{g}$ [YLC17]. ^{2} [FRNM12, LV12, LGW11, MCV11, NCMC+18, PBR18, RRCO11, She13, SLS+12, YLC17, ZCG+17]. $^{2+}$ [ASHF13, BJ17, CRB+12, CLMY12, GR11, LWL+12, MRT11, MG12, NZLG15, OPC17, RFEGPP+16, VO12, YLW+13]. $^{2-}$ [Fuk12, SBSD18]. $^{2\cdot-}$ [LGW11]. $^{2}\Pi$ [SZS+10, SLS+11]. $^{2}\Pi_{g}$ [SSAM13]. $^{2}\Pi_{u}$ [RS12a]. $^{2}\Sigma^{+}$ [SLZ+11a]. $^{2}\Sigma^{+}_{g}$ [ZCG+17]. $^{2}\Sigma^{+}_{u}$ [RS12a]. $^{2}\Sigma^{+}_{u}(2p\sigma_{u})$ [GWHH17]. ^{3} [ACMRN10, CdAFS+12, DVDBM11, DSSM19, GWZ+14a, HHL+12b, MCK17, OD12, ZCG+17, ZPB12]. $^{3+}$ [CRB+12, DSZB18, SS13]. $^{3-}$ [Bou12b, WZC+12]. $^{3}\Delta_{u}$ [SXS+12]. $^{3}\Pi_{g}$ [SXS+12]. $^{3}\Sigma^{-}$ [SSAM13, ZCG+17]. $^{3}\Sigma^{+}_{u}$ [SXS+12]. ^{4} [Kin13, RCGLV+14, SLS+12]. $^{4+}$ [NCMC+18, ZCG10]. $^{4}\Sigma$ [LDADB+15]. $^{6+}$ [DI18, ZCG10]. $^{\bullet+}$ [WSML16]. $^{\cdot}$ [CAAI12, PGG12]. ^{e} [DSSM18, DSSM19, SBMM11]. ^{II} [DS11, MC17]. ^{IV} [MLY+16, ZSHL16, ZLY+14]. $^{n-}$ [MLY+16, ZLY+14]. $'$ [KMK+16, LZFZ13, Qu13, UJSJ13, Con10, GWM11, JWG+12, LV12, RS11b, SC12a, SKM11, YLW+13]. $'3\Sigma^{-}_{u}$ [SXS+12]. $'_{3}$ [GWM11]. $''$

[Dau16, LZFZ13, MCV11]. ^{q} [BLdV19]. ^{R} [Pan16]. ^{V} [ZLY^{+}14]. ^{VI} [MLY^{+}16, ZLY^{+}14]. ^{VII} [ZLY^{+}14]. $_{0}$ [BMX^{+}19, CMCN11]. $_{0.5}$ [MGP16]. $_{1}$ [BMX^{+}19, MKD19, RDM^{+}11, SY10, VF13a, YXM^{+}18]. $_{1-x}$ [KA13]. $_{1-x/3}$ [Oni12]. $_{1.5}$ [MGP16]. $_{10}$ [LZW^{+}15]. $^{2+}_{10}$ [MCK17]. $_{11}$ [CS18, MLY^{+}16]. $_{12}$ [GAPK^{+}19b, GKGM18, HWL16, KGK13, MJ16a, MPD^{+}10, VPFD10, XCY15]. $_{120}$ [CTDOLA10]. $_{13}$ [MMBK12, SFA19, TW10, VDG13]. $_{144}$ [BDF^{+}16]. $_{15}$ [HLMO11]. $_{16}$ [CS18, TFB11]. $_{1}8$ [BDF^{+}18, yBZfC18, GKGM18, JL12a, MLY^{+}16, SCTW10]. $_{19}$ [GKGM18]. $_{1\sim2}$ [XZZ^{+}10]. $_{2}$ [AO12a, ATS15, ALA15, BDFM10, BPG^{+}10, BAP12, BDF^{+}18, BAMA12, BL11, BGFD14, BAA^{+}18, BBYZ18, BZZ15, yBZfC18, BXZ^{+}19, BG11b, BB10, BLKB11, BAB^{+}18, BJ17, Buc12a, BSPK11, CP10, CRSB12, CTW12, CCS13, CS17, CC11b, Cor16, CWSZ13, CS18, DMAB12, DLCB15, DVDBM11, DTVP^{+}12, DCDD10, Den13, DPDR11, DMG10, DZO11, DLM12, DQZF12, ESS13, EFO11, EO11, EMSB15, Esr18, FLCHL10, FBRBR12, FTB11, Fuk12, GP13a, GWM11, dDGNB10, GC18, GKT^{+}12, GR10, GD11, HV11, HDC^{+}11, HSYM11, HHL12a, HHL14, HYH^{+}10, HCL13, HHL^{+}12b, JL12a, JL12b, JLZ^{+}17, JWG^{+}12, JLG^{+}12, KWC10, Kal18, KAR12a, Kan11, KMF^{+}11, KI12, KLK13, KK14b, KSSK16, Kim19, KSST12, KLZQ15, KDOR17, KF17, KN15, KRG^{+}13, LZ12, Les12, LV12, LLG^{+}12, LCT14, LC16, LLL16, LZW^{+}18, LFP^{+}19, LCZ15, LLW^{+}12, LCS^{+}11a, LXLL11, LLLB13, LEU^{+}11]. $_{2}$ [MLY^{+}16, MLW10, MFK^{+}12, MTR^{+}19, MMP^{+}18b, MMC^{+}19, MC12, MFZ^{+}18, MBA^{+}13, MPD^{+}10, MKD19, MKM11, Mit11a, MZLM17, MPRCEG12, MPGGS19, MPTZ13, MCV11, MKW11, MGP16, MOH^{+}12, NW12, NTNL10, NL11, NMIP14, NH11, OCL^{+}18, Oni12, OGvSG18, PTS^{+}11, Pan16, PWL^{+}10, PC16, PCK19, Per10b, PK13b, PRPU^{+}13, PL18b, Puz10, QSLY10, Qu13, QCB^{+}10, RS12a, RS12b, RSL10, RFEGPP^{+}16, RWW^{+}19, RNB^{+}10, RGR12, RRB12, RBTL19, ŞBAT16, SK14, SD16a, SCLCPB12, SR19, SÁBA^{+}12, SVPTM^{+}10, Sat11b, SMEH15, SSAM13, SXS^{+}12, SR18, SPIL14, SZZZ11, STL12, SLZH12, Sri18, Sri19, STU19, SYQ^{+}10, SCTW10, SW12, SZ15, TOSN12, TSKN12, Tan13, TFSRM11, TNN16, TD11, TMC18, TSL11, Tob19, VV18, VPFD10, VPA11, Vik11a, Vik11b, VLK^{+}11, WSCL11, WLL11, WLG^{+}11, WZM^{+}13, WZHZ13, WZC^{+}12, WLWL14, WWGW18, WRW^{+}18]. $_{2}$ [XMZ^{+}12, XZL^{+}12, XDM^{+}10, XWCY11, XF19, YY18a, YIY^{+}13, YSK^{+}12, YLWrL12, YGLL10, YLZ^{+}17, YC13, YLC17, YLYC18, ZZ15, ZPR10, Zha10, ZK12, ZH12, ZQJW13, ZLWY13, ZGSM15, ZWL18, ZHL^{+}19, ZFS^{+}11, ZLWZ16, ZLY^{+}14, ZDZL11, dHLdS12, dOR10]. $_{20}$ [yBZfC18, CWL^{+}13, GB13, WSL^{+}11]. $_{24}$ [CJMC19, HLB19, JB18, MMBK12, MC18a, MC18b, YL11]. $_{2}5$ [BDF^{+}18]. $_{28}$ [MC18a, YLH^{+}19]. $^{4-}_{28}$ [MC18a]. $^{+}_{2}$ [AC12, Ber13c, Che12, OPC17, RS12b, RAN18, SSP14, VLFG12]. $^{+\cdot}_{2}$ [FBRBR12]. $^{-}_{2}$ [SSAM13]. $^{-/2-}_{2}$ [YGLL10]. $^{2+}_{2}$ [FBRBR12]. $_{2A}$ [CSSK^{+}12]. $_{2C}$ [CSVCB12, CSSK^{+}12]. $_{2n}$ [WLZ^{+}12a, BBYZ18, EML^{+}11]. $_{2/12}$ [Kim19]. $_{3}$

[XCL+18, lAyL14, ACMRN10, AM18, BCP10, BGFD14, BAA+18, BZZ15, BXZ+19, Bou12b, CCL+13, CdAFS+12, CRSB12, CWS15, CDL+19, CS18, DS11, DS12, DPDR11, DZ11a, DQZF12, DSFT17, EMSB15, EMS16, EAV16, FRNM12, GWM11, GMT18, GZMC11, GMP+11, JCCZ12, JLG+12, KWC10, Kal18, KAR12a, KG17, KCK14, KLZQ15, Lan10, Les12, LJL+11, LZZ+11, lLBqD+19, LFP+19, LGW11, LL19, LXLL11, LdAA+11, MWH15, MFK+12, Men10, MFZ+18, MPD+10, MEEA+13, MPRCEG12, MPGGS19, Mor11, NBL12, NH11, dMOB12, Oni10, Oni12, OH12, OH13, OCGM+19, PC16, Per10b, PP14, RLTAT19, RSN12, RB11b, SMC18, SK14, SKS11, SD12, Sik18, SSP14, SZZ+12, STL12, SM17, SYQ+10, TSL11, TL15, UV18a, UV18b, VV18, VPFD10, VVY18, VLK+11, WCY+10, WLZ+12a, WLZ+12b, WZM+13, WZHZ13, WCL+17, WTP+19, WZC+12, XZL+12, XZZ+10, XWC11a, XWCY11, XCL+18]. $_{3}$ [XF19, YLWrL12, ZHL+19, ZJC+13, dHLdS12, dOR10, dOdCMUdALR11]. $_{3--5}$ [CS17]. $_{3-n}$ [SKS10]. $_{30}$ [FBO+11]. $_{36}$ [LBY+14, MS17]. $_{38}$ [MC18b, YLH+19]. $\overset{+}{}_{3}$ [MSAB19, RR11]. $\overset{-}{}_{3}$ [Sat11b]. $\overset{2-}{}_{3}$ [GPM+15, WZC+12]. $_{4}$ [BDFM10, BDF+18, BAA+18, BAB+18, CJMC19, CCL+10, DWX+16, DLM12, ESS13, FBRBR12, HLMO11, HSN+11, HHL+12b, JCCZ12, KI12, Kim13, KLK13, KSSK16, KMM16, LGHL11, LL18, LFP+19, LXD13, LW18, LKLW11, MBKH19, MPD+15, MLW10, MOE+11, MBA+13, MPRB+10, MC18a, NMIP14, OCL+18, OPP+14, PAKA15, PL18b, RPBB11, RRRV19, RFEGPP+16, RTT10, ŞBAT16, SYK+12, Sat11b, TZD+19, TGA+11, VF13a, VDG13, WWGW18, XWC11a, XWCY11, XXJ+16, XF19, YYI+13, YIY+13, YSK+12, YLWrL12, ZLY+14, dHLdS12]. $_{40}$ [LZW+15, YLH+19]. $\overset{+}{}_{4}$ [WWGW18]. $\overset{-}{}_{4}$ [Sat11a, YGLL10]. $\overset{2+}{}_{4}$ [MCK17]. $\overset{2-}{}_{4}$ [Sat11a]. $_{4/3}$ [OA12]. $_{5}$ [BDF+18, Bou12b, BDR12, CRSB12, DCDD10, Den13, DZO12b, DQZF12, GWM11, HSYM11, KMM16, LCL+10a, LFP+19, MLY+16, MBA+13, Mor11, NBL12, NTNL10, NL11, PTS+11, PP14, SYK+12, WCY+10, WCS+13, WLWL14, XZZ+10, YYI+13, YSK+12]. $_{540}$ [CCEGK12]. $_{58}$ [SCTW10]. $\overset{-}{}_{5}$ [KMM16, LFP+19]. $_{6}$ [BD14, BDF+18, BGFD14, BLdV19, BLKB11, CS18, DWPK14, ESDO16, GWM11, Kal18, KI12, KLZQ15, LCL+10a, LGHL11, Mor11, MCK17, NBL12, NH11, PP14, RLTAT19, RRRV19, Sri19, TCSD12, TZD+19, TG13, WZW17, dHLdS12]. $_{6(10-n)}$ [PAKA15]. $_{6-\delta}$ [MGP16]. $_{6-x}$ [GLF+12]. $_{60}$ [BDF+16, BCP10, DFK16, FBO+11, IMS+13, KN15, MSS11, MIN13, Nik11, PAKA15, RR11, TKSK17, XCY15, YK11, ZLWL16]. $\overset{+}{}_{6}$ [BD14]. $\overset{-}{}_{6}$ [BD14]. $\overset{2-}{}_{6}$ [KMM16]. $\overset{3-}{}_{6}$ [GGJD13]. $_{7}$ [DSFT17, LdAA+11, Sik18]. $_{72}$ [GZW16]. $_{74}$ [USL+13]. $_{76}$ [JLL+18]. $_{78}$ [ZW15]. $\overset{+}{}_{7}$ [LdAA+11]. $\overset{-}{}_{7}$ [GGJD13]. $_{8}$ [Nes11]. $_{80}$ [WLZ+12b]. $_{82}$ [SUL+11]. $_{84}$ [KK12a]. $_{86}$ [KK11b]. $_{88}$ [YLZ+17]. $\overset{+}{}_{8}$ [WWGW18]. $\overset{-}{}_{8}$ [KBF+13]. $_{8/12}$ [Kim19]. $_{9}$ [MLY+16]. $\overset{3+}{}_{9}$ [BSPK11]. $_{A}$ [TOSN12, TSKN12, BMK+14, CPL15, COCF+14, ÇT14, DQZF12, GCDNGS12, KSS12, LZ12, RZG12]. $_{\alpha}$ [FNBK17]. $_{b}$ [KSS12, LZ12, SB18, SSB19]. $_{\beta}$ [FNBK17]. $_{d}$ [YGLL10]. $_{FH}$ [CDT12]. $_{g}$ [FRNM12]. $_{H}$ [Zha14, CJMC19]. **0–14** [XF19]. $_{im}$ [WB17]. $_{\infty h}$ [YGLL10]. $_{k}$ [KYLC19]. $_{l}$ [KYLC19, PAPCMM+16]. $_{m}$ [CTW12, CD12, GWJ12, KYLC19,

LKN13, MHHPR$^+$17, PAPCMM$^+$16, UKF$^+$11]. $_N$
[DVDBM11, EHKD11, EKD12, GGD12, GD11, LJK$^+$18, MEEA$^+$13, RWW$^+$19, SM16, Ali14, BPG$^+$10, BGMD15, BEM11, BLRdA$^+$10, BJdlMAV12, CDSK12, CAZ$^+$11, CTW12, CWSZ13, CD12, DTEMK11, EML$^+$11, FTB11, GR11, GAPK$^+$19b, GGJD13, GP13b, GB13, GWJ12, HDQ$^+$13, KSSK16, Kuz19, LRKM10, LKN13, LGHL11, LWL19, LCZ15, LHL$^+$15, MCP10, Men10, MJ14, MMV$^+$19, MHHPR$^+$17, MMRRA10, NW12, PAKA15, PAPCMM$^+$16, QSLY10, RGR12, SKS10, SJZ$^+$18, SR13, SBB16, SLZ$^+$12, SM14b, SM14c, SM14d, UKF$^+$11, UDVD10, WJL$^+$11, WCS$^+$13, WJL$^+$10, XYL$^+$18, YC13, ZRR$^+$11, ZCTG18, ZCP11]. $_{n-1}$ [MCP10]. $_{n-2}$ [LCZ15]. $_n^{(n-4)-}$ [KMM16]. $_N^+$ [GGD12]. $_N^-$ [RWW$^+$19]. $_n^{-/0}$ [LL11]. $_n^{0/-/2-}$ [DHYC19]. $_n^{2+}$ [LL18]. $_n^{q-}$ [SM14c]. $_x$
[BCGC12, GLF$^+$12, HCL13, KA13, Oni12, RLW$^+$13]. $_y$ [BCGC12]. A [ASW13]. α [BWB$^+$18, HZZ$^+$19, KSAK17, MFZ$^+$18, OPAVM18, LZZ12, PEA$^+$12, QTCL10, SVRGV12]. α_2 [EPS$^+$16]. β
[AC19, GCZ$^+$14, Jeo18, JSLH14, KZZ13b, LSG$^+$14, OPAVM18, WHS$^+$13, NMHPVG12, NRP$^+$11, PEA$^+$12, SJW13, TPdMB12]. β_2 [CSVCB12]. $\cdot$ [BLWJ17, BTH18, XF19, Men10, TBHL11, XLGA12]. $\cdots$ [TG13, JLG$^+$12]. $\cdots$ [MZLM17, SPIL14, WZW17, YZZ16]. χ_1 [DSCO$^+$13]. D
[IIH16, PGMGRM15, CWW$^+$16, MVG18, MW16, OVT$^+$16]. d^{10} [DLJT14]. Δ [CC11b, Yam10]. Δ_{rxn} [DE18]. ℓ [ZHF12]. ϵ [VLM$^+$10]. η^2 [MSBF18]. η^5 [DZO12b]. f [MW16]. G [ATPRV11, DKS11, VATPR11, VAT12, SPO$^+$11]. γ [BWB$^+$18, CC11b, MFK$^+$12, PEA$^+$12]. h [PUGSFM18]. J [AAHN16]. $j = 0$ [LZFZ13]. $k(T)$ [CP11]. K_+ [GBK18]. K_+^2 [GBK18]. l [WC14]. $l + m + n = 6$ [PAPCMM$^+$16]. $l, m, n > 0$ [PAPCMM$^+$16]. λ [AM13a]. λ^5 [TM19]. $LDA + U$ [HFdGC14]. $\leftarrow$ [SB18]. M [XYL$^+$18, KC11]. $m, n = 1$ [LKN13]. $m = 1$ [CD12, GWJ12]. $m = 1{-}{-}2$ [FTB11]. m^* [Dw13]. M^{VI} [HNBS18]. μ [ESS13]. N
[CZJZ12, CPL15, DDÇY12, DPRK12, DDF$^+$12, ES17, GW18, KC11, KSAK17, MOSK10, MAN15, NJA$^+$12, Pan16, RWW$^+$19, SFW12, CMCN11, CSK12, DFK16, DHYC19, GE12b, KSSK16, KMM16, LWL19, ZYZ$^+$11]. $n + m \leq 5$ [CD12]. N, N [dAVdM17]. $n =$ [LHL$^+$15, SM14b]. $n = 0$ [GAPK$^+$19b]. $n = 0, 1, 2$ [SKS10]. $N = 1$
[SM16, CWSZ13, GGJD13, GB13, HDQ$^+$13, SR13, SM14d, WCS$^+$13, YC13, BGMD15, PAKA15, SBB16, SM14c, BJdlMAV12, CD12, GWJ12]. $n = 1, 2$ [BPG$^+$10]. $n = 1, 4{-}{-}7$ [FTB11]. $n = 2$
[Ali14, HDQ$^+$13, MJ14, MMV$^+$19, CDSK12, GGD12]. $n = 2, 3, 4$ [GP13b]. $n = 20$ [SLZ$^+$12]. N' [CZJZ12, DDÇY12, Tav11]. $n \geq 2$ [SM14c]. o [KSAK17, SR18]. p [AGJ12, AMAC12, CSK12, DLJT14, HLZ$^+$14, RRK16, SR18, SRA$^+$11, ZSASS13, ZYZ$^+$11]. π
[BWE16, CCS13, DWZZ15, HIL19, KPL$^+$17, LDKB15, LW18, LB18, MC17, MANP17, NCMC$^+$18, NIK19, NMV$^+$14, OCGM$^+$19, PC16, PNC19, SSB19, SPD$^+$18, SSS15, Szc18, TK16b, YZZ16, YD17, ZHL$^+$19, CC11b, SLS$^+$12,

AEKGZ12, BMR$^+$13, DB15, FV11, GNM$^+$12, LCB10, MMA10, Nik11, NRGS11, RVNP12, RNV$^+$12, SD13a, VSS11, Yam10, ZZL$^+$11]. Π_u [HHL$^+$12b]. $\pi \cdots \sigma$ [WLC$^+$17]. $\pi\sigma^*$ [KGVG11]. pK_a [PWY$^+$18]. $\prime$ [Dau16, SAHAA16]. Ψ^α [GS10]. q [Agb12]. $q = 0$ [SM14c]. $\rightarrow$ [Buc12a, Coo12, GKT$^+$12, LCB10, MPRCEG12, NWQX11, YGL$^+$11, YZ10, ZH12]. $rmSU(2)$ [Bra10]. S [HR12, MMM19]. $S = 1/2$ [KLZQ15]. σ [LW18, SPIL14, SC18, ZHL$^+$19, CC11b, Ang10, Che12, DCdG10, JLG$^+$12, Yam10]. Σ^- [SLS$^+$12]. σ_{hole} [VVJ15]. $\sigma\pi$ [ZXY13, DMWY11]. sp^2 [OCGM$^+$19, PNC19]. $\sqrt{3} \times \sqrt{3}$ [OD16]. T [XCL$^+$18]. $\times$ [PWL$^+$10, ZWWY10]. $\rightarrow$ [GW18, KMM16, ZWL18]. $v = 0, 1$ [LZFZ13]. $v = 0, j = 0$ [YZ10]. φ [CC11b]. $W(l, m, n; \alpha, \beta, \gamma)$ [LWY13]. $\wedge$ [ZQJW13, LYL$^+$12]. X [AGOP18, AM18, BHA19, Kuz19, SB18]. $x = 0$ [HCL13]. $x = 1$ [RLW$^+$13]. $x = 2$ [BCGC12]. X^- [Kuz19]. X_2 [BHA19]. Y [Kuz19]. Z [XCL$^+$18].

***** [LCB10].

-1 [CPL15, LL17, TAY11, YZW$^+$15a]. **-1-methyl-1H-benzo** [ÖEDB11]. **-2** [ZWWY10, JWG$^+$12]. **-2-** [KDÇ12, KAOB11]. **-2-ethoxy-benzamide** [DPRK12]. **-3** [Tan12]. **-3-methyl-cyclopentanone** [PCR$^+$11]. **-3-methyl-divinylene** [FO10]. **-4** [RS11b]. **-4-phenylphenol** [NVPCJ$^+$13]. **-5** [SAHAA16]. **-6-** [KAOB11]. **-7** [PWL$^+$10]. **-A** [SSS15]. **-acceptor** [MANP17, KPL$^+$17]. **-acetyl** [Tav11]. **-activation** [Sri19]. **-Al** [MFK$^+$12]. **-alanine** [ZPR10]. **-aminophenanthridine** [VBO$^+$15]. **-anharmonic** [VOAH18]. **-arylamides** [DDF$^+$12]. **-arylcarbamates** [DDF$^+$12]. **-azauracil** [MPE15]. **-based** [MGP16]. **-benzene** [JW19]. **-benzoin** [ZSHL14]. **-benzoyl-** [LD17]. [**?**]benzylidene-Demir:2012:ETI. **-bidipyrrins** [JWG$^+$12]. **-bis** [SAHAA16]. **-bithiazole** [SAHAA16]. **-bithiazoline** [Qu13]. **-bonded** [SPIL14, DB15]. **-bonding** [LW18]. **-Br** [DVDBM11]. **-butene** [IK14]. **-C** [CJMC19, LdAA$^+$11]. **-calix** [Pli18]. **-carbon** [OCGM$^+$19]. **-carboxylate** [KSAK17]. **-catalysed** [ZYSW17]. **-catalyzed** [LYR$^+$17, LTL18]. **-CF** [lAyL14]. **-chain** [EPS$^+$16]. **-chloro** [PSKV19]. **-chloro-acetic** [DDÇY12]. **-chloroaniline** [HLZ$^+$14]. **-chlorobenzaldehyde** [SRA$^+$11]. **-cluster** [GP13b]. **-conjugated** [MMA10, GNM$^+$12]. **-cyano-biphenyl** [RS11b]. **-cyclic** [Con10]. **-cyclodextrin** [NMHPVG12, SVRGV12]. **-cyclodextrins** [PEA$^+$12]. [**?**]cyclohexyl-Cao:2012:RBM. **-cysteinato** [ADR$^+$18]. **-D** [BEM12, BMX$^+$19, HGB08]. **-D-glucan** [PTD$^+$12]. **-deformed** [Agb12]. **-deoxyguanosine** [SKM11]. **-diketonato** [AC19]. **-dimensional** [SPD$^+$18, PGMGRM15]. **-dimensions** [IIH16]. **-dimethylnitrosamine** [dAVdM17]. **-dioxy-2** [KMK$^+$16]. **-donation** [DCdG10]. **-doped** [AGOP18, ASW13]. **-Electron** [RVNP12, DLJT14, GAPK$^+$19b, MW16, NIK19, NRGS11, NMV$^+$14, SPD$^+$18, RNV$^+$12]. **-electron-poor** [NCMC$^+$18]. **-electron-rich** [NCMC$^+$18]. **-electronic** [HIL19]. **-element** [OVT$^+$16]. **-elements** [RRK16]. **-encapsulated** [ZLWL16]. **-ETO** [GS10].

-F12 [BL12]. **-FARMS** [MC17]. **-formyl** [KSAK17]. **-formylformamide** [NJA+12]. **-generalized** [GE12b]. **-glucosidase** [WHS+13]. **-glycine** [CWL+13]. **-heterocyclic** [MAN15, Pan16]. **-HMX-based** [Jeo18]. **-hole** [JLG+12, SC18, WLC+17, ZHL+19]. **-homodesmotic** [MMM19]. **-hybrid** [MCK17]. **-hydrazono-1** [SC12b]. **-hydrogenase** [BAA+18, MG10, DMG10, BGFD14]. **-hydroxy-2** [YLW+13]. **-hydroxypropanal** [SSdS17]. **-hydroxyquinoline** [CHV14]. **-IEPOX** [KZZ13b]. **-iminothiolate** [WRW+18]. **-induced** [DSZB18]. **-initiated** [LLW+12]. **-interaction** [TK16b]. **-iodane** [TM19]. **-kaempferol** [DSD18]. **-like** [She13]. **-M** [YLWrL12]. **-macrocycle** [CJMC19]. **-matrix** [AAHN16]. **-mediated** [SGL19]. **-membered** [ABTW14]. **-metalloenzyme** [dCDC+11]. **-methoxyphenyl** [ZSASS13]. **-methyl** [KSAK17]. **-methyl-** [IK14]. **-methylacyl-CoA** [LZZ12]. **-methylene** [HZZ+19]. **-methyloxaziridine** [CPL15]. **-methyloxirane** [CPL15]. **-Mg** [MSBF18]. **-molecular** [Nik11]. **-MoO** [MFZ+18]. **-N** [SC12a]. **-N-biaryl** [TPdMB12]. **-nitramines** [MOSK10]. **-nitroaniline** [KC11]. **-nitrosoureas** [CZJZ12]. **-nitrostyrene** [JSLH14]. **-nonmetal** [WCY+10]. **-ones** [HMA+19]. **-orbital** [PNC19]. **-oxide** [KC11]. **-oxodithioesters** [GCZ+14]. **-particle-hole** [ATPRV11, VATPR11, VAT12]. **-path** [WB17]. **-penicillamine** [MVG18]. **-peptide** [QTCL10]. **-phenyl** [YWJ+11]. **-phenyl-acrylonitrile** [LD17]. **-phenylpropyl** [DFK16]. **-propyl** [CMCN11]. **-pyridin-3ylmethylene-hydrazine** [SC12a]. **-pyridyl** [YLW+13]. **-quinone** [KSAK17]. **-Rg** [BPG+10]. **-RS** [ESS13]. **-salicilydenemethylfurylamine** [GW18]. **-scission** [LSG+14]. **-SCR** [MWH15]. **-semiregular** [Bib13]. **-sheet** [SJW13]. **-space** [PC16]. **-splitting** [GWM11]. **-stacking** [LB18]. **-sulfinyl** [SFW12]. **-supported** [BAB+18]. **-systems** [BWE16]. **-tert-butyl-anisol** [AMAC12]. **-tetrad** [DKS11]. **-tetrads** [DKS11]. **-thiazol-2-yl** [DDÇY12, SC12a, SC12b]. **-thioaminoacrolein** [NRP+11]. **-thioguanine** [SS18a]. **-type** [AGJ12, YD17, ZZL+11]. **-unsaturated** [OPAVM18]. **-vacancy** [ES17]. **-vertex** [GAPK+19a]. **-wave** [WC14, ZHF12, HR12]. **-xylene** [SR18]. **-yl** [WLS+19].

/D [XLLZ10]. **/halogen** [YZZ16]. **/HD** [SZ15]. **/NaTaO** [WCL+17]. **/OH** [LIK15]. **/Ph** [XCL+18]. **/S** [BMX+19]. **/T** [XLLZ10]. **/TiO** [MFZ+18]. **/trans}** [GLOGM+11]. **/Z** [LBM11].

1 [PP19b, IK14, KDÇ12, LKZ+16, MGK+12, MKD19, PP19b, SKHN13, Shi13, ZPB12, Ban12]. **1-** [KDÇ12]. **1-Aza-2-azoniaallene** [WLWT12]. **1'-Azobis** [PP19b]. **1-butene** [ZPB12]. **1-butyl-3-methylimidazolium** [MFK+12, WZZL10, dOLdlV13]. **1-chloroalkenes** [MLB+12]. **1-decanethiol** [FFF10]. **1-Phenyl-1** [IK14]. **1-proton** [LZZ12]. **1-styrylnaphthalene** [Bud12]. **1-substituted** [TT10]. **1.9Å** [SYK+12]. **10-phenanthroline** [YZW+15a]. **11** [GSB10, SACA18]. **115** [HS15, dFR15a]. **116** [COP16, Man16]. **12-vertex** [FSQ+11]. **13th** [Tch13]. **14th** [Ano13-49].

16th [DC12]. **1A** [Dau16]. **1H** [ÖEDB11, YB11]. **1H-imidazo** [YB11].

2 [Boe12, EKD12, KK14a, LJK+18, LV12, Men10, MEEA+13, SAHAA16, Tan12, WWX+11, Zha14]. **2-** [KAOB11, NVPCJ+13, ÖEDB11, YLW+13, Tan12]. **2-adamantyl-thiazolidine-4-one** [MBBT+12]. **2-amino** [RJY+10]. **2-amino-3-methylimidazo** [MLPT10]. **2-azidoethanamines** [SM10b]. **2-carboxylic** [KC11]. **2-chloroethyl** [CZJZ12]. **2-diazo-4** [LDW+11]. **2-dichloromethylbenzimidazole** [PMC11]. **2-dihydro-3H-pyrazol-3-one** [TAY11]. **2-dione** [OPP+14]. **2-dioxetanone** [dSdS13b]. **2-ethoxypyridine** [MCC12]. **2-furoic** [GIO12]. **2-hydroxy-3-methylbenzylidene** [TAY11]. **2-hydroxybenzylamine** [AFC+10]. **2-methyl-3-hydroxylbutyryl-coA** [MFR10]. **2-methyl-4-nitroaniline** [KC11]. **2-pyridone** [HHCA10, MCC12]. **2-RDM** [KK14a]. **2-substituted** [Tug13]. **2.0** [CYC+15]. **200** [KAR12a]. **2D** [BCNR18]. **2E** [KDÇ12]. **2H** [FRNM12, VHTEG15]. **2R** [CPL15].

3 [CWW+16, LKZ+16, SC12b]. **3-** [SC12b]. **3-alkylthiophene** [BMR+13]. **3-aminoacrylaldehyde** [NRS+11]. **3-bisphospo-D-glyceric** [SLA12]. **3-butadiene** [SKTI15]. **3-butadiene-ethene** [SKTI15]. **3-cyclohexadiene** [ZWWY10]. **3-dichloropropene** [ASMP15]. **3-diene** [EI11]. **3-Dienes** [LKZ+16]. **3-dihydro-** [SC12b]. **3-dihydrobenzimidazole-2** [KKG12]. **3-dihydropyridines** [ZYSW17]. **3-dimethylallene** [CPL15]. **3-diphenyl-4-** [YWJ+11]. **3-dipolar** [BL11, YNLD18]. **3-disubstituted** [fXxBhD19]. **3-imino-propen-1-ol** [HNH+12]. **3-imino-propenylamine** [RJA+10]. **3-mesityl-3-methylcyclobutyl** [KDÇ12]. **3-methyl-1-pyridin-2-yl-5-pyrazolone** [PGG12]. **3-Methyl-3-phenyl-cyclobutyl** [SC12a, SC12b, DDÇY12]. **3-methyl-4-nitropyridine** [KC11]. **3.5** [Jan13]. **32** [Tas14]. **34th** [RA10b]. **3A** [LZFZ13]. **3C** [TCCI10]. **3C-SiC** [TCCI10]. **3d** [GE12a, BL19, CLC10, XFW+14]. **3D-aromaticity** [BL19]. **3D-QSAR** [XFW+14]. **3G** [GZSMFN16, VRO+12]. **3H** [TAY11]. **3ylmethylene** [SC12a].

4 [EKN10]. **4-** [DDÇY12, RS11b, SC12a, SC12b, TAY11]. **4-addition** [LW13]. **4-butanetriol** [LL17]. **4-chloro-3-** [DPRK12]. **4-chlorophenol** [ASW13]. **4-chlorophenyl** [ÖEDB11]. **4-dieniminium** [BMX+19]. **4-dienone** [KAOB11]. **4-dihydrolutidine** [TM13]. **4-dimethyl-aminobenzonitrile** [NMHPVG12]. **4-dimethylaminophenyl** [FO10]. **4-dimethylcyclobutene** [MB13]. **4-Dimethylphenyl** [Tan12]. **4-dinitrophenyl** [RNdA+10]. **4-diols** [SBEH11]. **4-dioxane** [Cha10]. **4-dithio-5-fluorouracil** [NA12]. **4-fluoro** [YWJ+11]. **4-hydrogen** [SMRK18]. **4-hydroxylbutyloxy** [RS11b]. **4-methylcyclohexylidene** [KGVG11]. **4-phenylazoaniline** [NVPCJ+13]. **4-triazol-3-one** [CLY12]. **4-triazole** [LLW+11]. **4-triazolin-2** [IK14].

4-trifluoromethylphenyl [SAHAA16]. **4-X-2-hydroxybenzaldehydes** [EKN10]. **400K** [KAR12a]. **4965** [SKHN13].

5
[YTY19, SAHAA16, CSVCB12, CSSK+12, IK14, JLL11, KDÇ12, SZ11, Tan12]. **5-** [MJ11]. **5-Aryl-2-pyrones** [CM12]. **5-benzodiazepin-** [HMA+19]. **5-bromo-9-hydroxyphenalenone** [OA13]. **5-c** [YB11]. **5-d** [CC11a]. **5-diacetyl-1** [TM13]. **5-diamino-1** [LLW+11]. **5-diazadiborinine** [GC18]. **5-dihydropyrrolones** [VGGPdL19]. **5-dihydrothiophene** [HL19]. **5-dimethoxyphenol** [Tan12]. **5-dimethyl-2-phenyl-1** [TAY11]. **5-dimethyl-pyrazole-1-carbodithioic** [SJZL12]. **5-dione** [IK14, KDÇ12]. **5-diphenylformazans** [TT10]. **5-f** [MLPT10, YZW+15a]. **5-fluorouracil** [MR11, NA12]. **5-HT** [CSVCB12, CSSK+12]. **5-methylhydantoin** [SF13]. **5-nitro-1** [CLY12]. **5-triazine** [CLH14, TJS17]. **5-trinitro-1** [MJ11, TJS17]. **5'-triphosphate** [YTY19]. **5-tris** [FO10]. **503** [COP16]. **5d** [GE12a]. **5H** [LW13]. **5H-oxazol-4-ones** [LW13].

6 [BWB+18]. **6-acylbenzothiazolon** [SSTÖ11]. **6-diaminoanthraquinone** [DKS11]. **6-diazaadamantane** [KMK+16, KMM+18]. **6-dien-** [WLS+19]. **6-dinitrophenol** [LDW+11]. **6-distyrylpyridine** [MUPC10]. **6-fulleroid** [Iku17]. **6-hexafluorocyclohexane** [HWWW18]. **6-tetranitrooctahydroimidazo-** [CC11a]. **6-trinitro-1** [CLH14]. **66** [MLW16]. **68-84** [ZCTG18].

7 [Men10, PWL+10]. **7-trimethylxanthines** [SMGZ13]. **7-trinitro-9-fluorenone** [Men10]. **770** [HS15, dFR15a].

8 [WWX+11]. **8-dioxabicyclo** [VOK+18]. **8-naphthalimide** [QHS11]. **8-oxoguanine** [YM12]. **8-substituted** [SMGZ13]. **8-TCDD** [WWX+11].

9- [CRSB12].

= [AGOP18, AM18, BLL+13, BHA19, BBYZ18, CWS15, CDL+19, DPDR11, DD17, DHYC19, EMSB15, EMS16, EAV16, GWM11, HNBG15, HNBS18, HWL16, JLG+12, KSSK16, KMM16, Kuz19, LJL+11, LC16, LL18, LWL19, LGW11, LXD13, MLY+16, MLW10, MZLM17, NBL12, PSK+16, PP19a, Pan16, PCD14, PAKA15, RWW+19, RBTL19, SB18, SMC18, SKS10, SPIL14, SM17, SYQ+10, TW10, TL15, VO12, WSML16, WZW17, WLL19, XYL+18, XZL+12, XCL+18, YLWrL12, ZHL+19, ZCTG18, ZLY+14, dOR10]. **=4** [BEM11]. **=H** [RLTAT19].

A- [XLGA12]. **A/H5N1** [KRH13]. **Ab-Initio** [CS13, RRRV19, TK16a]. **ABAD** [MFR10]. **ABEEM** [DMWY11, ZXY13]. **ABEEM-** [DMWY11]. **ability** [Fin14b, LL18, NCMC+18, NIK19, PSK+16]. **abnormal** [Pan16].

absorbance [RKM12]. **Absorption** [JPPA10, JPP+11, PSK+13, BS11, BDR12, BPK19, CRSB12, CS17, Eil14, FBO+11, HMH+13, ILBS10, JCC10, LWL+12, LXW+14, LC19, Men15, SB10a, SCL19, TZ11, TT10, TCM+12, TG13, WWC17, WLZ+12b, YWR+18, ZQCJ10, ZWLC12, ZQJW13, Zha17, ZI19, dARAV12]. **abstraction** [FRNM12, LGW11, OD12, PM17, SKM11, SCBP17, TIN13, WWHZ13, WZHZ13]. **abundant** [RR11, SG19]. **AC** [RYW+15]. **accelerate** [BR15]. **Accelerated** [KPCV18, ZH15]. **Accelerating** [KFJ+18, TKN13]. **accelerator** [KCDC15]. **acceptor** [ABA11, BLdV19, CMR13, HSS18, IIS+17, KPL+17, KDA+11, LQ13, LYS+19, MANP17, SSK11, ScBsR+10, TSBSM12, ZYL+14]. **acceptors** [PWP+18]. **accessible** [TBST10]. **accompanying** [HSN18]. **account** [Var14]. **accuracy** [KPH+12, ZRLV10]. **Accurate** [LV12, MJ16a, MS14c, Puz16, RVO+14, SLC+18, SYL+18, ZZ18, BBB16, CHH+19, CH17, KS18, LBdV16, Mas10, OK16, SZZ+19, SRMB15, WZW17, WZX15b]. **accurately** [Kub12]. **ACE** [KRC+16]. **ACE-molecule** [KRC+16]. **acenes** [MMF+13]. **acetaldehyde** [AG10b]. **acetic** [DDÇY12]. **acetone** [AMMK11, LdBF+12, TYL10]. **acetonitrile** [JWJ+12, NTGC19, ZDZL11]. **acetyl** [Tav11]. **acetylacetone** [DP12, WZZL10]. **acetylcholine** [Ser11b]. **Acetylcholinesterase** [KMRG13]. **acetylene** [AKC10, BLR12, BL11, NKF+13, TL15]. **acetylene-linked** [NKF+13]. **AChE** [PK13a]. **achievement** [CKYR18]. **acid** [AEKGZ12, BLR12, CF17, DSCO+13, DJB10, DDÇY12, DLM+11, ENV15, EMSB15, GI14, GIO12, GORW19, GCZ+14, Jal10, JCC10, KS11, KB13, KC11, KBF+13, KSS12, KUTS10, LSR+10a, LSR+11, LGM+18, LBM11, LFS+11, LCZL11, MC11a, MZB+13, MK10b, MNE+13, Mit11b, MPGGS19, NHG+12, NHB12, PMEP19, PM17, PP14, PL18b, QZH13, RDB19, Rua10, SPPT15, SMRK18, SJZL12, SHL+13, SACA18, SLA12, SCS15, TV13, TBST10, TPT+13, VF13b, WJ11, YDW13, YSW11, Yu13, ZYL+13, dLdOdAD12, dM13]. **acid-4-nitropyridine-1-oxide** [KC11]. **acid-catalysed** [SMRK18]. **acid-catalyzed** [GCZ+14, KUTS10, LGM+18]. **acid-functionalized** [SPPT15]. **acidic** [EAK+10b, EAK+10a]. **acidities** [SK12a, TWR15]. **acidity** [JLL11, NHG+12]. **acids** [AM13b, Cza18, DWZZ15, KK11a, KyH13a, Kuv10, Pog12, PSK+13, SAG13, SN12, VF13a, WHM14, ZDZO10]. **acridine** [CRSB12]. **acridine/silica** [CRSB12]. **across** [KB12, MK10a, NBZG16]. **acrylamide** [PDNC14]. **acrylate** [LD17, LSG+14, NAK+17]. **acrylonitrile** [LD17]. **act** [PWP+18]. **acting** [ZZZ+18]. **actinide** [Gag11, JLL+18, Mag14, RMY+13]. **actinide-based** [Mag14]. **actinides** [MZST16]. **actinyl** [ZQXP17]. **action** [PRG+10, PM17, TTD13, WLD+10]. **activated** [GMM+18, HB14, Yak10]. **activating** [SBSD18]. **Activation** [MFOH18, Che12, GLT13, GZBH18, LNGW14, LCM+11, NZLG15, PRPU+13, SS18b, Sri19, YYI+12, YS18]. **activator** [YSA+11]. **Active** [SKTI15, WCGD12, DPRK12, EM19, GRD11, KM12b, KSY+11, LKd+16, PK13a, RDB18, SBL11, TYN13, VMR11, dCDC+11, Rus14]. **activities**

[BD14, Hat13, MPMCM+11, RCM+19]. **activity** [ASD18, BGJSM+18, CZJZ12, CWL+13, CJGTL12, DSD18, DMBJ15, ESBVJY12, GTSC+19, HSYM11, JB11, LCG12, LWH+12, MLC+11, PGG12, RCM+19, SSTÖ11, SSB+12b, ZYL+13]. **acute** [PI13]. **acyclic** [BBKO16]. **acylbenzothiazolon** [SSTÖ11]. **acylhydrazones** [Cao17]. **acylium** [FDMR11]. **acylphloroglucinols** [KM12b, MK10a, MK12]. **adamantane** [BBKO16, GZ14]. **adamantane-based** [GZ14]. **adamantyl** [MBBT+12]. **adapted** [Ali19b, ANC+15, CB10, SR12, TPCJ+12, VRO+12, WH12, YKN13]. **Adaptive** [BG11a, BR15, Lya14, MBSMJC18, ZKW17]. **adatoms** [PP10, WDJ+17]. **added** [Fuk12]. **Addition** [DI11, Buc11b, CAAI12, DP12, DFK16, Dum12, GW13, GMT18, JSLH14, LCM+11, LW13, MXC18, PDNC14, SHL+13, SDR+13, TIN13, TBHL11, WZZL10]. **addition-substitution** [Buc11b]. **additions** [SFW12]. **additive** [KF19]. **additives** [YZZH15]. **Additivity** [BMB16, RLER10, Dob14]. **address** [VVJ15]. **adduct** [DWGX12]. **Adducts** [MK10a, BAB+18]. **adenine** [MYZ+10, SOM10, TSH17, XSLF12, YTY19]. **adenine-thymine** [XSLF12]. **adenine-uracil** [MYZ+10]. **adenosine** [DSWL11, PRG+10, WYWL13, YTY19]. **adenosylmethionine** [WYWL13]. **adhesion** [dOdONM12]. **adiabatic** [Bud12, CH17, DMAB12, DM12, HGB08, HZW18, KB12, LV12, MPT11, MPTZ13]. **adiabatic-to-diabatic** [DMAB12, DM12]. **adjustable** [SZZ+19]. **Adjusting** [TW10]. **admissible** [TÁ10]. **ADP** [KTI+12]. **adrenoceptor** [CSVCB12]. **adsorbates** [BWW10, LRKM10]. **adsorbed** [Hog13, JCCZ12, RFMC19, TTM16]. **Adsorption** [CA17, DI18, IK18, NA12, SQ10, UDS19a, UMS13, BGMD15, BAP13, CTW12, CAO18, EFO11, EO11, FFF10, FTB11, GP13b, HLZ+14, HCL13, Kim18, KF17, LV19, LZ12, LWX+14, LIK15, NBL+14, ONBP11, PK16, RD14, RJLPGH+13, SD16a, SR19, SM19, VSMK13, VDG13, WJY15, WLH+19, WZC+12, WH18, ZDZL11, dLdOdAD12, GD11]. **adsorptions** [FZH+18]. **adsorptive** [HCH+18]. **Advances** [AK11, MCCGM+19, Nag16a, Liu15a, Ped16, Ban12, Mor13]. **aerobic** [KBF+13]. **aerogen** [EAV16]. **aerogen-bonding** [EAV16]. **affected** [VGS10]. **affects** [GJ18]. **affinities** [DTEMK11, KKT13, KKT14, VF13a]. **affinity** [CSSK+12, DPK18, DJ18, ESLM19, KKM+12, Kry11b, Kry12b, Shi13, dCSDdMC13]. **after** [GD11]. **Ag** [MSOV13, OD16, PAPCMM+16, SZZZ11, SYQ+10, XWC11a, ZPR10, AGG+18, ESBVJY12, JFT13, LRKM10, PSK+16, RK14, SQ10, WLL19, ZRR+11]. **against** [FMP+17, GAI19, KF19, SBKJ18]. **AgBr** [RS12a, RS12b]. **agenda** [SG14]. **agent** [MB14, PPK+13]. **ages** [Nic14]. **aggregates** [ATS+11, TFB11, WKE17, ZLE17]. **Aggregation** [YLH+19, GDM+10, MAD12]. **aggregations** [BBKO16]. **AgOH** [KSST12]. **agonists** [Ser11a, Ser11b]. **agostic** [HHL12a, HHL14, WLS+19]. **AgSi** [ZCP11]. **ahead** [HJK14]. **AHHCF** [dOR10]. **aided** [GbZA10]. **AIM** [GWZ+14b, NRHJ11, PK13a, RJY+10, RJA+10, UDVD10, ZZL+11].

Aiming [BBB16]. **Al** [CWS15, CDL+19, HHL12a, HHL14, JLL11, LXD13, MLW10, MFK+12, Oni12, Sat11b, TW10, XWC11a, CRB+12, DCDD10, DSZB18, KYLC19, LLZZ10, MCP10, NH11, Pan19, Sat11a, SUL+11, TZD+19, VDG13, WJL+10, PS13b]. **Alanine** [VO12, ZPR10]. **AlB** [RRRV19]. **alcohol** [Pli18, SCL19, dCDC+11]. **alcoholamines** [LCT14]. **alcohols** [MMM+12, SGKG12, SK12a, ZZC12]. **AlCoN** [AAAM12]. **aldehyde** [AG10a, LCS+11a, PWH+12, ZSS+13]. **Alder** [CM12, Iku17, LW11, MIKH19, ZLWL16, ZXY13]. **aldose** [SSdS17]. **aldose-ketone** [SSdS17]. **Algebra** [RW12, Lya14]. **algebraic** [SCLCPB12, SÁBA+12]. **algebras** [WH12]. **algorithm** [AFM+10, CGG18, GI11d, IG11, MCP10, SGH10]. **algorithms** [CL08, TB15]. **AlH** [NH11, SLZ+11c]. **aligned** [HV11]. **alignment** [CLL+11]. **aliphatic** [PI13, SN11]. **Alkali** [ČFČ11, Ber13a, HWL16, HWWW18, SHE10, SM14c, UDS19a, UDS19b]. **alkali-atoms** [UDS19a]. **alkali-based** [UDS19b]. **alkalide** [SM17]. **alkalides** [XWCY11]. **alkaline** [Ali14, BL10, CZCW19, DTEMK11]. **alkaline-earth** [DTEMK11]. **Alkalized** [STM18]. **alkaloid** [LMCZ11]. **alkaloids** [JSLH14]. **alkanes** [GZBH18]. **alkene** [ZSS+13, ZFW+13]. **Alkene-3-quinolinecarbonitriles** [ZFW+13]. **alkenes** [CAAI12, KBJ17, YZZ16, ZYSW17]. **alkyl** [ESS13, LYW11]. **alkylaromatics** [BMR+13]. **alkylation** [IUMVB10]. **alkylidene** [VGGPdL19]. **alkylthiophene** [BMR+13]. **alkynes** [LW15, SLS+15]. **all-** [HWWW18, LCB10]. **all-electron** [MPD+10, MPZWD10, NDM+12]. **all-metal** [MLW10]. **all-nonmetal** [JHL+18]. **allenoates** [XZG+18]. **allosteric** [ŚKB18]. **alloxan** [KB13]. **alloy** [BXR+13, VDG13, XGH+18b]. **AlN** [AAA12, RJLPGH+13]. **AlNiN** [AAAM12]. **AlO** [SZ11]. **along** [IKS08, IKS10, KRG+13]. **AlOOH** [MMC+19]. **alpha** [MBTVR12, SLS+10]. **Al —** [TZD+19]. **alternant** [DB13b]. **Alternative** [CSTA16, COCF+14, GZF14, MJ16a, PCK19, SKLC19, Szc18]. **alumino** [Ped16]. **alumino-silicate** [Ped16]. **aluminosilicate** [PBM10]. **aluminosilicates** [DCFD10]. **Aluminum** [ALK18, AGB19, ALK19, HTM10, IIW+11, Kar12b, MMC+19, MS14b, MM11, PMH+16, SM19]. **aluminum-bismuth-nitrogen** [MS14b]. **Aluminum-poor** [ALK18]. **Alzheimer** [Bal16, MPTR12]. **Am** [PKK14]. **AM05** [MA10]. **AM1** [PI13]. **ambient** [Ma14, WCGD12]. **ambiguity** [Fin14b]. **ambiphilic** [MAN15]. **America** [CJBMMAPR19, MCCGM+19, MMCNV19]. **American** [GRCGRRHT19]. **amide** [TPT+13]. **amido** [JLS13]. **amido-amine** [JLS13]. **amidogene** [Met11]. **amine** [HS11b, JLS13, LCM+11]. **amine-imine** [HS11b]. **amines** [KSAK17, LSR+10a, LSR+11, LW15, RZG12, TV13]. **Amino** [DSCO+13, AM13b, Coo12, CF17, Cza18, DJB10, Jal10, KyH13a, KSS12, MLPT10, Mit11b, NHG+12, Pog12, QZH13, RJY+10, Ril10, TAY11, VHTEG15, WHM14, YSW11, ZCC11]. **amino-2H-imidazole** [VHTEG15]. **aminoacetonitrile** [CdLdSC18, NC11]. **aminoacrylaldehyde** [NRS+11]. **aminobenzonitrile** [NMHPVG12]. **aminocarbonothioyl** [KDÇ12].

aminoguanidine [RCM+19]. **aminonitropyrazole** [RGST12]. **aminonitropyrazole-2-oxides** [RGST12]. **aminophenanthridine** [VBO+15]. **aminopyridine** [NFQ+11]. **aminopyridine-containing** [NFQ+11]. **ammonia** [EO11, MNV+17, MFOH18, NZLG15, RRVJ10, VPOG19, ZMB+17]. **amorphous** [LRKM10, RKM12]. **amphiphile** [KKH+13]. **amplification** [MJM19]. **amplifier** [Val13]. **amplitude** [XXJ+16]. **amplitudes** [MPT11]. **amyloidogenic** [MAD12]. **analog** [DC14a]. **Analogies** [SBD+16]. **analogous** [BB16, GI11f, XLZ+19]. **analogs** [ALK19, ALB18, Buc12a, For12, MGK+12, SLA12, ZWZK19, dSdS13a, TFMC19]. **analogue** [PWP+18, VFCSC17, ZRY+13]. **analogues** [HHYC+18, KMMS17, LLZ+14, NIK19, ZKWZ17]. **analyses** [KTI+12, Tsu15, XXbX+13, Yu13]. **Analysis** [CMCN11, FC19, HITU16, RPBB11, RS11b, VLG12, dSdS13a, AB16b, AC19, AOT+18, AOLB12, Ang10, ALRAE11, BF11, BDFM10, BEM12, BL10, BG13, BWE16, CTVA12, CP11, CDT12, CP13, CC11b, Dil13, DP16, ED16, EMED+12, FT15, FKC12, FDG18, GWZ+14b, GN19, GDM+10, GKT+12, GWME18, GMP+11, HCH+18, Haj18, Han19, HLMO11, HMH+13, HYD11, HW12, JN13, JAB12, Kar12b, KRG+13, LNGW14, LB18, LZ10, MFR10, MHT+08, MMCN+11, MGB18, MEEA+13, MBTVR12, Mor11, MOH+12, NH18, NZ13, NZLG15, OAT+13, OA13, OSJ+12, PH12, PCK19, Per10a, PMEP19, PWP13, RCM10, RAMB18, SAS+12, SA18, SGB11, SDP+16, SBEH11, SD12, SRA+11, TM19, TCS10, UDVD10, VV18, WJ11, XHZXXZ10, dA12, dOdCMUdALR11, AGNS14, SJW13, TD11]. **Analytic** [CSG14, Kry12a, MAF19, RW11]. **Analytical** [BLB+18, BVA+14, FKBG19, MPRCEG12, NDP10, SMV11, ZHF12, AEÖ12, HYZS12, HYZS19, ISN13, Mam13, Pit12, SZZ+19, ZRLV10, Cam10]. **analyze** [HEVMSA+19, RSCS10]. **analyzed** [CSSK+12]. **Analyzing** [Ale13, MBSMJC18, BCGC12, HXDY16, Luz11b]. **Anatase** [JK12, ATS15, EO11, GP13a, HCL13, OGvSG18, VS19, ZK12]. **anchor** [Jan10]. **anchoring** [LPO+12]. **anchors** [Jan10]. **ancillary** [YZW+15a, ZLLS10]. **andradite** [MPZWD10]. **Andrés** [Mer11]. **anesthetic** [PSPS11]. **angelicin** [EG10]. **angiotensin** [dSSdSGA12]. **angle** [DMAB12, DM12, DSCO+13, LZFZ13]. **angular** [Ash18, AKR12, HSN18, MOY13, SVPTM+10, TÁ10, YM14]. **Anharmonic** [CM17, AF19a, BBB+12a, CK13, DK13, IROW10, Kaw15, Tou11a, VOAH18, VBC+12a, VBC+12b, VV12, VV13]. **aNHC** [Pan16]. **anhydride** [DNCKCS+12, ZPW16]. **anhydrous** [CTVA12]. **aniline** [Zha15]. **animated** [Ash18]. **anion** [BDF+18, CWZ+10, DWZZ15, GXZ+14, HFL+17, LWZ+14, MTS15, ONBP11, Pat15, PM17, RGPZD13, RGR12, YM12, YT14, ZLWL16, ZLWZ16]. **anion-** [DWZZ15]. **anion-based** [LWZ+14]. **anionic** [BMB12, CADSG18, DHYC19, GLPA10, TD19, WTP+19, XZL+12]. **anions** [Bar11, DZO12c, HFA+19, LCL+10b, MPM15, MMSC19, RWW+19,

TZD+19, XSLF12]. **anisol** [AMAC12]. **Anisotropic** [BMTT11, LDZG16]. **anisotropy** [Ali14, MOY13]. **annealing** [MOE+11, TCG17]. **annealing-based** [TCG17]. **annelated** [PPK+13]. **annulation** [HZZ+19, XZG+18, ZQW+17]. **anode** [UDS19b]. **anomaly** [Kar12c]. **ansatzes** [Fin17]. **Answers** [Tas14]. **anthranilic** [MC11a]. **anthropogenic** [Mor11]. **anti** [CCC19, Iku17, MPE11, ScBsR+10, Zag11]. **anti-Bragg** [Zag11]. **anti-Bredt** [Iku17]. **anti-inflammatory** [MPE11, ScBsR+10]. **antiaromatic** [RBZ15]. **antibiotics** [LSR10b]. **antibonding** [CCL+16, CFV18]. **anticancer** [CZJZ12, DSD18, MKHM11, PPK+13, XZ11]. **Antidot** [YMY+13]. **antiferromagnetism** [Fuk12]. **antiinflammatory** [YINM13]. **antimalarial** [AB16b, LTdSJ+10, RDM+11]. **antimicrobial** [ESBVJY12]. **Antioxidant** [XLZ+19, KDA+11, KK11d, ZYL+13]. **antioxidative** [TIKN11]. **antiparallel** [SJW13]. **antisense** [UJSJ13]. **antisymmetric** [TKN13]. **antitrypanocidal** [MLC+11]. **antitrypanosomal** [LWH+12]. **antitubercular** [SD13a]. **antitumors** [CCL+10]. **antiviral** [MB14]. **any** [FMPM+14, RMC19]. **AP** [NYS+10]. **AP-UBD** [NYS+10]. **AP-UCC** [NYS+10]. **apoptosis** [QZH13]. **applicability** [BJ17, FCS13a, FCS13b, WKE17, ZT13]. **Application** [ASK15, DSL15, ENV15, JH15, NMSR14, OVT+16, PBR18, RZG12, Rom10, SCBP17, TGRP19, TLC+17, TPCJ+12, AVG19b, Cha11, GfWlZ11, HW12, KLK13, LLLT12, LVP12b, MPD+15, MT10, dMOB12, SKV12, XWC10, AEM+12, DLRMFY10, HBMM11, IKS08, IKS10, KPH+12, Luz11b, LKd+16, MPRCEG12, MJ11, PCR+11, RC11, SR12, SS12]. **Applications** [CW11, HFBC19, Lar11, MSNP18, Ném14, SDP+16, AMAM18, AMMC19, CJBMMAPR19, CC12, GMM+18, HKZZ15, HIL19, Hil13, Kap12, LGL+19, LMZY15, MANP17, MPMCM+11, MML+16, MG12, MML11b, Nic11, RMC19, SSS15, TSvL+16, TSS+15, YKM+15, YFY17, ZSZ14, CW13b, ZDZO10, Mor13]. **applied** [BVRM10, CF11, CL08, FCC11, HM11, NS13, PIS18, SMV11, SXH18, SS19b, WR14a]. **Approach** [LFF+10, AV19, ATL+14, AK17, AB18, AOLB12, ART08, AT18, ALB18, BPVDB11, BLB+18, BvWG14, BVP14, BLKB11, BAB+18, CGG18, DVDBM11, DLM12, DMBL16, DLP17, Exn11, FAFR12, Fri12, FUE+12, GBK18, GFPAV19, GR10, GRD11, HR19, JLL11, KP10, KC18, Kit17, KYLC19, KSO19, LBW11, LSR10b, LSR+13, LdAA+11, Mak15, MGK+11, MNP19, MGN14, MSVMCI10, MBBT+12, Mor12, NSN17, NNSN17, NTGC19, NVPCJ+13, OT14, OPC17, OGvSG18, PT13, Pir13, PBR18, RZ17, RBGGM18, RMC19, RNC+14, RC11, RdPW+12, SCLCPB12, SÁBA+12, SB10a, SC12b, SPSA11, SSB12a, SD13b, SC10a, SSA18, Sri19, SKL10, Tou11a, TPCJ+12, UYN+13, WZ10a, WWB+14, WR14a, XNL+14, Yam11, YK13, dSdS13b]. **approaches** [AV19, AMMK11, BBA+16, Cap16, CKL16, DC14b, EML+11, IAK13, ILBS10, Jia15, LMZY15, MDC15, Men15, NYS+10, PBB15, PJP08, Sko16, TKSK17]. **appropriate** [FSB16]. **approximants** [DB13a]. **Approximate** [FKBG19, HYZS12, HYZS19, ZLJ11, AST16, HMH10b, KYH+13b, Tou11a, ZRLV10]. **approximately** [KSN+10]. **Approximating** [Fin16b]. **approximation**

[AY15, BC15, BC16, BR12b, DVP18, Fin15, GZSMFN16, HMH10a, HVR18, IIH16, Kut13, PCV19, RAN18, SÁBA+12, SK17a, Sut12, VVN+16].
approximations
[CLXD15, FMMD+10, GZSMFN16, Per18, PBB15, RBD+10, SGL+16].
APSG [JNZ+14]. **APSG-based** [JNZ+14]. **aq** [DSZB18]. **aqua**
[BSPK11, MGK19]. **aqueous**
[AMMK11, CTVA12, DZO12c, GCDNGS12, JCC10, KS11, KSS12, LGZC15, MB14, MNE+13, MPL+11, PS10a, RZG12, RCM10, SM10b, TIKN11]. **AR20**
[CWB+13]. **Arbitrary** [IAA15, WC14, ZHF12]. **archea** [SLS+10].
Architectures [AH19, GAPK+19a, Lya19]. **area** [TBST10]. **arene** [Pli18].
argon [Lan10, SH19]. **arising** [JMPP19, SGG+10, TFZ+15]. **armchair**
[GMT16, SD16a]. **Armiento** [MA10]. **Armiento-Mattsson** [MA10].
AROCM [ZPW16]. **Aromatic** [CJMC19, TKS11, BRS10, BG13, Bla15, CA17, CAO18, DI18, GMT18, KUTS10, KKS+11, LV19, LL18, LW18, LVP12b, MLW10, MSS11, NHG+12, PCML08, RVNP12, RB18, RBZ15, Ril10, SFM13, Sat11a, SMR14, VC13, VRO+12, WvRSW+11, Yam10].
aromatically [Ril10]. **Aromaticity** [ALB18, XWC10, ATM17, BL19, CYL+19, EMK14, HM10a, Luz11b, MSOV13, PS13a, RB18, WCY+10].
aromatics [HBMM11]. **arranged** [KMK+16]. **arrangements** [Coo12].
arrays [CKB+19, XMZ+12]. **Arrows** [Brä13, ABM+19]. **arsenate**
[HCH+18]. **arsenide** [KP11, UDS19b]. **art** [NBZG16, PB10]. **articaine**
[PSPS11]. **Article** [NT15]. **artificial** [FCC11, YYI+12]. **aryl**
[BMF13, LW15, MHZ18, MSY+12, CM12]. **arylamides** [DDF+12].
arylation [SH18b, SGL19, Zha15]. **arylcarbamates** [DDF+12]. **ASA**
[TBST10]. **ascorbic** [ZYL+13]. **Asia** [WZ10a]. **Asn** [ScBsR+10]. **AsP**
[LJSS12]. **asparagine** [GSZ10]. **aspartame** [OT14]. **aspects**
[Hop15, IK14, LEU+11, Luz12, PK13b]. **aspirin** [EA12]. **assembled**
[KKH+13, QTCL10]. **assemblies** [GFRdG11]. **assembly**
[FFF10, JW19, LYW11, VFCSC17]. **Assessing**
[AM13b, DGA+13, PK13b, TCA10, LYD+18]. **Assessment**
[CC19, LCT14, SBKJ18, Vie17, BVCAP12, DVP18, JHSG18, KKH18, KSS12, LKDC11, OKR12, PSK+16, PI13, ZST+10, ZT13]. **Assignment** [LCL+10a].
assignments [LYR+17]. **associated**
[DW12, GI11a, Han19, MBTVR12, WJ11, YKM+15, dCSDdMC13].
association [NWQX11]. **assumptions** [PIS18]. **astrochemical** [For17b].
astrochemistry [For17a]. **astromolecule** [CdLdSC18]. **Astronomical**
[Puz17]. **astrophysical** [dSCC12]. **asymmetric**
[Hop15, JSLH14, LMCZ11, LW13, MMP11, PBB15, SHL+13]. **Asymptotic**
[BEM12, Han19, RBD+10]. **Atmospheric**
[HYZ13, BZZ15, BXZ+19, CGIAI12, LLW+12, MXC18, MPGGS19, Var14].
atmospherically [MTS15]. **atom**
[AD17, Bay19, CC11b, DWJZ11, DLG12, DSSM19, Esr18, EM19, FAFR12, GI14, GAMM10, GV11, HWWW18, HXX15, Ign11, Ign12, JWJ+12, JZZH17, KH10, KKL+16, Kin13, KDA+11, KFS13, LGHL11, LNGW14, LKLW11,

MFLK11, MAPS18, MNS11, MR18b, Pea11, PSC15, Pup11a, PJ19, RZ17, RZSZ18, RAFR18a, RAFR18b, Roy15, Roy16, RRCO11, RR19, SRPD16, SK17a, SKM11, SL13, SS12, TBB+19, TW10, WWHZ13, Zak13, ZS12].
atom-bond [AD17]. **atom-centered** [KFS13, Zak13]. **atom-pairwise** [KKL+16, PSC15]. **Atomic** [AST19, Ols11b, PNC19, SV11, ABS11, ALRA10, ALRAE11, CRA+11, CF11, CB10, Fin14a, Fin15, Fuk12, Gra08, Gra11, GE12b, HST13, IFT14, Lai11, LRMAA19, MGK+12, Mam14, MC11b, May14, MS17, NDH10, Nic11, NE11, PUH+11, RLER13a, RAGM10, Rom10, SLG11, SMV11, Sch15, SD13c, STM17, TMC+13, ZY13, ZLWY13, ZZZ+18, vLRRK15]. **atomic-wire** [SD13c]. **Atomistic** [AGG+18, Mai14, BMR+13, CLKD15, MMP+18a, vL13, Zha17].
atomization [Vyb08]. **Atoms** [LSC+18, OA13, TBRIS12, AMK10, AM10, BHMN19, BAX+19, BSO11, Dil13, DSSM18, EMSB15, GBS17, GLT13, GZSMFN16, GI10, GI11b, GI11c, GI11e, GS11, Gra11, HMP+11, HMA+18, IG11, JEA13, JMX+15, Joh17, Leh19c, LKJ13, LZW+15, LHX+19, LLH15, Luz11b, MOY13, MFLK10, MJ11, NS10b, NIT16, ONBP11, OD12, PRPU+13, PWP13, PNC19, RLW+13, RD14, RBVAG18, SBMM11, SBM16, SR19, Sha18, Sto18, SKL10, TBRIS10, TBRIS11, TH12, TXK+19, TFMC19, TLC+17, UGWL18, UDS19a, WLS+19, YJ17, ZS11, ZCG+16, ZHI17, ZZZ+18, ZJS13, dSTH17, dCGAMV12, Leh19a].
Atoms-in-molecules [OA13]. **ATP** [BGJSM+18]. **attached** [HMP+11].
attachment [DSVP15, Kry12b]. **attack** [LZFZ13]. **attending** [GWME18].
attenuated [NDP10]. **attenuating** [CF14]. **Attosecond** [Vik11a, SVPTM+10]. **attraction** [MSRn+11, SYQ+10]. **attractive** [DCD11, WH18]. **Au/SAPO** [GSB10]. **Au/SAPO-11** [GSB10]. **AuCl** [SM14b]. **augment** [BDG17]. **augmented** [CLKD15, D'y16, KRC+16, SZS+10, SLZ+11c, SLZ+11a]. **AuO** [SM14c].
aureusidin [KK11d]. **aurones** [XLZ+19]. **AuSi** [BCK19]. **Autler** [HYH+10]. **autocatalysis** [Pie12]. **Autocatalytic** [dM13]. **autocorrelation** [MPV+11]. **AutoDock** [CRFR11]. **autoignition** [MOH+12].
autoionization [DE18]. **autoionizing** [Cor16]. **automated** [KMNSP19, MHO+15, NKWT19, PBB15]. **Automatic** [MML+16, CW11].
AuX [LC16]. **auxiliary** [CEFMK12, GS10, KFJ+18].
auxiliary-density-matrix [KFJ+18]. **averaged** [ABLT11, CP13, RS12b, RSN12]. **avian** [KRH13, PCML08, WZ10a, ZBK15].
axial [LGS+16]. **axiomatic** [AK17]. **axis** [Lad14, XTLA13, XTLA14]. **aza** [DC14a, VGGPdL19, WWL+11, WLWT12]. **aza-Möbius** [WWL+11].
aza-oxypentadienyl [VGGPdL19]. **azanaphthoquinone** [PPK+13].
azauracil [MPE15]. **azide** [Per10b]. **azides** [AEKGZ12]. **azidoethanamines** [SM10b]. **aziridination** [MCC13b]. **azo** [MNP19]. **azo-bridged** [MNP19].
azobenzenes [JPP+11]. **Azobis** [PP19b]. **azochromophores** [FSB16].
azocompound [NVPCJ+13]. **azodicarboxylate** [KI15]. **azoles** [SK12a].
azomethine [DI10, LFTL18, XZG+18, ZQW+17]. **azoniaallene** [WLWT12].

azopyrroles [Jac12]. **azosulpha** [EAK+10b].

B [AGOP18, BCGC12, CWS15, CDL+19, GWM11, JLL11, Kal18, LCZ15, MLY+16, MKD19, PP14, VVAO12, WCS+13, XYL+18, YGLL10, ADB10, CWSZ13, CD12, HWL16, HZS14, KGK13, LCL+10a, LL18, LFP+19, RLTAT19, SB18, SSB19, SXS+12, SCZG12, TCSD12, XLGA12, YLH+19, YGLL10, ZYL+14]. **B-H** [SB18, SSB19]. **B-like** [SCZG12]. **B-spline** [HZS14]. **B-type** [XLGA12]. **B/PR** [GWM11]. **B2** [PP19a]. **B2-type** [PP19a]. **B3LYP** [JdOS16, Lu15, NDM+12, WZX15b]. **Ba** [MPD+15]. **BACE1** [VHTEG15]. **back** [LBdV16]. **back-donation** [LBdV16]. **Backbiting** [LSG+14]. **backbone** [PT13]. **bacteriochlorophyll** [MSBF18]. **bacteriochlorophyll-a** [MSBF18]. **BaFe** [WSCL11]. **baicalein** [MMMM12]. **balance** [AZD+11]. **Balancing** [TMC+13, NMSR14]. **band** [BA13, CRSB12, DM16, IMS+13, KA13, Lad14, RKCK19, SSB12a, VLM+10, XTLA13, XTLA14, YHL+13, ZQCJ10]. **Bandgap** [WCL+17, VVY18]. **bandgaps** [GbZA10]. **bands** [BW15]. **bandstructure** [MMA10]. **bang** [CF11, MSAB19]. **barium** [MMR+10]. **barrier** [CYK17, Cho19, DLM12, DDF+12, DCR10, LLF+12, NTCG18, TCG17]. **barrierless** [DSZB18, dMOB12]. **barriers** [DI18, SR19, SH18a, SCBP17]. **Base** [SM13, ACF+11, AZD+11, BTH18, CPF12, CW16, EMSB15, KSS12, Kuv10, LSR+10a, LSR+11, Lad14, MSH13, OM13b, PP14, SMEH15, XSLF12, XTLA13, XTLA14, ZKWZ17, ZBG+19, ZSQ+10, dSTH17]. **base-free** [ZBG+19]. **based** [AB16a, AV19, AOT+18, ATM17, AVG19b, AVG19a, AMMB+18, BP13, BMRM19, BSSS19, BBYZ18, yBZfC18, Bra10, Buc11b, BSO16, CWW12, CLC10, CwCW+11, CLL+11, CJBMMAPR19, CGG18, CC19, CKYR18, CL08, DKZ+10, DTVP+12, Dw13, DB13b, Exn11, FM16, FT15, FKC12, FSST16, GZ14, GZMC11, HR19, HJK14, HW12, HAX+18, HVR18, JMX+15, Jeo18, JNZ+14, KKM+12, Kim18, Kim19, KSAK17, KYH+13b, KF19, Kry12c, KM19, LPO+12, LCL+10a, LV12, LQZZ12, LXW+14, LYW+19, LCK+16, LXD13, LLZ+14, LWZ+14, LEU+11, MXC18, Mag14, MDC15, MANP17, MCP10, MGP16, NKF+13, NTGC19, NZ13, OPS10, OPAVM18, OAT+13, OK19, PI13, PABSK16, Pir13, PSPS11, PMAP12, PSK+13, RI19, RS11b, SYK+12, SMGZF19, SKHN13, ST15, Shi18, SK11, SLZ+12, SSS15, TCG17, TMC+13, TK16b, TGRP19, Tsu15, UDS19b, WKE17, WJY15]. **based** [WYM15, XWP+18, YZ13, YZZH15, YKN13, YSW11, ZZZ+18, ZKW17]. **bases** [BS14, EG10, EAV16, GGP13, JS18, MMR+10, PS10a, XZ11, Yak11, YDW13]. **basic** [GI11b, GI11c, BM16, KK14a, Nic11]. **basicities** [VF13a]. **basicity** [HFL+17, SM16]. **Basics** [Bae16, Mos14]. **basins** [HS11c]. **Basis** [JA12, KYS13, KB19, Rud12, VPA11, YFY17, Ali14, ANC+15, ABA11, BŁ16, BVCAP12, CHH+19, CC19, CML+16, DCZ17, Fuk12, GBK18, GTR11, HH18, Hil13, Hog13, JH15, KRC+16, KPCV18, KUY16, Kut13, Lai11, LV12, LWL+12,

MSNP18, MG12, NDM+12, PCD14, PBR18, RZSZ18, RLER14, RVO+14, RLZ12, SKTI15, SXH18, SZS+10, SLZ+11c, SLZ+11a, SLS+11, TCG17, TWR15, UGWL18, UV18b, VSS11, VRO+12, WSV10, YM14, Zak13, ZF15]. **bath** [YK13]. **batteries** [Ali19a, AVG19a, KLK13, Kim18, UDS19b]. **battery** [KJ15, Oni12]. **BAu** [LL11]. **Baylis** [ZQW+17]. **BaZrO** [GMP+11]. **BB** [YGLL10]. **bc** [RDM+11, RRB12]. **BCl** [MPM15, SLZ+11b]. **Be** [BLL+13, GCD13, NW12, RFEGPP+16, WCY+10, XZZ+10, YLW+13, Kuz19, Lu15, Met11, Nes11, Sza13, AM18, DTEMK11, DZO12b, GPM+15, Mit11a, RSN12, dOR10]. **beam** [AGG+18]. **Bean** [BMB12]. **bearing** [CMR13, CJMC19, MCK17]. **BEC** [GdLT12]. **beginnings** [QBRA18]. **Behavior** [GST11, DSC+11, DLM+11, LG12, MC18a, PNC19, RF10, RGS+13, SHE10, SM14c, SMGZ13, YLH+19]. **behaviors** [HKLW13, VSL+15]. **BeN** [UDS19a]. **Benchmark** [AV19, JZZH17, OH19, PB10, HM12, LP10b, OKR12, RS12a, RS12b, RSN12, Vie17, WZW17, YWH12a, YWH12b]. **benchmark-quality** [OKR12]. **Benchmarking** [CKB18, KDOR17, MXC18, Man16, MBSAG16a, PRFR17, MBSAG16b, Rus14, VBJK18]. **benchmarks** [Lat13, LJ13]. **bending** [GFB12a, IMS+13, ZZ15]. **bent** [HV11]. **Benveniste** [WSV10]. **benzal** [YWJ+11]. **benzal-5-pyrazolone** [YWJ+11]. **benzaldehyde** [ZSHL14]. **benzamide** [DPRK12]. **Benzene** [CGM12, CL11, CCS13, DKZ+10, DJ18, FZH+18, HAX+18, HhGqZZ17, JW19, KBMM10, SPSA11, Sch12a, SGL19, TG13, VC13, WDSL14, Yu13, ZS12]. **benzenes** [JW19]. **benzenoid** [ACT19, HIL19]. **benzenoids** [BR08, BR12a, RB08, RB11a, RVNP12]. **benzimidazole** [WLL+13]. **benzimidazoles** [LZB10, XFW+14]. **benzimidazolyl** [SHW+13]. **benzo** [ÖEDB11, ZLS+18]. **benzoazacrown** [FBU+11]. **benzoazacrown-containing** [FBU+11]. **benzocatafusenes** [MA12]. **benzochalcogenadiazole** [BSSS19]. **benzodiazepin** [HMA+19]. **benzofuran** [ASMP15]. **benzoic** [PMEP19, SN12, SHL+13]. **benzoin** [ZSHL14]. **benzonitrile** [ZRGE+19]. **Benzothiadiazoles** [Net12]. **benzoxazole** [YLW+13]. **benzoyl** [LD17]. **benzyl** [EHKD11, EKD12, SJZL12]. **benzylidene** [DDÇY12]. **BeO** [Ali14]. **BEPOX** [KZZ13b]. **Berry** [DMAB12]. **Beryllium** [NW12, AM18, DZO12b, Nic11]. **BeS** [DAR+11]. **Best** [Ish14, CB10]. **beta** [MBTVR12, PTD+12]. **better** [BLL+13]. **between** [ASHF13, AD17, ALMY18, BLR12, BHA19, BL11, BLWJ17, BWB+18, BTH18, BWE16, BB16, CZJZ12, CCL+13, CCC19, Cha10, CCS13, CDL+19, CF17, DNCKCS+12, EKN10, EHKD11, EKD12, EEMSS14, EAV16, Fin16a, Fin17, GXZ+14, Gra08, Gra11, GE12a, HCH+18, Han19, HMH+13, HIL19, JEA13, JLS13, Kan11, KdPNNS16, KMMS17, Kim16, LKOS17, LdMCdA+12, LMZ+11, LLG+12, LFTL18, LFP+19, LBdV16, LWC+10, LZD+11, LCS+11a, LCH+11, LCS+11b, LXLL11, MYZ+10, MFK+12, MSY+12, NBL12, NZ13, NAK+17, NBI+10, NL11, NRGS11, OKK10, PDNC14, PM12, RYM12, RFN+12, RMJ11, RNB+10, RS13, SSI+10, SD16b, SKHN13, Sch15, SM17,

SBD+16, SCZH16, SC18, Tav12, TDOD17, TYL10, TXL10, TL15, UV18b, WWC17, WLL11, WLWT12, WWD+15, WHM14, WWX+11, XZYS10, XCL+18, YM12, Yak11, YWY+12, ZLWZ16, ZMB+17, dCSDdMC13, dSdSPG11, dCDC+11, dLRR11]. **Beyond** [Chu12, DCD11, Dob14, EAA17, ZWE12, CTVA12, MA10, RB18, SK17a, Var14, VVN+16]. **BGlu1** [WHS+13]. **BH** [Kim13, XZZ+10, SLZ+11a]. **bi** [MMR+10, MHHPR+17]. **bi-cations** [MMR+10]. **biaryl** [TPdMB12]. **Bias** [BVRM10, CCC19]. **Bias-exchange** [BVRM10]. **BiBO** [MLK17]. **bicyclam** [SK11]. **bicyclic** [DZ11b, JA12, MMM19]. **bicyclo** [Sat11b, WLS+19]. **bidipyrrins** [JWG+12]. **biexciton** [LEU+11]. **BiFeO** [lLBqD+19]. **bifunctional** [XZ11]. **bifurcate** [dOdCMUdALR11]. **bifurcation** [MHO+15, YW11b]. **Big** [CF11, MSAB19]. **Biginelli** [LCZL11]. **bilayer** [KMT+12, SMK+12, SIT+12, YINM13]. **bilayers** [MP12, MCKD11]. **bilinear** [MPMCM+11]. **bimetallic** [GB18, MHHPR+17]. **Bimolecular** [LQ13, DAA16, WLWL14]. **binary** [AD17, CLL+11, GE12a, Kan18, LMC19, MS14b, RKCK19]. **Binding** [ESLM19, GB18, RWW+19, ZFW+13, ATS+11, BLB+18, BBM17, BJ17, CSSK+12, DPK18, DTF+11, DMG10, EKN10, FYhC11, GM11, GGD12, KKM+12, KB19, LCT14, LNI12, MS14a, MZB+13, MPTR12, MS14c, OT14, PSK+16, PP14, SH19, SAHA12, Shi13, ŚKB18, SW12, SJW13, VBJK18, WTH+11, WDJ+17, XZ11, dCSDdMC13]. **Binuclear** [RALK18, SS19a, WLS+19, ZLY+14]. **bio** [Swa13]. **bioactivation** [MMÅ13]. **bioactive** [MKHM11, dSSdSGA12]. **bioactivity** [MKHM11]. **Biochemistry** [AM13a, KRH13, KyH13a, KGK13, LSR+13, OM13b, PSK+13, PPK+13, SKHN13, Shi13, TYN13, XTLA13, YYI+13, YIY+13]. **biodiesel** [MCRS16]. **bioenergetics** [Blo15]. **biogenic** [MBTVR12]. **bioinformatics** [RNP13]. **bioinorganic** [BBA+16]. **biological** [Brä11a, CWL+13, CAPGAIG18, Chu12, LB14a, MG12, MMP11, XHZXXZ10]. **biologically** [ASHF13, KM12b, KSD10, VO11]. **bioluminescence** [CYLL11]. **biomimetic** [ADR+18, WRW+18, ZSHL16]. **biomolecular** [Mit11b, SKV12]. **biomolecules** [BMTT11, Dum12, IKS08, IKS10]. **biophysical** [WSV10]. **Biophysics** [AM13a, KRH13, KyH13a, KGK13, LSR+13, OM13b, PSK+13, PPK+13, SKHN13, Shi13, TYN13, XTLA13, YYI+13, YIY+13]. **biorelated** [LGZC15]. **biorthogonal** [BVP14]. **bipartition** [Du12]. **Biphenyl** [JMX+15, BMF13, RS11b]. **bipolar** [RS11b, Sil14]. **bipolaron** [PFdM13]. **bipyramid** [SALK19]. **bipyridine** [LKZ+16]. **bipyridine-ligated** [LKZ+16]. **biradical** [KMK+16, KMM+18, KSN+10, KYH+13b, ZZW11]. **bird** [WLZ18]. **birefringences** [RC11]. **Bis** [BSM+15, Jac12, LYW11, LWJL10, LZZ+17, MCC13b, Pli18, RNdA+10, SDR+13, SAHAA16, ZQCJ10, ZQXP17, dARAV12, JWG+12]. **bis-actinyl** [ZQXP17]. **bis-azopyrroles** [Jac12]. **bis-dithiolene** [SDR+13]. **bis-furylfulgimide** [LZZ+17]. **bis-heterocyclic** [LWJL10]. **Bis-imino** [BSM+15]. **bis-tert-alcohol-functionalized** [Pli18]. **bisadduct** [LYS+19]. **biscycloheptatrienyl** [ZFC+17]. **bisdiselenolene** [BB16]. **bisdisphenoid** [SALK19]. **bisdithiolene** [BB16]. **Bishop** [Ano11c, Ano11b, RC11, Sau11].

bisimide [JR19]. **bismuth** [MS14b, MHHPR+17, MLK17]. **bisphenol** [BLWJ17]. **bisphenol-F** [BLWJ17]. **bisphenyls** [SN11]. **bisphospo** [SLA12]. **Bistability** [SS19a]. **bit** [Ish14]. **bithiazole** [SAHAA16]. **bithiazoline** [Qu13]. **BiVO** [DWX+16]. **Björn** [Pyy11, SA11b, Sha11b, SL11]. **block** [GDM+10, JHL+18, KS19, MMA10]. **block-copolymer** [GDM+10]. **blockade** [ZX12]. **blocks** [LLZ+14, Sza13, XWP+18]. **blue** [Kry10, LXW+14, SLS+14, SHW+13, TU10, dOR10]. **blue-emitting** [SHW+13]. **blue-green** [SLS+14]. **blue-shifted** [Kry10]. **blue-shifting** [dOR10]. **BN** [LGHL11, BSS15, FKL+12, GLT13]. **BnHn2** [LCZ15]. **BnHn2-** [LCZ15]. **bodipy** [TPT19]. **body** [ARG11, BSO16, DLP17, Fri12, GR11, Hog13, IM15, KRG+13, LV12, Lin14, Lya14, Per10a, RAN18, RAGM10, SK17b, SIB+13, SHKS15, Zak16]. **body-fixed** [IM15]. **Bond** [CP13, FC19, GRLA18, HS15, Mar11, MPMCM+11, RL12, SB10b, ZZC12, ZFC12, dFR15a, AV19, AGB19, ABKJ18, AD17, AG19, ASK15, AMMB+18, BCP10, Bla15, Bou12b, BWB+18, CC11a, Che12, CYC+15, Coo12, CF17, DLP17, EKN10, EMS16, FGD+19, FKC12, GIO12, GI11b, Gin10, GWME18, GPM+15, GZBH18, HNH+12, HHL12a, HHL14, HAX+18, JLG+12, JE10, Kal18, KZA+17, Kan18, KK14a, KK11a, KM12c, KN15, Kuz19, LZZ+11, LW18, LW15, MNV+17, MTR+19, MGB18, MBSMJC18, MBA+19, MML11b, ND11, Nal12, NHB12, NRGS11, NRP+11, NRHJ11, OKR12, OK16, OHDA13, PCMG12, PCK19, RJA+10, RI19, RB11b, RKCK19, SS10, SSK+12, SH18b, Sch10b, Sch13, SMEH16, SRA+11, SCL19, SBSD18, SC18, TL15, Tob19, TCA10, VVJ15, WCGD12, WTW+15, WLC+17, XHZXXZ10, XX12, XCD18, YIY+13]. **bond** [YL10, YS18, YZZ16, ZAE10, ZZX10, ZCC11, ZYL+14, dFR15b, dSNBG08, LCM+11]. **Bond-dissociation** [SB10b]. **Bond-extended** [MPMCM+11]. **bonded** [CdLdSC18, CCP18, DLM12, DMBL16, DB15, GCD13, IKS08, IKS10, KS18, LJL+11, LJW+11, MT10, Mit11a, MS14c, OA13, RNE10, SGKG12, SPIL14, ZLZ+14, ZFS+11, dSCC12]. **Bonding** [Con10, Mil12, TFMC19, XWC11a, ZPR10, ABM+19, AMK10, AG19, BHA19, BMX+19, BG11b, Buc10, CLXZ12, CPF12, CG12, CCL+16, Cha10, CNSK11, DMS+10, DB15, EPS+16, EAV16, Fin14b, FC19, GI14, GLXL18, Gin10, GORW19, GPM+15, HSYM11, HYD11, JN13, KK13, KdPNNS16, Kry10, KM19, LYR+17, LFP+19, LWL19, LW18, LBdV16, LYD+18, MCCGM+19, MS14a, MPD+15, MT10, MC12, MKM11, NZLG15, NE11, Pan16, PK13b, RJY+10, Riv11, RSCS10, SM19, SJZ+18, SYY16, SC18, UDVD10, WSML16, WJ11, XZYS10, YZW15b, YRN+11, ZFC+17, dOdCMUdALR11, CFV18, GAPK+19a]. **Bonding/** [CFV18]. **bonding/antibonding** [CCL+16]. **bondons** [PO15]. **bonds** [ABS13, AKHS13, AM18, ALHC18, BLR12, BL11, CG12, CDL+19, DR18, DLM12, DLLA10, ED16, EEMSS14, HB14, IROW10, JLZ+17, KKC14, KKG12, LLF+12, LLG+12, LZD+11, LLZ+12, MK11, MK12, MAT19, MJ16b, MGB18, MB15, NBL12, NZ13, OS10b, PRFR17, RRVJ10, Ril10, SSI+10, SSK+12, Sch13, SMP10, SIS+08, SPIL14, SS11, SM14a, SW12, SCZH16,

TKS11, XCL+18, YSS+10, YYI+13, YGLL10, YWH+12c, ZZL+11, ZHL+19, ZLWZ16, ZYL+14, ZJS13, dAVdM17, dLRR11, dOR10]. **Book** [Ban12, Brä12, Kry11a, Li11, Lin12, Mas11, Mor13, Mue12, SGJ10, Sch10a, Tay12]. **boosters** [HEVMSA+19]. **borane** [LCZ15, MFOH18, MC12]. **boranes** [GWM11]. **borazine** [Kal18, RLTAT19, STM18, ZHL+19]. **border** [AGOP18, CN12, GMT16]. **borides** [ČFČ11]. **Born** [BPL13, GVPCK10, RSM12, RAN18, SK17a, Sut12, VVN+16]. **borofullerenes** [YLH+19]. **boron** [ALHC18, BCGC12, Buc10, DWGX12, ES17, Esr18, FZX18, For12, GWZ+14b, GAMM10, HIL19, HNBG15, KC19a, LQ13, LC12, Mar11, MJSC18, OVT+16, PPDF11, RRCO11, TNT18, TCSD12, UDS19b, WG18, XYL+18, ZDF13, ZCG+16, YGLL10]. **boron-** [HNBG15]. **boron-arsenide** [UDS19b]. **boron-nitrogen** [KC19a]. **boron-rich** [TCSD12, WG18]. **boroxine** [Kal18]. **boroxol** [LFP+19]. **Bose** [DCD11]. **Bound** [Agb12, AY15, PGMGRM15, TD19, DSSM19, Fin16b, FDA16, FRGC10, GWHH17, KH10, LDADB+15, ONK+13, Ril10, WC14]. **Bound-states** [Agb12]. **boundaries** [WLH+19]. **Boundary** [LZ12, CW13b, MFLK11, UYN+13]. **bounded** [LLP17]. **Bounds** [MC11b, PR10a]. **Box** [GZSMFN16, NCMC+18, GZF14, Lun13a, Lun13b, Roy15, Tou13]. **boxed** [RAFR18a, RAFR18b]. **bpy** [DS11]. **Br** [DVDBM11, EMSB15, EMS16, HNBG15, JLG+12, Kuz19, LCL+10a, LMZ+11, LLG+12, RLTAT19, SB18, SZL+14, TL15, WZW17, XZL+12, JLZ+17, LWL19, OK16, TSL11]. **bracteatin** [KK11d]. **Bragg** [Zag11]. **branched** [SPD+18]. **branching** [MOY13, RSL10, TSL11]. **Brändas** [Ban12]. **Bravyi** [TSS+15]. **Brazilian** [DC10, DC12]. **Br —** [LLG+12]. **BrBr** [LGW11]. **BrCl** [JLZ+17]. **BrCN** [BMBD10]. **breaking** [AGB19, DLCB15, SSK+12, SC18, Tob19, WLZ18, YIY+13]. **Bredt** [Iku17]. **BrF** [JLZ+17, Wu11]. **BrF-HX** [Wu11]. **BrHBr** [GRLA18]. **bridge** [CLMY12, HSS18, KyH13a, Nal12, Nal13, SSK11]. **bridge-acceptor** [SSK11]. **bridged** [MNP19, ZZR+12, ZLS+18]. **bridges** [ATS+11]. **bridging** [MG10]. **Brief** [Ano11a, BC15, BC16, Mai14, YZ13]. **Brillouin** [BG11a]. **broad** [FCS13a, FCS13b, TZ11]. **Broder** [PR11a]. **Broken** [FDNR10, SC10a, CR18, GFRdG11, Tob19]. **broken-symmetry** [CR18, GFRdG11]. **brominated** [MFB11]. **bromine** [FGD+19]. **bromo** [OA13]. **Brønsted** [GI14, RDB19]. **brookite** [GP13a]. **BS** [YGLL10]. **BSE** [RAMB18]. **B —** [MGB18]. **bt** [Qu13]. **Bu** [GWM11]. **buckyballs** [GKGM18]. **buckybowl** [LZW+15]. **Buckycatcher** [DI15]. **build** [GBK18]. **building** [JHL+18, KS19, LLZ+14, MDC15, MSOV13, Sza13, XWP+18, CNBPR+11]. **bulk** [TFB11]. **bundle** [GWME18, JE10]. **bupivacaine** [MP12]. **butadiene** [SKTI15]. **butadiynol** [ŞBAT16]. **butadiynyl** [KI12]. **butanetriol** [LL17]. **butatrienone** [ŞBAT16]. **butene** [IK14, TFA10, ZPB12]. **butyl** [AMAC12, MFK+12, WZZL10, dOLdlV13]. **bzq** [ZQJW13].

C [AM18, Ban12, BDF+18, BCP10, BGFD14, BBYZ18, yBZfC18, CJMC19, DQZF12, GWM11, GZW16, GB13, GCD13, JLL+18, JLG+12, Kal18, KI12, KN15, LKN13, LCS+11a, MLY+16, MGD11, NBL12, OGvSG18, PAKA15, PP14, SUL+11, USL+13, VF13a, VLK+11, WLZ+12a, WLZ+12b, WZW17, WSL+11, YK11, YZL+10, YLZ+17, YL11, ZQJW13, ZHL+19, ZW15, ZLWZ16, ZCTG18, TSKN12, YB11, BHA19, yBZfC18, CCEGK12, CWL+13, CRSB12, CTDOLA10, DFK16, DSFT17, EML+11, FBRBR12, FBO+11, GB13, HV11, HLB19, HHL+12b, IMS+13, JB18, JCCZ12, KWC10, KZA+17, Kan11, KK11b, KK12a, KI12, LCL+10a, LBY+14, LZW+15, LCZ15, LXD13, LW15, LdAA+11, MNV+17, MSS11, MIN13, MS17, MPGGS19, MC18a, NL11, NMIP14, Nik11, OCL+18, PTS+11, PAKA15, RR11, RRCO11, ŞBAT16, Sat11b, Sri19, SCTW10, SW12, SZY17, SC18, TZD+19, TG13, TKSK17, WCS+13]. **C** [WZW17, WWGW18, XCY15, XCD18, XZG+18, YS18, ZPM10, ZLWL16, ZJC+13, DZO12b]. **C-H** [YS18]. **C1s** [LdBF+12]. **C2h** [KS18]. **C60** [DI10, GHGF12]. **C=S** [JLG+12, JLG+12]. **Ca** [VO12, WCY+10, XZZ+10, YLW+13, CRB+12, CLMY12, DTEMK11, GR11, MPD+10, MPTZ13, SBB16, VPFD10, YYI+13]. **Caballol** [dGR14]. **CACA** [Ser11a]. **cacao** [dAGNJT12]. **CaCuO** [Fuk12]. **caffeine** [LCG12, PRG+10, ST15, PRG+10]. **cage** [yBZfC18, CS13, DI18, GAPK+19b, JL12a, SL10, WLZ+12a, KK12a]. **cage-like** [JL12a]. **caged** [PAKA15]. **cages** [NW12, XYL+18]. **calcite** [SC11]. **calcium** [Ish14, RCGLV+14]. **calcium-doped** [RCGLV+14]. **calculate** [ZLE17]. **Calculated** [SPO+11, Dw13, FKL+12, MFK+12, VMC11, WWC17]. **Calculating** [FYhC11, KC11, WB17, ARH+13, CML+16, MGK+11, SA11a]. **Calculation** [FZC14, KKS+11, MHO+15, Rit12a, SHS+13, VLFG12, VO11, YŞÖ12, AM12, BVCAP12, BBYZ18, Boe12, CP10, DK13, FLCHL10, FBM+10, FSB16, GWZ+14a, GCDNGS12, HMI+15, Han19, IK18, KMK+16, KHH10, Kri13, lLBqD+19, LIK15, LSKM19, MGK+12, Mam13, MA12, Mit11c, dMOB12, PS10a, Per10b, PCR+11, Rit12b, SBM16, SMGZF19, ST15, SRASZ16, TTT13, VF13a, WZHZ13, XCD18, YK13, YM14, YH14b, YLYC18]. **calculational** [SC12a]. **Calculations** [KH10, KV11, LKJ13, SR19, TWHZ14, dHLdS12, AV19, AK17, AFA13, ADB10, ACMRN10, AGG+18, BCK19, Bas11, BB10, Bou12b, BJ12, Buc11b, Bud12, COCF+14, CK17, CSTA16, ČFČ11, Dau16, DSL15, DAE+12, DWX+16, DZO12c, DZO12a, DFF+13, ESS13, Eng16, FSK+11, GAPK+19b, GVPCK10, GSaY11, GZF13, Glu13, GJ18, GE12b, HK11, HHCA10, HH18, HS11b, HL19, HNBS18, HZS14, IKC18, JH13, KAR12a, KK14a, KG17, KRK+17, KPCV18, KSS12, Kim13, KJ15, KJ16a, KJ16b, Kin13, KYH+13b, KPH+12, KKG12, LRP+11, Leh19a, Leh19b, Leh19c, LCL+10a, LC16, LYW+19, LCK+16, LLZ+12, LNI12, MCCGM+19, MJ16a, MVC13, Mit11b, Mit11a, MFLP12, MSY+12, MPT11, MPTZ13, MJM19, NS19, NKWT19, NMSR14, NZLG15, yOITn15, OKK10, OCGM+19, OPP+14, OH19, OSJ+12, Pan19, PP19a, PK16, PBR18, PB10, RS12a]. **calculations**

[RZG12, RLER14, RAMB18, RCGLV+14, RVO+14, Rud12, RRCO11, RTT10, RMY+13, SH19, SMEH15, SAHG11, SAHA12, SJZ+18, SL13, Sko16, STL12, SRA+11, SN11, SW12, SJW13, SCBP17, Tan13, TNN16, TSH17, TWR15, UTTn13, UGWL18, USL+13, VVVB10, Wag14, WWC17, WYM15, WZW17, YYI+12, YIY+13, YSK+12, YKM+15, YHL+13, Zak13, ZST+10, ZQCJ10, ZCC11, ZF15, ZZC12, ZZZ+18, dSM19a]. **calix** [Pli18]. **CAM** [JdOS16]. **CaMn** [SYK+12, YYI+13, YIY+13, YSK+12]. **Can** [ADR+18, Kuz19, Lu15, Met11, Nes11, Sza13, TFA10, Blo15, Luz11a, PWP+18, WLZ18, ZLWL16]. **cancer** [LB14a]. **candidate** [AB16b, XWP+18]. **candidates** [Ali19a, KMRG13]. **Canonical** [GW13, CCL+16, JH15, Jør15, Jør18]. **Canuto** [Ano11a, RdA11]. **CaO** [SAHA12]. **capabilities** [AG19, OCGM+19]. **capability** [CJSNLM11]. **capacities** [GVPCK10, UDS19b]. **capacity** [KDA+11]. **capped** [SALK19]. **capsules** [KKH+13]. **capture** [GSaY11, Mai14, PRPU+13, Sri19]. **carbazol** [MUNZVR12]. **carbazol-oxadiazole** [MUNZVR12]. **carbazole** [ZBBB17]. **Carbene** [CDL+19, HZZ+19, LWC+10, LCS+11a, LCH+11, LCS+11b, LXLL11, RMP+14, ZFS+11]. **carbenes** [ABTW14, ALB18, CDL+19, MAN15, Pan16, SZL+14]. **carbide** [NEEV15, RK14]. **carbides** [GM11]. **carbocyanine** [Mas10]. **carbodiimides** [WLWT12]. **carbodithioic** [SJZL12]. **carbohydrazide** [HZZW11]. **Carbon** [DSFT17, MPL+11, AKC10, AEM+12, ACT19, Bas11, BEPZ10a, Buc10, Buc11b, BSO11, CS13, CTDOLA10, DI10, DM16, EBR11, ETGLMJ+19, FC19, GAMM10, GT13, GZBH18, GGP13, HCH+18, HNBG15, HNBS18, Hog13, JW19, JR19, KKC14, KKT13, KKT14, KG08, LV19, LMC19, Mai14, MAT19, MSOV13, OPS10, OCGM+19, OD12, PP14, PNC19, RRK16, SA18, SD13a, SC10a, SQ10, TZD+19, TDOD17, TC10, Wan11, WW11, WHY+14, WJY15, WDJ+17, Yam10, ZCX+16, ZMB+17]. **carbon-carbon** [FC19]. **carbon-hydrogen** [GZBH18]. **carbonate** [DLO16, YM12]. **Carbonates** [RBLZ15, ZQW+17]. **carbonic** [dM13]. **carbonmonoxy** [CHSO13]. **carbonyl** [BLdV19, BH10a, DWJZ11, GGJD13, MTS15, MG10, RCM+19, WLS+19, YYS15, dCSDdMC13]. **carbonyl-coordination** [GGJD13]. **carbonyls** [LLW+12, RALK18]. **carborane** [FSQ+11, LCZ15]. **carborazine** [Kal18]. **carboryne** [HhGqZZ17]. **carboxaldehyde** [TBA13]. **carboxylase** [WLD+10]. **Carboxylate** [SCB+14, KSAK17, LYL+12]. **carboxylic** [KC11, LGM+18, MK10b, SAG13, TPT+13, VF13a, WJ11]. **carcinogenic** [DKZ+10]. **Carlo** [ÁFV12, ABG12, ANC+15, ASK15, Cal10, CKB+19, CCC19, CP16, HCH+18, Hog13, HB14, HM12, JCCZ12, PDR+14, PIS18, RCGLV+14, SGC13, SCBP17, Wag14, WCM14, ZLR15, ZCC11]. **Carlos** [HS15]. **carrier** [GNM+12]. **carriers** [NMV+14]. **Cartesian** [GMR18]. **cascade** [Fra17]. **case** [AGRI+12, BDF+16, Bas11, BBM17, BLdV19, CCL+16, DMAB12, DVDBM11, DAA16, DCDD10, DFF+13, GS11, GB18, GWME18, KLE+19, Kuz19, Mar12, MVG18, MSC10, MURR13, Oni10, Ped16, PK13b, SS10, TC12, TWR15, YLZ+17, CTVA12, DB12]. **cases**

[Zak13]. **CASPT2** [BDFM10, BDR12, ČFČ11, GLOGM+11, KZZ13a, LCL+11, LGP+12, MR11, Pul11, RS12b, SKTI15, SZZ+12]. **CASPT2//CASSCF** [GLOGM+11]. **CASSCF** [BDFM10, DAR+11, GLOGM+11, Lar11, Ols11a, PE11, RS12b, RSN12, SZZ+12, SBL11]. **CASSCF/CASPT2** [SZZ+12, BDFM10]. **CASSCF/MRCI** [DAR+11]. **Catacondensed** [RB08, RB11a]. **catalysed** [SMRK18, ZYSW17]. **catalysis** [BvWG14, KJ14, MMM+12, MCRS16, PIS18, Sic16, SLS+15, XDM+10]. **catalyst** [ENV15, Esr18, EM19, GB18, Hog13, JXX+15, LCM+11, TM19, Var14, ZQW+17, ZBG+19]. **catalyst-free** [ZBG+19]. **catalysts** [BAB+18, TFZ+15, WR14a]. **Catalytic** [BD14, PM17, SS18b, AGOP18, BGFD14, CLY12, DMBJ15, ED16, GGZZ16, GSB10, HSN+11, HSYM11, LPOP12, MLW+14, MMP+18b, NEEV15, TK16a, TTD13]. **catalyze** [XGH18a]. **catalyzed** [AKC10, AZD+11, CAPGAIG18, CWZ+10, Che12, GCZ+14, HZZ+19, JL12b, JSLH14, KUTS10, LGM+18, LZZ12, LQ13, LYR+17, LLF17, LD17, LTL18, LFTL18, LMCZ11, LCZL11, LW13, LW15, LKZ+16, MPGGS19, MCC13b, PRFR17, SH18b, SHL+13, SR11a, SLS+15, TTD13, TFA10, WML10, WWLZ17, WZZL10, WRW+18, XZG+18, YS18, ZCZ+12, ZSHL14, ZZC15, ZQW+17, ZSS+13, ZLY+14, ZPW16]. **catechin** [MKHM11]. **catecholamines** [MBTVR12]. **cathode** [KLK13, Kim18]. **Cation** [ZLWZ16, ATS+11, Ber13a, BMX+19, DWJZ11, DAE+12, HV11, LCL+10a, LLC+11, MMMM12, MS14c, ONBP11, Oni10, OCGM+19, PDR+14, PvS10, SPSA11, SZZ+12, XZL+12, YM12, ZFC12]. **cation-** [OCGM+19]. **cation-exchange** [PDR+14]. **cation-exchanged** [PvS10]. **cationic** [BCGC12, FTB11, ZQJW13]. **cations** [BMF13, ESLM19, GK12, HFA+19, IGMK11, LGP+11, LPG+12, MMR+10, MKM11, NKWT19, PDR+14, SHE10, WLWT12, YLW+13, ZLWZ16]. **caused** [HYH+10]. **causes** [ABP13, MFM18]. **causing** [MFR10]. **cavernous** [CJMC19]. **cavities** [MGK19, Pup11a]. **Cavity** [PCR+11, OPC17, RAFR18b, RAFR18a]. **CBr** [WZHZ13]. **CBS** [CFOC+10, VF13a]. **CBS-Q** [VF13a]. **CBS-QB3** [CFOC+10]. **cc** [SLS+11]. **cc-pV5Z** [SLS+11]. **CCH** [EMS16, LZZ+11]. **CCl** [SKS11, LGW11]. **CCSD** [CK13, VV13, BL12, CPF+11, DVP18, JdOS16, SLS+11, TD19, VV12]. **CD** [SZY17, ASHF13, XZZ+10, XWC11a, LKLW11, XWC11a]. **CDO** [ADR+18, SAHG11]. **CdS** [XWC11b]. **Ce** [WLG+11, WSL+11]. **cefotaxime** [LBM11]. **Cell** [KMT+12, CWB+13, JK12, LGS+16, MANP17, QJ13, SSS15, TGRP19, WLL+13, WWB+14]. **Cell-penetrating** [KMT+12]. **cells** [AGJ12, BDG17, FFPD16, FM16, cLqFtW+14, LYS+19, MY17, PMAP12, SG19, TZ11, ZSAP11, Zha17]. **cellular** [Kuv10]. **cellulose** [FNBK17]. **center** [Buc10, Buc11a, CRSB12, CN12, Hog10, HZS14, Koc13a, MSNP18, Tal11, Yam10, YD17]. **centered** [GAPK+19a, KFS13, Zak13]. **centers** [ASD14, YGLL10]. **centrifugal** [CLXD15, IIH16, ZLJ11]. **centrosymmetric** [KPL+17]. **century** [Pup11b]. **CeO** [QCB+10]. **ceria** [KJ14]. **ceric** [BSPK11]. **cerrado** [CCA+12]. **cesium** [MMR+10]. **CF** [lAyL14, Mor11, Mor11]. **CFCl** [dOdCMUdALR11]. **CFP** [KyH13a]. **CGR**

[HXDY16]. **CH** [ACMRN10, CdAFS+12, CRSB12, DQZF12, LJL+11, LXLL11, Men10, NBL12, dMOB12, TSL11, XWCY11, BMR+13, BHV+11, BZZ15, BXZ+19, DS12, DZ11a, FRNM12, GZMC11, HHL+12b, KAR12a, Les12, LP10b, LKLW11, MEEA+13, dMOB12, Puz10, SK14, SD12, SZZ+12, STL12, SLZH12, TSL11, VLK+11, WZHZ13]. **CH/** [BMR+13]. **chain** [Cal10, DSCO+13, DW12, EPS+16, IKS08, IKS10, Lak10, LGL+19, PP19b, WW11]. **chains** [BEM11, CEM14, CEV10, CFGC11, DSFT17, MAT19, NRI15, PL18a, TIKL13, WZ10b, Yak10, ZY13]. **chalcogen** [BHA19, EMSB15, EMS16, MZLM17, Sch13, ZFS+11]. **Chalcogen-bonded** [ZFS+11]. **chalcogen-chalcogen** [EMS16]. **chalcone** [EM17]. **chalcones** [XLZ+19]. **chalcopyrite** [dLdOdAD12]. **challenge** [Li15]. **Challenges** [DE18, KO14, KJ14, FAK19, NBZG16, Pie11]. **chameleonic** [SSK+12]. **change** [DSWL11, KCK14, MSK+12]. **changes** [FBD+13, GMP+11, YSG10]. **changing** [DLG12]. **channel** [AGRI+12, LZFZ13]. **channel-charybdotoxin** [AGRI+12]. **channels** [Les12, RBGGM18, STL12]. **chaos** [KC18]. **chaos-driven** [KC18]. **chaotic** [Gan14, YW16]. **character** [CCL+16, CFV18, CJMC19, CAO18, MHOG18]. **characteristic** [KK12a, MKHM11, OCL+18]. **characteristics** [BF11, BSO11, EBH11, Nic11, Ril10, SM17, SMGZ13, YZW15b, ZLS+18]. **Characterization** [EA12, JLL11, AT18, DAA16, Den13, JLL+18, LMC19, MC11a, NC11, PWP+18, ŞBAT16, TTM16, ZWZK19]. **characterize** [GfWlZ11]. **characterizing** [MAW+18]. **characters** [CC11a, MMF+13, XWC11a, YMY+13]. **Charge** [CS17, DPRK12, EPS+16, GI11a, GWME18, GHS12, JdL08, KT12b, MHOG18, SSKS12, SM14a, TMM+14, Zen11, AS19, BHV+11, CLMY12, DTFK15, DS11, ELC08, FSBA12, Gao12, GNM+12, Gin10, GGD12, GHCMCMQ17, JR19, KUS19, KBMM10, LYS+19, LXW+12, MGK+12, MSG16, MANP17, MPL+11, NDH10, NMV+14, OK19, PK13a, PSC15, PETB18, QJ13, RS12a, SSK11, Sch15, SRA+11, TCG13, TCS10, WDJ+17, WDS19, ZY13, ZB18, dCDC+11]. **charge-bond** [Gin10]. **charge-dependent** [PSC15]. **charge-dipolar** [ELC08]. **charge-solvated** [CLMY12]. **Charge-transfer** [Zen11, FSBA12, TCG13, ZB18]. **Charge-transfer-to-solvent** [CS17]. **charge-transport** [ZB18]. **Charged** [TGRP19, BGMD15, BMF13, CAZ+11, DCBB11, EPS+16, HITU16, KWWH18, LZ12, MMBK12, RTG+19, SS10]. **Charged-cell** [TGRP19]. **charges** [CG12, CB10, GSR12, GFRdG11, KKS+11, Sch15, TMC18, TC12, ZZZ+18]. **CHARMM** [HSS+11, PSPS11]. **CHARMM-based** [PSPS11]. **charybdotoxin** [AGRI+12]. **CHBr** [WZHZ13]. **CHCHCF** [lAyL14]. **CH**$\cdots$ [EAA17]. **Checking** [HMH10a]. **chelate** [MHZ18]. **chelate-aryl** [MHZ18]. **chelated** [ZPW16]. **chelates** [NZAVR10]. **chelating** [NFD+10, NFQ+11]. **chelation** [Bal16]. **chelator** [DP16]. **chelators** [MPTR12]. **chelotropic** [CJGTL12]. **Chem** [BR16, COP16, HS15, Man16, dFR15a]. **Chemical** [AGNS14, Brä14, DVC14, Joh17, KKH+13, LLM13, MNE+13, NYA+13, NDLC19, PM16, SC10b, TIN13, TM13, TCCI10, Tsu15, Zil14, ABS13,

ASMP15, AD17, AMMB+18, BF11, Bal16, BL10, BL11, BG11b, Brä13, BVRM10, CJBMMAPR19, CKL16, CLXD15, CFGC11, CPAT11, DKZ+10, DPK18, DSL15, DPRK12, DFK16, DMS+10, DLM+11, DMBL16, DSFT17, EAK+10b, EML+11, EMED+12, EMEPD15, FBO+11, FBD+13, Gag11, GP13a, GRCGRRHT19, GFPAV19, GA19, GI11a, GbZA10, Gru17, HMA+19, Hop15, HAX+18, JN13, KWC10, Kal18, KBGC12, KMK+16, KM12c, KUTS10, KK11d, LZZ12, LYR+17, LL17, MC11a, MPE15, MTR+19, MC14, MG12, MQA17, MKM11, MBBT+12, MML11b, MGP16, NC11, Nal12, NZ13, Ném14, NVPCJ+13, NRP+11, NJA+12, OS10b, OWD18, OSJ+12, ÖEDB11, PWY+18, PO15, Qu13, RLW+13, RGTS11, RNE10]. **chemical** [RMP+14, RR19, RBTL19, SSI+10, SSK+12, SAG13, SBEH11, SKHN13, SC12a, SW10, SN15, SM19, SC10a, She14, Shi13, SIS+08, SKM11, SR13, Sko16, SFY12, SBKJ18, SRA+11, SK10, SSB+12b, TFBG14, TYN13, Tap15, TMC18, TKSK17, UTTn13, UJSJ13, VOK+18, VO11, VO12, WYM15, WLD+10, WLWL14, YNLD18, YSS+10, YYI+13, YB11, ZBK15, ZZC12, dHLdS12, vL13, vLRRK15]. **chemiexcitation** [dSM19a]. **Chemiluminescence** [dSdS13b]. **Chemisorption** [OD16]. **chemistries** [Vie17]. **Chemistry** [AH19, ÁIGVZW12, Brä13, Hog13, IFT13, KYS13, KYH+13b, TBRIS12, ZJS13, Ban12, Bar16, BMRM19, BZBZ13, Blo15, BHH+13, BT15, Buc12b, Cav13, CAA19, CM16, CSG14, DC12, Gag11, GGZZ16, HR13, HEVMSA+19, IK14, Jia15, Kap12, Kar09, Kar10, KC19b, KN15, LSR+10a, LSR+11, LJ16, LFS+11, LCZL15, LSKM19, Luz11a, MMŁ+16, MEF+15, MMCNV19, MQG13, MPGGS19, Mor13, NBZG16, NTCK13, Nic11, Nic14, NMSR14, OM13b, PTH11, Pup11b, Puz17, Rei15, RNB+10, SDP+16, She13, SG14, SPM+15, Tch16, TBB+19, TBRIS10, TBRIS11, Tri14, TB15, VVN+16, VMR11, VBJK18, WYWL13, WWX+11, WR14b, YZ13, ZLWY13, ZWSF16, DC10, SG14, BT17, Tch13]. **Chemists** [RA10b]. **chemogenomics** [IAK13]. **chemometric** [LSR+10a, LSR+11]. **chemosensor** [LWZ+14]. **CHF** [STL12]. **Chiral** [YWR+18, BdTG11, CPL15, KGVG11, LPM+11, LMCZ11, LW13, QCW+12, SFW12, WTZ+11, YWY+12, ZSS+13]. **chirality** [Luz11b, SD13a]. **chiroptical** [Cap16]. **chirp** [GRLA18]. **CHITEL** [RA10b]. **chloramine** [SZL+15]. **chloride** [EHKD11, EKD12, MMM+12, SKS11, dOLdlV13]. **chlorides** [BLM+12, HSN+11]. **chlorinated** [FBO+11, KZA+17]. **chlorine** [DWGX12, cLqFtW+14, MOY13, XXbX+13]. **chlorins** [CJSNLM11]. **chloro** [DDÇY12, DPRK12, PSKV19]. **chloroalkenes** [MLB+12]. **chloroaniline** [HLZ+14]. **chlorobenzaldehyde** [SRA+11]. **chlorobenzene** [SGL19, SC18]. **chlorobenzofuran** [ASMP15]. **chloroethyl** [CZJZ12]. **chloroethylnitrosoureas** [ZMZ13]. **chlorophenol** [ASW13]. **chlorophenyl** [ÖEDB11]. **chloroquine** [KdPNNS16]. **chlorotrifluoroethylene** [OCB+10]. **CHN** [RB11b]. **CHNC** [DW12]. **CHO** [DZ11a, Sch10b]. **choice** [AGPDZ13, FSB16]. **Cholesky** [BVA+14, CPF+11]. **Choosing** [KBJ17]. **Chou** [QZH13]. **chromites** [Zen11]. **chromium** [HM12]. **chromogens** [JA12]. **chromophore** [BF11, BSM+15, GLOGM+11, LORR+12, TCM+12].

chromophores [HSS18, LDKB15, LXW+12, PJP08, ZWLC12]. **CI** [ADB10, MdAdCS12]. **cinchona** [JSLH14, LMCZ11]. **cinnamates** [PSK+13]. **cinnamic** [AEKGZ12, PSK+13]. **cinnamoyl** [AEKGZ12]. **circular** [DLRMFY10, PCR+11, SB10a]. **circumscribed** [ACT19]. **cis** [BSM+15, Bud12, FMKJ14, GLOGM+11, HWWW18, KZZ13b, TMC18, CC11a, LCB10, LZ10]. **cis-** [FMKJ14, KZZ13b, TMC18]. **cis}-1** [CC11a]. **cis}-11** [LCB10]. **cis}-13** [LCB10]. **cis}-7** [LCB10]. **cis}-9** [LCB10]. **cis-trans** [BSM+15]. **CK2** [DPK18]. **Cl** [DS12, EMSB15, EMS16, FBO+11, GB13, HJRO13, HNBG15, JLG+12, Kuz19, LMZ+11, LLG+12, LWL+12, LCS+11a, MZLM17, MEEA+13, MPRCEG12, RLTAT19, SB18, SKS10, SD12, SPIL14, SYQ+10, SZL+14, TL15, WZW17, XZL+12, DZO11, KZA+17, LLLB13, LdAA+11, Ma14, MGB18, SM14b, SC18, XZYS10, YGL+11]. **Claisen** [EM17, YY18b]. **clam** [CHL+19]. **Clar** [RB18]. **Clarification** [CHSO13]. **class** [GMGRMP12, HS11c, KM12b, Mar12]. **Classes** [TÁ10, VOK+18]. **Classical** [BM16, KC16, BTH18, Cho16, Cho19, CP11, DW12, Dw13, Liu15a, Mak15, MLB+10, SPSA11, XLLZ10, YZ10, Zak16, Men15]. **classical-map** [DW12]. **Classification** [AA11]. **classifications** [LQZZ12]. **clathrate** [LB19]. **Claus** [SR18]. **ClCl** [LGW11, MZLM17]. **cleavage** [KRH13, LW15, QZH13, SRA+11]. **ClF** [SPIL14, SCZH16]. **climbing** [SSB12a]. **close** [FSQ+11, HNH+12]. **close-carborane** [FSQ+11]. **closed** [JEA13, KK13, MSRn+11, STM18, dSdS13b]. **closed-** [JEA13]. **closed-shell** [MSRn+11, STM18, dSdS13b]. **closo** [LYR+17, SALK19]. **closo-dodecaborate** [LYR+17]. **closure** [YY18b]. **cloud** [FT15]. **clouds** [BN12]. **clue** [PSKV19]. **Cluster** [TC10, AHC+18, Ali19b, BN12, BDFM10, BP13, BVP13, BVP14, BBB+12b, BA13, BAB+18, BJ12, Cam10, Cam12, Car19, DZO12c, DMBL16, EFO11, EO11, Fer11, GLF+12, GZW16, GP13b, GD11, HCH+18, HFBC19, KP11, LP10b, LSR+13, Luz08, MMBK12, MPT11, MC18b, NW12, PWL+10, PCV19, PB10, RSN12, RFEGPP+16, RWW+19, RMY+13, SR12, SYK+12, SSK+12, SZS+10, SS18b, Sto18, Sza13, THL+15, TCSD12, Tob19, TGA+11, Var11, VVAO12, VVVB10, WWC17, WWQG17, YY18a, YYI+13, YIY+13, YKN13, YT14, ZE18, ZW15, ZCTG18]. **cluster-configuration** [Ali19b]. **cluster-continuum** [RFEGPP+16]. **clusters** [AGCVG15, ATL+14, AGB19, ALHC18, BD14, BCGC12, BPT12, BGMD15, BvWG14, BGL+16, BPSM12, BJdlMAV12, CDSK12, CAZ+11, CF11, CCP18, CTW12, CD12, DVDBM11, DPK18, DTEMK11, DHYC19, DQZF12, ESDO16, EBH11, FTB11, FMCA11, GR11, GP13a, GAPK+19b, GGD12, GKGM18, GD11, GFRdG11, GWJ12, HDQ+13, HLZ+14, HJ13, HFBC19, IIW+11, JFT13, JB18, Jen13, JL12a, KP11, Kar12b, KSSK16, KYLC19, KSG+12, KRG+13, LKN13, LL11, LFP+19, LCZ15, LMC19, LG15, LSCMSFC19, LHL+15, MJ16a, MBKH19, MLW10, MCP10, MJ14, MMV+19, MJSC18, MD11, MPRB+10, MURR13, MMRRA10, MW15, MCK17, NG11, Nes11, OKK10, PMH+16, Pop19, PAPCMM+16, QSLY10, Riv11, RF10, RCGLV+14, RGR12, SFA19, SJZ+18, SIB+13, SR13, SBB16, SCS15, TZD+19,

TW10, TFMC19, TPCJ+12, UKF+11, VSMK13, WJL+11, WCS+13].
clusters [WJL+10, XGH18a, XWC11a, XWC11b, XF19, YSK+12, YGLL10, YZW15b, YJ17, YZ12, YC13, ZWSF16, ZRR+11, ZCW16, ZCP11].
clusters-continuum [DQZF12]. **CN**
[EMSB15, LZZ+11, Oni12, ZLWZ16, CP10]. **CNaY** [LZZ+11]. **CNC** [Zha10].
CNH [Tap15]. **CO**
[BGFD14, BAA+18, BDR12, DPDR11, DWPK14, GGJD13, WZC+12, WRW+18, Kim19, VDG13, YL11, BD14, BGFD14, BLdV19, CRSB12, CCS13, Esr18, EM19, FTB11, GSB10, HDC+11, LCT14, LZW+18, MPM15, MMP+18b, RDB18, RDB19, RBTL19, SCLCPB12, SAHA12, SLSZ13, Sri18, Sri19, SCTW10, WLG+11, WZC+12, ZCW16, AAA12, CRB+12, GZMC11, Kim18, MRT11, NKWT19, ZYSW17, WRW+18]. **Co-** [GZMC11]. **Co-based** [Kim18]. **CO-photolysis** [BGFD14]. **CO/** [WRW+18]. **Co/Ni** [AAA12].
CoA [LZZ12, MLW+14, MFR10]. **coadsorptions** [SR19]. **cobaloxime** [JL12b]. **cobaloxime-catalyzed** [JL12b]. **cobalt** [JL12b, SS19a]. **COCH** [Men10]. **COCl** [SKS11]. **cocrystal** [DGR+16, LZZ+13]. **cocrystallization** [KAOB11]. **code** [FMPM+14, GCK+17, MMŁ+16, dMOB12]. **Coding** [FAK19, CLC10, CLL+11]. **codoping** [YHL+13]. **coefficients** [AFM+10, FLCHL10, FBM+10, KH12]. **coenzyme** [SLS+10]. **cofactor** [LZZ12]. **cofactor-independent** [LZZ12]. **cofactors** [KGK13]. **cognition** [Val13]. **coherence** [She14, SMMT13, ZBK15]. **Coherent** [Coo12, Mar13, SMMT13]. **coinage** [DMBJ15]. **cold** [ZJS13]. **collagen** [EPS+16, PWH+12, SGG+10]. **colleague** [Sau11, SL11]. **collected** [RA10b]. **Collective** [MLDP10, BM10]. **collinear** [SÁBA+12]. **Collins** [Sit15]. **collision** [LWWZ13, LPM+11, MGK+11, SÁBA+12]. **collisions** [BMTT11, BHV+11, DSC+11, dDGNB10, LdAA+11]. **comb** [MPC10]. **Combination** [KYH+13b, SN15, Buc10, CK13, DQZF12, SZS+10, SLZ+11c, SLS+11, VV12, VV13]. **combinations** [Boe12]. **combine** [Lin14].
Combined
[IK18, SJZL12, TAY11, KP11, MLDP10, NZ13, Tan13, ZLWY13, BBB+12b].
combines [WZX15b]. **Combining** [PC16]. **combustion** [MPGGS19].
CoMFA [MGK+12]. **Comment** [BR16, CK13, Cin20, COP16, FKBG19, Fer19, HS15, KBG17, Lad14, Lun13a, Man16, MBSAG16b, MMM20, PS14, Tou13, VUC13, dSSF16a, dFR15a, HYZS19, PS13b, VV13, XTLA14].
commentary [Ols11a]. **comments** [Brä11b]. **commercial** [FT15].
Common [VSL+15, ESLM19, LCH14]. **compact** [LQZZ12, LLZaH14].
compactification [DTF+11]. **Comparative** [BLRdA+10, BO11, CLH14, DTEMK11, FDG18, LJL+11, LL19, LL17, MMF+13, NS10a, PI13, SD16a, dAGNJT12, CCBR+12, FFF10, HNH+12, KM12a, KKM+12, LCCH10, LLZZ10, ONBP11, PRPU+13, RS11b, YM13, ZLZ+14, ZLY+14, dSdSPG11].
comparing [HXDY16]. **Comparison** [AM13a, BPT12, CDSK12, Han19, JdOS16, MR11, RALK18, SSP+17b, SMMT13, UV18b, YF16, ZHL+19, ABLT11, BLL+13, BGKK16, CCC19, GP13a, HDQ+13, Kan11, KC16, LdBF+12, LZFZ13, OKR12, dSMPRSF18, SD13a, Sch13, SG19, SBKJ18,

VOK+18, FMCA11, FC19, RCM+19, SCZH16, ZZL+11]. **Comparisons** [CA17, PGG12]. **compass** [ZBK15]. **compatibility** [Fin17]. **compensating** [FUE+12]. **compensatory** [Chu12]. **Competition** [GE12a, SM17, TL15, GHS12, LFP+19, NRGS11, YZZ16]. **Competitive** [LLG+12, AMMB+18, SBKJ18]. **compilation** [TB15]. **complementary** [Yak11]. **complemented** [WJY15]. **complete** [CHH+19, CC19, GS10, LV12, SGB11, SXH18]. **Complex** [GLT13, IA13, JH13, KBF+13, ONK+13, BSS16, Bou12b, Cho16, DSD18, DI15, DZO12b, FDNR10, GRLA18, GR10, IKC18, JLG+12, JR19, KRG+13, LZ12, LV16, LLG+12, LSR+13, LBdV16, LDADB+15, LKZ+16, MNC12, MIN13, MMT+13, MSBF18, NS10a, NTGC19, NBI+10, NMIP14, OAA19, PEA+12, PWY+18, Puz17, Qu13, RW11, SS19a, SY10, Sat11b, Sic16, SLS+15, VDG13, VPOG19, WRW+18, XZ11, XCD18, XCL+18, YSS+10, YYI+13, YSK+12, YS13, YW16, ZSASS13, ZSHL16, dCSDdMC13, dOdCMUdALR11]. **Complex-scaling** [JH13]. **complex-valued** [YW16]. **complexant** [XWCY11]. **Complexation** [ESLM19, SHE10, ZKKR11, ZAE10]. **Complexes** [ALMY18, GHGF12, AC19, ADR+18, AM18, BHMN19, BPG+10, BAP12, BHA19, BZBZ13, BLdV19, BPK19, BCS+12, BB16, BSV12, CRB+12, CPF12, CTW12, Con10, CLMY12, CADSG18, DSD18, Den19, DPDR11, DG19, DCdG10, DdG+11, ED16, ESS13, EMSB15, EMS16, FBRBR12, For12, FBD+13, HS11b, HL19, HYD11, HZZW11, JW19, KRK+17, KV11, Kry12c, KBMM10, LJL+11, LYW11, LXW+14, LYR+17, LYL+12, LXD13, Lu10, MZB+13, MCE11, MNV+17, MC17, MGK19, MC12, Men10, MG12, MKM11, MS14c, MPRCEG12, ND11, NFD+10, OAC17, OPP+14, OVT+16, Owe17, PCMG12, PRG+10, PAKA15, RFEGPP+16, RB11b, SS10, SVRGV12, SG19, SGKG12, SRASZ16, SAHA12, SLS+14, SK11, SSP+17b, SPIL14, SHW+13, SM17, SK12b, SS13, TTD13, TMM+14, TL15, UDVD10, VO12, WLS+19, WXB+11, WZW17, WHM14, Wu11]. **complexes** [YZL+10, YZL+11, YZW+15a, YWH+12c, YZZ16, ZPR10, ZQCJ10, ZLLS10, ZQJW13, ZLZ+14, ZZC15, ZHL+19, ZSQ+10, ZFS+11, ZLWZ16, ZSZ14, ZQXP17, ZBBB17]. **Complexity** [GN19, EMED+12, LRMAA19, SMOD11]. **compliance** [NH18]. **component** [AB18, CW16, FZC14, KKT13, KKT14, MHT+08, MM19, SN15]. **components** [LVP12a, NIK19, Nal12, RLZ12]. **composed** [TK16a]. **Composite** [KO10, ZJS13, CC19, Mor12]. **Composite-system** [KO10]. **composites** [KT12b]. **composition** [GLF+12, GbZA10, IBA+11, Lad14, LKN13, QZH13, XTLA13, XTLA14]. **composition-dependent** [LKN13]. **Compound** [ZST+10, KWC10, LLLB13, MQA17, PGG12, RCM+19, SKS10, SSW16, TYL10, TXL10, WR14b, vL13]. **compounds** [AMK10, ASD18, BG13, BH10a, Buc11b, CCA+12, CHV14, FC19, GZMC11, HZG12, KM12b, LOHB13, LV19, LTdSJ+10, LTL18, LWJL10, MLC+11, MPMCM+11, MW16, Mor12, MSRn+11, OPAVM18, OG19, Pan19, PP19a, PI13, PH12, Pie11, PP19b, RDM+11, RRK16, RR19, SMC18, SLC+18, Shi13, TSvL+16, TWR15,

VPGC12, WCY+10, WWQG17, WLL19, YLWrL12, ZFC+17].
Comprehensive [LKN13, RYM12, WJY15, BTH18, FKC12, KI15, SL10].
compressed [Man16, MBSAG16a, MBSAG16b, SBM16]. **compression** [GSPR19]. **Compton** [Kar12c, Kar15]. **Computation** [ČW13a, Sic16, YÇÖ11, AF19a, CHH+19, ILBS10, Kar12b, KYS13, KZZ13a, KMNSP19, MMM19, RBD+10, WKE17, Zen11, GI11c]. **Computational** [AM13a, AH19, AMK10, BYAT13, BGJSM+18, BJ17, BBA+16, BCS+12, CAA19, CSK12, CLY12, ÇT14, EM17, EBH11, FFPD16, For17a, FNIT16, GAI19, GGJD13, HNBG15, Hog13, HCL13, IMS+13, KRH13, KYS13, KyH13a, KBJ17, KYH+13b, KFS13, KGK13, LKOS17, LJK+18, LPOP12, LFS+11, LSR+13, LCCH10, LCCH11, MSG16, MK12, MANP17, MMF+13, NKF+13, Nym14, OAC17, OH13, OM13b, PS13a, PRG+10, PAPCMM+16, PSK+13, PPK+13, RW11, ŞBAT16, SK14, SB10a, SKHN13, She12, She13, Shi13, SR11a, TYN13, TV13, THSR13, VSMK15, VGGPdL19, WXZ+11, WG18, XYL+18, XTLA13, XZYS10, XZCH11, YYI+13, YIY+13, YS18, YMY+13, ZK12, ZQJW13, ZWZK19, ATPRV11, AASU+17, AKC10, ASW13, AVG19a, Bar16, BDF+18, BSSS19, BDG17, BB16, CLXZ12, CPL15, DLO16, DGA+13, EA12, Esr18, GWM11, GZBH18, GLPA10, HFL+17, JK12, KDÇ12]. **computational** [Kry10, LLF+12, LFTL18, LBdV16, Lya19, MK10b, MMW19, MEF+15, MM11, NBZG16, Ném14, PDNC14, Ped16, PZ19, PIS18, SGB11, SDP+16, SMRK18, Ser11a, SJZL12, Shi18, SMA11, TAY11, Tan12, Tch13, TT10, TU10, VV18, VS19, WML10, WLL+13, YBMK12, ZZC15, Zha15, ZYL+13, ZCG+16, ZBBB17, ELC08, JLL+18]. **Computations** [GLT13, IA13, KBF+13, KKH+13, KKT13, LLM13, MOY13, McC13a, MNE+13, ONK+13, OA13, TIN13, TM13, BBB+12a, CP11, PB10, Rus14, TTM16, Yu13]. **compute** [SGH10]. **Computed** [SUL+11]. **Computer** [PDR+14, CTDOLA10, FFF10, Ish14, yOITn15, VVN+16]. **Computing** [AGJ12, Tra19, CKB+19, DCOC+19, Ezz10, FT15, Lya19, PJP08, TY17]. **concave** [ONK+13]. **concave-bound** [ONK+13]. **concentration** [LV19, Pan19]. **concentration-dependent** [LV19]. **concept** [GI11b, GI11c, Kry11b, Kry12b, KN15, Kry10]. **Concepts** [Brä13, Hor13, IFT13, MSH13, Mar13, WR14b, YK13, ZJS13, BM16, GFPAV19, Gru17, PIS18, Sit15, Tch16, TFMC19]. **conceptual** [BCGC12, GHCMCMQ17, KP10, PC13, SMGZF19]. **concerted** [ACF+11, Met11]. **Concluding** [LF15]. **Concurrent** [EMED+12]. **condensate** [DCD11]. **condensation** [Chu12]. **condensed** [AF19b, GCK+17, Mak15]. **condensed-matter** [AF19b]. **condition** [BS16, HMH10b, IKN13, RTG+19]. **conditions** [CW13b, DKR10, PM12, RLER14]. **Condon** [Mam13]. **conductance** [KM12c, OPS10, RBGGM18]. **conducting** [CEV10, ZLWZ16]. **conduction** [IKS08, IKS10, MGP16]. **conductivity** [NMS+10, Oni10]. **conductor** [LSKM19, Oni12, SLS+19]. **conductor-like** [LSKM19, SLS+19]. **conductors** [PFdM13]. **cone** [MFLK11]. **Conference** [Ano13-49]. **Configuration** [RRCO11, Ali19b, BEM11, CGG18, CP16, DVDBM11, GBK18, HFD11,

JH15, KUY16, Luz08, NVI10, PBR18, SYL+18, Sha11b, SLZ+11c, SWS12, SZL+14, TG16, VVVB10, YKN13, ZST+10]. **configuration-interaction** [JH15]. **configurations** [Buc12b, FM16, RSN12]. **confined** [CKB18, CB19, FAFR12, GT13, JZZH17, KSC15, MNS11, MR18a, MR18b, OPC17, PJ19, RBVAG18, SA18, SL13]. **Confinement** [Bay19, GBS17, HS15, dFR15a, BPSM12, CDS+18, COP16, GZF13, GKGM18, MAPS18, Roy15, Roy16, TFSRM11, dSSF16b, dSSF16a, dFR15b, dSMT+18]. **conflicting** [Yam10]. **conflicts** [She14]. **confluent** [PMGMGR12]. **conformation** [Ire12, PK13a]. **Conformational** [BLWJ17, BCF+11, BSV12, EAH13, JN13, JB18, NRS+11, OSJ+12, YSG10, AB16b, AM13a, BTH18, CCC19, DSWL11, DFV+12, GSR12, GJ18, HHYC+18, KM12b, LBM11, MMW19, MUPC10, NJA+12, OMÐ13a, Pie12, SAS+12, WZX11, RCM10]. **conformationally** [UJSJ13]. **conformations** [BMR+13, CLMY12, MKSG13, NRI15, ZFW+13]. **conformer** [KKH18]. **conformers** [OPP+14, RJY+10, WZX11]. **confused** [HM10a]. **Congested** [Dil13]. **Congress** [NYA+13, RA10b]. **Conical** [MSH13, BMX+19, GSaY11, HV11]. **Conjecture** [Koc13b, Sit15]. **conjugate** [JSLH14, LCM+11]. **conjugated** [ALRAE11, DI18, FZH+18, GNM+12, MSG16, MMA10, RNV+12, TKS11, Wan11]. **conjunction** [KDOR17]. **connected** [TKS11]. **connecting** [Pat15]. **connection** [CH17, KUY16, MBA+19, PL11]. **connectivity** [AD17, Pog12, ZCTG18]. **conquer** [SKHN13, SN15, YKN13]. **consequences** [CFV18, Coo12, Fer19, Joh17, Kar15, Nas19, LNI12]. **conservation** [RS09, RS11a]. **consideration** [Fuk12, HYZ13]. **considerations** [GAPK+19a, NGS11, PMC11]. **considering** [Sut12]. **consistent** [Fin15, GRD11, ISN13, Mor12, SY10, SZS+10, SLZ+11c, SLZ+11a, SHMR11, WDJ+17]. **consisting** [KKH+13]. **constant** [Buc12a, DNCKCS+12, MVC13, Nag17, NZLG15, Shi18, WFS13]. **constants** [ATL+14, BCHN16, BJ12, CAAI12, CCP18, CFGC11, CSP+10, CDT12, CGIAI12, CJOOW11, Cyb11, DCOC+19, KP10, Kin13, LJSS12, MPTZ13, NH18, NB17, dMOB12, Per10b, RRK16, SGB11, SYL+18, SLZ+11b, SXS+12, SLS+12, SS12, SM10b, SWS12, UV18b, VLFG12, VO11, WZHZ13, Wit18]. **constituent** [MKHM11]. **constrained** [Lev10, SSB12a, WCM14]. **constrained-search** [Lev10]. **constraint** [PSMD16]. **constraints** [CM16, Fin17, MB12, Oht13]. **Constructing** [Beh15, KFY+12]. **construction** [Pop15, SX15, WR14a, MPB11, RVO+14]. **Contact** [LJK+18, DK13, XZYS10]. **contacts** [EAA17, GI14]. **containing** [Con10, DLLA10, FBU+11, HZG12, LWJL10, MPD+15, MB15, NCMC+18, NFD+10, NFQ+11, RRK16, RR19, SDM12, SCTW10, YGLL10, YZZ16]. **contamination** [Bla15, GXZ+14]. **content** [ALRA10, Sha11a, TRZ+19]. **context** [BBM17]. **continuation** [RW11]. **continuous** [Ale13, Ban12, Mor13]. **Continuum** [AF19b, JCC10, Cam10, Cam12, Cap16, Car19, COCF+14, CML+16, DZO12c, DQZF12, FRGC10, GMA+19, Kit15, Li15, LSKM19, PCR+11, RTG+19, RFEGPP+16, SL10, SLS+19, WML11].

contracted [SGH10]. **contraction** [Cin11a, FS11, HSN18]. **Contrasts** [SBSD18]. **contribution** [COdF+11, FKL+12, KL11, KC19b]. **contributions** [BWE16, GRCGRRHT19, RC11, RdA11]. **Contributors** [Ano12p, Ano12q]. **Control** [DP16, CZCW19, DLCB15, GV19, LW13, TCG17, vL13]. **controllability** [DKR10]. **controlled** [KPH+12]. **Controlling** [GLXL18, NTGC19, CKL16]. **contryphan** [FMKJ14]. **contryphan-Sm** [FMKJ14]. **conventional** [BH10a, MMM19, MPM15, Mar12]. **Convergence** [ATPRV11, Sil14, KB19, MBTVR12, TKN13, VPA11]. **conversion** [Buc12b, Mat02, Mat10, MMP+18b, Pha19, TFBG14, VGGPdL19, WRW+18]. **converting** [dSSdSGA12]. **Cooked** [MLPT10]. **Cooked-food** [MLPT10]. **cooling** [MPC10]. **Cooper** [SMR14]. **cooperation** [SJZ+18]. **Cooperative** [SW12, SJW13, LSR10b]. **cooperativity** [AKHS13, EEMSS14, EMS16, KK11a, LJW+11, MS14a]. **coordinate** [AHT12, CP11, HSN18, Laz14, MHO+15, YK13, dAB17]. **coordinated** [AM18, LVdSdM14]. **coordinates** [Kaw15, NH18, RPBB11, RCP14, WDSL14, dAB17]. **coordinating** [CCL+16, YZL+10]. **Coordination** [DLO16, BZBZ13, GGJD13, LYD+18, MSBF18, MSRn+11, OG19, dSMPRSF18, SLC+18, WR15, dCSDdMC13]. **copernicium** [DR18, ZT13]. **copolymer** [GDM+10]. **copolymers** [BSSS19, DSRGD12, GbZA10, MMA10, OCB+10]. **Copper** [AKC10, BBA+16, CPF12, CAPGAIG18, CWZ+10, FRNM12, LXW+14, LSCMSFC19, MVG18, MHHPR+17, UDVD10, UMS13, ZSZ14, dARAV12, MCC13b]. **Copper-catalyzed** [AKC10, CAPGAIG18]. **copper-exchanged** [UMS13]. **copper-zinc** [CWZ+10]. **coprocessing** [CKB+19]. **core** [CW16, CL18, Eng16, Glu13, HH18, KMM+18, MPTZ13, MZST16, MCK17, NBI+10, PZ19, SDY16, TOSN12, TSKN12, ZCG10]. **core-excited** [CL18, ZCG10]. **core-expanded** [PZ19]. **core-ionized** [Glu13]. **core/shell** [SDY16]. **cores** [LFP+19]. **coronene** [SR19, RNV+12]. **correct** [Kri13, TWR15]. **corrected** [HFdGC14, KPH+12, MIN13, MS17, SA18]. **correction** [IN15, KDOR17, KF19, Mas10, PSC15]. **corrections** [Cyb11, DAC12, DB11, KKL+16, MM19, SKY+13, WZX15b]. **Correlated** [ARG11, AF19a, AOT+18, BLdV19, CDS+18, DFV+12, Dun15, GBS17, HFdGC14, Jia15, KH10, KPH+12, Kry12c, MBA+19, OH19, SR12, TH13, Zak13]. **Correlation** [HIL19, Kan18, Lat13, Per18, RKCK19, WWD+15, AM13b, Ali14, AB18, Ali19b, AGPDZ13, AK11, DLJT14, Dw13, EM16, FMMD+10, Gra08, Gra11, HMH+13, Hog13, Hor13, Ign11, Ign12, LCT14, Liu15a, LG12, Lu15, Luz12, MSNP18, Mor12, PTH11, RPVM10, SFC16, She12, SXH18, SZS+10, SLZ+11c, SLZ+11a, SP19, TÁ10, Tob19, YKM+15, YDW13, dCDC+11]. **correlation-consistent** [SZS+10, SLZ+11c, SLZ+11a]. **correlation/dispersion** [dCDC+11]. **correlations** [CD15, DB13b, KK13, SMEH16, Sit15]. **Correspondence** [SSI+10]. **corresponding** [MAT19]. **Corrigendum** [HHL14, KJ16a, KKT14, SDS20]. **corrole** [SSS15]. **corrole-based** [SSS15]. **corrosion**

[EAK+10b, EAK+10a, EI11, THSR13]. **corrosion-inhibition** [THSR13]. **cosine** [GH11, GE12b, LLH15]. **Coulomb** [SS12, CF14, ARG11, BPL13, BBL12, Fin16b, FRGC10, Fuk12, GH11, IOO18, JH13, KH12, KWWH18, KK13, LLH15, Luz12, Nag16b, NDP10, PGGRMP10, Rit12b, Roy13, Roy16, SMOD11, Sil14, TC12, WWGW18, ZX12]. **Coulomb-attenuated** [NDP10]. **coulomb-attenuating** [CF14]. **Coulomb-like** [PGGRMP10]. **Coulombic** [Roy15, YW11b]. **Coulombic-like** [YW11b]. **coumarin** [MNP19, MDNDO+16]. **coumarins** [GTSC+19]. **Counter** [XLGA12, ZLWL16, MMSC19, Oni10]. **Counter-ion** [XLGA12]. **counterpart** [KC16]. **counterpoise** [KPH+12]. **counting** [JL12a]. **Coupled** [BJ12, Cam10, Cam12, Car19, PCV19, Sto18, VVVB10, WWC17, BVP13, BVP14, BSM+15, CSVCB12, DMAB12, DLM12, LRP+11, LP10b, Luz08, MPT11, PB10, RS12b, RSN12, SZS+10, Sza13, Tob19, Var11, XDM+10, YK13, ZE18]. **Coupled-cluster** [Cam10, Cam12, PCV19, LP10b, PB10, SZS+10, Sza13]. **coupling** [ATL+14, Ash18, BJ12, BSV12, CCP18, CFGC11, CSP+10, CDT12, IROW10, Kry10, Lar10, LKOS17, LW15, MKD19, MC18b, PM12, RCP14, SSI+10, Shi18, SHS+13, WTP+19, Wit18, YSS+10, YH14b, ZLS+18]. **couplings** [HKLW13, Kaw15, LB19]. **course** [HSYM11]. **covalency** [MML11b]. **covalent** [ABS13, AB16a, MURR13, NE11, YLH+19, KK13]. **covariant** [Luz08]. **Cover** [Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g, Ano12h, Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n, Ano13k, Ano13q, Ano13r, Ano13s, Ano13t, Ano13u, Ano13v, Ano13w, Ano13a, Ano13b, Ano13c, Ano13d, Ano13e, Ano13f, Ano13g, Ano13h, Ano13i, Ano13j, Ano13l, Ano13m, Ano13n, Ano13o, Ano13p, Ano13x, Ano13-35, Ano13-41, Ano13-42, Ano13-43, Ano13-44, Ano13-45, Ano13-46, Ano13-47, Ano13y, Ano13z, Ano13-27, Ano13-28, Ano13-29, Ano13-30, Ano13-31, Ano13-32, Ano13-33, Ano13-34, Ano13-36, Ano13-37, Ano13-38, Ano13-39, Ano13-40, Ano13-48, Ano14a, Ano14b, Ano14n, Ano14t, Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14z, Ano14c, Ano14d, Ano14e, Ano14f, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14o]. **Cover** [Ano14p, Ano14q, Ano14r, Ano14s, Ano14-27, Ano14-37, Ano14-43, Ano14-44, Ano14-45, Ano14-46, Ano14-47, Ano14-48, Ano14-28, Ano14-29, Ano14-30, Ano14-31, Ano14-32, Ano14-33, Ano14-34, Ano14-35, Ano14-36, Ano14-38, Ano14-39, Ano14-40, Ano14-41, Ano14-42, Ano15a, Ano15b, Ano15c, Ano15d, Ano15e, Ano15t, Ano15x, Ano15y, Ano15z, Ano15-27, Ano15-28, Ano15-29, Ano15-30, Ano15-31, Ano15-32, Ano15-33, Ano15-34, Ano15f, Ano15g, Ano15h, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n, Ano15o, Ano15p, Ano15q, Ano15r, Ano15s, Ano15u, Ano15v, Ano15w, Ano16a, Ano16s, Ano16t, Ano16n, Ano16u, Ano16v, Ano16w, Ano16x, Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16b, Ano16c, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m]. **Cover** [Ano16o, Ano16p, Ano16q, Ano16r, Ano17a, Ano17b, Ano17m, Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x, Ano17y, Ano17z, Ano17c, Ano17d,

Ano17e, Ano17f, Ano17g, Ano17h, Ano17i, Ano17j, Ano17k, Ano17l, Ano17o, Ano17p, Ano17q, Ano17r, Ano17s, Ano18a, Ano18r, Ano18s, Ano18t, Ano18b, Ano18o, Ano18u, Ano18v, Ano18w, Ano18x, Ano18y, Ano18z, Ano18-27, Ano18-28, Ano18-29, Ano18c, Ano18d, Ano18e, Ano18f, Ano18g, Ano18h, Ano18i, Ano18j, Ano18k, Ano18l, Ano18m, Ano18n, Ano18p, Ano18q, Ano19a, Ano19t, Ano19b, Ano19c, Ano19d, Ano19o, Ano19u, Ano19v, Ano19w, Ano19x, Ano19y, Ano19z, Ano19-27, Ano19e, Ano19f, Ano19g, Ano19h, Ano19i, Ano19j, Ano19k, Ano19l, Ano19m, Ano19n, Ano19p, Ano19q]. **Cover** [Ano19r, Ano19s, Ano12o]. **coverage** [ZCW16]. **COX** [MPE11]. **COX-2** [MPE11]. **COXIB** [OSJ+12]. **Cr** [HNBS18, MPD+10, VPFD10, XWC11a, CRB+12, KMU+13, NKWT19, Pan19, RRRV19]. **CrCl** [AM12, HK11]. **created** [Bae14, CD15]. **creation** [Kar15]. **Cremer** [KC19b]. **Crick** [PS10a]. **Crick-type** [PS10a]. **Criegee** [SMRK18]. **criteria** [GI14]. **criterion** [AOT+18, Fin16a, OAT+13]. **criterium** [ALB18]. **Critical** [CDT12, Exn11, Roy16, SDS19, TC12, ABLT11, AOLB12, DVP18, Kar12b, Kuz19, PCK19, SDS20]. **CrN** [AGCVG15]. **Cro** [AM13a]. **cross** [CK13, MGK+11, NA14, PWH+12, VV12, VV13]. **cross-linking** [PWH+12]. **cross-sections** [MGK+11]. **crosscoupling** [LTL18]. **crossed** [GV11, PL18a]. **crossing** [MMG15, RMJ11]. **crossings** [LKd+16]. **crosslinks** [ZMZ13]. **crossover** [DS11, DCdG10, SRASZ16, SSP+17b, ZSQ+10]. **crown** [DC14a, LJK+18, Pli18]. **crown-** [Pli18]. **Crown4** [CFP+10]. **Crown5** [CFP+10]. **crucial** [CG12]. **cruzi** [SLA12]. **Crystal** [BA13, FLvLA15, Kim13, TD11, BWB+18, DCDD10, DWGX12, GIO12, LZZ+13, NHB12, TSvL+16, VBC+12a]. **CRYSTAL06** [MPZWD10]. **Crystal14** [DOE+14]. **crystalline** [Bon17, DOE+14, EBR11, EA12, LRKM10, MMA10, SSKS12, SMEH15, STM17]. **crystalline-orbital** [MMA10]. **crystallinity** [JHSG18]. **crystallization** [BLKB11, ISRK12]. **Crystallographic** [HMA+19, WTW+15]. **crystallography** [PMHM19]. **crystals** [ABS13, AB16a, BWB+18, KC11, KG08, SMEH16, VBC+12b, ZSASS13, ZB18]. **Cs** [ČFČ11, DIOG12, MLW10, RBTL19, YK11, RK14]. **CSCH** [ZFS+11]. **C** — [ED16, SH18b]. **Cu** [MHHPR+17, MSOV13, SZZZ11, SYQ+10, VO12, XWC11a, YL11, Bal16, CRB+12, CDSK12, DWPK14, EM19, JFT13, KLZQ15, LYW11, LLZZ10, MGK19, MM10, NKWT19, PSK+16, PAPCMM+16, RYW+15, TOSN12, TSKN12, Tan13, WLL19, WZC+12]. **Cu/AC** [RYW+15]. **cubane** [NVI10, YYI+13]. **cubic** [QCB+10]. **cucurbit** [MGK19]. **cucurbituril** [VSMK15]. **CuH** [UDVD10]. **cumulant** [Kon11, Pir13, SIB+13, SHKS15]. **cumulative** [LS17]. **cuprate** [DB13b, SM10a]. **cuprates** [Lar10, Lar12]. **Curcumin** [Bal16]. **curly** [ABM+19]. **Current** [GEL18, HJK14, HKIH13, Vik13, ATM17, ALB18, BL19, GKS10, HMH10a, MAT19, Nal15, PS10b, PS14, PL11, RLTAT19, RBZ15, SM19, SZ15, VUC13, dA12]. **Current-density** [HKIH13, Vik13, HMH10a]. **currents** [RVNP12, RNV+12, SMR14]. **Curriculum** [Ano11a, Ano11c, KK12b]. **Currier** [LD17]. **Currier/cyclization** [LD17]. **curve**

[LQZZ12, MPT11, MPTZ13, LLZaH14]. **curved** [DI18]. **curves** [DHZS11, GM11, PPDF11, SAS+12, Vik11b]. **cusp** [RLER14]. **CuT1** [VLG12]. **cutoff** [KdSM+10]. **cutting** [LCK+16]. **CX** [LGW11]. **cyanates** [LKOS17]. **cyanide** [CMCN11, DR18, GZW16, WWLZ17, ZW15]. **cyanins** [ESLM19]. **cyano** [KPL+17, RS11b]. **Cyanoacetaldehyde** [KS19]. **cyanobenzenes** [EMK14]. **cyanogen** [BMBD10]. **cyanospherands** [ELC08]. **cyanuric** [DWZZ15]. **cyclacene** [OCGM+19]. **cyclacenes** [BLB+18]. **cycle** [KB13]. **cycles** [BvWG14, COCF+14, Sic16]. **cyclic** [ABM+19, BBKO16, DGA+13, FMKJ14, GHGF12, HL19, Jan10, JB18, LMCZ11, Luz11a, MZLM17, MMF+13, OB19, QTCL10, SB16, XZG+18, Con10]. **cyclization** [ALMY18, KSAK17, LD17]. **cycloaddition** [ABM+19, BL11, CJGTL12, DI10, KI15, LLF17, LFTL18, LWC+10, LCS+11a, LXLL11, NAK+17, SKTI15, WLWT12, YNLD18, ZRGE+19, ZWWY10]. **cycloalkanes** [DFV+12]. **cycloalkanone** [HZZ+19]. **cyclobutadiene** [LXD13, ND10]. **cyclobutane** [LSL+08]. **cyclobutene** [QB15]. **cyclobutyl** [DDÇY12, SC12a, SC12b]. **cyclodextrin** [NMHPVG12, SVRGV12]. **cyclodextrins** [PEA+12]. **cyclododecane** [DFV+12, SAS+12]. **cyclohexa** [KAOB11]. **cyclohexadiene** [TXK+19, ZWWY10]. **cyclohexane** [WWGW18]. **cyclohexyl** [CZJZ12]. **cyclometalated** [CADSG18, YZL+11]. **cyclometallated** [WXB+11]. **cycloparaphenylenes** [GMM+18]. **cyclopenta** [EI11]. **cyclopenta-1** [EI11]. **cyclopentadiene** [VV18]. **cyclopentadienyl** [ONK+13, ZFC12]. **cyclopentadienyltitanium** [RALK18]. **cyclopentane** [OPP+14]. **cyclopentane-1** [OPP+14]. **cyclopentanone** [PCR+11]. **cyclopentene** [ALMY18]. **cyclopentenols** [VOK+18]. **cyclopentyne** [ALMY18]. **cyclopropane** [TBA13]. **cyclopropenyl** [ÇT14]. **cyclotetrazenes** [fXxBhD19]. **cyclotridecane** [DFV+12]. **Cycloundecane** [DFV+12]. **cylindrical** [D'y16]. **Cys** [ScBsR+10]. **Cys-Asn-Ser** [ScBsR+10]. **cysteinate** [WHM14]. **cysteinato** [ADR+18]. **cysteine** [ASD18, CLMY12, HYD11, SKS10, YWH+12c, dAGNJT12]. **cysteine-Ca** [CLMY12]. **cysteine-formaldehyde** [YWH+12c]. **cysteine-thymine** [HYD11]. **cytochrome** [RDM+11, TSKN12]. **cytosine** [CTVA12, Cyb11, JS18, KUS19, YM13].

D [IIS+17, Kan11, STL12, SZY17, TSL11, XLLZ10, ZGSM15, CC11a, ÖEDB11, BEM12, BMX+19, BAB+18, DLRMFY10, HGB08, KH10, KSO19, LCL+10a, LQZZ12, LLZaH14, NF11, OD12, PTD+12, QTCL10, SLA12, SSS15, SK10, VVY18, WTH+11, YGLL10, YSW11, ZH12, Cys11]. **D-** [SSS15]. **D-dimensional** [DLRMFY10]. **D-wave** [KH10]. **D3** [SSB19, SA18]. **DABA** [Ser11a]. **DABCO** [LLF17, LD17]. **DABCO-** [LLF17]. **DABCO-catalyzed** [LD17]. **damage** [CAPGAIG18, FMP+17, POLV12, SS18a]. **dance** [FK18]. **Darmstadtium** [DR18]. **data** [CFV18, EKN10, LLH15, OKR12, SAG13, SDP+16, SMEH15, SBKJ18, VLG12]. **data-base** [SMEH15]. **database** [TBST10]. **dataset**

[OK16]. **Dative** [AM18]. **David** [Ano11c, Ano11b, RC11, Sau11]. **Davydov** [BEPZ10a, BEPZ10b, Lak10]. **DBUH** [RI19]. **dC** [XLGA12]. **DDQ** [YYS15]. **deacetylase** [dSMPRSF18]. **deactivation** [MR11]. **deal** [PBB15]. **Dealing** [AAHN16]. **deamination** [AASU+17]. **dear** [Sau11]. **Debye** [KWLS15, LKJ13, MGK+11, SMV11, Win10]. **decades** [Nes10]. **decahedral** [VS19]. **decanethiol** [FFF10]. **decapeptide** [DGA+13]. **decarboxylation** [EAH13]. **Decay** [AC11, ASD14, Cao17, CCM08]. **Decisive** [SC18]. **decoherence** [Brä11b]. **decomposition** [ÁFV12, CPF+11, CWS15, DWPK14, ENV15, HSN+11, LPOP12, LdAA+11, MCC12, MOSK10, MML+11a, MJ11, NB19, NEEV15, PWL+10, PMEP19, RLW+13, SKS11, SZ11, SLS+19, WLWL14, Yu13, ZL10, ZDZL11, dM13]. **decompositions** [BVA+14]. **Deep** [MVC13]. **defect** [BXR+13]. **defective** [ATS15, BAP13, Esr18]. **defects** [ES17, KC19a]. **deficiency** [MFR10]. **defined** [Fin16a, Gru17]. **Definition** [LVP12a, Kon11, MBTVR12]. **definitions** [Tch16]. **Deflation** [MQG13]. **deflection** [AOLB12]. **deformation** [GMP+11, KK12a]. **deformations** [KMT+12]. **deformed** [Agb12, MJ11]. **deg** [FDG18]. **degeneracies** [Lev10, RMG+19]. **Degeneracy** [MSC10]. **degenerate** [BDPT12]. **deglycosylation** [WHS+13]. **degradation** [HYZ13, SZL+15, dlLIAI+12]. **Degree** [YIY+13, CAAI12, GV19, LSW19, LWY19, PR11b, PL18a]. **degree-Kirchhoff** [LSW19, LWY19, PR11b, PL18a]. **dehalogenase** [ZCZ+12]. **dehalogenation** [PSKV19, ZCZ+12]. **Dehydration** [MMM+12]. **dehydrofulvene** [LVP12b]. **dehydrogenase** [SSB+12b, dCDC+11]. **dehydrogenation** [HSYM11, NTNL10, WZM+13]. **Delayed** [SGG+10, GMM+18]. **Deletion** [Cin11a]. **delivery** [RdPW+12]. **Delocalization** [DZO11, LNI12, ARH+13, AT18, LDKB15, MJ16b, NE11, NRGS11, RBVAG18, WDSL14, WWD+15]. **delocalized** [ALK18, DG19, Joh17]. **delta** [DAC11]. **demon** [CD15]. **denaturation** [BMB12]. **Deng** [Roy14]. **denoising** [SRMB15]. **denominators** [CPF+11]. **dense** [BN12, DW12, Ng12]. **densities** [ALRA10, ALRAE11, BPL13, Fin15, LS17, MAT19, MT11, MNZPT19, SS19b, WGLX10, ZL12]. **Density** [Ano13-49, BHA19, BGBV12, BJdlMAV12, CCL+13, CM12, CD12, DCBB11, DSZB18, DQZF12, EM16, ED16, FZX18, GMR18, GGD12, HLZ+14, HKLW13, HYD11, ISN13, IKN13, JS17, Kar13, KCC13, KK14b, KSAK17, Kit14, Kit17, Lae14, LWL+12, LWX+14, LBY+14, MLC+11, MW16, MUNZVR12, MIN13, MLB+12, MM13, MCRS16, MOH+12, NTNL10, NZAVR10, PS10b, PS14, PMH+16, RGPZD13, SA18, SVRGV12, SKY+13, SS13, TOSN12, Tan12, TIN13, TDOD17, TFZ+15, UMS13, VUC13, WJL+11, Wit18, YKM+15, YL11, ZCX+16, ZRR+11, dCSDdMC13, AC19, ABLT11, AK17, AM13b, AB18, ATM17, AGPDZ13, AST16, BMK+14, BD14, BCGC12, BVCAP12, BL19, BDF+16, BDF+18, BLdV19, BLKB11, CDSK12, CEFMK12, CM15, CNSK11, CH17, CZLD17, CLH14, CC19, CK17, CF14, CC11b, CSTA16, DWJZ11, DKS11, DPRK12, DW12]. **density** [Dil13, DZ11a, DGR+16, DG19, FO10, FDNR10, Fin16a, Fin17, FA17,

FSB16, GFPAV19, GCK+17, GM11, GJ18, GHCMCMQ17, GWME18, GD11, GCZ+14, HMA+19, HR19, HHCA10, HZZ+19, HMH10a, HMH10b, HKIH13, HZZW11, IN15, JR12, JPP+11, Jan13, JW18, Jeo18, JW19, Jou13, KK13, KME+18, KPCV18, KJ16a, KJ16b, KKL+16, Kit15, KYLC19, KDOR17, KJ14, Kri13, KFS13, KG08, KMU+13, KFJ+18, Kuz19, Lat13, LPO+12, LSR10b, Leh19a, Leh19b, LW11, LC16, LSP+16, LLW+11, LCK+16, LDZG16, LNI12, MYZ+10, MLW+14, MJ16a, MFK+12, Mas10, MKSG13, MLK17, MJ11, MBBT+12, MBSMJC18, MNS11, MKW11, MJM19, Nag15, Nag17, NAK+17, NDP10, NL11, NMIP14, NMSR14, NIT16, OD16, POLV12, PI13, PK13a, PABSK16, PP16, PTH11, PL11, PCV19, PR10b, PSMD16, PRFR17, PFdM13, Per18, PBR18, PJP10]. **density** [PMAP12, PI16, PC13, QHS11, RLER13a, RCM+19, RPVM10, RGTS11, RAMB18, RBVAG18, Rud12, RSCS10, RLZ12, RS13, RKCK19, SS10, SLG11, SB18, SFC16, SLC+18, SN12, SAHG11, SHL+13, SJZ+18, SIS+08, SDM12, SSP+17b, Sri19, SRA+11, SK12b, SX15, Tan13, TÁ10, TCA10, TGRP19, TLC+17, TRZ+19, UV18a, VPGC12, Vik13, VBO+15, VSL+15, WKE17, WW11, WJY15, WDJ+17, WTZ+11, WR15, XNL+14, XSLF12, fXxBhD19, XGH+18b, YLH+19, YWH12a, YWH12b, YRN+11, Yu13, YF16, ZT13, ZKKR11, ZQCJ10, ZLWY13, ZBG+19, ZMZ13, ZCG+16, ZSZ14, ZKW17, ZZ18, Zho18, dCGAMV12, CTDOLA10, LLZ+12, Ven12]. **density-based** [ZKW17]. **density-dependent** [IN15]. **Density-functional** [FZX18, BDF+16, BDF+18, BLKB11, CF14, DW12, JR12, LNI12, MYZ+10, WR15]. **Density-functional-theory** [SVRGV12]. **Density-matrix** [EM16, Kit14, Kit15]. **deoxygenated** [TYN13]. **deoxyguanosine** [SKM11]. **deoxyribonucleoside** [MB14]. **Dependence** [AG10a, BLWJ17, Buc12a, BN11, BSV12, CAAI12, GLF+12, KP11, KSG+12, KKH+13, LZFZ13, Mar11, MIN13, MKSG13, PMMGL+11, Rud12, WR15]. **dependent** [ASD18, Bae16, Bae14, BDF+16, BDF+18, CP10, CEFMK12, CW11, CW13b, DCZ17, DM16, FMMD+10, GFPAV19, GSR12, HS11a, HHCA10, HKZZ15, IN15, ILBS10, IG11, JPP+11, LKN13, LV19, lLBqD+19, LMZY15, Luz13, MJM19, NMS+10, NSN17, NNSN17, NDP10, Oht13, PVS11, PVS12, PSC15, PJP10, PMAP12, PI16, SFC16, SLC+18, SSAM13, SL13, Sko16, SHW+13, Vik11a, Vik11b, WKE17, WYWL13, YLYC18, ZQCJ10, ZCG+17, ZLE17, ZSZ14, ZZ18, Zho18]. **dephasing** [Gan14]. **Depicting** [LBdV16]. **depolarization** [AEM+12]. **deposited** [SAHG11, SAHA12]. **deposition** [TFBG14]. **deprotonation** [CFOC+10, Kry12b, PUGSFM18, Shi18, WXB+11]. **depth** [LYS+19]. **Depurated** [Cin20, MMM16, MMM20]. **derivation** [BR10, BR16, Bra10]. **Derivative** [HSN18, BSSS19, DWPK14, KGVG11, LWZ+14, TPT19, WLZ+12b]. **derivatives** [ALMY18, BSS15, CWL+13, CCL+16, CFV18, CWB+13, CSG14, DKZ+10, DWZZ15, DNCKCS+12, EI11, FSQ+11, GTR11, GB13, HNH+12, HMA+19, HS11b, HLB19, ILBS10, JLZ+17, JB11, JFDD10, KZA+17, KKM+12, KSN+10, KKG12, LGM+18, LWL+12, LYS+19, LWY19,

LCCH10, LWH+12, LCH+11, LCS+11b, LW15, MLY+16, MNV+17, MLPT10, MDNDO+16, MBBT+12, NRHJ11, OAA19, PPK+13, QHS11, RYM12, RBZ15, RMP+14, SF13, SSTÖ11, SRMB15, TZ11, TKSK17, Val17, VV18, VMC11, VHTEG15, VBO+15, WGLX10, WLL+13, WJ11, YWR+18, ZSAP11, ZZX10, ZZR+12, ZYL+13, ZMB+17, ZFC12]. **derived** [CADSG18, MAN15, NH18, PAKA15]. **describe** [CB10, MMG15, PABSK16, Sza13]. **describing** [Gar08, JCC10, dGR14]. **description** [AB18, DVDBM11, DCFD10, DMBL16, Fer19, FGD+19, GC19, HFdGC14, KO14, LORR+12, MPMCM+11, MBA+19, Nas19, NGS11, SIM14, SFL+10, TCA10, TRZ+19, ZZ18]. **descriptions** [PC16, PCK19]. **descriptor** [AKR12, FDG18, PUGSFM18]. **descriptors** [GI10, GI11b, GI11c, GI11e, JS18, LV19, LNV+18, Nag16b, Nal15, OPAVM18, PH12, Pog12, TFA10]. **Design** [FZH+18, HSS18, IIS+17, cLqFtW+14, Val17, BJ17, CAA19, DC14b, GbZA10, HM10b, LLZ+14, LZZ+17, MY17, MSM16, Ném14, Oni12, OWD18, SRASZ16, SAHAA16, Sik18, SLA12, SSS15, STM18, THL+15, TK16b, VVY18, WWB+14, WR14a, WR14b, XFW+14, YZZH15, YHLC15, ZFW+13, ZWZK19]. **designed** [NTGC19, OAA19]. **designing** [SSB12a, ST15]. **desorption** [ÁFV12, FTB11, GD11]. **Dess** [TM19]. **destructuring** [KRG+13]. **desulfurization** [VPGC12]. **detachment** [DZO12c, DZO12a]. **Detailed** [Sch13, Fin14a]. **Details** [Lar10]. **detector** [BMB10]. **determinant** [RLZ12]. **determinants** [CSSK+12]. **Determination** [ATL+14, GI11b, GI11c, IKN13, SN12, Ali14, AGPDZ13, AST16, MLW10, PT13, Ser11b, GBK18]. **determine** [SFW12, Tob19]. **determined** [Mor12]. **Determining** [MGM11, AGB19, Bon17, IKN13]. **detonation** [LZZ+13, RGTS11, WGLX10, ZZX10, ZL12]. **Detours** [DB13a]. **deuterium** [NHB12]. **deuterons** [HITU16]. **developed** [AY15]. **Developing** [AV19]. **Development** [KSN+10, Lin14, NSN17, NNSN17, SR11b, SKV12, SZ15, GEL18, Kap12, KKL+16]. **developments** [AMMC19, HJK14, Jør18, Mur12]. **device** [yBZfC18]. **devices** [Jan10]. **dfppy** [ZQJW13]. **DFT** [YSK+12, AEKGZ12, AFC+10, ACF+11, BVCAP12, BPVDB11, BP13, Bas11, BZBZ13, BLRdA+10, BAA+18, BS14, BDR12, BAB+18, BJ12, BO11, BW13a, BW13b, BSV12, BSPK11, CRB+12, CR18, CPF12, ÇAS13, CRSB12, CW16, CCL+10, CKYR18, CKB18, CFGC11, DSCO+13, DSD18, DCDD10, DCFD10, Dw13, DAE+12, DPDR11, DP16, DdG+11, DB15, DFF+13, EG10, ESDO16, ESS13, EFO11, EO11, ES17, EM19, ESBVJY12, FSQ+11, FV11, FRNM12, FPRGMHGB12, GAPK+19b, GC18, GJ18, HS11b, HFdGC14, HNBS18, HhGqZZ17, JPPA10, Jan10, JL12b, JB11, JLL11, KMS+11, KP10, KP11, Kar12b, KBF+13, KAG08, KMM+18, KG17, KI15, KKG12, KBMM10, LJ13, LGM+18, Les12, Lev16, LYW11, LLP+13, LLF17, LZW+18, LTL18, LYW+19, LGW11, DVMC19, LKZ+16, LGS+16, MXC18, MCP10, Mar12, MCC12, MGK19, Mas10, MMP+18b]. **DFT** [MMC+19, MFZ+18, MCL11, MS17, MML+11a, MMM+12, MAN15, Nag16a, NEEV15, OKK10, OGvSG18, OCB+10, OCGM+19, OPP+14, OVT+16, PS10a, PTS+11, PK13a, PWL+10,

PAD+10, QCW+12, RK14, RRVJ10, RGST12, RFEGPP+16, RDB19, RYW+15, RNdA+10, RFMC19, RS11b, Rua10, SSP+17a, SSB19, SMGZF19, Sat11b, Sch12a, SMEH15, Ser11a, Ser11b, SAHA12, SHE10, SM13, SS18b, SB10b, SBB16, SHW+13, SMGZ13, SWS+14, Tas14, Tav12, TGRP19, TG13, Tug13, TKSK17, UV18b, VF13a, VV18, VLG12, VSN+11, Vie17, WLWT12, XX12, XZ11, XZG+18, YNLD18, YYS15, YY18a, YY18b, YYI+12, YIY+13, YZL+11, YWY+12, YZW+15a, YZZ16, ZSAP11, ZLWL16, ZL10, ZQXP17, ZLY+14, ZPW16, ZCP11, ZDZL11, dSdS13a, dSdS13b, dSM19a].
DFT-based [BP13, Dw13, MCP10]. **DFT-D** [BAB+18]. **DFT-D3** [SSB19]. **DFT-treatment** [AEKGZ12]. **DFT/M08** [Vie17]. **DFT/M08-HX** [Vie17]. **DFT/TB** [ZCP11]. **DFT/TD** [LGS+16]. **DFT/TD-DFT** [LGS+16]. **DFT/TDDFT** [BAA+18, YZW+15a, ZSAP11]. **DFT/UFF** [JLL11]. **DFTB3** [PSC15]. **dG** [XLGA12]. **di-anionic** [DHYC19]. **di-enol** [Val17]. **di-lanthanide** [OAC17]. **Diabatic** [CHM+17, ART08, DMAB12, DM12, KUY16, MHOG18, MKD19, SHS+13]. **diacetyl** [TM13]. **diagonalization** [GBK18, Man16, MBSAG16a, MBSAG16b]. **diagonalizations** [CKYR18]. **diagrams** [FMKJ14, Jen13]. **dialkaline** [BHMN19]. **dialuric** [KB13]. **diamagnetic** [Pit12, RP11a]. **diamantane** [BBKO16]. **diamines** [LKOS17]. **diamino** [LLW+11]. **diaminoanthraquinone** [DKS11]. **diamond** [GZ14, ZWWY10]. **diamond-like** [GZ14]. **dianions** [TIN13]. **diarylethenes** [MPJ12, YXM+18]. **diarylethylenes** [Bud12]. **diastereocontrol** [SFW12]. **diastereoselectivities** [TFZ+15]. **diasteroisomers** [BCF+11]. **Diatom** [CNBPR+11]. **diatomic** [Agb12, BKM15, BB10, CP13, CJOOW11, GM11, GS11, HRT12, HVR18, Ish14, JZP17, KBGC12, KBG17, Leh19c, LLP17, MPM15, NDH10, RC11, Roy14, SYY16, Tou11a, VOAH18, Leh19b]. **diatomics** [GI11b, GI11c, IM15]. **diaza** [ZLS+18]. **diaza-benzo** [ZLS+18]. **diazaadamantane** [KMK+16, KMM+18]. **diazadiborinine** [GC18]. **diazine** [BHA19, CW16]. **diazo** [LTL18, LDW+11]. **diazonium** [Bon17]. **diazotization** [LLW+11]. **dibenzothiophene** [VPGC12]. **dibenzothiophene-like** [VPGC12]. **diborane** [ZYL+14]. **diborane···** [SSB19]. **dicarbon** [FC19]. **dications** [Buc12b, GNM+12]. **dichalcogen** [KM19]. **dichloro** [LCS+11a]. **dichloro-germylene** [LCS+11a]. **dichloroketene** [CHH+19]. **dichloromethylbenzimidazole** [PMC11]. **dichloropropene** [ASMP15]. **dichlorosilylene** [LLLB13]. **dichotomy** [GMT18]. **dichroism** [PCR+11, SB10a]. **diclofenac** [KK19]. **dicopper** [BH10b, RNdA+10]. **dicyclobutadieno** [LWY19]. **dielectric** [CN12, KP10, KT12b, Ng12, NDM+12, OA13, RTG+19, Ser11a, Ser11b]. **dielectron** [LB19]. **Diels** [CM12, Iku17, LW11, MIKH19, ZLWL16, ZXY13]. **Diels-Alder** [MIKH19]. **dien** [WLS+19]. **diene** [EI11]. **dienes** [LW11, LKZ+16]. **dieniminium** [BMX+19]. **dienone** [KAOB11]. **diethyl** [KI15]. **diethyldichalcogens** [Dum12]. **difference** [AD17, Fin16a, Kim16, LCZ15, WH18]. **differences** [ALK19, BWB+18, BB16, MK10a]. **Different** [MAT19, ABP13, ABA11,

BS16, CW16, CP11, FM16, GI11e, GGP13, HGB08, JdOS16, KP10, LZZ+17, MNP19, MIKH19, TW10, TFZ+15, YŞÖ12, ZCW16, Zil14]. **differential** [Ali14, yBZfC18, CRA+11, HVR18, Nag10]. **differentiation** [CW11]. **difficult** [KLE+19, Mar12]. **difficulties** [Sut12]. **diffraction** [ÖEDB11]. **diffuse** [SZS+10, SLZ+11c, SLZ+11a]. **Diffusion** [JCCZ12, PP10, ABG12, BR12b, HKZZ15, LWX+14, MFOH18, RJLPGH+13, SR19, UDS19a, WLH+19]. **difluorohydroxyborane** [MMCN+11]. **dihydro** [SC12b, TAY11]. **dihydrobenzimidazole** [KKG12]. **dihydrobenzoxazoles** [ZBG+19]. **Dihydrogen** [dOR10, AKHS13, GD11, GT13, MS14c]. **dihydrolipoic** [PM17]. **dihydrolutidine** [TM13]. **dihydrolysergol** [RGS+13]. **dihydropyridines** [ZYSW17]. **dihydropyrrolones** [VGGPdL19]. **dihydrothiophene** [HL19]. **dihydroxyacetone** [BGJSM+18]. **dihydroxybenzene** [YY18a]. **diimide** [HSS18]. **diiso** [LKOS17]. **diketonato** [AC19]. **diketone** [SKS10]. **diketopyrrolopyrrole** [MSG16, PWP+18, WWB+14]. **diketopyrrolopyrrole-analogue** [PWP+18]. **diketopyrrolopyrrole-thiophene** [MSG16]. **dilauroyl** [MKSG13, TTM16]. **Dimensional** [DTF+11, ART08, Beh15, BEPZ10b, Cho15, CYK17, Dau16, DLRMFY10, DBTA19, Dw13, DMS+10, Mam13, MPD+15, MDC15, MSC10, MLDP10, PGMGRM15, RZSZ18, RNC+14, SPD+18, SD13b, SSAM13, VBC+12a, VBC+12b]. **dimensionally** [Yam11]. **dimensions** [IIH16, RPVM10, RAK10]. **dimer** [AM13a, BF11, CHL+19, GIO12, HM12, KS18, MPT11, NTGC19, NVI10, NHB12, PMMGL+11, SH19, SXH18, SKY+13, SS13, TNN16, TBB+19, Zak13]. **dimeric** [Rua10]. **Dimerization** [LSR10b, LS19, Rua10, SKTI15, TFA10]. **Dimers** [TBRIS12, BCF+11, Cas15, CZCW19, FSB16, GORW19, KM12a, KK11a, KSS+19, KDOR17, MT10, PP10, PMEP19, RPBB11, RNE10, SZZ+19, TBRIS10, TBRIS11, TPT+13, VSS11, WJ11, dSCC12]. **dimetal** [ZFC+17]. **dimetallocene** [LYD+18]. **dimethoxyphenol** [Tan12]. **dimethyl** [JSLH14, JAB12, LdBF+12, LXLL11, NMHPVG12, Owe17, SJZL12, SSP14, SCZH16, TAY11, TXL10, WXZ+11]. **dimethyl-germylidene** [TXL10]. **dimethyl-silylene** [LXLL11]. **dimethylallene** [CPL15]. **dimethylamine** [LLZZ10]. **dimethylaminophenyl** [FO10]. **dimethylaminopropanol** [WZX11]. **dimethylcyclobutene** [MB13]. **dimethylmethylene** [LWC+10]. **dimethylnitrosamine** [LVdSdM14, dAVdM17]. **Dimethylphenyl** [Tan12]. **dinitrogen** [VPOG19]. **dinitrophenol** [LDW+11]. **dinitrophenyl** [RNdA+10]. **dinitrosamine** [JN13]. **dinuclear** [FDNR10, PEA+12]. **dinucleoside** [PAD+10]. **dinucleotide** [Cys11]. **dinucleotides** [HW12]. **dioctahedral** [PDR+14]. **diodes** [MUNZVR12, NZAVR10]. **diols** [LKOS17, SBEH11]. **dione** [OPP+14, QJ13, IK14, KDÇ12]. **dioxabicyclo** [VOK+18]. **dioxane** [Cha10, CNSK11]. **dioxetanone** [dSdS13b]. **dioxetanones** [dSM19a]. **dioxide** [JLS13, KKT13, KKT14, MPL+11, PP14, TDOD17]. **dioxin** [MSY+12]. **dioxolene** [DG19]. **dioxy** [KMK+16, KMM+18]. **Dioxygen** [MMÅ13]. **dioxygenase** [ASD18]. **Dioxygenation** [ADR+18, ASD18].

diperfluorophenyl [WDS19]. **diperoxide** [SRA+11]. **diphenyl** [YWJ+11]. **diphenylamino** [CRSB12]. **diphenylcarbene** [GLXL18]. **diphenylformazans** [TT10]. **diphenylopolyenes** [MMWA11]. **diphosphinito** [ED16]. **dipolar** [BL11, DI10, ELC08, YNLD18]. **dipole** [AM12, Ber13a, Ber13c, BVP14, GFB12b, GI11a, GI11c, HK11, IMS+13, KA11, LKJ13, MA11b, MD11, MVA19, MNS11, SS12]. **dipoles** [SMEH15]. **Dirac** [DJ12, Agb12, Bay19, BCNR18, DJ95, NF11, RW12, Rit12b, SS12]. **diradical** [MMF+13, NYS+10, PCK19, Shi18, YSS+10]. **Diradicalology** [NKF+13]. **diradicals** [BSM+15, CKL16, ZLS+18]. **Direct** [ARH+13, CP11, FLCHL10, HHL+12b, KyH13a, LKLW11, Nal12, SSdS17, TK16a, ZZW11, Haj18, Nal13, Sha11b, SGL19, VPGC12, WWHZ13]. **direct-potential-fit** [Haj18]. **Directed** [DKR10, ABS13]. **direction** [IAA15]. **Directional** [SMP10]. **directionality** [KUTS10]. **directly** [Kri13, WWL17]. **disarms** [NP18]. **discontinuously** [GB10]. **discotic** [SSKS12, ZSASS13]. **discovered** [VVY18]. **discovery** [CAA19]. **Discrete** [DTFK15, GMA+19, JCC10, TIKL13]. **discussion** [Yos20]. **disease** [Bal16, MPTR12]. **diselenide** [Dum12]. **diselenide-linked** [Dum12]. **dismutase** [CWZ+10, PM17]. **disorder** [PDR+14, Wan13]. **dispersing** [ISRK12]. **Dispersion** [KH12, SA18, Dob14, ISN13, IN15, KDOR17, LCT14, MS17, PSC15, Pit12, SKY+13, WJY15, dCDC+11]. **dispersion-corrected** [MS17]. **dispersion-improved** [LCT14]. **dissipative** [Cho19, PD11]. **dissociated** [MTL+12]. **Dissociation** [CK17, GM11, PW10, SSW16, SM10b, BMBD10, Bla15, CC11b, DSZB18, GSaY11, GLT13, GRLA18, GD11, KWC10, KZA+17, KTI+12, KMM16, LLL16, MMBK12, MNE+13, OKR12, OK16, dMOB12, RPBB11, Rua10, SLZ+11b, SB10b, SQ10, SYS14, SDY16, SCS15, TJS17, VSMK13, VO11, XX12, ZZX10, ZCC11, ZSHL14, ZZC12, dSNBG08]. **dissociations** [TCA10]. **dissociative** [DLCB15, Kry12b]. **dissolution** [KLK13]. **distance** [GI11b, LSS19, SXH18]. **distances** [GST11]. **distillation** [TB15]. **Distinguishing** [ZR13]. **distortion** [CL11, YYI+13]. **distortions** [GFB12a, GHCMCMQ17, PK13b]. **distributed** [RAMB18]. **distribution** [ABP13, DPRK12, EPS+16, GGD12, LGHL11, PK13a, RCM10, SACA18, SM14a, TMM+14, WZX11, vLRRK15]. **distributions** [GV19, LSS19, LBdV16, SVPTM+10]. **distyrylpyridine** [MUPC10]. **disubstituted** [fXxBhD19, dOdONM12, dSNBG08]. **disulfide** [Jan10, KKT13, KKT14, WXZ+11, WHY+14, ZMB+17]. **disulfides** [GSaY11]. **dithio** [NA12, PS13a]. **dithio-substituted** [PS13a]. **dithiolene** [SDR+13, ZLWZ16]. **dithiols** [LKOS17]. **dithione** [QJ13]. **divalent** [NFD+10]. **divergence** [ALRAE11, Rit12a, Rit12b]. **divergence-free** [Rit12a, Rit12b]. **divergent** [DB13a, SWS+14]. **Divide** [SKHN13, YKN13, SN15]. **divide-and-conquer** [SN15]. **Divide-and-conquer-based** [SKHN13, YKN13]. **divided** [HS11c]. **divinyl** [dlLIAI+12]. **divinylene** [FO10]. **division** [FDG18]. **DJ** [Shi13]. **DJ-1** [Shi13]. **DMABN** [CFP+10]. **DMABN-Crown4** [CFP+10].

DMABN-Crown5 [CFP+10]. **DMAP** [LLF17]. **DMAP-catalyzed** [LLF17]. **DMC** [RYW+15]. **DMRG** [MFLP12]. **DMSO** [VLK+11, CCL+10, SK12a, Ven12, YZZ15]. **dmso-S** [CCL+10]. **DNA** [Lad14, XTLA14, ACF+11, BS14, BBM17, BTH18, CLC10, CW16, Che13, Coo12, DTFK15, DSVP15, EG10, FV11, GfWlZ11, HW12, JS18, KZA+17, KUS19, KKS+11, LCH14, LQZZ12, LLZ+14, MMR+10, MS10, Net12, OM13b, POLV12, PAD+10, PPK+13, RAK10, SM13, Sza13, TD19, XLGA12, XTLA13, Yak10, Yak11, ZMZ13, ZTC11, CAO18]. **DNA-based** [LLZ+14]. **DNA-bases** [EG10]. **DNA-binding** [BBM17]. **DNA/** [CAO18]. **DNA/RNA** [BS14, KZA+17]. **DNT** [LPOP12]. **do** [HST13]. **Docking** [LdMCdA+12, Net12, CSVCB12, CSSK+12, RdPW+12, YWY+12]. **DOD** [YFY17]. **DOD-PBEP86-NL** [YFY17]. **dodecaborate** [LYR+17]. **dodecyl** [CAPL12]. **Does** [BN12, Bud12, DPK18, MBA+19, Fin14b, OG19]. **Domain** [ABLT11, Lya19, CP13, Pat15, SLS+19, ZLE17]. **Domain-averaged** [ABLT11, CP13]. **domain-restricted** [ABLT11]. **Domain-specific** [Lya19]. **donation** [DCdG10, LBdV16]. **Donor** [BLdV19, ABA11, BLL+13, BGJSM+18, BAB+18, CMR13, HSS18, IIS+17, KPL+17, LQ13, LGS+16, MANP17, SSK11, ScBsR+10, TSBSM12, WLS+19, ZKKR11, ZFS+11]. **donor-** [MANP17, KPL+17]. **donor-acceptor** [ABA11]. **donor-peptide** [SSK11]. **donors** [CN12, MNP19, VVJ15, WTW+15, XZYS10]. **donut** [ACT19]. **dopamine** [RFMC19]. **dopant** [RMTG11]. **dopants** [VSMK13, WTP+19]. **Doped** [XMZ+12, AGOP18, ASW13, BSS15, CSK12, CWW+16, DVDBM11, DWX+16, DHYC19, ENV15, EM19, FFPD16, FTB11, GAMM10, GMM+18, HLMO11, HNBG15, HWL16, HWWW18, KJ14, LSCMSFC19, LHL+15, NW12, Oni10, OGvSG18, RKM12, RZC13, RYW+15, RCGLV+14, SD16a, UDS19a, ZCX+16]. **doped-gold** [FTB11]. **doping** [BHAH+18, BGL+16, Fer11, GAPK+19b, KSS+19, Kim19, OH13, PPDF11, TZD+19, TW10, YYI+13, ZK12]. **dot** [CSK12, CN12, LEU+11, MR12, OK19, RP11a, YH14a, ZX12]. **dots** [HGB08, OPS10, SD13b, SS19b, YÇÖ11]. **Double** [CF14, SLZ+12, WTP+19, AF16, Ali19a, AG19, yBZfC18, CF17, ETGLMJ+19, KKC14, KMT+12, LV12, DVMC19, MAT19, NBL+14, NTCG18, PAD+10, PM17, Sri18, SDL+15, VAT12, WZX+15a, Xu16, Xu19, Yu13, YF16, ZX12]. **double-cage** [yBZfC18]. **double-electron** [Sri18]. **double-excitations** [VAT12]. **Double-hole-mediated** [WTP+19]. **double-hybrid** [AF16, Ali19a, Yu13, YF16]. **double-shell** [DVMC19]. **double-well** [SDL+15, Xu19]. **doubles** [HFD11, PCV19]. **doubly** [BMF13, Cor16, DSSM18, KT12a, SX15]. **Douglas** [SN15]. **down** [RF10]. **doxorubicin** [Bas11]. **Dr.** [Mer11]. **drawbacks** [PIS18]. **Dressed** [MMWA11]. **Drigo** [COP16, HS15, dFR15a]. **driven** [AS19, Coo12, EM16, GB10, KC16, KC18, MS12, SPSA11, WR14a, Xu16, Xu19]. **driving** [Pan19]. **drug** [AB16b, BJ17, CAA19, HM10b, IAK13, KKS+11, MS10, RdPW+12, SD13a, SSTÖ11, SK11, HM10b]. **drug-DNA** [MS10]. **drugs** [EAK+10b, GCDNGS12, YINM13]. **Ds** [OM13b]. **DSD** [YFY17].

DSD-PBEP86-NL [YFY17]. **dT** [XLGA12]. **dual** [EMSB15, NH18, UDS19a, WWHZ13, YK13, JLG+12]. **dual-level** [WWHZ13]. **ductile** [KG17]. **due** [ALA15, CAO18, ZSZ14]. **duplex** [PPK+13]. **during** [HSYM11, MNC12, MSAB19, Tob19]. **Duschinsky** [Mam13]. **dyads** [MUNZVR12]. **dye** [AGJ12, BDG17, ÇAS13, FM16, FSBA12, cLqFtW+14, MY17, MFB11, MANP17, PMAP12, QJ13, SG19, SSS15, WKE17, WWB+14, Zha17]. **dye-aggregates** [WKE17]. **dye-sensitized** [AGJ12, FM16, cLqFtW+14, PMAP12, QJ13, SSS15, WWB+14, Zha17]. **dyes** [AGJ12, BBM17, FM16, FBU+11, GMA+19, JPPA10, JWG+12, cLqFtW+14, MY17, Mas10, PJP10, WWB+14, ZSAP11]. **Dynamic** [ÁFV12, DLG12, KWLS15, AM13b, Ang10, BŁ16, CCEGK12, CEFMK12, FKL+12, FC19, KYS13, LKJ13, MNS11, NH18, RC11, RVO+14, Tob19, TSH17, TPCJ+12, YKM+15, ZWLC12, dWLC14]. **Dynamical** [AFM+10, BR10, BR16, GWZ+14a, Sko16, ZZ15, EML+11, Ign11, Ign12, KMF+11, NE11, PETB18, VVY18]. **Dynamics** [KKH+13, LLM13, MNE+13, PPK+13, RDB18, SRPD16, SPPT15, TIN13, TM13, AS19, BM16, BBB+12b, BR15, BWB+18, CTVA12, CCC19, CW13b, Cho19, CLXD15, CAPL12, Dau16, DGR+16, DLZ11, DP11, EAH13, Fra17, FUE+12, GKS10, GVPCK10, GW18, GSPR19, HDÖS12, HXX15, HHL+12b, IKC18, JHSG18, KTI+12, Kaw15, KCC13, KSC15, Kit14, Kit15, Kit17, KF17, KUY16, LWWZ13, LC19, LPM+11, LKLW11, MAD12, MMG15, Mak15, MSH13, MDC15, MP12, MCARL11, MOE+11, MMBK12, MKD19, MMT+13, MRS15, MSK+12, MPL+11, MLB+10, MBS+18, MMP11, NTGC19, Nym14, OHDA13, PD11, PP10, PMH+16, PI16, RSM12, RP16, Rit11, SMK+12, SIT+12, SPSA11, SMEH15, SIB+13, SHKS15, SLS+10, SKV12, SZ15, SZY17, SBL11, TK16a, TPdMB12, UTTn13, Vik11a, VGS10, WWHZ13, XZJ+16, Xu16, Xu19, Yak10, Yak11, YGL+11]. **dynamics** [YAF+15, YT14, YINM13, YLC17, Zak16, ZPM10, ZZW11, ZGSM15, ZH15, ZCG+17, ZWL18, ZRLV10]. **dynamics-friendly** [MDC15]. **dynamics/quantum** [BBB+12b, EAH13]. **Dyson** [DZO11, SOM10].

E-C [LXD13]. **Early** [Kap12, LJ16]. **earth** [Ali14, BHMN19, CZCW19, DTEMK11, SG19, ZQCJ10]. **easy** [PR10b]. **echo** [HST13]. **Eckart** [PKK+16, TCG17, VOAH18]. **Economical** [ZF15]. **EDA** [ŚKB18]. **edaravone** [PGG12]. **edge** [PE11]. **edged** [WWL+11]. **edges** [BBKO16]. **edited** [Ban12]. **Editor** [CK13, Lad14, PS14, VV13, XTLA14, COP16, HS15, Lun13a, Man16, MBSAG16b, PS13b, Sha11a, Tou13, VUC13, dSSF16a, dFR15a]. **Editorial** [Ano18-30, Bar16, Brä14, Cav17, For17a, LJ16, LV16, MEF+15, Nag16a, Tch13]. **E**$\cdots$ [WSML16]. **edt** [BAA+18]. **Effect** [ALRA10, BSSS19, CdLdSC18, Eil14, KP10, KMM+18, KT12b, KM19, MFB11, MMC+19, Mit11b, MTS15, RP11a, Sch10b, Shi18, SYS14, WLZ+12a, YLW+13, ZCZ+12, dOLdlV13, AC19, BMTT11, BdTG11, BS14,

BGL+16, Bra10, BEPZ10b, CNBPR+11, CCC19, CYLL11, COP16, DKS11, DK13, GWZ+14b, GZMC11, HV11, HR19, HSN+11, IGMK11, JN13, JLG+12, Lad14, LSR10b, LZ12, LPOP12, LWL+12, LLC+11, LWJL10, LB19, MNP19, MG12, MS10, MSK+12, MPT11, MW15, NTCG18, ND10, OKK10, OA13, PCMG12, RY12, RMTG11, RRK16, RR19, SD13a, SIM14, SM19, SAHAA16, SPIL14, SK10, STU19, TYN13, TMC18, TJS17, WWL+11, XTLA13, XTLA14, XWCY11, XZJ+16, YRN+11, YKN13, YD17, ZGSM15, ZKWZ17, dSSF16b, dSSF16a, dAVdM17, Jan10, JWG+12, ZAE10].
Effective [AST19, CEM14, Liu15b, May14, TSvL+16, Vik11b, YHL+13, BCGC12, CCBR+12, Dw13, GbZA10, KUY16, MPTZ13, MZST16, PGGRMP10, TG16, ZE18, Liu16]. **effectively** [ABM+19]. **Effects** [ABA11, BS16, Bla15, CAO18, KSAK17, LLZ+12, MSRn+11, PETB18, AGOP18, ACF+11, Ali14, AEM+12, ALMY18, BHMN19, BH10a, BSO16, Chr10, CFGC11, DCD11, DPDR11, DWZZ15, DLLA10, EHKD11, EKD12, EEMSS14, EAV16, Fer11, GR11, GBS17, GWM11, GZF13, GR10, GRCATG19, HZW18, Ire12, IROW10, IK14, JA12, JHSG18, KI15, KRG+13, LDKB15, LGHL11, LDW+11, MNZPT19, MZLM17, MKHM11, MURR13, MPE11, NG11, NMHPVG12, Oni10, OGvSG18, OK19, PCR+11, PWP13, QHS11, RLTAT19, RP11b, RFN+12, RS12a, RSN12, RSM12, RdA11, Ril10, SH18a, SKTI15, SP19, TK16a, TV13, TFSRM11, TH12, Tob19, VFCSC17, VSMK13, WDR+11, WLC+17, XX12, XLGA12, XDM+10, YZW+15a, YMY+13, YT14, YFY17, ZH12, ZLS+18, ZBG+19, ZYL+13, ZBBB17, ZFC12, dCDC+11, dSMT+18, dSNBG08, SMK+12]. **Efficiency** [Cal10, AGOP18, ATPRV11, BDG17, Mai14, THSR13, VRO+12]. **Efficient** [BŁ16, KI15, SHW+13, SCBP17, YM14, ZWSF16, ZRLV10, CKB+19, FZH+18, FM16, IIS+17, LCK+16, OAA19, SKLC19, SGH10, SAHAA16, WTP+19, WZX15b, ZCX+16, ZKW17, dSM19a]. **EGEE** [LG10]. **Ehrenfest** [KUY16]. **eigenfunctions** [PMGMGR12, PBR18]. **eigenstates** [KB12]. **eigenvalue** [Mit11c]. **eigenvalues** [Mit11c]. **eigenvector** [LHX+19]. **eight** [SALK19]. **eight-vertex** [SALK19]. **Einstein** [DCD11]. **elastic** [Per10b, UV18b]. **Electric** [CB19, MJM19, SS12, BŁ16, CHL+19, CKB18, DB15, EBR11, GMR18, GV11, KA11, KT12b, LB19, MM19, PCD14, SMEH15, SMEH16, SM19, VRO+12, YŞÖ12, Zha17]. **electrical** [GKS10]. **electride** [OCL+18]. **electrides** [HWL16]. **electrocatalysis** [MLW16]. **electrocatalytic** [FFPD16]. **electrochemical** [AVG19b, NBZG16]. **electrochemistry** [FFPD16]. **electrode** [KJ15, Tug13]. **electrodes** [Che13]. **electrodynamics** [FNIT16, IFT14, Lin14, Liu15b, Liu16]. **electrolyte** [DLO16]. **electrolytes** [AVG19a, MNE+13, Pha19]. **electromagnetic** [Bae14, NTGC19]. **Electron** [Bas11, DZO12c, DJ18, DSVP15, LC16, LRMAA19, LZ10, MT11, PUH+11, PI16, RVNP12, RBVAG18, SLG11, VBC+12a, AA11, AOT+18, Ali14, AEM+12, AGG+18, ALRAE11, AM18, ARH+13, AST16, AT18, BLL+13, BHMN19, Ber13a, BL10, BL11, BSSS19, BKM15, Buc10, Buc11a, CMR13, ČW13a, CM15, CG12, CH17, CSMZ10, CSTA16, DLCB15, DAA16, DLJT14, DTEMK11, Dil13, DZO12a, DLLA10,

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electron [OAT+13, POLV12, PL11, Pir13, PNC19, RBGGM18, RNV+12, RCM10, RAGM10, RS13, RKCK19, SDS19, SDS20, SS10, SBMM11, SBM16, SYK+12, SPD+18, SSAM13, SHS+13, SM12, Sit15, SL13, ScBsR+10, SBKJ18, Sri18, SP19, Tob19, TC12, VF13a, VBC+12b, WLS+19, WWD+15, WH12, XZYS10, YNLD18, YM14, YRN+11, YHLC15, YD17, ZDZO10, ZFS+11, ZZZ+18, ZSZ14, ZJS13, dA12, dCDC+11]. **Electron-density** [RBVAG18]. **electron-group** [WH12]. **electron-muon** [RAGM10]. **electron-N** [SSAM13]. **Electron-pair** [LRMAA19, MT11, WH12]. **electron-proton** [DLCB15]. **electron-rich** [YNLD18]. **electron-withdrawing** [BSSS19]. **electronegativity** [CG12, GI11b, GI11c, GI11e, GI11f, Kan18, TSBSM12]. **Electronic** [AB16b, AC19, AGB19, AVG19b, BZBZ13, Ber13b, BVP14, BBYZ18, BBAL12, BG11b, BG11c, CZLD17, CJGTL12, DZO12b, DLLA10, FBO+11, FMCA11, GZF13, HHCA10, IA13, KK11b, KLZQ15, KP13, LVdSdM14, MLY+16, MFZ+18, MS14b, MKM11, NBL+14, NDM+12, Pup11a, RKM12, RZC13, SGC13, SBB16, TNT18, TSKN12, TSH17, VSN+11, VBO+15, XTLA13, XTLA14, YW11a, YH14a, AEKGZ12, AO12a, Ale13, ART08, AST16, BVCAP12, BPVDB11, BPL13, BS11, BL10, BW15, BBB16, BSV12, CWL+13, Cas15, CMCN11, CWW+16, CHSO13, COP16, DIOG12, DAR+11, DDÇY12, DD17, DWX+16, DG19, DCHC11, DHYC19, DHZS11, DSH+13, DB13b, Dun15, D'y16, ETGLMJ+19, Fin14b, FSK+11, GBS17, GAPK+19b, GSZ10, GWM11, GFB12b, GP13b, GMT16, GEL18, GJ18, GB13, GMM+18, GC19, HMI+15, HTM10, HIL19, HJ13, HWWW18, HhGqZZ17, IGMK11, IK18].
electronic [JL12a, KG17, KRK+17, KMF+11, KCK14, KJ15, KJ16a, KJ16b, KSD10, Kle11, KYLC19, KSY+11, KFY+12, KZZ13a, KHH10, KAOB11, KMM16, Kri13, KO12, KUY16, Lai11, Leh19c, LL11, lLBqD+19, LMZY15, LL19, LLZ+14, LBdV16, DVMC19, LHL+15, LZ10, Lya14, MSG16, MLC+11, MC11b, May14, MMWA11, MUNZVR12, MBA+13, MPZWD10, MGB18, Mil12, MS17, MKD19, MA11a, MA11b, MMRRA10, MJ11, MB13, MPT11, MPTZ13, MM13, MW15, MSRn+11, MCRS16, MC18b, NS19, NA12, NIT16, NZAVR10, OGvSG18, PE11, PCR+11, PAKA15, PMAP12, QJ13, QCB+10, RMLPGGGH16, RS12a, RMJ11, RRRV19, RNC+14, RMTG11, Rus14, RMY+13, SRPD16, SR12, SD13a, SB10a, SLC+18, SYL+18, SLS+14, SXS+12, SLS+12, SLSZ13, SIS+08, SRS+17, SSTÖ11, SR11b, SZZ+12, ScBsR+10, SSW16, SK12b, TYN13, TZ11, TV13, TD11, TBB+19, TFB11].
electronic [TRZ+19, TG13, UTTn13, Var14, VPA11, VLFG12, WWC17, WFS13, WDS19, WJL+10, YZL+10, YZL+11, YZW15b, YH14b, ZQCJ10, Zha10, ZLLS10, ZZR+12, ZCG+16, ZQXP17, Zho18, ZCP11, dSSF16b,

dSSF16a, Bou12b, Lad14]. **electrons** [BEM12, BMB10, BB10, BMB16, Dw13, Fer19, Ign11, Ign12, ISRK12, KK13, KK14a, KV19, Kry12c, Nas19, Nes10, QCB+10, RP11a, RPVM10, RS13, SALK19, She12, SS19b]. **electrons-Nd** [BB10]. **Electronuclear** [SL13]. **electrophilic** [Buc11b, YSA+11]. **Electrophilicity** [PC13, IG11]. **Electrostatic** [HL19, NMHPVG12, TH12, TCS10, AC19, CDSK12, DPRK12, IG11, KKS+11, KRG+13, PK13a, TYN13, ZCZ+12]. **electrostatics** [BWE16]. **element** [OVT+16, SHS+13]. **elementary** [EMED+12, EMEPD15, SOF+10, Zil14]. **elements** [AÖ12b, ČW13a, GI10, LXD13, NZ13, RRK16, SW10, TMC+13]. **eleven** [DCFD10]. **ELF** [Fin14a]. **eliciting** [TPT19]. **elimination** [BLM+12, FZC14, MM19, MLB+12, Zha10]. **elliptical** [MFLK11]. **elongated** [ALHC18]. **Elongation** [KdSM+10, XLGA12]. **else** [Kry10]. **Elso** [COP16, HS15]. **elucidating** [Kaw15]. **elucidation** [MMP+18b, SBKJ18]. **elusive** [SSP14]. **elymoclavine** [RGS+13]. **embedded** [BA13, Lan10, LC19, SMV11, SRN+19, JLL11]. **Embedding** [ABS11, DB13a, QB15, AB16a, GCK+17, HJK14, SRN+19, TGRP19]. **embeddings** [AF19b]. **emeraldine** [RMTG11]. **Emergence** [LFP+19]. **emergent** [SMMT13]. **Emerging** [AH19, GP13a]. **emission** [BS11, BSO11, CFP+10, LXW+14, ORJ18, PSK+13, dSdS13a]. **emissive** [ZKWZ17]. **emitter** [OAA19]. **emitting** [MUNZVR12, NZAVR10, SHW+13]. **empirical** [Hat13]. **Employing** [Tob19]. **enable** [LSKM19]. **enal** [HZZ+19]. **enantiomeric** [LW13]. **enantiomers** [MP12]. **enantioselective** [LCZL11, QCW+12, WTZ+11]. **enantioselectivity** [LCM+11]. **encapsulated** [CWL+13, JL12a, KG08, TPT+13, WW11, ZLWL16]. **Encapsulation** [RR11]. **endic** [ZPW16]. **Endo** [Jal10]. **Endohedral** [JW19, ACL12, BBYZ18, GAPK+19a, HLB19, JLL+18, LYW+19, MS17, SCTW10, WLZ+12a, WSL+11, YL11]. **endohedrally** [NW12]. **endohedrals** [YK11]. **ene** [IK14, Sat11b]. **Energetic** [GB13, GAMM10, HLB19, HM11, HZZW11, Kar15, LCCH10, LL17, MTS15, SRA+11, TCSD12]. **Energetics** [MNC12, ACMRN10, CdAFS+12, CdLdSC18, DCBB11, GCD13, KUTS10, PMMGL+11, Puz10, QTCL10, TBA13]. **Energies** [BBKO16, LBW11, SCZG12, ASHF13, AC12, Ali19a, ABA11, BVCAP12, Bla15, CFOC+10, CHH+19, DZO12c, DZO12a, EKN10, FLvLA15, FYhC11, FC19, GMA+19, GM11, GFRdG11, HNH+12, HIL19, HM10b, IKN13, Kin13, KKS+11, KB19, LDKB15, LORR+12, MMM19, Mas10, MS14c, NA14, Nal13, NVI10, OKR12, OK16, Pea11, PBB15, SH19, SR19, SOM10, SZL+14, Tsu15, VF13a, VLFG12, WWC17, WZW17, WR15, XX12, YÇÖ11, YWH+12c, ZZX10, ZCC11, ZZC12]. **Energy** [CC11b, FDA16, AV19, AG10b, AK17, AB18, AOLB12, AEM+12, ART08, AZD+11, AST16, ALK19, BXR+13, BPVDB11, BP13, BAP12, BSS16, BBL12, Ber13c, BVA+14, Bou12b, Bud12, CPF+11, CWW12, CNBPR+11, CDS+18, CCL+16, CFV18, CLH14, CSG14, COP16, DK13, DB11, DHZS11, EMK14, Fin16a, FMMD+10, GST11, Gra08, Gra11, HR19, Han19, HJRO13,

HFD11, HMH10b, HFdGC14, HM10b, HM11, HBMM11, ISN13, IK18, Jeo18, JZP17, KKH18, KyH13a, Kim16, KSN+10, KMNSP19, KMM16, KPH+12, Kri13, Kuz19, LFF+10, LSR10b, LV12, LWWZ13, LDZG16, LG12, LDADB+15, LVP12a, LSC+18, MZB+13, MGK+11, MDC15, MCP10, MHT+08, MA12, McC13a, MOE+11, MOLF11, MIN13, MAF19, MJSC18, MGD11, MPRCEG12, MLB+10, NA12, Ném14, Ng12, NDP10, NIT16, OPAVM18, OH19, PML+11, Per18, PMEP19, Pha19, PP14]. **energy** [RBGGM18, RPVM10, RGTS11, RCP14, RLER10, SAS+12, SIM14, SFC16, SGL+16, SCLCPB12, SA11a, SB16, SXH18, SLZ+11b, SRS+17, SK11, SGC13, SS19b, SSW16, STU19, SZ15, SZY17, SC18, TNN16, TSL11, Tou11b, VPA11, Vik11b, Vyb08, Wag14, WKE17, WWL17, WH18, fXxBhD19, XZZ+10, YH14b, YLC17, YLYC18, ZWL18, ZS12, ZRLV10, dHLdS12, dSSF16b, dSSF16a, Yu13]. **energy-based** [SK11]. **energy-dependent** [FMMD+10]. **energy-loss** [AEM+12]. **energy-relevant** [Wag14]. **Energy-surfaces** [FDA16]. **engineering** [RI19, WCL+17]. **enhance** [ZLWL16]. **Enhanced** [BGL+16, TZD+19, DSD18, LLZ+14, Mas14, MS14c, MPE11, SKV12, Sri19, TFSRM11, TSBSM12]. **Enhancement** [GV19, KKT13, KKT14, SJW13]. **enhancements** [ATPRV11]. **enhancing** [MZLM17, WLC+17]. **enol** [AZD+11, Coo12, GW18, MPGGS19, VF13b, Val17]. **enol-imine** [Coo12]. **enols** [MPGGS19]. **enones** [LMCZ11]. **enough** [MSS11]. **ensemble** [AM13a, Jou13, PP16]. **Entangled** [Xu16, EMEPD15, SK17b, Xu19]. **Entanglement** [Kar15, Tap15, BT15, BT17, SPM+15, XZJ+16, ZZ15, ZBK15]. **Enthalpies** [Mor12, dSNBG08, HZG12]. **Entropic** [DTPC17, LSS19, SMOD11, LRMAA19, MR18b]. **entropies** [HN12, OH19]. **Entropy** [AZD+11, DBTA19, Gra08, Gra11, JZZH17, NTCG18, PD11, PKK+16, PSGK17, Sit15, SDL+15, WSV10]. **envelope** [MMA10]. **envelopes** [BW15]. **environment** [AG10a, GC19, JCC10, TYN13, MPL+11]. **Environmental** [OK19, RdPW+12]. **environments** [AM10, Mar13, MVA19]. **Enzymatic** [SCB+14, BMB12]. **enzyme** [DPRK12, ZST+10, dSSdSGA12]. **enzymes** [AHC+18, WYWL13]. **EOM** [DVP18, TD19]. **EOM-CCSD** [TD19]. **EOMCC** [DSVP15]. **E'Ph** [WSML16, WSML16]. **epoxidation** [LMCZ11, ZLY+14]. **epoxide** [KMS+11, KUTS10]. **eQE** [GCK+17]. **equalization** [GI11a, GI11f]. **Equation** [FKBG19, UV18a, Agb12, ATPRV11, Bay19, BKM15, BR10, BR16, Cam10, CW11, CW13b, Cho16, GMGRMP12, HYZS12, HYZS19, KC16, Kha16, Kri13, MNZPT19, Nag16b, NF11, PGGRMP10, PVS11, PVS12, PGMGRM15, RZ17, RW12, RA10a, VATPR11, VAT12, WC14, Zak16, ZLJ11]. **equations** [CRA+11, DSCO+13, Per10b, ZLE17]. **equilateral** [RSN12]. **equilibration** [Nes11]. **equilibria** [Kim19]. **equilibrium** [KS18, LDW+11, Nal15, NB17, SXH18, TSH17, Zak16]. **equivalences** [ZWE12]. **Equivalent** [GSZ10]. **era** [IAK13]. **Ergodicity** [NE11]. **Erratum** [BR12a, BC16, BT17, BW13a, DJ12, FCS13a, Ign12, IKS10, Kar10, LSR+11,

Liu16, Mat10, RB11a, RAFR18a, RS11a, TBRIS11, TBRIS12, Yur15]. **error** [KB19, VSS11]. **errors** [LNI12]. **Esteemed** [Sau11]. **ester** [HM11, SJZL12]. **esterification** [LGM+18]. **esters** [CGIAI12, QCW+12, WTZ+11]. **estimate** [BBL12]. **estimated** [EKN10, Kuz19]. **estimates** [CWF11, CDS+18, ÇT14]. **Estimating** [CCL+16, ZS12, Bla15]. **estimation** [Den19, EMK14, KFY+12, SK12a, VVN+16]. **Estrada** [HIL19]. **ethanol** [FFF10, HDQ+13, MOE+11, PSKV19]. **ethene** [Ang10, SKTI15, TGA+11]. **ether** [KI15, LJK+18, TPdMB12]. **ethers** [QCW+12, SCZH16, dlLIAI+12]. **ethoxy** [DPRK12]. **ethoxypyridine** [MCC12]. **ethyl** [KI15, KDÇ12]. **ethyl-pyrrolidine-2** [KDÇ12]. **ethylbenzene** [HWHZ11, SSB+12b]. **ethylbenzenes** [MOH+12]. **ethylene** [AKC10, DLO16, KI12, LCH+11, NA14, NIK19, SDR+13, TXL10, TFA10, WDR+11, dlLIAI+12]. **ethylene/linear** [NIK19]. **ethylenes** [YNLD18]. **ethyltoluene** [GK12]. **ethynyl** [ŞBAT16]. **ethynylpyridines** [SM12]. **ETO** [GS10]. **ETOs** [AA15]. **Eu** [XYL+18, BRBRS11, USL+13]. **Euler** [Nag16b]. **eupatilin** [LLP+13]. **eV** [NA14]. **evaluate** [CJSNLM11, HNH+12, PBR18]. **evaluating** [CKL16, GI11d]. **Evaluation** [GAPK+19b, GS10, Hat13, NJA+12, Sch12a, dWLC14, AA15, BŁ16, GTR11, GI10, HSN+11, IG11, JS17, RI19, SPO+11, TPdMB12, YZ13, ZRLV10, GI11b, MC18a, OCGM+19]. **event** [GI11a]. **events** [CSS16]. **evidence** [HV11, HHYC+18, WTW+15]. **evidences** [CG12]. **evolution** [ABM+19, BL11, IFT13, IFT14, JL12b, MLW16, RGR12, YSS+10, YSK+12]. **Evolutionary** [CGG18]. **evolving** [LSR+13, Vik11b, YYI+13]. **Ex** [NCMC+18]. **Exact** [GZSMFN16, HR12, HFZ12, Kha16, KUY16, RBD+10, RS13, Zak16, AM13b, Eng16, FA17, Hog13, IHG10, Kry12c, LEU+11, MPB11, PT13, SFL+10, Tou11a, FLCHL10]. **exact-exchange** [SFL+10]. **Exactly** [GMGRMP12, PGGRMP10, PMGMGR12]. **EXAFS** [LSR+13]. **examination** [Kan17]. **examine** [KJ14]. **example** [CP10, DMBL16, MSAB19, RBTL19]. **examples** [DLM12, Hop15, JA12, Mai14, MMP+18b, Sic16]. **ExCage** [DI18]. **excellence** [MEF+15]. **exceptional** [LA11]. **Excess** [BHMN19, JdL08, KM19, YHLC15]. **Exchange** [Dw13, Fin16a, MMM20, PTH11, ATL+14, AM13b, Ali19b, AGPDZ13, AK11, BHV+11, BVRM10, CWW12, Cin20, Eng16, FB17, IHG10, KMK+16, KMM+18, Kry12c, LZFZ13, LCT14, Lu15, MMM16, MEEA+13, Mys12, PDR+14, RPVM10, RFEGPP+16, RLER10, SPPT15, SFL+10, SFC16, Shi18, TÁ10, XZL+12, MRS15]. **exchange-correlation** [AGPDZ13, AK11, LCT14, RPVM10, SFC16, TÁ10]. **exchanged** [PvS10, UMS13]. **excimers** [Cas15]. **exciplex** [KB19]. **Excitation** [KyH13a, BVCAP12, BSS16, FMCA11, dDGNB10, GMA+19, IHG10, LWWZ13, LORR+12, Mas10, MIN13, SZL+14, WSCL11, YH14b, ZGSM15]. **excitations** [CD15, VAT12, VBC+12b, Zho18, ZB18]. **Excited** [Cha11, Glu13, ACF+11, Ali19b, Cam10, Cao17, CHM+14, CM16, CL18, Cor16, DSSM18, GWHH17, HMA+18, IGMK11, JA12, KT12a, KK14b,

KKT13, KKT14, LSL+08, LV16, LP10b, LGZC15, LZ10, MMWA11, MT11, MNS11, MB12, Nes11, NDP10, Nic11, PRPU+13, PMAP12, SBM16, SR11b, SK12b, Sza13, TTT13, TBB+19, TXK+19, WKE17, YÇÖ11, YXM+18, ZZ18, ZCG10, MQG13]. **excited-state** [ACF+11, Cao17, JA12, WKE17]. **excitons** [RP11b]. **exclusion** [CM15]. **execution** [Lya19]. **exhibiting** [Fin15]. **exist** [BN12]. **exohedral** [GB13, HLB19, JW19, WLZ+12b]. **ExoMol** [TY17]. **expanded** [CJBMMAPR19, LLZ+14, PZ19, ZRY+13, ZWZK19]. **Expansion** [Kut13, Nik11, HSN18, HMH10a, Kit15, LV12, LSC+18, Sil14, SS12, Win10]. **expansions** [Tal11]. **expectation** [MC11b]. **Experimental** [CSSK+12, DDÇY12, EI11, MLPT10, SC12a, AZD+11, CFV18, DSH+13, FPRGMHGB12, HHYC+18, KAOB11, MMV+19, RGS+13, SC12b, SRASZ16, SJZL12, SBKJ18, TAY11, VMC11, WWGW18]. **experiments** [LRP+11, WSV10, YS13, MM10]. **explained** [TM19]. **explanation** [XCD18]. **Explicit** [BH10a, Koc13a, JCC10, MAD12, MK10a, Pir13]. **Explicitly** [CDS+18, AF19a, GBS17, TH13]. **exploitation** [MPB11]. **Exploiting** [LSKM19, WH18]. **Exploration** [MOE+11, MBA+13, WCS+13, HSS18, MCP10, MOLF11, NH11, SSP+17a, Sic16, TCSD12, YS18]. **explorations** [WLL+13]. **explored** [JMX+15]. **Exploring** [AGOP18, ACF+11, DCR10, ESBVJY12, HJRO13, JMPP19, KB12, KC19a, LV19, MNP19, PK13a, SS18a, TMC18, ZCG+17]. **explosion** [WWGW18]. **explosive** [DGR+16, LZZ+13]. **explosives** [YZ13]. **exponent** [HITU16]. **exponential** [GMGRMP12, GH11, GE12b, Hog13, KH10, LLH15, PGMGRM15, PSGK17, Roy13]. **exponential-cosine-screened** [LLH15]. **exponential-screened** [Roy13]. **exponential-type** [GMGRMP12, PGMGRM15]. **expressed** [Glu13]. **Expression** [RA10b, Kuv10]. **expressions** [AEÖ12, GZSMFN16]. **Extended** [Koc13b, CLL+11, DQZF12, Haj18, HBMM11, Ire12, MPMCM+11, MSOV13, NZ13, PP19b, WML11]. **Extending** [AT18]. **Extension** [Kon11, WB17, BAP12]. **Extensive** [DSSM19, IM15]. **extensivity** [RS09, RS11a]. **extent** [LDKB15]. **External** [Hor13, Bae14, DSZB18, DB15, Glu13, KSC15, Kit14, RS13, TJS17]. **extractants** [VBJK18]. **extraction** [LCH+11, LCS+11b]. **extracule** [MT11]. **extrapolated** [ZE18]. **extrapolation** [CHH+19, CC19, LV12, SXH18]. **extrapolations** [KF19]. **extrema** [SRMB15]. **extreme** [Mit11c]. **Eyring** [BR16, BR10]. **Eyringpy** [DCOC+19].

F [yBZfC18, CS18, DPDR11, DSSM18, DSSM19, EMSB15, GWM11, GKT+12, GB13, HNBG15, JLG+12, KAR12a, KMM16, Kuz19, LJL+11, LGHL11, LZZ+11, LMZ+11, LLG+12, LC16, MEEA+13, PP14, RLTAT19, SB18, SKS10, SPIL14, SYQ+10, SZL+14, TMC18, TL15, WZW17, XZL+12, MLPT10, YZW+15a, BLWJ17, DMAB12, DZO11, GKT+12, LGHL11, Ma14, MGB18, Pup11b, Sik18, SZ15, TNN16, YGL+11, ZHL+19, ZCG10]. **F12** [BL12, yOITn15]. **Fabricio** [COP16]. **fac** [AC19]. **face** [DMWY11, DLG12]. **Factor** [Tri14, Kan17]. **factors**

[AGB19, BMX+19, Mam13, MK11, SPO+11, TZ11, VLG12]. **families** [GN19]. **family** [OOI+19, WZX15b]. **Fan** [Roy14]. **far** [Var14]. **FARMS** [MC17]. **Fast** [GFRdG11, PMHM19, PT13, PSC15, SAS+12, SLS+19, UDS19b]. **Fatigue** [YXM+18]. **fayalite** [NDM+12]. **FCu** [ALMY18]. **FCX** [SZL+14]. **Fe** [DMG10, ESS13, FTB11, MPD+10, MG10, MGP16, PAKA15, Qu13, YL11, Zha10, AM10, BGFD14, BAA+18, CRB+12, DS11, DCdG10, KSD10, LVdSdM14, NKWT19, OGvSG18, SSP+17b, ZSQ+10, ZSHL16]. **Fe/C/S** [OGvSG18]. **Fe/C/S-doped** [OGvSG18]. **feasibility** [JS17]. **features** [CD12, DLG12, Pie12, Sch10b, TC10]. **FeCp** [XCY15]. **feed** [FCC11]. **feed-forward** [FCC11]. **FeF** [KCK14]. **FeFe** [BGFD14, BAA+18]. **female** [MEF+15]. **FemEx** [MEF+15]. **femtosecond** [HYH+10, MPC10]. **Fenna** [BSS16, MSBF18]. **Fermi** [ABLT11, CP13, FA17, IROW10, KCDC15, KK13]. **fermion** [FYhC11, Lun13a, Lun13b, Tou13]. **Fermionics** [Kle11]. **Fernando** [COP16]. **ferrimagnet** [TD11]. **ferrocene** [DAA16, XCY15]. **ferrocenium** [DAA16]. **Ferrocenyl** [MMW19]. **ferroelectric** [DMS+10, DLM+11, OCB+10]. **ferromagnetic** [BXR+13]. **Feshbach** [WB17]. **Fe —** [SBSD18]. **Festschrift** [KN15]. **few** [Mai14, SLS+19]. **FF** [LGW11]. **fiber** [KFY+12]. **fictitious** [MVA19]. **Fidelity** [BCNR18, CKYR18, Luz11b]. **Field** [CKB+19, Bae14, BBB+12b, Bra10, BSO11, BN11, CL11, CHL+19, DCD11, DB15, EBR11, FKL+12, Fri12, FSST16, GZF13, GRD11, HSS+11, ISN13, KKH18, KSC15, KV19, Kit14, KC19b, Lae14, LB14b, LB19, MM19, Mit11b, MPL+11, MJM19, NTGC19, PVS12, PL11, PCR+11, Pop15, RP11a, SRPD16, SY10, SMEH16, SAHAA16, SS19b, SR11b, SV11, SHMR11, TSvL+16, Vik11a, Vik11b, Vik13, Zha17, dAB17]. **field-effect** [SAHAA16]. **field-emission** [BSO11]. **Field-programmable** [CKB+19]. **field-theoretical** [Fri12]. **fields** [Bae14, CSS16, FT15, GV11, HEVMSA+19, KT12b, PM12, SRPD16, SMEH15, Sto18, WYM15]. **file** [RAMB18]. **Filho** [COP16, HS15]. **film** [JK12]. **films** [GDM+10]. **filter** [Man16, MBSAG16a, MBSAG16b]. **Filtered** [MPV+11]. **Finding** [JHL+18, SRMB15, KB12]. **Fine** [RDB18, RAFR18b, SCZG12, RAFR18a]. **fingerprint** [vLRRK15]. **finite** [CS17, FKL+12, NS10b, PE11, TLC+17]. **finite-length** [PE11]. **firefly** [CYLL11]. **Firsov** [AOLB12]. **First** [BXR+13, DWX+16, FTB11, Fra17, Jia15, Kan17, KLK13, LLL16, lLBqD+19, LIK15, MBKH19, Per10b, RZG12, RJLPGH+13, RRB12, TZ11, Wan13, WLH+19, ZWLC12, vL13, AFA13, AGG+18, BZBZ13, Bon17, CEFMK12, CC11a, CWW+16, CJOOW11, FSB16, FT15, GXZ+14, HMA+19, IGMK11, JMPP19, KSS12, Kim13, LLM13, LBdV16, LSCMSFC19, MKM11, MJM19, Pan19, PP19a, RD14, RVO+14, TCCI10, TWR15, VVAO12, VDG13, XWCY11, XCD18, YHL+13, dWLC14, WZC+12]. **first-principle** [TCCI10]. **First-principles** [BXR+13, Fra17, Jia15, Kan17, lLBqD+19, LIK15, MBKH19, Per10b, RJLPGH+13, RRB12, Wan13, WLH+19, ZWLC12, AGG+18, Bon17, CC11a, CWW+16, CJOOW11, HMA+19, Kim13, LLM13,

LSCMSFC19, MJM19, Pan19, PP19a, XCD18, YHL+13, WZC+12]. **first-row** [BZBZ13, MKM11]. **first-shell** [JMPP19]. **Fischer** [MJ16a]. **fischeri** [PI13]. **Fisher** [LNV+18, MR18a, Nag15, OOI+19]. **fit** [Haj18]. **fitting** [KFJ+18, PCV19]. **five** [RNV+12, WLS+19]. **five-electron** [WLS+19]. **fixating** [WR14a]. **Fixation** [GC18]. **fixed** [IM15]. **flavonoid** [DSD18]. **flavonols** [FZX18]. **flavor** [Tch16]. **flavors** [Mat02, Mat10]. **flexibility** [LBM11, MFB11, OMÐ13a]. **flexible** [BAB+18, ZP16]. **flexible-cluster** [BAB+18]. **FLi** [YLWrL12]. **flow** [FUE+12]. **fluctuation** [NTCG18]. **fluence** [HMH+13]. **fluid** [TTM16, Vik11a]. **fluids** [SA18]. **fluorene** [BVCAP12, Shi18]. **fluorene-based** [Shi18]. **fluorenone** [Men10]. **Fluorescence** [AMMK11, CFP+10, GMM+18, Men15]. **Fluorescent** [BBM17, LDKB15, NTCK13, TCM+12, ZWLC12]. **fluoride** [HL19, LWZ+14, MdAdCS12, OCB+10, ZL10, dLRR11]. **fluoride-chlorotrifluoroethylene** [OCB+10]. **fluoride-mediated** [ZL10]. **fluorides** [KMM16, THVP14]. **fluorinated** [yBZfC18, SPIL14, SCZH16]. **fluorination** [Pli18]. **fluorine** [Ril10, SZL+14, VVJ15]. **fluorine-substituted** [SZL+14]. **Fluorines** [VVJ15, WTW+15]. **fluoro** [YWJ+11]. **Fluoroammonium** [VVY18]. **fluorochromic** [FBU+11]. **fluoroethylene** [KGVG11]. **fluoroionophores** [CFP+10]. **fluoromethane** [KGVG11]. **fluoroprotein** [BSM+15]. **fluoroquinolone** [BJ17]. **fluorouracil** [MR11, NA12]. **flux** [GKT+12, Han19, MNZPT19]. **fly** [UTTn13, WLZ18]. **Flying** [SRS+17]. **FMO** [ŚKB18]. **FMO-EDA** [ŚKB18]. **FNH** [VVY18]. **focal** [dOdONM12]. **Fock** [CC12, MdAdCS12, Tch13, AHT12, BVP13, FA17, GST11, HZS14, Leh19a, Leh19b, Luz11a, Luz13, Mys12, NSN17, NNSN17, PI13, RBVAG18, SZ11, TTT13, ZE18]. **focused** [Buc11b, NIK19]. **focusing** [BWB+18]. **fold** [VDG13]. **folding** [MAW+18]. **follow** [GAI19]. **Following** [dGR14, LHX+19]. **food** [MLPT10]. **force** [BBB+12b, FT15, HSS+11, KKH18, MGN14, Mit11b, Pop15, SR11b, SV11, WYM15, dAB17]. **forced** [DSZB18]. **forces** [BPG+10, FC19, STM17, TJS17, UTTn13]. **forecast** [MGK19]. **Foreword** [KN15, RSL11]. **form** [DR18, FCS13a, FCS13b, KI12, LW18, QZH13, She13, SWS+14, TCM+12]. **formal** [Jou13]. **formaldehyde** [Buc12b, For12, LWC+10, LXLL11, LLLB13, OD12, WML10, YWH+12c]. **formalism** [AHT12, MM19, Mos14, BDF+16]. **formamide** [CWF11, MYZ+10, NS10a, PCMG12, RY12]. **Formation** [ASMP15, AGG+18, MGK19, RBLZ15, ASD14, ALA15, BXR+13, BPT12, BRS10, CP13, CF17, ED16, EM17, FLvLA15, GI11a, HZG12, KZA+17, KS19, KRG+13, KSO19, LLF+12, MS10, Mor12, PP19b, Pop19, PL18b, RYW+15, RMP+14, SS10, SSK+12, SR19, TM13, TXL10, VVAO12, VGGPdL19, ZZX10, ZMZ13, ZCTG18, ZQXP17, YM12]. **Formazan** [Tav12]. **formed** [MNV+17, Met11, MSAB19, TFB11]. **Formic** [MPGGS19, BLR12, ENV15, GORW19, KBF+13, Yu13]. **forming** [LLLB13, TYL10]. **formohydrazide** [Tav11]. **forms**

[AFC+10, BWB+18, CTVA12, DAC11, HMH10b, SOM10]. **formula** [PR11a, SXH18, SZZ+19]. **formulas** [CC19, Gar08]. **formulation** [CAPL12, DP11, Fin17, KUY16, PD11, SK17b, ZLE17]. **formyl** [KSAK17]. **formylformamide** [NJA+12]. **forward** [FCC11]. **Foster** [Cin11b]. **Foundations** [AMAM18, NS10b, Sha18]. **Four** [Hog10, BPL13, BMB16, Buc10, Buc11a, DM12, MSK11, VVS+18]. **four-** [Buc11a]. **Four-center** [Hog10]. **four-membered** [MSK11]. **four-particle** [BPL13]. **Fourier** [SA11a, YŞÖ12, vLRRK15]. **Fourteen** [PR10b]. **FOX** [LCCH10, LCCH11]. **FOX-7** [LCCH10, LCCH11]. **Fpg** [ZTC11]. **Fr** [ČFČ11]. **fractional** [BLKB11, Gan14, MNZPT19, TMC18]. **fragment** [Exn11, MAF19, MSY+12]. **fragment-based** [Exn11]. **fragmentation** [BDFM10, GK12, SBKJ18, YKN13]. **fragments** [ABKJ18, DWPK14, Luz11b, ZDZO10]. **frame** [IM15, NF11, SVPTM+10]. **framework** [BVP14, BR15, CLKD15, Sic16, Tap15, VAT12]. **frameworks** [MLW16, RdPW+12]. **francium** [KP13]. **Franck** [Mam13]. **FrAr** [Ber13b]. **Free** [AG10b, LCG12, MLB+10, AK17, BDG17, CFOC+10, ENV15, Esr18, FM16, Fin17, FA17, GAI19, Kle11, KDA+11, LSR10b, LSG+14, Luz11a, Luz12, LGS+16, MR18b, Nag15, RCM+19, Rit12a, Rit12b, SX15, TPT+13, ZBG+19]. **free-radical** [LSG+14, RCM+19]. **frequencies** [AF19a, MCE11, RDB18, Rud12, ŞBAT16, SZL+14, WHY+14, YWH+12c]. **frequency** [HH18, MPC10, TU10, ZPZ15, ZLE17]. **FRgXF** [LWL19]. **friend** [Sau11]. **friendly** [MDC15]. **fringes** [YS13]. **frontier** [ABA11, LSR+11, YZZH15, LSR+10a]. **Frontiers** [HKLW13, ISN13, IKN13, Kut13, MIN13, NS13, OHDA13, SIB+13, SHS+13, SKY+13, TKN13, TH13, UYN+13, UTTn13, YKN13]. **frozen** [Mas10]. **FT** [ÇAS13]. **FT-Raman** [ÇAS13]. **FTIR** [ÇAS13]. **fuel** [FFPD16, Sic16]. **Fukui** [Boc17, MJ11, PUGSFM18, SKL10]. **Fulfilling** [MC18a]. **fulfillment** [RLER14]. **Full** [BEM11, Dau16, SR12, YIY+13, DVDBM11, XS18]. **Full-configuration-interaction** [BEM11, DVDBM11]. **Full-dimensional** [Dau16]. **full-shell** [XS18]. **Fullerene** [DJB10, yBZfC18, CCEGK12, CJMC19, DI15, DFK16, FBO+11, KP11, KSS+19, KK11b, KK12a, LYS+19, MSS11, MS17, Nik11, PAKA15, RR11, RGPZD13, TKSK17, Var11, ZW15]. **fullerene-buckycatcher** [DI15]. **fullerene-derived** [PAKA15]. **fullerenes** [ARH+13, BBYZ18, DI11, Den19, GZW16, JLL+18, LBW11, DVMC19, MNS11, MC18a, YLZ+17, ZCG+16, ZCTG18]. **fulleroid** [Iku17]. **Fully** [Leh19a, Leh19b, RTT10, AC12, Leh19c, RVNP12]. **fulvene** [HMA+18, Val17]. **Function** [Kut13, NS13, TKN13, TH13, YKN13, AB16a, AV19, AÖ12b, AOT+18, AOLB12, BL10, BL11, Gao11, Han19, KL11, Kub12, Liu15a, MGB18, MRS15, Ng12, OAT+13, PUGSFM18, RZ17, SGH10, Sta10, SS12, SD13c, Tob19, Tou11a, UYN+13, WWL17]. **function-based** [AV19]. **Functional** [Ano13-49, BHA19, HKLW13, ISN13, IKN13, MIN13, SKY+13, TK16b, AC19, AK17, AM13b, AB18, AGPDZ13, BMK+14, BD14, BCGC12, BVCAP12, BDF+16, BDF+18, BGBV12, BLKB11, BJdlMAV12, CCL+13,

CNSK11, CH17, CM12, CZLD17, CC19, CK17, CF14, CTDOLA10, CSTA16, CD12, DWJZ11, DCBB11, DKS11, DW12, DZ11a, DGR+16, DG19, DSZB18, DQZF12, ED16, FCS13a, FCS13b, FZX18, FO10, FDNR10, Fin17, FA17, FSB16, GFPAV19, GCK+17, GMR18, GM11, GGD12, GHCMCMQ17, GD11, GCZ+14, HMA+19, HR19, HHCA10, HLZ+14, HZZ+19, HMH10a, HMH10b, HKIH13, HYD11, HZZW11, IN15, JR12, JPP+11, JA12, JS17, JW18, KME+18, Kar13, KPCV18, KK14b, KKL+16, KSAK17, KYLC19, KSG+12, KJ14, Kri13, Kry12c, KG08, KMU+13, Lat13, LPO+12, LSR10b, Leh19a, Leh19b, LW11, LWL+12, LWX+14, LBY+14, LLW+11, LCK+16]. **functional** [LDZG16, LLZ+12, LSC+18, LNI12, MYZ+10, MLW+14, MJ16a, MLC+11, MFK+12, MA10, MW16, MUNZVR12, MG12, MKSG13, MLK17, MLB+12, MBBT+12, MM13, MKW11, MJM19, MCRS16, MOH+12, Nag15, Nag17, NH18, NDP10, NTNL10, NL11, NMIP14, NMSR14, NDM+12, NZAVR10, OD16, POLV12, PS10b, PS14, PI13, PMH+16, PABSK16, PP16, PTH11, PR10b, Pir13, PU14, PJP10, PMAP12, PI16, PC13, QHS11, RGPZD13, RS12b, RCM+19, RPVM10, RAMB18, Rud12, RSCS10, SB18, SA18, SGL+16, SVRGV12, SLC+18, SN12, SAHG11, SHL+13, SJZ+18, SIS+08, SDM12, SRMB15, Sri19, SK12b, SS13, TOSN12, Tan12, TIN13, Tan13, TDOD17, TFZ+15, TLC+17, UV18a, UMS13, VPGC12, Ven12, VUC13, Vik13, VBO+15, WKE17, WJL+11, WW11, WJY15, WDJ+17, WTZ+11, WR15, Wit18, XNL+14, XSLF12, XGH+18b, YLH+19, YWH12a, YWH12b]. **functional** [Yu13, YL11, ZT13, ZKKR11, ZQCJ10, ZLWY13, ZCX+16, ZBG+19, ZRR+11, ZMZ13, ZCG+16, ZSZ14, ZZ18, Zho18, dCSDdMC13]. **functionality** [ATS+11]. **Functionalization** [ZWWY10, JNY17, YLH+19]. **functionalized** [LRKM10, MSOV13, MLW16, OD16, Pli18, SPPT15, TDOD17, WLZ+12b, ZK12, ZBG+19]. **functionals** [AF16, Ali19b, AK11, DCDD10, DCFD10, Fin16a, HFdGC14, Jan13, Jou13, KDOR17, Lae14, LCT14, LSP+16, LORR+12, Lu15, MXC18, PSMD16, PRFR17, SFC16, SMOD11, SOF+10, SSP+17b, SGC13, SX15, TÁ10, TCA10, UV18b, VSL+15, YF16, YFY17, dSdS13a]. **Functions** [GLT13, IA13, KBF+13, ONK+13, CSMZ10, CML+16, FRGC10, GBK18, GBS17, GTR11, GN19, GS10, HITU16, HGB08, Hog13, Hor13, KH10, Kar13, MPV+11, MSNP18, MJ11, NS13, NDLC19, Oht13, OH19, PABSK16, RZSZ18, SPO+11, SZS+10, SLZ+11c, SLZ+11a, SKL10, VSL+15, WH12, YM14, vLRRK15]. **Fundamental** [Brä13, Hor13, IFT13, MSH13, Mar13, YK13, ZJS13, Blo15, CK13, GI11b, GI11c, GI11e, VVVB10, VV12, VV13]. **fungal** [VGS10]. **furoic** [GIO12]. **Further** [Jør18, ZLWL16]. **furylfulgide** [LZZ+17]. **furylfulgimide** [LZZ+17]. **fused** [RGTS11, WDS19, Yam11]. **future** [BJ17, MGN14, Sic16]. **fuzziness** [Tch16].

G [KK12b, CSVCB12, DE18, ZR13]. **G1** [PWP13]. **G3** [DCR10]. **G3B3** [LVP12a]. **G4MP2** [VF13a]. **Ga** [CWS15, JLL11, LXD13, MLW10, BXR+13, CCM08, GWJ12]. **Ga-like** [CCM08]. **GABA** [Ser11a]. **gain** [Luz11a]. **Gaining** [RNdA+10, vL13].

galactosyl [LQ13]. **galanthamine** [PK13a]. **gallium** [ALK19, KP11]. **gamma** [MMC+19]. **gamma-AlOOH** [MMC+19]. **GaN** [CWW+16, KO12]. **gap** [RKCK19, SSB12a, SSP+17b, YHL+13]. **GAPDH** [SLA12]. **garnet** [VPFD10]. **garnets** [MPD+10, MPZWD10]. **Gas** [DD17, DZ11a, FDMR11, LNGW14, NZLG15, ZDF13, AEAS+19, BGL+16, BLM+12, CFOC+10, CRSB12, Che12, CF17, DLG12, DCOC+19, EHKD11, FBRBR12, GMT18, HDC+11, HDQ+13, IKC18, JEA13, JWJ+12, KS11, KZZ13b, KDOR17, LGZC15, LWL19, LGW11, LG12, LdAA+11, MPD+15, MCC12, MB14, MOSK10, MB15, MURR13, MML+11a, MLB+12, MMM+12, MJ11, Mor11, NKWT19, PSK+16, PK16, PB10, RP16, RCM10, RNE10, SF13, SMC18, SD16b, Ser11a, Ser11b, SK12a, SZZ+19, SYS14, SSdS17, TWR15, VF13a, VV18, VSMK15, WXZ+11, WZX11, WLG+11, WWLZ17, WLL19, XGH18a, YJ17, YC13, ZL10, dSdSPG11, dSMT+18]. **Gas-phase** [DZ11a, FDMR11, LNGW14, NZLG15, AEAS+19, BLM+12, CFOC+10, CRSB12, GMT18, LGW11, MCC12, MOSK10, MML+11a, WXZ+11, WZX11, WWLZ17, ZL10, MJ11]. **GaSb** [KMU+13]. **gases** [BAP12, JMPP19]. **gate** [CKB+19, TB15, TPT19]. **gates** [MR12, ZPR10]. **Gauge** [Kub12, ALB18, Bra10]. **gauge-including** [ALB18]. **Gaussian** [AS19, BC15, BC16, Boe12, CML+16, GTR11, HITU16, Hil13, Kut13, Mat02, Mat10, MSNP18, NDM+12, OHDA13, PCD14]. **Gaussian-type** [HITU16]. **Gbar** [Boe12]. **GC** [NMS+10]. **Gd** [WSL+11, XYL+18, CWL+13]. **Gd-encapsulated** [CWL+13]. **GDP** [MMT+13]. **Ge** [LCS+11a, MPD+10, XCL+18, ZHL+19, LLLB13, MSVMCI10, UKF+11, ZCX+16]. **Ge-** [ZCX+16]. **gear** [KKH+13]. **gear-shaped** [KKH+13]. **GeCNT** [SD16a]. **geminal** [Tok16]. **geminals** [TKN13]. **GEN1INT** [GTR11]. **General** [GBK18, PIS18, Rit12b, FRGC10, MMG15, Pie12, QZH13, YAF+15]. **general-purpose** [YAF+15]. **generalization** [HXDY16]. **Generalized** [ACL12, ALRAE11, ART08, Cin11b, LMZY15, MGK+11, MPTZ13, MZST16, PMGMGR12, PBB15, CM15, CM16, Gra11, GdLT12, GE12b, Mit11c, SS12, ZLJ11]. **generated** [NH18, PE11]. **Generating** [AÖ12b, BW15, Fuk12, LLC+11, MJSC18]. **generation** [BAX+19, CML+16, GFRdG11, HMA+18, KYLC19, LHX+19, MMŁ+16, OD12, TXK+19, ZLR15]. **generator** [AHT12]. **genetic** [AFM+10, CL08]. **genome** [Kuv10]. **Geometric** [KMM16, MR12, Sjö15, CD12, GTR11, LW13, LB18, RW12, Sch10b]. **Geometrical** [CSMZ10, GHCMCMQ17, WJL+10, EKN10, KK12a, LL11, MBBT+12, MM13]. **Geometries** [SZL+14, Buc11a, MHT+08, ZYL+13, ZCP11]. **Geometry** [CL11, CWSZ13, Jør15, Jør18, MCE11, Cyb11, GP13b, KYH+13b, LWJL10, MG12, MJ14, MMV+19, NBL+14, Sch15, SN11, WJL+11, YIY+13, ZBBB17]. **germanene** [BHAH+18]. **germanic** [TXL10]. **germylene** [LCS+11a, LCS+11b]. **germylidene** [LLLB13, TXL10]. **GFP** [KyH13a, LORR+12]. **GFP-like** [LORR+12]. **GFP-X-CFP** [KyH13a]. **GGA** [FCS13a, FCS13b, KSG+12]. **ghost** [PP16]. **giant** [ZX12]. **GIAO**

[CFGC11]. **GIAO-DFT** [CFGC11]. **given** [Du12, MM19]. **glasses** [Ped16]. **Global** [BPVDB11, GTSC+19, HJ13, OPAVM18, YLC17, GI10, GI11b, GI11c, KYLC19, KMNSP19, Kut13, MCP10, MDNDO+16, SRS+17, YLYC18, ZWL18]. **globular** [MSK+12]. **Glu** [TK16a]. **glucan** [PTD+12]. **Glucose** [JFT13]. **glucosidase** [WHS+13]. **glutamate** [ŚKB18]. **glutaric** [NHB12]. **glyceric** [SLA12]. **glycinamide** [KKG12]. **glycine** [CWL+13, CCP18, CLMY12, LRP+11, SJZ+18]. **glycine-** [CLMY12, SJZ+18]. **glycine**· · · [KRG+13]. **glycol** [dlLIAI+12]. **glycolaldehyde** [BYAT13]. **glycosidases** [PRFR17]. **glycosidic** [PRFR17]. **glycosylation** [LQ13]. **Glyoxal** [SMA11]. **glyphosate** [CRB+12]. **goals** [Brä14]. **Gödelian** [Brä11a]. **goethite** [HCH+18]. **gold** [BvWG14, FTB11, LC16, LTL18, LIK15, MFOH18, ONBP11, RWW+19, SDY16, ZT13, ZRY+13, ZHI17]. **Goldstone** [PO15]. **good** [TSBSM12]. **Gould** [ABKJ18]. **GPCRs** [CSSK+12]. **GpG** [Cys11]. **GPUs** [HEVMSA+19]. **GQSD** [ZH15]. **Gradient** [WR14a, ISN13, KF19, MM19, MAF19, MBA+19, SRMB15, dCGAMV12]. **gradient-based** [KF19]. **Gradient-driven** [WR14a]. **gradient-regulated** [MBA+19]. **gradients** [BVA+14, Cam10, NDP10, SGH10]. **grafted** [DSRGD12]. **grain** [WLH+19]. **gramicidin** [SMK+12, SIT+12]. **graph** [Bib13, GRD11, XXJ+16]. **graphene** [AGOP18, ABP13, ASW13, BAP13, BSO16, CA17, CAO18, DI10, ENV15, EM19, FFPD16, GMT16, HBMM11, ISRK12, JNY17, KK19, LWX+14, MFM18, NBL+14, PPDF11, RD14, SPD+18, SC10b, She12, She14, UDS19a, WWL+11, YMY+13, OK19]. **graphene-based** [BSO16]. **Graphenic** [TBRIS12, TBRIS10, TBRIS11]. **Graphenic-Type** [TBRIS12, TBRIS10, TBRIS11]. **graphic** [ZH15]. **graphical** [CLC10, HW12, LQZZ12, LLZaH14, LSKM19, PUGSFM18, RNP13, WH12, YSW11]. **graphically** [SGH10]. **graphs** [CDSK12, DZ11b, Du12, GA19, PR10a, Pal10, PL11, Tra19]. **graphyne** [BSS15, CA17]. **green** [BSM+15, MKHM11, SLS+14, SD13c, ZWLC12, RZ17, SS12]. **green-function** [SD13c]. **greenhouse** [Mor11]. **grid** [CKYR18, FLCHL10, GMR18, LG10, LCK+16, SA11a]. **grid-based** [CKYR18, LCK+16]. **grid-cutting** [LCK+16]. **grids** [RL12]. **Grignard** [BPT12]. **Grimme** [KDOR17, SA18]. **Ground** [MM13, RAGM10, ADB10, BPVDB11, BG11b, BG11c, CHM+14, DGA+13, HM12, HMA+18, Ign11, Ign12, KK14b, KYLC19, Kri13, LP10b, LJSS12, LdAA+11, MPM15, MQG13, MPT11, MPTZ13, Nic11, OH19, RRCO11, SFM13, SGC13, SR11b, SS12, SK12b, SZY17, TBB+19, TXK+19, THVP14, Zak13, CJOOW11, MNS11, VPA11]. **ground-state** [Ign12, KYLC19, THVP14, Zak13]. **group** [AG10a, AMK10, BLdV19, BLM+12, CWS15, EAA17, ED16, Eng16, GAPK+19a, GRD11, JLG+12, LSR10b, LdMCdA+12, LZB10, LXD13, LYD+18, NZ13, PBR18, SH18a, SSA18, TMC+13, THVP14, WH12, YKM+15, YD17, ZZC12]. **group-12** [THVP14]. **group-13** [LYD+18]. **groups** [ATS+11, ABA11, BSSS19, CMR13,

FNBK17, KPL+17, KSAK17, LPO+12, NHG+12, Ril10, ScBsR+10, Tri14]. **growing** [CD12]. **growth** [LVP12b]. **Grx3** [Dum12]. **Grx3-like** [Dum12]. **GTP** [MMT+13]. **guanidine** [LW13]. **guanidine-catalyzed** [LW13]. **Guanine** [SL10, BSV12, KMMS17, POLV12, YM12, ZRY+13]. **guess** [LCK+16]. **Guest** [DC14a, XXbX+13]. **guests** [NCMC+18]. **guide** [SLS+19]. **guided** [SRS+17]. **Guseinov** [Mam14]. **Gutzwiller** [YWH12a, YWH12b]. **GW** [RAMB18].

H [BDF+18, BGFD14, BJ17, BTH18, Buc12a, BSPK11, CRSB12, CS17, DMAB12, DPDR11, DZO11, DZO12b, DQZF12, EML+11, EMS16, FBRBR12, GWM11, GB13, GR10, GKGM18, HJRO13, JCCZ12, JLG+12, KWC10, Kal18, Kan11, KI12, KSSK16, KSST12, KRG+13, LZ12, LCL+10a, LJL+11, LZZ+11, LMZ+11, LBY+14, LZW+15, LCZ15, LXD13, LdAA+11, LEU+11, MLY+16, MC12, MMBK12, MPRB+10, MC18a, NBL12, NL11, NMIP14, NH11, OCL+18, PTS+11, Pan16, QSLY10, RLTAT19, RFEGPP+16, RGR12, ŞBAT16, Sat11b, SZZZ11, SCTW10, SZL+14, SZ15, SZY17, TBRIS12, TG13, VLK+11, WCY+10, WZW17, WLWL14, WWGW18, XLLZ10, XCL+18, XF19, YIY+13, YSK+12, YLYC18, ZGSM15, ZCG+17, ZWL18, ZHL+19, AC12, AST19, BN12, BDFM10, BPVDB11, BP13, BPG+10, BAP12, BEM11, BHV+11, Buc12a, CLXZ12, CP10, CC11b, Cor16, DLCB15, DSD18, Den13, DMS+10, DLM12]. **H** [DMBL16, FBM+10, GWM11, GZSMFN16, GMT16, GKT+12, GJ18, GD11, HV11, HSYM11, IKS08, IKS10, IROW10, JL12b, KWC10, KH12, KdPNNS16, KMF+11, KI12, KDA+11, KF17, LZ12, LZZ+11, LZFZ13, LWWZ13, LGW11, LKLW11, LCM+11, MMC+19, MKW11, MSAB19, NW12, NWQX11, OPC17, PWL+10, PL18b, RLW+13, RR11, RNB+10, Roy15, Roy16, RR19, SB18, SSB19, SD16a, SR19, SH18b, SVPTM+10, SMEH15, SMEH16, SSP14, SL13, SS11, SK10, STU19, SCTW10, Tan13, TBRIS10, TBRIS11, VVAO12, VPA11, Vik11a, Vik11b, VLFG12, WZC+12, XDM+10, XCL+18, YY18a, YS18, YZ10, YLC17, ZWL18, ZJC+13, GLT13]. **H-abstraction** [LGW11]. **H-atom** [KDA+11]. **h-BN** [GLT13]. **H-Bond** [LCM+11, SMEH16]. **H-bonded** [DLM12, DMBL16, IKS08, IKS10]. **H-bonding** [CLXZ12, DMS+10, KdPNNS16]. **H-bonds** [IROW10, SS11]. **H-passivated** [GMT16]. **H/D** [SK10]. **H2** [ZCG+17]. **H5N1** [KRH13, WZ10a]. **HAl** [Sat11a]. **HALA** [RRK16]. **Half** [KMS+11, AAAM12, AAA12, DZO12b, SMOD11, Pup11b]. **Half-a-century** [Pup11b]. **half-line** [SMOD11]. **half-metallicity** [AAAM12, AAA12]. **half-sandwich** [DZO12b]. **halide** [DZO12c, HNBG15, LGM+18, XZL+12]. **halide-exchange** [XZL+12]. **halides** [BMBD10, For12, LC16, MML+11a, RYM12, RKCK19]. **Hall** [Bra10]. **halo** [EMK14, LGP+11]. **halo-** [EMK14]. **haloalkane** [ZCZ+12]. **haloammonium** [XZL+12]. **Halogen** [DLP17, SC18, VVY18, BLL+13, Buc11b, CLXZ12, DPK18, DWZZ15, EMSB15, FGD+19, GLXL18, JLZ+17, KKC14, Kuz19, LJL+11, LLG+12, LDZG16, LZD+11, LLZ+12, MS14c, Sch13,

SMP10, SPIL14, SYY16, SCZH16, TL15, VVJ15, WTW+15, XZYS10, YZZ16, ZZL+11, ZLWZ16, ZYL+14, dOdCMUdALR11]. **halogen-bonded** [LJL+11]. **halogen-bonds** [JLZ+17]. **halogen-hydride** [BLL+13]. **halogen-oxygen** [dOdCMUdALR11]. **halogen-substituted** [CLXZ12]. **halogenabenzene** [WLZ18]. **halogenated** [GHS12, LLW+12, TL15]. **halogen**$\cdots$ [LDZG16]. **halomethanes** [HLJZ11]. **halonitrenes** [SYL+18]. **halopyridinium** [ZLWZ16]. **HAlS** [LPG+12]. **Hamiltonian** [Bra10, FYhC11, IM15, Kry12c, Mos14, SPSA11, SA11a, SKG11, TD11, TSvL+16, YYI+12]. **Hamiltonians** [Liu16, Cal10, CCBR+12, Liu14, Liu15b, MQA17, SR12, ZE18]. **Hammett** [DNCKCS+12]. **happens** [Tou11b]. **hardness** [Bar11, GI10, GI11a, GI11b, GI11c, GI11d, GI11e, GI11f, VO11]. **HArF** [GWZ+14b]. **harmful** [dSMT+18]. **harmful-gas-sensing** [dSMT+18]. **harmonic** [CB19, CML+16, DTPC17, DBTA19, MR18a, PVS12, PABSK16, YK13]. **harmonicity** [CTVA12]. **harmonics** [BAP12, Kit15, MFLK10, Nik11, RLER13b]. **Hartree** [AHT12, CC12, FA17, GST11, HZS14, Leh19a, Leh19b, Luz13, MdAdCS12, Mys12, NSN17, NNSN17, PI13, RBVAG18, SL13, SZ11, TTT13]. **HAu** [CS18]. **HAuF** [CS18]. **having** [BB10, KP10, RNV+12, SALK19, SN11]. **HB** [XZZ+10]. **HBeN** [LCL+10b]. **HBN** [LCL+11]. **HBNH** [BL12]. **HBr** [LGW11, SLS+11, WZHZ13]. **HC** [EAA17]. **HCCH** [BL11]. **HCF** [dOR10]. **HCl** [LGW11, SPIL14, YGL+11, EI11, MPRCEG12, SZS+10]. **HCN** [JLG+12, Tap15]. **HCN/CNH** [Tap15]. **HCNO** [MKW11]. **HCNS** [KZZ13a]. **HCO** [WB17, WZC+12, YL10]. **HCOOH** [XDM+10]. **HCu** [ALMY18]. **HD** [ZGSM15, GWZ+14a, GWHH17, Kan11, SZ15]. **HDCH** [SZY17]. **H**$\cdots$ [DB15, MNV+17]. **healing** [ES17]. **Heat** [MMP11, FUE+12, GVPCK10]. **Heats** [PP19b, ZZX10]. **heavier** [ALB18, YD17]. **heavy** [BMRM19, ND10, RRK16, RR19]. **HeH** [NWQX11, OPC17, Vik13]. **HeI** [DTVP+12]. **Heisenberg** [ATL+14]. **Heitler** [CC12]. **helical** [MCE11, NRI15]. **Helium** [Var11, AC11, CS13, HMP+11, Ign11, Ign12, KH10, KWWH18, KT12a, LLH15, OH19, Pop19, SXH18, YÇÖ11]. **Helium-fullerene** [Var11]. **helium-like** [KWWH18, YÇÖ11]. **helix** [PAD+10]. **Helmholz** [Koc13b]. **hemagglutinin** [KRH13]. **heme** [LVdSdM14, LdMCdA+12, SBSD18]. **hemerythrin** [TYN13]. **hemispherands** [SHE10]. **heptagon** [SCTW10]. **heptagon-containing** [SCTW10]. **herbicides** [CRB+12]. **Hermitean** [Brä12]. **heroin** [RCM10]. **Hess** [SN15]. **hetaryl** [MMW19]. **hetarylazo** [ÇAS13]. **heteroaromatic** [WWQG17]. **heteroatom** [GAPK+19a]. **heteroatom-centered** [GAPK+19a]. **heterocycles** [VOK+18]. **heterocycles-6** [VOK+18]. **heterocyclic** [ABTW14, CYL+19, CDL+19, GZ14, HZZ+19, LWJL10, LZD+11, LLLB13, MAN15, Pan16, WLL19]. **heterogeneous** [Lya19, MCRS16, PCV19, PIS18]. **heterojunction** [OKK10, WCL+17]. **heterojunctions** [IMS+13]. **heteroleptic** [SK12b]. **heterolytic** [GWM11]. **heteronuclear** [GI11b, GI11c, LYD+18].

heteropentamers [MOE+11]. **heteropolycyclic** [TXL10]. **heteroporphyrins** [RBZ15]. **heterostructures** [MFZ+18]. **hex** [Sat11b]. **hex-2-ene** [Sat11b]. **hexaazaisowurtzitane** [DGR+16]. **hexaazaisowurtzitane/nitroguanidine** [DGR+16]. **hexacarbalane** [ALK18]. **hexafluoroacetylacetonate** [dARAV12]. **hexafluorocyclohexane** [HWWW18]. **hexagonal** [KC19a, LFP+19, NBL+14, PL18a, UV18a, UV18b]. **hexahydro** [MJ11]. **hexahydro-1** [MJ11]. **hexanal** [BCS+12]. **hexanuclear** [PAPCMM+16]. **HF** [GKT+12, LGW11, SPIL14, YGL+11, YZ10, AFM+10, SYY16, SCZH16, Bou12a]. **HFC** [Tas14]. **HFC-32** [Tas14]. **HFE** [KAR12a]. **HFE-161** [KAR12a]. **HfF** [BLKB11]. **Hg** [NFQ+11, WHM14]. **HgClOH** [RSM12]. **HGGGW** [MRT11]. **HH** [Che12]. **HI** [LGW11]. **hidden** [YLZ+17]. **Hierarchy** [ZLE17, PC13]. **HIF** [MGK+12]. **HIF-1** [MGK+12]. **High** [Dun15, Kin13, MPRB+10, ZCG10, Beh15, BHH+13, CKB+19, CRFR11, CLH14, CKYR18, CML+16, DBTA19, DSFT17, DSSM18, Fer11, HSN18, Jeo18, JW19, KG17, KMU+13, LCL+10a, cLqFtW+14, LMC19, Luz08, Lya19, Mai14, MDC15, Mil12, NKKN15, RGTS11, RNE10, SSP+17b, SZL+14, WCGD12, fXxBhD19, XZZ+10, XCD18, YYI+12, YZ13, YM14]. **high-** [Fer11]. **high-density** [JW19]. **high-dimensional** [Beh15, DBTA19]. **high-efficiency** [Mai14]. **high-energy** [CLH14, XZZ+10]. **high-energy-density** [Jeo18, fXxBhD19]. **high-harmonic** [CML+16]. **high-level** [LCL+10a, RNE10, SZL+14]. **High-lying** [ZCG10, DSSM18]. **high-order** [Luz08]. **high-performance** [BHH+13, CKB+19, cLqFtW+14, Lya19, NKKN15]. **High-precision** [Kin13]. **high-pressure** [KMU+13]. **high-resolution** [DSFT17]. **High-spin** [MPRB+10]. **High-temperature** [Dun15, WCGD12]. **high-throughput** [CRFR11, KG17]. **high-valent** [YYI+12]. **higher** [LBW11, SMRK18]. **highest** [SM14b]. **Highly** [KPH+12, KS18, WZW17, EM19, KRH13, LLZaH14, NDH10, OK16, OAA19, SMEH16, YAF+15]. **hill** [SSB12a, RA10a]. **Hillman** [ZQW+17]. **hindered** [SBEH11]. **Hirsch** [MC18a]. **Hirschfelder** [Haj18]. **Hirschfelder-long-range** [Haj18]. **histidine** [NHG+12]. **histone** [dSMPRSF18]. **Historical** [Hop15]. **hitting** [PR11a]. **HIV** [KKG12, SKHN13]. **HIV-1** [SKHN13]. **HL** [CCL+10]. **HM** [BDR12]. **HMgH** [WLL11]. **HMgO** [LGP+12]. **HMH** [BLL+13]. **HMX** [Jeo18, LZZ+13]. **HMX/NTO** [LZZ+13]. **HNB** [LCL+11]. **HNBe** [LCL+10b]. **HNCH** [XDM+10]. **HNgBeF** [SMC18]. **HNO** [BL11, YL10]. **HOAl** [LGP+11]. **HOCl** [RNE10]. **Hoff** [Buc10]. **HOH** [SW12]. **Hohenberg** [LB14b, Lev10]. **holding** [NIK19]. **hole** [ATPRV11, ABLT11, FV11, JLG+12, MCL11, SC18, VATPR11, VAT12, WTP+19, WLC+17, ZHL+19]. **hole-transporting** [MCL11]. **holes** [CP13]. **hollow** [MC18a, PAKA15]. **hollow-caged** [PAKA15]. **Holstein** [DTFK15]. **HOMg** [LGP+12]. **HOMO** [MA12]. **homodesmotic** [MMM19]. **Homodimers** [ZS12]. **homogeneous** [CSTA16, Lak10, MLB+12, MMM+12, Sic16, Yak10]. **Homology**

[PTD+12, SLS+10, CSVCB12]. **homolytic** [KZA+17, OKR12, OK16]. **Homonuclear** [EMS16, KBGC12, NZ13, SZZ+19, SM14a]. **HONPAS** [QSX+15]. **HOO** [YL10, ZZW11]. **Hooke** [BPL13]. **Hookean** [LEU+11]. **hopping** [MMG15]. **horseradish** [ZST+10]. **HOSO** [STU19]. **host** [DC14a, MSS11, OCGM+19, XXbX+13, YBMK12]. **hot** [BW15]. **HOX** [LLG+12]. **Hras** [MMT+13]. **Hras-GDP** [MMT+13]. **Hras-GTP** [MMT+13]. **HRh** [DPDR11]. **HS** [dDGNB10, LZFZ13]. **HSAB** [ZXY13]. **HSAl** [LPG+12]. **HSH** [SKS10]. **Hsp90** [KTI+12]. **HT** [CSVCB12, CSSK+12]. **Hua** [FKBG19, HYZS19, KBG17, AAHN16, HRT12, HYZS12]. **hubbard** [LNI12, HFdGC14, WDJ+17]. **Hubbard-corrected** [HFdGC14]. **hubbard-like** [LNI12]. **Hückel** [Koc13b]. **Huge** [FBD+13]. **Hulburt** [Haj18]. **Hulthén** [Roy15]. **Human** [CSVCB12, WTH+11]. **humans** [KRH13]. **Hund** [KT12a, MHT+08]. **HX** [SPIL14, HNBG15, SPIL14, Vie17, Wu11]. **hybrid** [AV19, AF16, Ali19a, AK11, CF14, FCS13a, FCS13b, HZZW11, Kry12c, KSO19, LPO+12, MCK17, NMSR14, SB10b, SX15, TFSRM11, XCY15, YYI+12, YIY+13, Yu13, YF16, ZPR10, MPE15, SIS+08, YSK+12]. **Hybrid-density** [SIS+08]. **hybridization** [ABS11]. **hybrids** [MJM19]. **hydantoin** [ND11]. **hydratase** [MLW+14]. **hydratase-lyase** [MLW+14]. **hydrate** [XXbX+13]. **hydrated** [BMF+14, EPS+16, MNC12, SMEH16, SCS15]. **hydrates** [LB19]. **Hydration** [Ma14, Pat15, PBM10, RGR12, RBTL19, SL10]. **hydrazide** [DDÇY12]. **hydrazine** [SC12a]. **hydrazono** [KDÇ12, SC12b]. **hydride** [BLL+13, Ber13a, HMI+15, JL12b, Mar11, MHOG18, OA12, YYS15]. **hydrides** [AO12a, BDR12, CP13, EAA17, SH18a, SSA18]. **hydroacylation** [WML10]. **hydroaminations** [ZSS+13]. **hydroboration** [SLS+15]. **hydrocarbon** [MSY+12, WLS+19]. **hydrocarbons** [BRS10, Bla15, CA17, DI18, FC19, GMT18, GHS12, HIL19, LVP12b, RNV+12, SFM13, VRO+12]. **hydrochloric** [dLdOdAD12]. **hydrofluoropolyethers** [Vie17]. **Hydrogen** [AO12a, BLR12, BAP13, Cha10, CTDOLA10, GZ14, HS15, JLG+12, KK11a, MSVMCI10, MURR13, ND11, NBL12, OA12, PCMG12, SGKG12, SJZ+18, SKM11, WWGW18, YL10, dFR15a, dLRR11, AV19, AKHS13, BCGC12, BN12, Bay19, BL11, BWB+18, CdLdSC18, CDS+18, CNSK11, CCP18, CC11a, Coo12, COP16, DAC11, DAC12, Den13, DLG12, DLM12, DLP17, DB15, EKN10, EPS+16, FAFR12, FRNM12, FMCA11, FKC12, GI14, GIO12, GH11, GORW19, GZBH18, GZMC11, HNH+12, HL19, HNBG15, HYD11, IAA15, IK18, JN13, JCCZ12, JZZH17, Kar12c, KKG12, KS18, Kry10, LLF+12, LJW+11, LLG+12, LWX+14, MS14a, MdAdCS12, MK11, MK12, MNV+17, MCARL11, MTL+12, MT10, MFOH18, MFLK11, MMBK12, MS14c, MMM+12, MAPS18, MNS11, MR18b, NW12, NG11, NMIP14, NH11, NHB12, NRGS11, NRP+11, NRHJ11, NEEV15, OH12]. **hydrogen** [OH13, OHDA13, OA13, PM17, Pup11a, RZ17, RZSZ18, RJY+10, RJA+10, RYM12, RI19, Ril10, Riv11, RAFR18a, RAFR18b, RNE10, RB11b, SRPD16,

SS10, SMRK18, Sch10b, Sch13, SK17a, SM19, SMP10, Sic16, SSP14, SPIL14, SYS14, SS12, SCL19, SW12, SCZH16, SCBP17, TL15, UDVD10, Var14, VSMK13, WLS+19, WCGD12, WWHZ13, WZHZ13, WWLZ17, WJ11, WH18, XDM+10, YW11a, YWH12a, YWH12b, YRN+11, YWH+12c, ZAE10, ZZL+11, ZLZ+14, ZL10, dSCC12, dSSF16b, dSSF16a, dFR15b, dAVdM17, dOR10].
hydrogen-bond [OHDA13, SCL19]. **Hydrogen-bonded** [SGKG12, CdLdSC18, CCP18, KS18, LJW+11, MT10, OA13, RNE10, ZLZ+14, dSCC12]. **hydrogen-bonding** [DB15]. **hydrogen-like** [SS12]. **hydrogenase** [BGFD14, BAA+18, MG10, DMG10]. **hydrogenated** [IIW+11]. **hydrogenation** [TGA+11, VPGC12, XSLF12, ZZC15]. **hydrogenic** [DLRMFY10, DBTA19]. **hydrolysis** [CCL+10, DSZB18, KFS13, PRFR17, PMC11, RNdA+10, YTY19]. **Hydronium** [DE18]. **hydrophobic** [NHG+12, SMK+12]. **hydroquinone** [NP18]. **hydrosulfide** [HLJZ11]. **hydroxamates** [TPdMB12]. **hydroxamic** [KK11a]. **hydroxide** [DE18, RGR12, WZZL10]. **hydroxides** [DCDD10]. **hydroxy** [TAY11, YLW+13]. **hydroxyacetone** [SSdS17]. **hydroxyanthraquinone** [JB11]. **hydroxybenzaldehydes** [EKN10]. **hydroxybenzenes** [ATM17, KM12a]. **hydroxybenzylamine** [AFC+10]. **hydroxycarbene** [Buc12b]. **hydroxycarbonyls** [SSdS17]. **hydroxycinnamoyl** [MLW+14]. **hydroxycinnamoyl-CoA** [MLW+14]. **hydroxyfullerene** [KK11c]. **Hydroxyl** [TWHZ14, CGIAI12, FNBK17, KAR12a, LLP+13, LCM+11, Ril10, XNL+14, YM13, YY18a, ZZC12]. **hydroxyl-thiourea** [LCM+11]. **hydroxylapatite** [UV18a, UV18b]. **hydroxylated** [MDNDO+16]. **hydroxylations** [SSI+10]. **hydroxylbutyloxy** [RS11b]. **hydroxylbutyryl** [MFR10]. **hydroxymatairesinol** [SBEH11]. **hydroxymethyl** [KAOB11]. **hydroxyphenalenone** [OA13]. **hydroxypropanal** [SSdS17]. **hydroxyquinoline** [CHV14]. **Hylleraas** [OH19, PSGK17]. **Hyper** [LXW+12, DW12, FKL+12, KP11, Kha16, Mar12, XWCY11]. **hyper-netted-chain** [DW12]. **hyper-radial** [Kha16]. **hyperbolic** [AY15, GE12b, SDL+15, dAB17]. **hyperbolic-type** [AY15]. **hyperbolical** [WC14]. **hyperconjugative** [CSP+10]. **hyperfine** [Bou11, Bou12a, Kin13, Wit18]. **hypergeometric** [PMGMGR12]. **hyperpolarizabilities** [AK11, CEFMK12, NKF+13, OCL+18, YMY+13, dWLC14]. **hyperpolarizability** [BHMN19, FSB16, GXZ+14, Kar12b, Mar11, RVO+14, WWL+11]. **hyperspherical** [BAP12, PML+11, RPBB11]. **hypersurfaces** [PBM10]. **hypervirial** [ATPRV11, VATPR11, VAT12]. **hypochlorous** [TV13]. **hypoelectronic** [SALK19].

I-converting [dSSdSGA12]. **i-motifs** [KUS19]. **I.** [KK12b]. **IB** [DWX+16]. **ibuprofen** [XNL+14]. **ice** [Mil12, Wan13]. **ices** [LRP+11]. **ICN** [BMBD10, McC13a]. **iconicity** [Tch16]. **icosahedral**

[DVMC19, SR12, XCY15]. **icosahedron** [SLZ+12]. **icosahedron-based** [SLZ+12]. **identical** [XZL+12]. **identifies** [ST15]. **identify** [MVG18]. **Identifying** [BB16]. **identities** [Cin11a, Cin11b]. **Identity** [RDB19, Buc10, Buc11a, GI11b, GI11c]. **IEO** [FYhC11]. **IEPOX** [KZZ13b]. **II** [Bal16, DSD18, DCdG10, FBD+13, LYW11, LGW11, LGS+16, MGK19, NNSN17, NFQ+11, OAA19, RNdA+10, SLC+18, SG19, TFA10, WHM14, WRW+18, YZL+10, ZSASS13, ZLLS10, dCSDdMC13, dARAV12, dCDC+11, ADR+18, Bou11, Bou12a, Cam10, CPF12, Ire12, Jør18, Kry12b, Leh19b, LSR+13, MS12, OH13, PD11, PEA+12, PVS12, QD10, SGL19, YYI+13, YIY+13, YSK+12, YWR+18]. **IIB** [Eng16]. **III** [CADSG18, EG10, LVdSdM14, MSOV13, MMSC19, PCD14, RMP+14, SLS+14, SSP+17b, SHW+13, WXB+11, ZQCJ10, ZQJW13, ZYSW17, ZSQ+10, AC19, AMK10, Cam12, CWS15, LYR+17, NMS+10]. **IIIA** [Eng16]. **Ill** [Gru17, BMB12]. **Ill-defined** [Gru17]. **ill-posed** [BMB12]. **illustration** [LP10b, MHOG18, ZSZ14, RBD+10]. **illustrative** [Mai14]. **Image** [Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g, Ano12h, Ano13k, Ano13q, Ano13r, Ano13s, Ano13t, Ano13u, Ano13v, Ano13w, Ano13a, Ano13b, Ano13c, Ano13d, Ano13e, Ano13f, Ano13g, Ano13h, Ano13i, Ano13j, Ano13l, Ano13m, Ano13n, Ano13o, Ano13p, Ano13x, Ano13-35, Ano13-41, Ano13-42, Ano13-43, Ano13-44, Ano13-45, Ano13-46, Ano13-47, Ano13y, Ano13z, Ano13-27, Ano13-28, Ano13-29, Ano13-30, Ano13-31, Ano13-32, Ano13-33, Ano13-34, Ano13-36, Ano13-37, Ano13-38, Ano13-39, Ano13-40, Ano14a, Ano14b, Ano14n, Ano14t, Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14z, Ano14c, Ano14d, Ano14e, Ano14f, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14o, Ano14p, Ano14q, Ano14r, Ano14s, Ano14-27, Ano14-37, Ano14-43]. **Image** [Ano14-44, Ano14-45, Ano14-46, Ano14-47, Ano14-48, Ano14-28, Ano14-29, Ano14-30, Ano14-31, Ano14-32, Ano14-33, Ano14-34, Ano14-35, Ano14-36, Ano14-38, Ano14-39, Ano14-40, Ano14-41, Ano14-42, Ano15a, Ano15b, Ano15c, Ano15d, Ano15e, Ano15t, Ano15x, Ano15y, Ano15z, Ano15-27, Ano15-28, Ano15-29, Ano15-30, Ano15-31, Ano15-32, Ano15-33, Ano15-34, Ano15f, Ano15g, Ano15h, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n, Ano15o, Ano15p, Ano15q, Ano15r, Ano15s, Ano15u, Ano15v, Ano15w, Ano16a, Ano16s, Ano16t, Ano16n, Ano16u, Ano16v, Ano16w, Ano16x, Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16b, Ano16c, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m, Ano16o, Ano16p, Ano16q, Ano16r, Ano17a, Ano17b, Ano17m]. **Image** [Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x, Ano17y, Ano17z, Ano17c, Ano17d, Ano17e, Ano17f, Ano17g, Ano17h, Ano17i, Ano17j, Ano17k, Ano17l, Ano17o, Ano17p, Ano17q, Ano17r, Ano17s, Ano18a, Ano18r, Ano18s, Ano18t, Ano18b, Ano18o, Ano18u, Ano18v, Ano18w, Ano18x, Ano18y, Ano18z, Ano18-27, Ano18-28, Ano18-29, Ano18c, Ano18d, Ano18e, Ano18f, Ano18g, Ano18h, Ano18i, Ano18j, Ano18k, Ano18l, Ano18m, Ano18n, Ano18p, Ano18q, Ano19a, Ano19t, Ano19b, Ano19c, Ano19d, Ano19o, Ano19u, Ano19v, Ano19w,

Ano19x, Ano19y, Ano19z, Ano19-27, Ano19e, Ano19f, Ano19g, Ano19h, Ano19i, Ano19j, Ano19k, Ano19l, Ano19m, Ano19n, Ano19p, Ano19q, Ano19r, Ano19s]. **imidazo** [YZW+15a, YB11]. **imidazole** [CC11a, NHG+12, ÖEDB11, VHTEG15]. **imidazoles** [Tug13]. **imine** [BH10a, ÇT14, Coo12, HS11b, LFTL18]. **imines** [SFW12, XZG+18, ZZC15, ZQW+17]. **imino** [BSM+15, HNH+12, RJA+10, dCSDdMC13]. **iminomethyl** [Tan12]. **iminothiolate** [WRW+18]. **Immersive** [SDP+16]. **Impact** [AFC+10, Bon17, KPL+17, NA14, NDLC19, OB19, PUH+11, SBKJ18, VSS11, Wan13, WDS19]. **impedes** [DMG10]. **impenetrable** [OPC17, RAFR18a, RAFR18b, Roy15]. **Implementation** [dMOB12, BDF+16, CRFR11, KI15, KUY16, Pon19, Yos20, ZPR10]. **implemented** [GRD11]. **implication** [PL18b]. **Implications** [ASD18, GFB12a, MSBF18, Tch16, MPGGS19]. **implicit** [DFF+13, Koc13a]. **Importance** [PRPU+13, ALMY18, GSaY11, KUS19, MFLP12, EBR11, Kar12b]. **important** [COdF+11, KZZ13b, KBMM10, MTS15, VO11]. **improve** [MBA+19]. **Improved** [JZP17, PABSK16, SIM14, TNN16, CAPL12, IIH16, LCT14, Lu15, MMP+18a, RMG+19]. **Improvement** [LCK+16, SOF+10]. **Improving** [AST16, NB17]. **impurities** [ESDO16, SYS14]. **Impurity** [Fer11, Kry12c, HGB08, PK13b, TGRP19]. **impurity-induced** [PK13b]. **In-depth** [LYS+19]. **inaccurate** [SRMB15]. **inactivation** [CRB+12]. **Ince** [RA10a]. **incident** [NA14]. **include** [Lev10]. **including** [ALB18, DK13, GFRdG11, RS12a, ZLJ11]. **inclusion** [PEA+12, SVRGV12]. **incorporated** [EM19]. **incorporating** [QZH13]. **incorporation** [LSC+18]. **increase** [WCY+10]. **increasing** [Kar12b]. **incredibly** [SLS+19]. **Increments** [SP19]. **independent** [CP10, ILBS10, LZZ12, ZSZ14]. **index** [AD17, Cha11, Cin11a, EMK14, FDG18, GA19, HIL19, LSW19, LVP12a, PR10a, Pal10, PR11b, PL18a, QB15, SHMR11, WZ10b, PR11a]. **indexes** [GTSC+19]. **indicator** [Fin14b, TSBSM12]. **indices** [ABKJ18, ACT19, DZ11b, Du12, DNCKCS+12, IG11, LWY19, MPMCM+11, MBSMJC18, PO15, SMGZF19, TYN13, Tra19]. **indirect** [BBL12, Nal12, Nal13]. **indium** [FSK+11]. **individual** [MMM19, YSW11]. **indol** [SC12b]. **indol-2-one** [SC12b]. **indole** [ÇAS13, LW15]. **indoles** [SH18b]. **indolylfulgides** [TCG13]. **induce** [DPK18]. **induced** [ATM17, ALB18, CSS16, DS11, DSWL11, DSZB18, GKS10, HV11, LCB10, MAT19, MMSC19, PM12, PL11, PK13b, RBZ15, SS18a, SK10, ZY13, ZMZ13]. **induces** [KMT+12]. **inducible** [WLL+13]. **inducing** [LSC+18]. **induction** [dCDC+11]. **industry** [DSL15]. **inelastic** [IAA15]. **Inequalities** [HN12, Per10a]. **InFeO** [LL19]. **infinite** [MFLK11, SN15]. **infinite-order** [SN15]. **inflammatory** [MPE11, ScBsR+10]. **Influence** [AGOP18, CR18, CAAI12, DWPK14, EMS16, GVPCK10, dDGNB10, GKGM18, KK19, KK11c, KP12, LWWZ13, MHZ18, PFdM13, RB11b, SBL11, BS11, BDG17, BLM+12, BSO11, Fin14b, Gan14, LS19, NHG+12, NMS+10, RBTL19, ScBsR+10,

SYQ+10, SW12, VC13, WXB+11, XWC11b, ZLLS10, ZHI17]. **Influences** [SKY+13, DLLA10, FBD+13, OG19, YTY19]. **influencing** [BMX+19]. **influenza** [KRH13, WZ10a]. **Information** [AB18, Ano17-42, Ano17-43, Ano17-44, Ano17-45, Ano17-46, Ano17-47, Ano17-48, Ano17-49, Ano17-50, Ano18-31, Ano18-32, Ano18-33, Ano18-34, Ano18-35, Ano18-36, Ano18-37, Ano18-38, Ano18-39, Ano18-40, 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, Ano19-28, Ano19-29, Ano19-30, Ano19-31, Ano19-32, Ano19-33, Ano19-34, Ano19-35, Ano19-36, Ano19-38, Ano19-39, Ano19-40, Ano19-41, Ano19-42, Ano19-43, Ano19-44, Ano19-45, Ano19-46, Ano19-47, Ano19-48, Ano19-51, DLRMFY10, LS17, MEEA+13, MR18b, SP19, ALRA10, Ano15-35, Ano15-36, Ano15-37, Ano15-38, Ano15-39, Ano15-40, Ano15-41, Ano15-42, Ano15-43, Ano15-44, 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, Ano15-58, Ano16-29, Ano16-30, Ano16-31, Ano16-32]. **information** [Ano16-33, Ano16-34, Ano16-35, Ano16-36, Ano16-37, Ano16-38, Ano16-39, Ano16-40, Ano16-41, Ano16-42, Ano16-43, Ano16-44, Ano16-45, Ano16-46, Ano16-47, Ano16-48, Ano16-49, Ano16-50, Ano16-51, Ano16-52, Ano16-53, Ano17-27, Ano17-28, Ano17-29, Ano17-30, Ano17-31, Ano17-32, Ano17-33, Ano17-34, Ano17-35, Ano17-36, Ano17-37, Ano17-38, Ano17-39, Ano17-40, Ano17-41, CHL+19, EMED+12, EMEPD15, IOO18, LNV+18, MAT19, MR18a, Nag15, Nal15, OOI+19, OH19, PKK+16, PSGK17, Rei15, SLG11, Sjö15, SDL+15, TBST10, TRZ+19, WSV10, YOS15, Ano19-37, Ano19-49, Ano19-50]. **Information-entropic** [MR18b]. **information-theoretic** [IOO18, YOS15]. **Information-theoretical** [MEEA+13, EMED+12]. **informed** [DC14b]. **Infrared** [CLMY12, ZQXP17, DSFT17, GIO12, IROW10, KV11, MTS15, NDM+12, UTTn13, VVVB10, YWR+18, dARAV12]. **Inheritance** [YDW13]. **inhibition** [EI11, PCF+18, THSR13]. **inhibitive** [LZB10]. **inhibitor** [SKHN13, SKS10]. **inhibitors** [DSWL11, EAK+10b, EAK+10a, KMRG13, KKG12, MGK+12, RDM+11, ST15, SLA12, TPdMB12, WLL+13, XFW+14, YWY+12, ZFW+13, dOdONM12]. **InI** [BD12]. **Initial** [BLWJ17, BS16, LCK+16, Liu15a, TJS17]. **initialization** [ZWSF16]. **Initially** [SWS+14]. **initiated** [LLW+12]. **Initio** [CS13, LC16, PMH+16, PK16, ABKJ18, AEM+12, ATS15, BLR12, BHV+11, BMB10, BR15, Bou11, BM10, Buc11a, Buc11b, CTVA12, CCBR+12, CHM+14, CCS13, CK17, DG19, DZO12a, DCdG10, DFV+12, DOE+14, DM16, EG10, For12, FBU+11, FSK+11, GW18, GMP+11, HMI+15, HHCA10, HFD11, HL19, HHL+12b, IKC18, KAR12a, KDÇ12, KP11, KK14b, KSST12, KMU+13, KUY16, LSR+10a, LSR+11, LVdSdM14, Les12, LJW+11, LL11, LV12, LYR+17, LLLB13, LdAA+11, MC11a, MHT+08, MPJ12, MOE+11, MMBK12, MPD+10, MPZWD10, Mit11a, MSY+12, MLK17, MLB+12, MLB+10, NS19, NDM+12, NRHJ11, OT14, ONBP11, Pha19, QSLY10, RLW+13, RRVJ10, RS12a, RRRV19, Ril10, RNC+14, RAMB18, Ser11a,

SAHAA16, STL12, SM14c, Sri18, SN11, SJW13, SPM+15, TK16a, TNN16, TSL11, THVP14, UGWL18, UV18b, VPFD10, Var11, WZX11, Wit18]. **initio** [Wu11, WLWL14, YKM+15, YZL+11, Yu13, ZDZO10, ZZL+11, ZLZ+14, ZF15, ZXY13, ZZZ+18, ZRLV10, DAE+12, GWJ12, MPM15, SW12, Wag14]. **initio-based** [LV12]. **injection** [ZQJW13]. **inner** [BB10]. **inner-transition** [BB10]. **innovator** [SL11]. **inorganic** [BMRM19, BMF+14, BGJSM+18, KSO19, MCCGM+19, Swa13, YSA+11]. **inserted** [KRH13, LWL19]. **insertion** [DPDR11, RRVJ10, SMC18]. **Insight** [DMWY11, HFL+17, She12, She13, TFZ+15, WLL+13, BGMD15, DGR+16, EM17, KCDC15, MNV+17, MC17, MMSC19, RNdA+10, SAG13, SACA18, SC11, VHTEG15, YWJ+11, AF16, Tan13]. **Insights** [CP13, CADSG18, GJ18, HNBS18, MS14a, MC18b, SLA12, TFBG14, VBO+15, Bal16, BHA19, DJB10, LXW+14, LKZ+16, MNE+13, NP18, Pan16, SMGZF19, SR11a, ŚKB18, XZYS10, XLZ+19, YHLC15, dSM19a, dARAV12, KMS+11, QTCL10]. **instability** [Pat15]. **instanton** [Buc12a]. **insulator** [BEM11, Lar12, SAHG11]. **insulators** [YZZH15]. **Int** [BR16, COP16, HS15, Man16, dFR15a]. **integral** [HSN18, HFBC19, KSST12, LWY13, Mak15, RCGLV+14, SGC13, YK13, ZLR15]. **integrals** [AEÖ12, AA15, GTR11, GS10, Hog10, YM14, YŞÖ12]. **Integrated** [Cap16, HCH+18]. **integration** [BG11a]. **integrations** [Koc13a]. **intelligence** [Ezz10, SRS+17]. **intense** [DLCB15, SRPD16]. **intensities** [VVVB10]. **inter** [Tav11]. **inter-** [Tav11]. **interact** [NCMC+18]. **interacting** [Cap16, DM12, Dil13, KWWH18, Nes10, RP11a, RS13, SGL+16]. **Interaction** [ASHF13, DWPK14, EG10, JLS13, MYZ+10, MRT11, RNB+10, SPD+18, SK11, TBRIS10, ZT13, Ali19b, Bae14, BLL+13, Bas11, BEM11, Ber13b, CAZ+11, CCL+13, CGM12, CGG18, CRSB12, Cha10, CC11a, CYL+18, CP16, DC14a, DVDBM11, DTVP+12, DLG12, DWZZ15, ELC08, Eng16, EBH11, EAV16, FZX18, GWZ+14b, GD11, HFD11, HM10b, JFT13, JH15, JLG+12, KMM+18, KV19, KPH+12, LLG+12, LBdV16, Luz08, MMR+10, Mar12, MMC+19, NL11, NVI10, NFQ+11, OA12, PSK+16, PBR18, RYM12, RFN+12, RFMC19, RS11b, RRCO11, SSB19, SA18, SD13a, SD16b, SKHN13, SYL+18, Sha11b, SLZ+11c, SS11, SM14d, SWS12, SZL+14, SYY16, SCZH16, TK16b, TG16, VHTEG15, VVVB10, WLL11, WZW17, WWQG17, WG18, Win10, XXbX+13, ZST+10, ZCZ+12, ZS12, ZMB+17, TBRIS11, TBRIS12, YL10]. **Interactions** [KMMS17, MFK+12, dCDC+11, AGRI+12, BMR+13, BAP12, BMRM19, BLWJ17, BDG17, BLdV19, BWE16, Buc12b, CNBPR+11, CdLdSC18, CNSK11, CCS13, CKL16, Chu12, CSP+10, Cys11, DJB10, Dob14, DLP17, EAA17, EA12, EMS16, FNBK17, FRGC10, FKC12, HCH+18, HMA+19, HYD11, Jal10, JEA13, JLZ+17, KdPNNS16, KMK+16, KP12, KKG12, Kry12a, Kuv10, Kuz19, LMZ+11, LC16, LYW+19, LZZ+13, LDZG16, LB18, MZB+13, MHZ18, MS12, MIKH19, MSNP18, MPD+10, MPZWD10, MS10, MSY+12, MZLM17, MAW+18, MURR13, MMSC19, NH18, Nal13, NRI15, OA13, PML+11, PABSK16, PP16, Pie12, PETB18,

RK14, Ril10, Riv11, RGR12, SB18, Sch15, SSAM13, SM14b, SM14c, SS13, TH12, TDOD17, TCS10, Var11, VBC+12b, VSMK15, Yak11, YJ17, Yu13, YF16, YFY17, Zak13, ZRY+13, ZFS+11, ZLWZ16, dCSDdMC13]. **interactions** [dOdCMUdALR11]. **intercalated** [CWF11]. **intercalation** [KKS+11, MS10]. **intercalators** [Net12]. **interchain** [FNBK17]. **interconversion** [AZD+11, SAS+12, SSdS17]. **interdigitation** [MCKD11]. **interelectronic** [ALRA10, PWP13]. **interest** [Sko16]. **Interesting** [KBGC12]. **interface** [DLZ11, LLM13, RTG+19, SFNC+18, MRS15]. **interfaces** [NBZG16, OK19, SFL+10, TTM16, WML11]. **Interfacial** [IMS+13, LYS+19]. **interference** [YS13]. **interhalogens** [LWL19]. **interleukin** [WLL+13]. **interleukin-2** [WLL+13]. **Intermediate** [RMP+14, JL12b, MPRCEG12, Tal11]. **intermediates** [GGZZ16, KZZ13b, SMRK18, SBSD18, VGGPdL19]. **intermetallic** [AO12a]. **Intermolecular** [EAA17, LZZ+13, MZB+13, Pie12, Yu13, ZRY+13, BPG+10, Buc12b, EML+11, EA12, KP12, KMNSP19, MB15, OA13, OD12, PML+11, SPIL14, TNN16, Tav12]. **Internal** [MPC10, DDF+12, NH18, Sch15]. **International** [Ano13-49, NYA+13, Brä14, SG14]. **internuclear** [GI11b, GST11]. **Interplay** [MK11, Sch15, dCDC+11]. **interpolated** [ZRLV10]. **Interpolating** [MQA17]. **Interpolation** [RP16, DTVP+12]. **Interpretation** [CFP+10, Kar12c, Mor13, DHZS11, DSH+13, MHT+08, MAW+18, ZPM10]. **interpreted** [Nes11]. **Interpreting** [LB18, ZP16]. **intersection** [MSH13]. **intersections** [BMX+19, GSaY11, HV11]. **Interstellar** [TBRIS12, BN12, BRS10, CM17, LRP+11, RR11, TBRIS10, TBRIS11, XDM+10]. **Interstitial** [LLF+12]. **interstrand** [ZMZ13]. **intersubband** [BN11]. **intersystem** [LKd+16, MMG15, RMJ11]. **intra** [EML+11]. **Intramolecular** [BMR+13, RJY+10, RJA+10, AV19, Buc12b, CNBPR+11, COdF+11, CKL16, EKN10, FSBA12, HNH+12, JN13, JS17, KMM+18, KSAK17, KAOB11, Kry10, LXW+12, MK11, MK12, MB15, MSBF18, NRGS11, NRP+11, NRHJ11, Tav11, Tav12, UTTn13, YRN+11, ZZ18, dSM19a]. **Intriguing** [LB19, WSML16, ZLS+18, YHLC15]. **Intrinsic** [Lai11, MHO+15, NH18, GJ18]. **Introduction** [CCC11, KKL+12, LP10a, ÖS10a, ÖS12a, PBL12, Sch12b, SE11, Tch11, BC15, BC16, KCK14, KSAK17]. **Intuitive** [OS10b]. **Invariance** [Laz14, Kon10]. **invariants** [LZ10]. **Inverse** [CCA+12, Kar09, LXD13, WR14b, BMB12, BN11, CYK17, JW18, KM12c, PT13, WR14a, Kar10]. **Inversion** [MMM20, Cin20, DI18, MMM16, NKWT19, PM12, SH18a]. **inverted** [AAHN16, BW18, KMT+12]. **investigated** [CP16]. **Investigating** [BS14, MB15, CHSO13]. **Investigation** [EAV16, Gan14, HLB19, HWWW18, KG17, KLK13, KCK14, SM12, VO12, ASMP15, ATM17, AAA12, AZD+11, BXR+13, BAA+18, BWE16, Buc11a, CZJZ12, CHM+17, CNSK11, CC11a, DDÇY12, DMG10, DOE+14, DSVP15, Exn11, GWJ12, HDQ+13, HWHZ11, HCL13, JFT13, KB13, KSSK16, Kim19, LB14a, LOHB13, LRP+11, LPO+12, LL11, LDW+11, LXD13, LZZ+17, LMCZ11, LCZL11, LW15, MWH15,

MCP10, MPTR12, MB14, MHOG18, MSK11, MJ14, MMV+19, MLK17, MLB+10, MKW11, NFD+10, OT14, ONK+13, PZ19, PJP10, PMAP12, PSK+13, QSLY10, RK14, RFMC19, RW11, RMP+14, Rua10, SAG13, SMRK18, SS18b, SR13, SAHAA16, SDM12, TZ11, THVP14, TD19, WGLX10, WXB+11, XZL+12, XCY15, XZG+18, XF19, YLH+19, YJ17, YLW+13, ZH12, ZR13, ZSHL14, ZZC15, Zha17, ZQW+17, ZL12, ZYL+13, ZMZ13, ZCG+16, ZMB+17, dCSDdMC13, dSdSPG11, dSTH17, GFRdG11, XWC10]. **Investigations** [Bou12a, BL12, Cas15, DSSM19, Kim13, KRG+13, Mag14, MSNP18, NMIP14, SZS+10, SLZ+11b, SLZ+11c, SLZ+11a, SLS+11, SM14c, SM14d, VSN+11, WFS13, YL11, ZZR+12, ZFS+11]. **involve** [Bud12]. **involved** [CLXZ12, MM10]. **Involvement** [LSL+08]. **involves** [ZZ18]. **involving** [LLLB13, Ril10, TCA10, YHLC15]. **iodane** [TM19]. **iodide** [MJ14, MMV+19, NTGC19]. **iodides** [LW15]. **Iodine** [MOY13, VKF+19]. **iodo** [LZD+11]. **iodo-perfluorobenzene** [LZD+11]. **ion** [ABS13, AB16a, Ali19a, BS14, CDS+18, COP16, DLO16, DCHC11, EHKD11, EKD12, FBRBR12, FDMR11, GFB12b, GH11, HMI+15, HLJZ11, HFL+17, IAA15, KMS+11, KME+18, KLK13, Kim18, KUS19, KHH10, LJK+18, MS14a, MHZ18, MPTR12, MHOG18, MNC12, Ng12, Oni10, Oni12, SSP+17a, SZS+10, SLZ+11a, SLS+11, SLZH12, Vik13, WFS13, XLGA12, YW11a, dSSF16b, dSSF16a, SSP14]. **ion-covalent** [ABS13, AB16a]. **ion-neutral** [FBRBR12]. **ion-pair** [SSP+17a]. **ion-stabilized** [KUS19]. **Ionic** [BWW10, AFC+10, AVG19b, AVG19a, Ber13c, Buc12a, DLZ11, HFL+17, KME+18, MFK+12, MHOG18, NDH10, RI19, RF10, WZZL10, XWC10, ZPZ15, dOLdlV13]. **Ionization** [MAPS18, VAT12, ABG12, CHH+19, DLCB15, DVP18, FMCA11, GZMC11, HMH+13, Kit17, LDKB15, PUH+11, PM16, SVPTM+10, SOM10, TGRP19, VF13a, YÇÖ11]. **ionized** [Glu13]. **ionochromic** [FBU+11]. **ions** [ASHF13, BMTT11, BSPK11, CCM08, DSC+11, DP16, FBRBR12, KWLS15, KWWH18, KLK13, KFY+12, LLZZ10, MGK+11, NC11, RP16, SB16, SKL10, WLG+11, WHM14, YYI+12, ZCG10]. **IPR** [KK12a]. **IQA** [JNY17, MC17]. **IQF** [MC17]. **Ir** [ZQJW13, BBB+12b, BWB+18, CWF11, DSD18, HMH+13, KBMM10, MSK11, ÖEDB11, RDB18, RDB19, VPFD10, ZQCJ10, SHW+13, TGA+11]. **IR-MALDI** [HMH+13]. **IrF** [SR13]. **iridium** [SK12b, WXB+11, ZQJW13, CADSG18, SLS+14]. **iron** [AC19, ADR+18, ASD14, ASD18, BBA+16, DB13b, FDNR10, GFRdG11, HFD11, Joh17, KO14, LMC19, LKZ+16, NBL+14, ONK+13, SS19a, SYS14, SGL19, TSvL+16, THSR13, VPOG19, WLS+19]. **iron-based** [DB13b]. **iron-carbon** [LMC19]. **iron-dependent** [ASD18]. **iron-porphine** [Joh17]. **irradiation** [AGG+18, WDR+11]. **irregular** [ZCG+16]. **Isatin** [CPF12]. **isatoic** [DNCKCS+12]. **isocloso** [SALK19]. **isocyanide** [LJW+11]. **Isodensity** [TMC+13]. **Isodensity-based** [TMC+13]. **isodesmicity** [LVP12a]. **isoelectronic** [KT12a, KA11, RZSZ18]. **Isolated** [TWHZ14, KK11b]. **Isolated-Pentagon-Rule** [KK11b]. **Isomeric** [VFCSC17, ŞBAT16]. **isomerism** [GPM+15, GCD13, LBM11, MMSC19].

isomerism-induced [MMSC19]. **Isomerization** [CFGC11, LVP12b, CWSZ13, GK12, GLOGM+11, MB13, NTGC19, PL18b, SSdS17, Tap15, VF13b, WCS+13, TTD13]. **Isomers** [OPP+14, CW16, CWSZ13, FBRBR12, FMKJ14, HM10a, KK11b, KK12a, LCB10, MCP10, Met11, Puz10, RJA+10, RNV+12, Rua10, USL+13, WWL+11]. **isomery** [Tav12]. **isomorphic** [ZKWZ17]. **isomorphously** [JLL11]. **isopropyl** [HYZ13]. **isotherm** [Boe12]. **isotope** [Bou11, Bou12a, HZW18, MURR13, SK10, YT14]. **Isotopic** [MD11, MVA19]. **isotopologues** [BL12, GJ18, WH18]. **isotropic** [MR18a, NB17]. **Israfil** [Mam14]. **Issue** [AH19, Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g, Ano12h, Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n, Ano13k, Ano13q, Ano13r, Ano13s, Ano13t, Ano13u, Ano13v, Ano13w, Ano13a, Ano13b, Ano13c, Ano13d, Ano13e, Ano13f, Ano13g, Ano13h, Ano13i, Ano13j, Ano13l, Ano13m, Ano13n, Ano13o, Ano13p, Ano13x, Ano13-35, Ano13-41, Ano13-42, Ano13-43, Ano13-44, Ano13-45, Ano13-46, Ano13-47, Ano13y, Ano13z, Ano13-27, Ano13-28, Ano13-29, Ano13-30, Ano13-31, Ano13-32, Ano13-33, Ano13-34, Ano13-36, Ano13-37, Ano13-38, Ano13-39, Ano13-40, Ano13-48, Ano14a, Ano14b, Ano14n, Ano14t, Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14z, Ano14c, Ano14d, Ano14e, Ano14f, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m]. **Issue** [Ano14o, Ano14p, Ano14q, Ano14r, Ano14s, Ano14-27, Ano14-37, Ano14-43, Ano14-44, Ano14-45, Ano14-46, Ano14-47, Ano14-48, Ano14-28, Ano14-29, Ano14-30, Ano14-31, Ano14-32, Ano14-33, Ano14-34, Ano14-35, Ano14-36, Ano14-38, Ano14-39, Ano14-40, Ano14-41, Ano14-42, Ano15a, Ano15b, Ano15c, Ano15d, Ano15e, Ano15t, Ano15x, Ano15y, Ano15z, Ano15-27, Ano15-28, Ano15-29, Ano15-30, Ano15-31, Ano15-32, Ano15-33, Ano15-34, Ano15f, Ano15g, Ano15h, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n, Ano15o, Ano15p, Ano15q, Ano15r, Ano15s, Ano15u, Ano15v, Ano15w, Ano15-35, Ano15-36, Ano15-37, Ano15-38, Ano15-39, Ano15-40, Ano15-41, Ano15-42, Ano15-43, Ano15-44, 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, Ano15-58]. **Issue** [Ano16a, Ano16s, Ano16t, Ano16n, Ano16u, Ano16v, Ano16w, Ano16x, Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16b, Ano16c, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m, Ano16o, Ano16p, Ano16q, Ano16r, Ano16-29, Ano16-30, Ano16-31, Ano16-32, Ano16-33, Ano16-34, Ano16-35, Ano16-36, Ano16-37, Ano16-38, Ano16-39, Ano16-40, Ano16-41, Ano16-42, Ano16-43, Ano16-44, Ano16-45, Ano16-46, Ano16-47, Ano16-48, Ano16-49, Ano16-50, Ano16-51, Ano16-52, Ano16-53, Ano17a, Ano17b, Ano17m, Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x, Ano17y, Ano17z, Ano17c, Ano17d, Ano17e, Ano17f, Ano17g, Ano17h, Ano17i, Ano17j, Ano17k, Ano17l, Ano17o, Ano17p, Ano17q, Ano17r, Ano17s, Ano17-27, Ano17-28, Ano17-29, Ano17-30, Ano17-31, Ano17-32]. **Issue** [Ano17-33, Ano17-34, Ano17-35, Ano17-36, Ano17-37, 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, Ano18a, Ano18r, Ano18s, Ano18t, Ano18b, Ano18o, Ano18u, Ano18v, Ano18w, Ano18x, Ano18y, Ano18z, Ano18-27, Ano18-28, Ano18-29, Ano18c, Ano18d, Ano18e, Ano18f, Ano18g, Ano18h, Ano18i, Ano18j, Ano18k, Ano18l, Ano18m, Ano18n, Ano18p, Ano18q, Ano18-31, Ano18-32, Ano18-33, Ano18-34, Ano18-35, Ano18-36, Ano18-37, Ano18-38, Ano18-39, Ano18-40, 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, Ano19a, Ano19t, Ano19b, Ano19c, Ano19d, Ano19o, Ano19u, Ano19v, Ano19w, Ano19x, Ano19y, Ano19z, Ano19-27, Ano19e, Ano19f, Ano19g]. **Issue** [Ano19h, Ano19i, Ano19j, Ano19k, Ano19l, Ano19m, Ano19n, Ano19p, Ano19q, Ano19r, Ano19s, Ano19-28, Ano19-29, Ano19-30, Ano19-31, Ano19-32, Ano19-33, Ano19-34, 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, NYA+13, NT15, ÖS12b, For17a, Kon10, LV16, Rei15, Rup15a, ÁIGVZW12, Ano12o]. **issues** [MMP11]. **Italy** [Bar16]. **iterative** [ATPRV11, Mit11c, MPT11, SHMR11]. **IV** [DdG+11, IKN13]. **IVA** [Eng16]. **IxV** [PPDF11].

J [BR16, COP16, HS15, Man16, dFR15a, CDT12]. **J.** [XTLA14]. **Jack** [BMB12]. **Jack-Bean** [BMB12]. **Jacob** [Jan13]. **Jaguar** [BHH+13, ZWSF16]. **Jahn** [AGPDZ13, DMAB12, GFB12a, RGPZD13, SBD+16, TPCJ+12, WLZ18, YYI+13, ZFC12]. **Janus** [CHL+19]. **jar** [TFBG14]. **Jensen** [ALRAE11]. **Johnson** [DJ12, DJ95]. **joint** [AZD+11]. **Jones** [CAPL12, RC11]. **Josimar** [COP16]. **Journal** [SG14]. **junction** [Jan10, SD13c, ZYZ+11]. **junctions** [XWP+18]. **Just** [Var14]. **justified** [RVO+14, SKL10].

K- [PUH+11]. **kaempferol** [DSD18]. **kaleidoscopic** [SG14]. **kaolinite** [CWF11, CGM12, WWQG17]. **Kaplan** [KK12b]. **Karlin** [PR11a]. **Karplus** [DSCO+13]. **KCl** [DLZ11]. **KD** [DLM12]. **KDP** [AFA13, DMS+10, DMBL16]. **Keggin** [TPCJ+12]. **Kepler** [DJ12, DJ95]. **Kernel** [HM10b, HM11, IHG10, PC13, VSL+15, HBMM11]. **kernels** [NDLC19]. **ketene** [ŞBAT16]. **keteneimine** [VGGPdL19]. **keto** [AZD+11, Coo12, GW18, MPGGS19, VF13b]. **keto-amino** [Coo12]. **keto-enol** [AZD+11, MPGGS19]. **ketone** [DP12, SSdS17, WZZL10]. **ketones** [WTZ+11]. **key** [SB16, TZ11]. **KH** [DLM12]. **kinase** [BGJSM+18, DSWL11, WLL+13, dOdONM12]. **kind** [PWP+18]. **kindling** [TCM+12]. **kinematic** [DKR10]. **kinematics** [PT13]. **Kinetic** [AK17, KAR12a, SFC16, Tav11, AB18, AST16, BW18, BR10, BR16, FDA16, Han19, HZW18, HMH10b, JAB12, KMU+13, LSC+18, NIT16, PIS18, SGL+16, SAG13, Sko16, SS19b, XNL+14, dlLIAI+12, MOH+12].

Kinetic-energy-density [SFC16]. **kinetic-energy-releases** [Han19]. **kinetically** [fXxBhD19]. **kinetics** [ACMRN10, BMB12, BLM+12, CdAFS+12, COdF+11, DS12, EML+11, HWHZ11, MXC18, MCC12, MPRCEG12, MML+11a, MLB+12, MMM+12, PRFR17, RLW+13, Var14, WLWL14, ZZW11]. **kinks** [Yak10]. **Kirchhoff** [Cin11a, LSW19, LWY19, PR10a, Pal10, PR11b, PR11a, PL18a, WZ10b]. **Kitaev** [TSS+15]. **KOH** [VLK+11]. **KOH/DMSO/CH** [VLK+11]. **Kohn** [AT18, BW18, Bar11, Gan14, KdSM+10, KFJ+18, LB14b, Lev10]. **kojic** [KS11]. **Kondo** [BRBRS11]. **Kondo-like** [BRBRS11]. **Korea** [LJ16]. **Kr** [KDOR17, EAV16]. **Kramers** [BMB16, GBK18]. **Kratzer** [Sta10]. **KRb** [LDADB+15]. **KRb-K** [LDADB+15]. **Kroll** [SN15]. **Kubo** [Hor13]. **Kubo-transformed** [Hor13]. **Kullback** [LSS19, LNV+18]. **kynurenine** [BS11].

L [CCL+10, DPDR11, MLW10, ZQJW13, WHM14, KSG+12, PUH+11, QTCL10, ZYL+13]. **L-** [PUH+11, QTCL10]. **L-ascorbic** [ZYL+13]. **l-cysteinate** [WHM14]. **L99A** [DFF+13]. **L99A/M102Q** [DFF+13]. **LaAlO** [Oni10]. **labile** [YIY+13]. **laboratory** [IM15]. **laboratory-** [IM15]. **ladder** [CEM14, Jan13]. **ladder-like** [CEM14]. **Ladik** [XTLA14]. **LaF** [Lan10]. **Lagrange** [Mit11c, KRC+16, OPC17, WWL17]. **Lagrange-mesh** [OPC17]. **Lagrange-sinc** [KRC+16]. **Lagrange-type** [Mit11c]. **Laguerre** [SMOD11]. **Lamb** [Rit12a, Rit12b]. **Lamé** [MFLK10]. **landscape** [DVC14, PP14]. **landscapes** [AG10b]. **language** [Tch16]. **LaNiInH** [OA12]. **Lanthanide** [XYL+18, FS11, OAC17, SSW16, TG13, VBJK18, WLG+11]. **Laplacian** [CWW12, LGL+19, LZZ19]. **Laplacian-based** [CWW12]. **Laplacians** [LWY19]. **Large** [DFF+13, SN15, BHMN19, BBB+12a, BBB16, CKYR18, DFV+12, GFRdG11, HSS18, KP11, KYH+13b, LSKM19, MSS11, Mit11c, OCL+18, PBB15, QSX+15, RAMB18, TY17, Tok16, UDS19b, XXJ+16, YFY17, ZWSF16]. **large-amplitude** [XXJ+16]. **Large-scale** [DFF+13, SN15, CKYR18, RAMB18]. **larger** [JLL+18, MSNP18, RVNP12]. **Laser** [BN11, RP11b, DLCB15, GV19, GRLA18, HYH+10, IAA15, NWQX11, SRPD16, SVPTM+10]. **later** [Mur12]. **lateral** [LEU+11, SIT+12]. **Latin** [CJBMMAPR19, GRCGRRHT19, MCCGM+19, MMCNV19, RA10b]. **lattice** [DTFK15, Ng12, PK13b, VBC+12b]. **lattices** [DB13b, VBC+12a]. **law** [BR10, BR16]. **layer** [Kim18, RTG+19]. **layer-structured** [Kim18]. **layers** [ATS15, Dw13]. **laying** [KHH10]. **LCAO** [Nal13]. **Lck** [XFW+14]. **LDA** [Fuk12]. **Lead** [VDG13, CAA19, MW15, Per10b, VVY18]. **Leading** [LG12, KMS+11, YY18a]. **Leading-order** [LG12]. **learned** [LSP+16]. **learning** [BR15, CLKD15, FLvLA15, MJSC18, NDLC19, Rup15a, Rup15b, SKLC19, STM17, vLRRK15]. **Lee** [LJ16]. **Legendre** [Win10]. **Leibler** [LSS19, LNV+18]. **length** [Mar11, PE11, RKCK19, Sch10b]. **Lennard** [CAPL12]. **lesion** [SM13]. **lessons** [PR10b]. **Letter** [HS15, PS14, Sha11a, dFR15a]. **Letters** [CK13, COP16, Lad14, Lun13a,

Man16, MBSAG16b, PS13b, Tou13, VV13, VUC13, XTLA14, dSSF16a]. **level** [AOT+18, AST19, BLdV19, KK13, KdSM+10, LCL+10a, MAN15, NBI+10, PAD+10, PWH+12, RNE10, Shi13, SZL+14, WWHZ13]. **levels** [CDS+18, DK13, Kin13, MA12, SA11a, Tou11b]. **levodopa** [EAH13]. **Levy** [SGC13]. **Lewis** [EMSB15, GCZ+14, PP14, dSTH17]. **Li** [BCGC12, BL10, ČFČ11, HHL12a, HHL14, HWL16, MLW10, MPRB+10, OCL+18, RFEGPP+16, Sat11b, SM17, Sri19, XWCY11, YK11, YC13, BGL+16, CDSK12, DLZ11, GGD12, HMP+11, HYH+10, JMPP19, JCCZ12, KH12, LKJ13, LdAA+11, MT11, MJ14, SM16, TL15, UDS19a, VVAO12, WCY+10, XWCY11, YZ10, YLC17, ZLWL16, ZCG10, dOR10]. **Li-B-H** [VVAO12]. **Li-like** [ZCG10]. **LiBH** [WZM+13]. **library** [DSM+19b]. **Lieb** [SGC13]. **LiF** [YZ10]. **life** [BHH+13]. **lifetimes** [Ber13a, SCZG12]. **ligand** [BZBZ13, BLdV19, BPK19, CPF12, CSSK+12, DS11, DPDR11, DCdG10, GZMC11, Joh17, KKG12, MCE11, SLS+14, WLS+19, WTH+11, XWC11b, YZW+15a, ZLLS10, CSVCB12]. **ligands** [AC19, ASHF13, Con10, CADSG18, DPK18, DG19, DdG+11, LYW11, LXW+14, LGS+16, SHW+13, SM14b, YZL+11, ZKKR11, dCSDdMC13]. **ligated** [LKZ+16]. **light** [ALB18, BSS15, CSS16, DS11, MUNZVR12, MGB18, NZAVR10, WCL+17, dSCC12, dSdS13a]. **light-emitting** [NZAVR10]. **light-induced** [CSS16, DS11]. **lignan** [SBEH11]. **LiH** [YLC17, FBM+10, LWWZ13, RAN18, SPO+11, SCTW10]. **like** [BRBRS11, CEM14, CCM08, DTPC17, Dum12, GZ14, JL12a, JHL+18, KWWH18, KP11, LORR+12, LSKM19, LC12, LNI12, PGGRMP10, She13, SLS+19, SS12, SCZG12, VPGC12, VBC+12b, WCY+10, YÇÖ11, YW11b, ZCG10]. **limit** [CHH+19, KYS13, LV12, RPBB11]. **limits** [Coo12, Kry11b, RBD+10, RBTL19]. **LiMn** [KLK13]. **LiN** [Per10b]. **line** [Bib13, BR12b, IROW10, SMOD11, TY17]. **Linear** [D'y16, UYN+13, ABA11, BEM11, Boe12, Buc10, CKB18, EBH11, GRLA18, KJ16a, KJ16b, LWY19, LZZ19, MMWA11, MM19, MMF+13, NIK19, NMV+14, OPAVM18, PVS11, PL18a, PCD14, PBB15, QSX+15, RSN12, RCP14, WZ10b, Yam11, ZY13, ZLE17, dOdCMUdALR11]. **linear-response** [Yam11]. **linear/cyclic** [MMF+13]. **Linearity** [IKN13]. **linearized** [Liu15a]. **linearly** [YF16]. **lineshape** [LC19, SB10a]. **LiNH** [WLL11]. **LiNi** [Kim19]. **linkage** [MMSC19]. **linked** [Dum12, LYW11, NKF+13]. **linking** [PWH+12]. **Lipid** [Kuv10, KMT+12, MCKD11, SMK+12, SIT+12, YINM13]. **lipids** [FMP+17]. **Lippmann** [DJ12, DJ95]. **liquid** [AMMK11, CSTA16, KME+18, MMP+18a, MFK+12, MPV+11, OHDA13, Pha19, Riv11, SSKS12, TGRP19, WZZL10, ZSASS13, dSdSPG11, dOLdlV13]. **liquids** [AVG19b, AVG19a, HFL+17, RI19, RdA11]. **LiRb** [GFB12b]. **List** [Ano10a, Ano10b, Ano10c, Ano10d, Ano11d, Ano11e, Ano12p, Ano12q, Ano12r]. **lists** [TY17]. **lithium** [Ali19a, AVG19a, BCGC12, DLO16, EEMSS14, HFBC19, KLK13, Kim18, Kin13, MJ14, Per10b, SD16a, SKY+13, WWL+11, WLH+19, YC13, ZLZ+14]. **lithium-iodide** [MJ14]. **lithium-ion** [Ali19a, Kim18]. **lithium-orientation**

[WWL+11]. **Liu** [LSC+18]. **living** [SB16]. **LiX** [DIOG12]. **LMFBR** [FUE+12]. **Ln** [BSPK11]. **LnO** [TG13]. **Load** [NMSR14]. **loaded** [LWX+14]. **Lobatto** [Rom10]. **Local** [AKR12, FSST16, IN15, RB18, ZXY13, ATL+14, AK11, CCL+16, DNCKCS+12, Fin17, FKC12, Glu13, ISN13, KK12a, Lya14, MDNDO+16, OS10b, OPAVM18, PK13b, PSPS11, RPBB11, RPVM10, SMGZF19, SN15, SACA18, Zha17, Kut13, YSS+10]. **Locality** [RCP14, LNV+18]. **Localization** [GB10, AOT+18, AT18, BEM12, BL10, BL11, GNM+12, KC18, MGB18, MFLP12, OAT+13]. **Localized** [ABS13, NB19, AEKGZ12, ALK18, BMB10, IK18, PABSK16, SSB19, DG19]. **localized-** [SSB19]. **locally** [KUY16]. **Locating** [QZH13]. **location** [NMV+14]. **logic** [TPT19, ZPR10]. **London** [CC12, Dob14]. **lone** [CCL+16, CFV18]. **Long** [RR19, SSK11, AM10, BR12b, Dun15, Haj18, HSN18, MIN13, MC18a, SKV12, SKY+13]. **Long-range** [RR19, SSK11, AM10, Dun15, MIN13, MC18a, SKY+13]. **long-time** [SKV12]. **long-wave** [BR12b]. **look** [PR11b]. **loop** [Dum12]. **loss** [AEM+12, DCHC11, NDLC19, NH11]. **Low** [LCZL15, TU10, ALK19, BG11b, BG11c, BEPZ10b, DAR+11, DLM12, DCHC11, DdG+11, Fer11, GFB12b, HFD11, JCC10, KKH18, Kan17, Kin13, Kon11, KZZ13a, KHH10, LLF+12, LVdSdM14, LP10b, LCL+11, LGP+11, LGP+12, LXD13, MCP10, MMWA11, MT11, MOH+12, NS19, SSB12a, SLSZ13, SSP+17b, SZZ+12, SSW16, WFS13, ZPZ15]. **low-barrier** [DLM12]. **low-dimensional** [BEPZ10b]. **low-doping** [Fer11]. **low-energy** [ALK19, HFD11]. **Low-frequency** [TU10]. **low-lying** [BG11b, BG11c, DAR+11, DCHC11, GFB12b, JCC10, Kin13, KZZ13a, LVdSdM14, LP10b, LCL+11, LGP+11, LGP+12, MMWA11, MT11, NS19, SLSZ13, SZZ+12, WFS13]. **low-temperature** [MOH+12]. **low-valent** [LXD13]. **LOWDIN** [FMPM+14, JH15, SG14, Yos20, dA12]. **Löwdin's** [Pon19]. **Lower** [DVP18]. **lowering** [GAPK+19b]. **lowest** [DAC12, MLW10, SYL+18, Zho18]. **Lp** [YZZ16]. **LRESC** [AMAM18]. **LSQC** [LCZL15]. **Lu** [ZHI17]. **Luis** [Mer11]. **luminescence** [SGG+10]. **luminescent** [CADSG18, KP12, LXW+14]. **LUMO** [MA12]. **Lungu** [Tou13]. **lyase** [MLW+14, ZSHL14]. **lying** [BG11b, BG11c, DAR+11, DCHC11, DSSM18, GFB12b, JCC10, Kin13, KZZ13a, LVdSdM14, LP10b, LCL+11, LGP+11, LGP+12, MCP10, MMWA11, MT11, NS19, SLSZ13, SZZ+12, WFS13, ZCG10]. **lysergol** [RGS+13]. **lysozyme** [DFF+13].

M [Ano11c, Ano11b, BLL+13, BL10, BDR12, DD17, FTB11, HWL16, JL12a, JLG+12, MLY+16, MLW10, PAKA15, Sau11, SZZZ11, SM17, SYQ+10, TFB11, VO12, WCY+10, XZZ+10, XWC11a, XWCY11, YK11, YLWrL12, ZLWZ16, ZLY+14, GBS17, JL12a, JLG+12, KJ14, MLW10, PUH+11, SY10, SLS+10, SZZZ11, TFB11, XWC11a, YK11]. **M-Cd** [XWC11a]. **M-doped** [KJ14]. **M-shell** [GBS17]. **M-shells** [PUH+11]. **M06** [KSG+12]. **M06-L** [KSG+12]. **M08-HX** [Vie17]. **M102Q** [DFF+13]. **Machine**

[Rup15b, SKLC19, STM17, BR15, CLKD15, FLvLA15, LSP+16, MJSC18, NDLC19, Rup15a, vLRRK15]. **machine-learned** [LSP+16]. **machine-learning-augmented** [CLKD15]. **macro** [RAK10]. **macro-dimensions** [RAK10]. **macrocycle** [CJMC19]. **macrocycles** [VSMK15]. **macromolecules** [Chr10, OVT+16]. **macroscopic** [DLM12, DP11, FUE+12]. **made** [Mas10]. **Magic** [TB15, MJ16a, MHHPR+17, TZD+19]. **Magnesium** [FMP+17, BPT12]. **Magnetic** [GKS10, KV19, KMU+13, MPD+10, MPZWD10, WSCL11, Zag11, AGCVG15, ATL+14, AC11, AK11, ALB18, AM10, BXR+13, Bou12b, CL11, CWW+16, CKL16, GE12a, GV11, JL12a, JHL+18, KSC15, KSG+12, KSY+11, KT12b, Lae14, LB14b, LL19, LMC19, LB19, Mag14, MZB+13, MC18a, NBL+14, OMĐ13a, PL11, RP11a, RZC13, SRPD16, SSI+10, Shi18, SS19b, SBB16, SS12, Sto18, SS13, TD11, TW10, Vik11a, Vik11b, Vik13, VRO+12, YZW15b, ZPM10, ZP16, ZLS+18, ZLWZ16, ZST+10]. **magnetic-field** [PL11]. **magnetic-resonance** [AK11]. **magnetically** [ATM17, ALB18, MAT19]. **magnetism** [ABP13, KLZQ15, SC10b]. **magnetization** [KLZQ15]. **magneto** [KG17]. **magneto-electronic** [KG17]. **magnetoelectric** [RC11]. **magnetoexcitons** [MLDP10]. **magnetoresistance** [ZX12]. **magnetotropicity** [TG13]. **magnets** [LL19]. **magnitude** [LZD+11]. **main** [TMC+13]. **main-group** [TMC+13]. **Major** [ALK19]. **Makarov** [CYL+18]. **make** [SLS+19]. **MALDI** [HMH+13]. **malonaldehyde** [NRHJ11, RJY+10]. **malonate** [DdG+11, JSLH14]. **maltolate** [DdG+11]. **manganese** [SSK+12]. **manifest** [GI11e]. **manifold** [MCV11]. **manifolds** [CC11b]. **manipulated** [CHL+19]. **Mannich** [TFZ+15]. **Mannich-type** [TFZ+15]. **Manning** [ZHF12]. **Many** [BSO16, GR11, CSMZ10, DLP17, Fer19, Fri12, Kha16, KRG+13, LV12, Lin14, Lya14, Nas19, Per10a, RBVAG18, SK17b, SIB+13, SHKS15, Sit15, Zak16]. **Many-body** [BSO16, GR11, DLP17, Fri12, LV12, Lin14, Lya14, Per10a, SK17b, SIB+13, SHKS15, Zak16]. **many-electron** [CSMZ10, Kha16, RBVAG18, Sit15]. **many-electrons** [Fer19, Nas19]. **map** [DW12, Dw13]. **mapped** [Sta10]. **mapping** [Kry12b, WWC17]. **maps** [GB18]. **Maria** [HS15, dFR15a]. **marker** [BCNR18]. **Markov** [Cal10]. **Markovian** [CW13b]. **Markovnikov** [DMWY11]. **Martin** [TM19]. **mass** [ABKJ18, Dw13, DdG+11, FUE+12, PGGRMP10, SBKJ18]. **masses** [GbZA10]. **Massively** [yOITn15, PCV19]. **match** [SMK+12]. **matching** [MGN14]. **material** [FFPD16, IKC18, LC12, Oni12, OA13, TFBG14, YBMK12]. **Materials** [Ném14, BCGC12, BHH+13, BCNR18, CLH14, DMBL16, Fer11, GNM+12, HNBG15, IIS+17, Jia15, KJ15, Kim18, LPO+12, MW16, MML11b, MSOV13, MGP16, NBI+10, PETB18, SSB12a, TK16b, UMS13, VVY18, Wag14, fXxBhD19, ZCX+16, ZWSF16, ZLWZ16]. **Mathematical** [Gar08, Lev16, Sha11a, Yos20]. **matrices** [ABLT11, Boc17, Gin10, Mit11c, Per18, WH12, Yur13, Yur15]. **Matrix** [Luz08, AAHN16, AÖ12b, ČW13a, CM15, EM16, GBK18, HMH+13, KK13,

KJ16a, KJ16b, Kit14, Kit15, Kit17, KFS13, KFJ+18, Lan10, Lat13, SHS+13, YKM+15]. **Matrix-covariant** [Luz08]. **matter** [AF19b, DW12, Ng12, Tap15]. **Matthews** [BSS16]. **Matthews=** [MSBF18]. **Matthews=-Olson** [MSBF18]. **Mattsson** [MA10]. **MAu** [FTB11]. **Maximum** [EMEPD15, GGJD13]. **Maxwell** [CD15]. **May** [LW18]. **mazzite** [RDB19]. **MCCH** [DD17]. **MCI** [TIKN11]. **MCI-186** [TIKN11]. **MCSCF** [OD12]. **MD** [AHC+18, Eil14, MFB11, SLA12, YWY+12]. **MD/QC** [Eil14]. **MD/QC-simulated** [Eil14]. **MD/QM** [MFB11]. **Me** [ČFČ11, GWM11, HHL14, RBTL19, HHL12a]. **mean** [DCD11]. **mean-field** [DCD11]. **Meaning** [Gao11]. **means** [AGNS14, BL10, Ném14, OK16, RNdA+10, TH12, ZXY13]. **measurement** [Ezz10]. **measurements** [Bra19, KDA+11, ZPM10]. **measures** [Ale13, DTPC17, IOO18, Kan18, LS17, LSS19, Lat13, LRMAA19, Luz13, MR18b, SLG11, YOS15, ZYL+14]. **MeB** [ČFČ11]. **mechanical** [CPAT11, DKR10, DC14b, LV19, MMP+18b, MPD+10, MPL+11, Pan19, PP19a, RDM+11, SSA18, VPFD10, XS18, YZ12]. **mechanics** [BBB+12b, EAH13, IAK13, Ma14, MPE15, MSC10, Rup15a, Rup15b, SK17b, SIB+13, UV18b, Brä12]. **mechanics/molecular** [Ma14]. **Mechanism** [KBF+13, MCC13b, Pli18, SH18b, WML10, ZQW+17, ZL10, AG10a, Bal16, BCP10, BL11, BLWJ17, yBZfC18, CCL+10, CWS15, DS12, DP12, DZ11a, DSZB18, EAH13, EM17, FZX18, FDMR11, HWHZ11, HhGqZZ17, JSLH14, LGM+18, LJK+18, LLL16, LZW+18, lLBqD+19, LS19, LWJL10, LWC+10, LCM+11, LCS+11a, LCH+11, LCS+11b, LXLL11, LLLB13, MLW+14, MOSK10, MR11, MML+11a, MKW11, NE11, OH12, OH13, PL18b, PO15, RY12, RFMC19, SAS+12, SSI+10, SAG13, SKS10, SKS11, SDR+13, SDM12, SR18, SLS+15, SZL+15, SSdS17, TM13, TYL10, TXL10, VPGC12, VLK+11, VOK+18, WGLX10, WXZ+11, WHS+13, WWLZ17, WWX+11, WLD+10, XDM+10, XZCH11, YM12, YNLD18, YWJ+11, YZZH15, ZRGE+19, Zha10, ZZW11, ZCZ+12, ZBK15, ZBG+19, ZSS+13, ZCTG18, ZTC11, ZLY+14, ZPW16]. **Mechanisms** [CGIAI12, LLF17, LFTL18, PWL+10, XZG+18, AGNS14, CWZ+10, FTB11, HLJZ11, HZZ+19, HNBS18, HYZ13, JLS13, LNGW14, LD17, MXC18, MMP+18b, MLB+12, NKWT19, NZLG15, OD12, PTS+11, PRG+10, RFEGPP+16, SYK+12, SSK+12, SS18a, VHTEG15, WLWT12, YSS+10, ZPB12, ZMZ13, ZSHL16]. **Mechanistic** [Buc12b, GMT18, LTL18, LKZ+16, NP18, SGL19, WRW+18, dSM19a, AASU+17, AEAS+19, RNdA+10, VPOG19, dlLIAI+12]. **mechanochemical** [TJS17]. **mechanochemistry** [QBRA18]. **media** [CPL15, Ser11a]. **mediated** [Dau16, FDMR11, SGL19, WTP+19, ZL10]. **mediating** [Var14, ZYL+14]. **Medium** [TBRIS12, BRS10, BBB16, EAK+10b, EAK+10a, MPMCM+11, PBB15, Puz16, Ser11b, TV13, TBRIS10, TBRIS11, XDM+10]. **medium-sized** [Puz16]. **medium-to-large** [BBB16, PBB15]. **MEDT** [ZRGE+19]. **meeting** [Tch13]. **Meetings** [ÁIGVZW12]. **meets** [Puz17]. **melamine** [AASU+17]. **member** [RNV+12]. **membered** [ABTW14, BBKO16, MSK11, WvRSW+11, Zha14]. **membrane**

[FMP+17, KMT+12, SMK+12, YINM13, MMP11]. **memory** [BXR+13]. **Mentor** [SL11]. **MePIm** [MKM11]. **mer** [AC19]. **Mercury** [KG08]. **merits** [ZSZ14, MGN14]. **merocyanine** [MFB11]. **Mes** [Pan16]. **mesh** [OPC17]. **mesityl** [KDÇ12]. **Meso**
[IMS+13, MMF+13, NKF+13, OH13, She13, YMY+13, VSN+11]. **Meso-**
[IMS+13, MMF+13, NKF+13, OH13, She13, YMY+13]. **meso-substituted**
[VSN+11]. **mesogen** [RS11b]. **mesoscopic** [Lun13a, Lun13b, Tou13]. **Meta**
[KSG+12]. **Meta-GGA** [KSG+12]. **metabolism** [DKZ+10].
metabolism-based [DKZ+10]. **metabolites** [LCG12]. **metabotropic**
[ŚKB18]. **metadynamics** [BVRM10, MBS+18]. **Metal**
[RdPW+12, ZFC+17, ASHF13, ADR+18, BWW10, BHMN19, BEM11,
BZBZ13, BDG17, BLdV19, BB10, BDR12, CPF12, CWW+16, CP13, ČFČ11,
DS11, DSD18, DMBJ15, DD17, DP16, ENV15, Esr18, ESLM19, FM16,
GM11, GZBH18, HSN+11, Hog13, HWWW18, JHL+18, KWC11, KFY+12,
KT12b, Kry12c, Lar12, LYW+19, LKd+16, MHZ18, MLW10, MC17,
MPTR12, MVG18, MBA+19, MLW16, NKWT19, NZ13, NFD+10, OKK10,
PSK+16, RCM+19, RZC13, SFL+10, Sat11a, SG19, SHE10, SK11, SM14c,
TTD13, VSMK13, WCY+10, WLL19, WR15, XS18, XGH18a, YLW+13,
YLZ+17, ZK12, ZLWZ16, ZHI17, ZSZ14, HZZW11]. **metal-** [WCY+10].
metal-flavonoid [DSD18]. **metal-free** [BDG17, ENV15, Esr18, FM16].
metal-insulator [BEM11]. **metal-ligand** [CPF12]. **metal-organic**
[MLW16]. **metal-pentagon** [LYW+19]. **metal-sulfur** [LKd+16].
metal-to-ligand [DS11]. **metalated** [MSOV13]. **metallaboranes**
[SALK19]. **metallic** [AM10, CRB+12, Nic11, VDG13]. **metallicity**
[AAAM12, AAA12, Kan18]. **metallo** [Jal10]. **metallocene** [OD16].
metallocyclophanes [BH10b]. **metalloenzyme** [dCDC+11].
metalloenzymes [SSI+10, SSK+12, SIS+08, YSS+10]. **metallofullerene**
[HLB19, SUL+11]. **metallofullerenes** [LYW+19, WLZ+12a, WSL+11, YL11].
metallophilic [LC16]. **metallophthalocyanines** [ZDZO10].
metalloporphyrins [CCL+13]. **metals** [BMRM19, DWX+16, HNBS18,
JEA13, JL12a, MKM11, Pie11, SAHG11, TMC+13, XYL+18, ZFC+17].
metals-encapsulated [JL12a]. **metastable** [DSSM19, MTS15].
metastable-bound [DSSM19]. **methacrylate** [DSRGD12, IBA+11].
methamidophos [SZL+15]. **methanation** [LZW+18]. **methane**
[AGB19, BPSM12, CAPL12, SSI+10, YRN+11, Zak13]. **methanogenic**
[SLS+10]. **Methanol** [VLK+11, XGH+18b, BCF+11, GB18, KBF+13,
LGM+18, LCB10, RYM12, RFN+12, SCBP17, ZSHL16]. **methionine**
[TBHL11]. **Method**
[MMM20, AAHN16, AHT12, ANC+15, BDF+16, BW15, Boe12, Buc12a,
Cam10, CLC10, CLL+11, CR18, CFOC+10, CNSK11, CC19, CYK17, Cin20,
CC12, CF14, DK13, DW12, Dil13, DCR10, DSSM18, D'y16, FYhC11, FKL+12,
FZC14, FRGC10, FNIT16, GRD11, HKZZ15, HSN18, Hor13, HZS14, HM10b,
HM11, HBMM11, IFT13, IFT14, ISN13, IN15, JH15, KRC+16, Kar12b,
KSS12, KLK13, KCK14, KYH+13b, Kit15, KFJ+18, LdMCdA+12, MMM19,

MMG15, MdAdCS12, MMM16, MR11, MAF19, Mit11a, MBSMJC18, MMA10, MB12, NZ13, NL11, Ols11a, Pon19, Pul11, SBMM11, SY10, SA11a, SSB12a, SN15, SGH10, SLZ$^+$11a, SHMR11, Szc18, TKN13, VAT12, WWL17, XLGA12, Xu16, Xu19, YKN13, YŞÖ12, ZE18, ZCG$^+$17, ZL10, SP19]. **Methodologies** [RSCS10]. **methodology** [CF11, FCC11]. **Methods** [Brä13, Hor13, IFT13, MSH13, Mar13, YK13, ZJS13, dGR14, AF19a, BLRdA$^+$10, CP10, CCC19, CC19, CKB18, DGA$^+$13, DFV$^+$12, Exn11, Gag11, HCH$^+$18, HNH$^+$12, Hat13, HJK14, HJ13, JW18, KKH18, Kon10, LP10b, Lya14, MPM15, MC17, Mar12, MBA$^+$13, Mit11c, MMP11, NC11, NDP10, NMSR14, Nym14, PDR$^+$14, PI13, Pie11, dSMPRSF18, RFEGPP$^+$16, RS11b, RSCS10, SGB11, SOF$^+$10, Sch12a, Sza13, SPM$^+$15, Tok16, TG13, UYN$^+$13, Var11, WKE17, WH12, WCM14, WZX15b, YZ13, YKM$^+$15, YWY$^+$12, ZDZO10, ZXY13, ZKW17, dHLdS12]. **methoxy** [BLM$^+$12, KAOB11]. **methoxyalkyl** [BLM$^+$12]. **methoxyphenol** [KAOB11]. **methoxyphenyl** [ZSASS13]. **Methyl** [SC12a, SC12b, CMCN11, DDÇY12, DP12, FO10, HYZ13, IBA$^+$11, IK14, KC11, KSAK17, LD17, LSG$^+$14, MFR10, NAK$^+$17, NZAVR10, Owe17, ÖEDB11, PGG12, PCR$^+$11, SLS$^+$10, SHW$^+$13, WZZL10, Zha14, KAOB11]. **methyl-5-methoxyphenol** [KAOB11]. **methyl-substituted** [NZAVR10]. **methylacyl** [LZZ12]. **methylallenoate** [LLF17]. **methylamine** [LLZZ10]. **methylation** [BS14, CAAI12, JS18, WYWL13, YPDW14]. **methylbenzylidene** [TAY11]. **methylbutenol** [AEAS$^+$19]. **methylcyclobutyl** [KDÇ12]. **methylcyclohexylidene** [KGVG11]. **methyldiazonium** [BS14]. **methylene** [ES17, HZZ$^+$19, MHT$^+$08, Met11, RJY$^+$10, RRVJ10, KAOB11]. **methylene-3-methoxy-cyclohexa-2** [KAOB11]. **methylenecyclopropane** [LMZ$^+$11]. **methyleneindolonone** [LLF17]. **methylenesilylene** [TYL10]. **methylhydantoin** [SF13]. **methylhydrazine** [WWHZ13]. **methylimidazo** [MLPT10]. **methylimidazolium** [MFK$^+$12, WZZL10, dOLdlV13]. **methyloxaziridine** [CPL15]. **methyloxirane** [CPL15]. **methylphosphonate** [HYZ13]. **methylsubstituted** [KBMM10]. **methylsulfonyl** [SK14]. **MeX** [RBTL19]. **Mexican** [ÁIGVZW12]. **Meyer** [WCGD12]. **Mg** [BLL$^+$13, PAKA15, Sik18, TW10, WCY$^+$10, XZZ$^+$10, YLW$^+$13, ZWL18, BJ17, CRB$^+$12, DTEMK11, MSBF18, SC11, dOR10]. **MgB** [PK13b]. **MgC** [LZ12]. **MgCl** [BAB$^+$18]. **MgH** [ZWL18, HSYM11, ZWL18]. **MgO** [SAHG11, SAHA12]. **MH** [BLL$^+$13]. **micelle** [KMT$^+$12]. **Michael** [DP12, PDNC14, SHL$^+$13, WZZL10]. **micro** [RAK10]. **micro-** [RAK10]. **microequilibrium** [SGB11]. **microhydration** [MTS15, PSKV19, VKF$^+$19]. **microiterations** [MOLF11]. **microkinetic** [PIS18, Tan13]. **microporous** [FZH$^+$18, UMS13]. **Microscopic** [DVDBM11, Lar12, RSL10, SM10a, DP11, MSG16, Pat15, SGB11, ZLR15]. **microscopy** [ZLWY13]. **Microsolvation** [HFA$^+$19, Ire12, Ven12, JMPP19, LG15]. **might** [GAI19]. **migration** [WWGW18]. **Mikheev** [BdTG11]. **mild**

[EAK+10b, EAK+10a, EI11, GMT16]. **Milestones** [RNP13]. **mimic** [VPOG19]. **Mind** [TWR15]. **Mini** [MMA10]. **Mini-bandstructure** [MMA10]. **minima** [MCP10, PBM10, SRS+17]. **minimal** [Lai11]. **minimum** [MJSC18]. **Minnesota** [Ali19b]. **mise** [Kry10]. **mise-en-scènes** [Kry10]. **misuses** [PIS18]. **mixed** [CP11, DKS11, FDNR10, HFBC19, KL11, KSY+11, Lad14, LJW+11, ST15, SN12, TPCJ+12, XTLA13, XTLA14, YIY+13, YSK+12]. **mixed-quantum** [CP11]. **mixed-quantum/classical** [CP11]. **mixed-valence** [FDNR10, KSY+11, TPCJ+12, YIY+13, YSK+12]. **mixtures** [HFL+17]. **Mk** [NYS+10, SKHN13]. **MK-4965** [SKHN13]. **MLi** [SM17]. **M'M** [MLY+16, AHC+18, AHC+18, AMMK11, Cap16, DMG10, Exn11, GFRdG11, MOLF11, MG10, RNC+14, SDP+16, SD16a, SD16b, ST15, SLA12, UYN+13, VHTEG15, ZKW17, dAGNJT12]. **MM-ER** [TIKN11]. **MM/continuum** [Cap16]. **MMPs** [TPdMB12]. **MN** [PAKA15, BXR+13, BDR12, YL11, KLK13, Kim19, MRT11, NKWT19, PM17, SAHA12, TMM+14, YYI+12]. **Mn-superoxide** [PM17]. **MnXMn** [YIY+13]. **MO** [ZLY+14, HNBS18, MLY+16, MGP16, PP19a, BB10, Bou12b, Nal13, DWPK14, GD11]. **MoB** [BG11c]. **mobile** [SL13]. **mobilities** [UDS19b]. **Möbius** [GXZ+14, LGL+19, WWL+11]. **Mode** [DJ95, DJ12, LYD+18, PVS12, SSI+10, ST15, SD12]. **Model** [LEU+11, ASD18, AMAM18, BPL13, BEM11, BGFD14, BAA+18, BKM15, BH10a, Buc11a, Buc11b, CPF+11, Cam10, Cam12, Cap16, Car19, COCF+14, CNSK11, CSVCB12, Cys11, DZO12c, DQZF12, FMP+17, FB17, FS11, GLOGM+11, Haj18, IMS+13, JK12, JZP17, KyH13a, KBJ17, KKG12, Kub12, LLF+12, LDKB15, LSR+13, LKJ13, Liu15a, LNI12, Lya19, MYZ+10, MMP+18a, MSH13, MGK+11, MRT11, MPE15, MA12, MT10, MIN13, PABSK16, PWL+10, PCR+11, RTG+19, SPPT15, SMGZF19, SSK11, SPSA11, SKS10, SL10, SM10a, SLS+19, SRN+19, SSdS17, TGRP19, Vie17, VGS10, WML11, WWQG17, Zen11, ZLJ11, ZZZ+18, dOR10]. **modeled** [MMBK12]. **Modeling** [BRS10, IBA+11, Kry12a, LBM11, LC19, Men15, MRÅ11, NBZG16, dSMPRSF18, Pog12, TBB+19, TCM+12, ZPZ15, ZI19, AHC+18, BGFD14, Buc10, CRSB12, CSSK+12, DSM+19b, DFK16, DLM+11, DDF+12, FBO+11, GMA+19, HL19, KMS+11, KBJ17, KGK13, LTdSJ+10, LZZ12, Mai14, MPJ12, MCV11, OVT+16, PTD+12, PIS18, RDB19, RBTL19, SJZL12, Sic16, SLS+10, SR18, SBKJ18, SM14a, SSB+12b, TAY11, YBMK12, YJ17, ZP16, ZK12, dAGNJT12, dSSdSGA12, KMRG13]. **Models** [FFF10, AM13a, ADR+18, AS19, Ali19a, BMR+13, BM16, Buc12b, CWW12, CPAT11, CSTA16, EPS+16, FLvLA15, GMT16, HVR18, JCC10, KO10, LVdSdM14, Li15, LORR+12, LSKM19, LWH+12, LZ10, Luz13, MPV+11, NS10b, OPAVM18, PI13, PL11, QBRA18, RFEGPP+16, SKTI15, SJW13, TD11, VLG12, WYM15, WH18, YYI+12, vLRRK15]. **modern** [Hat13, Lya19, TBB+19]. **modes** [CLXZ12, FKC12, HAX+18, PM12, RPBB11, RA10a, TU10]. **modification** [KK19, Wan11]. **modified** [DJ18, HFZ12, LZW+15, PSGK17]. **modulated**

[HGB08]. **Modulation** [MS14a, GV19]. **MODYLAS** [YAF+15]. **Moeller** [EG10]. **MOFs** [PK16]. **moieties** [Cha11, NCMC+18]. **moiety** [BS14, ELC08, SKM11]. **Moiseyev** [Brä12]. **Molecular** [Buc11b, CSS16, CSSK+12, CHV14, DGR+16, DLZ11, FKBG19, FUE+12, Hor13, IHG10, KTI+12, KM12c, KKT13, MY17, MAD12, MSH13, Mar13, MP12, MOY13, McC13a, MMT+13, MBS+18, NVI10, OHDA13, OA13, PvS10, PWH+12, PPK+13, RAK10, SMK+12, SIT+12, SVPTM+10, SIB+13, SHS+13, SSS15, TPdMB12, UYN+13, UTTn13, VHTEG15, WML11, WWB+14, YK13, YINM13, dSSdSGA12, AC19, AV19, AS19, ABA11, AA15, Bae14, BŁ16, BBB+12a, BPT12, BDF+16, BMF+14, yBZfC18, BMB10, BBB+12b, BR15, BWB+18, BWE16, BH19, CRA+11, CDSK12, Cam10, CZJZ12, CTVA12, CCC19, CCL+16, CFV18, CD15, CNSK11, CHL+19, CAPL12, COP16, Dau16, DSD18, DDÇY12, DI18, DMWY11, DLG12, DDF+12, DdG+11, DWGX12, Eil14, ESLM19, FZH+18, FBRBR12, FMPM+14, For12, Fra17, FK18, FBU+11, FSST16, Fuk12, FDG18]. **molecular** [GVPCK10, GFB12b, GI11d, GH11, GJ18, GSPR19, GR10, GHP11, GS10, HS11a, HYZS12, HYZS19, HLB19, Hil13, Hog10, HZS14, HFL+17, HVR18, HFBC19, IFT14, IA13, IKC18, Ish14, JdL08, Jan10, KLK13, KCK14, KHH10, KKH+13, KKT14, Kry12a, KRG+13, KUY16, LB14a, LG10, Lai11, Laz14, LLM13, LA11, LTdSJ+10, LFS+11, LJSS12, LG15, LC19, LKLW11, LNI12, LB18, Ma14, Mam14, MC11b, MHT+08, Mas14, MOE+11, MMBK12, MKSG13, MAF19, Mit11a, MSY+12, MSK+12, MVA19, MPL+11, MLB+10, MBTVR12, MBBT+12, MSAB19, MMP11, Mur12, NKKN15, NDH10, NAK+17, Nic11, Nik11, NB19, OT14, OB19, OWD18, PP10, PMH+16, PH12, PBB15, Pog12, PETB18, PRG+10, Puz16, RS12b, RSM12, RBGGM18, RAN18, RMC19, RP16, RLER14, Rit11, RC11, RAMB18, RdPW+12, RA10a]. **molecular** [SC12b, SLZ+11b, SXS+12, SLS+12, SLSZ13, Shi13, SRS+17, SACA18, SLS+10, SKY+13, SWS12, TK16a, TY17, TFA10, Tok16, TSH17, TIKL13, TRZ+19, TC12, TPT19, Vik13, WZ10a, WFS13, WC14, XFW+14, XXJ+16, Xu16, XWP+18, Xu19, YZZH15, YAF+15, YT14, ZSASS13, ZFW+13, ZPR10, ZLE17, ZLWZ16, ZRLV10, ZB18, dSSF16b, dSSF16a, dOdCMUdALR11, dWLC14, dOLdlV13, vL13, vLRRK15, Puz10, RI19, RdA11]. **molecular-dynamics** [PP10]. **molecular-level** [Shi13]. **Molecule** [ANC+15, AM12, ASK15, Ber13c, CAZ+11, CL11, CHM+14, CHM+17, CC11b, Cor16, DAC11, DAC12, DAR+11, DPRK12, DLG12, DCZ17, ES17, Esr18, Fra17, GWHH17, GI11a, GT13, HK11, IIS+17, KKH18, KSC15, KP12, KN15, Lan10, LJSS12, LEU+11, Luz11b, MGM11, MHT+08, MSS11, MKD19, MZLM17, MPTZ13, MJM19, MC18b, OT14, OCL+18, PK13a, RPBB11, SXS+12, SLSZ13, SLZH12, SRA+11, TFBG14, TH12, Tob19, VOAH18, Vik11a, Vik11b, WR14a, YW11a, ZZZ+18, KRC+16, TFSRM11]. **Molecule-adapted** [ANC+15]. **molecule-TiO** [TFSRM11]. **molecule-to-material** [TFBG14]. **molecules**

[Agb12, Ale13, Ali19a, ACL12, AT18, BMK+14, BdTG11, BCHN16, BRS10, BAX+19, BDG17, BBB16, BB10, Cam12, CM17, CPL15, CRSB12, CKB18, CB19, CK17, CF17, DIOG12, DK13, DSRGD12, Dil13, DCR10, EML+11, EMS16, GFB12a, GMR18, Gin10, GS11, GHP11, HRT12, HMH+13, HST13, HNBG15, HYH+10, HMA+18, Jen13, JMX+15, Jeo18, JZP17, JCCZ12, KBGC12, KBG17, KKL+16, Kim16, KKH+13, KKS+11, KKT13, KKT14, LKDC11, Leh19b, Leh19c, LHX+19, LSKM19, LPM+11, LLP17, Luz12, MSG16, MCE11, MK10a, Mar12, May14, MFLK10, MCL11, MGB18, MSM16, Mit11a, MB15, MJ11, MCK17, MPE11, Nal15, NS10b, OKK10, OA13, OD16, PL11, PWY+18, PKK14, PWP13, PB10, Puz16, Puz17, RBGGM18, RGTS11, RWW+19, RC11, Roy14, RAK10, SGB11, SD16b, SSKS12, SA11a, SKG11].
molecules [SMEH15, Sha18, SB16, SMR14, SRN+19, Sto18, SYY16, Sut12, SCZH16, SV11, THL+15, TK16b, TH12, TXK+19, TFMC19, Tou11a, UGWL18, VO11, XHZXXZ10, YZZ16, YD17, ZS11, ZDF13, ZP16, ZCC11, ZZZ+18, ZS12, ZI19, dSCC12, dSTH17]. **Møller**
[RS11a, BVA+14, NMIP14, RS09, TH13]. **molten** [BM10, DLZ11]. **moment**
[AM12, Ber13c, BVP14, HK11, KSG+12, Kri13, MdAdCS12, YŞÖ12].
moments
[AM10, Ber13a, DPRK12, GFB12b, GI11a, GI11c, LMC19, MD11, TW10].
Momentum
[SH19, ALRA10, Ash18, AKR12, HSN18, MOY13, TCG17, TÁ10, YOS15].
Moniliophthora [PTD+12]. **mono**
[Buc12b, DHYC19, Jac12, MMR+10, PS13a, ZQXP17, BL10]. **mono-**
[Buc12b, DHYC19, Jac12, MMR+10, PS13a]. **monoacetylides** [DD17].
monoamines [MBTVR12]. **monoanions** [CYL+19]. **monoatomic** [Bar11].
monoboronyl [MLK17]. **monobromide** [HTM10]. **Monochloride**
[MOY13]. **monoclinic** [DWX+16]. **monocyclic** [Du12]. **monodentate**
[ZKKR11]. **monofluorides** [KWC11]. **Monofunctional** [XZ11].
monofurazan [ZZX10]. **monohalogenated** [MNV+17]. **monoiodide**
[HTM10]. **Monolayer** [UDS19b]. **monolayers**
[KC19a, MDP12, RZC13, TTM16]. **monolithiated** [WWL+11]. **Monomer**
[Cas15, BHA19, JWG+12, MM13, BMR+13]. **monomeric** [Rua10].
monomers [MBA+13, UJSJ13]. **Monometallic** [ZW15, GZW16, ZCTG18].
monomolecular [MOSK10]. **mononitride** [DSH+13, HFD11, KLE+19].
monooxygenase [SSI+10]. **monophosphates** [PAD+10]. **monosulfur**
[WJ11]. **monovinyl** [dlLIAI+12]. **monoxide** [AKC10, Hog13]. **monoxides**
[TG13]. **Monte** [ÁFV12, ABG12, ANC+15, ASK15, Cal10, CKB+19, CCC19, CP16, HCH+18, Hog13, HB14, HM12, JCCZ12, PDR+14, PIS18, RCGLV+14, SGC13, SCBP17, Wag14, WCM14, ZLR15, ZCC11]. **montmorillonite**
[BJdlMAV12]. **MoO** [MFZ+18]. **moracin** [MGK+12]. **mordenite** [NL11].
Morita [ZQW+17]. **morphine** [RCM10]. **Morse**
[Agb12, PSGK17, Sta10, Tou11a, ZLJ11]. **MoS** [LZW+18]. **most** [GI10].
Mostar [ACT19]. **motif** [SLZ+12, YD17]. **motifs** [CJMC19, KUS19, Kry10].
motion

[Cam10, DKR10, KCDC15, KC18, MMCN+11, MMSC19, SRPD16, Sut12]. **motions** [HZW18, XXJ+16, YW11a]. **motors** [OWD18]. **moving** [FAFR12]. **MP2** [KBMM10, LKLW11, NMIP14, yOITn15, RSM12, SZ11, Tav12, Yu13]. **MP2-F12** [yOITn15]. **MP4** [SZ11]. **MPI** [CwCW+11]. **MPI-2** [CwCW+11]. **MRCC** [NYS+10]. **MRCI** [DAR+11, LJSS12, Mit11a, ONBP11, SLZ+11b, SLZ+11a]. **MRI** [GSPR19]. **MRPT2** [ONBP11]. **MS** [BDR12, MR11]. **MS-CASPT2** [BDR12, MR11]. **Mu** [GJ18]. **Mu/H** [GJ18]. **Multi** [KKT13, KKT14, Koc13a]. **multi-center** [Koc13a]. **Multi-component** [KKT13, KKT14]. **multiband** [PK13b]. **multicenter** [CwCW+11]. **Multichannel** [DS12, SD12]. **multicharged** [MGK+11]. **multicolor** [CYLL11]. **Multicomponent** [STU19, GJ18, Kar13, OT14]. **multiconfiguration** [DCHC11, LCL+10b, LPG+12, SL13]. **multiconfigurational** [Gag11, HJK14, KK14b, Luz13, NS13, PP16, Pie11, SY10, VMR11]. **multidimensional** [Kha16, SIB+13]. **multielectron** [Kry11b, Kry12b]. **multiexcited** [SCZG12]. **multimode** [RGPZD13]. **multiobjective** [SSB12a]. **multiparameter** [GMGRMP12, IIH16]. **Multipartitioning** [RS09, RS11a]. **Multiphoton** [NWQX11]. **Multiple** [HhGqZZ17, PBM10, PP14, DB12, GFRdG11, Ish14, JW19, MGB18, NMV+14, RWW+19, YGLL10]. **Multiple-pathways** [PP14]. **Multiplets** [BMB16]. **Multiplicative** [LSW19, LWY19, PL18a]. **multiplicities** [Nal12]. **multiply** [HDÖS12]. **multiply-valued** [HDÖS12]. **Multipole** [Tal11, LBW11, YŞÖ12]. **multipoles** [TH12]. **Multireference** [CYLL11, KB19, LP10b, RMG+19, SWS12, BVP13, GSaY11, HFD11, JNZ+14, Kon10, MdAdCS12, SYL+18, SLZ+11c, SZL+14, dSM19a]. **Multiscale** [AHC+18, Mas14, ZP16, CLKD15, CwCW+11, MGN14, TTM16]. **Multistep** [SAS+12, Sic16]. **Multithreaded** [MAF19]. **multitopic** [SSP+17a]. **multivacancy** [MFM18]. **multiwalled** [LV19, MNS11]. **multiwavelet** [HS11a]. **munchnöne** [GHCMCMQ17]. **muon** [RAGM10]. **muonic** [UGWL18]. **muscimol** [Ser11a]. **mustard** [VSMK15]. **mutagenesis** [CSVCB12]. **mutagens** [MLPT10]. **mutant** [dAGNJT12]. **mutation** [SSB12a]. **mutations** [DMG10, MFR10, MG10]. **mutipathways** [SWS+14]. **Mutual** [Mat02, MAT19, Mat10]. **Mycobacterium** [ST15]. **myoglobin** [CHSO13].

N [AGOP18, BBYZ18, BJ17, CJMC19, CWS15, CWSZ13, GC18, HWL16, JLG+12, Kal18, LYL+12, Men10, MC18a, OCL+18, PCK19, Per10b, RLTAT19, SB18, SÁBA+12, SSAM13, WLZ+12a, WLZ+12b, XZZ+10, XXJ+16, XCL+18, Zha10, ZH12, ZQJW13, SC12a, ARG11, BEM11, LL18, LWY19, XYL+18, XWC10, ZCTG18, ABTW14, CJMC19, CTW12, CDL+19, Esr18, FLCHL10, GMM+18, HZZ+19, HM10a, HXX15, KMK+16, KMM+18, LYL+12, LW15, MNV+17, MBA+13, PRPU+13, PL18b, Puz10, RRB12, SÁBA+12, SC12a, SSAM13, SXS+12, TMC18, Tob19, TPdMB12, WZX11, XMZ+12, XZL+12, XZG+18, YZL+10, YWJ+11, Zha10, ZH12, ZGSM15, ZCG10]. **N-** [SC12a].

N-confused [HM10a]. **N-coordinating** [YZL+10]. **N-cyclic** [XZG+18]. **N-dimethylaminopropanol** [WZX11]. **N'-dioxy-2** [KMM+18]. **N-Doped** [XMZ+12, GMM+18]. **N-haloammonium** [XZL+12]. **N-heterocyclic** [ABTW14, CDL+19, HZZ+19]. **N1** [KS18]. **N1-to-O2** [KS18]. **NaAlH** [HSN+11]. **NaAlO** [Oni12]. **NaH** [Ber13a]. **NaNbO** [WTP+19]. **Nano** [IMS+13, KO14, MMF+13, NKF+13, OH13, She13, YMY+13, JLS13, KFY+12, RAK10]. **nano-** [RAK10]. **nano-fiber** [KFY+12]. **Nano-Science** [IMS+13, MMF+13, NKF+13, OH13, She13, YMY+13]. **nano-silicon** [JLS13]. **nanocages** [LBY+14]. **nanocapsules** [ZDF13]. **nanoclusters** [Ali14, AF16, MS14b, MHHPR+17, MA11a, MA11b, XS18, ZRY+13]. **nanocrystals** [TCCI10]. **nanodroplets** [HMP+11]. **nanoflakes** [YMY+13]. **nanographene** [LC12, SR19]. **nanographene-like** [LC12]. **nanohorns** [MSOV13, TC10]. **nanohybrid** [MSOV13]. **nanomagnets** [Mag14]. **nanomaterials** [Sik18]. **nanoparticle** [KO14, PW10, VS19]. **nanoparticles** [AGG+18, ALA15, BLRdA+10, ESBVJY12, GE12a, KT12b, LIK15, RAK10, SDY16, TFSRM11, ZHI17]. **nanopores** [BMF+14]. **nanoribbons** [DMBJ15, GMT16, PPDF11]. **nanorings** [KAG08]. **nanorods** [KO12]. **nanoscale** [RF10]. **nanoscience** [CJBMMAPR19]. **nanosheet** [CWW+16, Esr18]. **nanosheets** [ES17]. **nanosilicons** [She13]. **nanostructure** [CTDOLA10]. **nanostructured** [GP13a, PETB18]. **nanostructures** [ACT19, GAMM10, HNBS18]. **nanosystems** [BEPZ10b, DKR10]. **nanotube** [JW19, JR19, LSW19, OPS10, SD13a, SD16b, WW11, WJY15, XMZ+12]. **nanotube-based** [OPS10]. **nanotubes** [AEM+12, Bas11, BEPZ10a, BSO11, DI10, DM16, D'y16, EBR11, ETGLMJ+19, ES17, FZH+18, FZX18, FKL+12, GWZ+14b, GT13, HCH+18, HIL19, HNBG15, JW19, KG08, LV19, MM11, NEEV15, PE11, RRB12, SA18, SD13a, SD16a, SC10a, TNT18, Wan11, WG18, ZCX+16]. **nanowire** [SM19]. **nanowires** [LLZ+14, MSVMCI10, YZW15b, dSMT+18]. **Nap** [WSML16]. **naphthalene** [IBA+11, QJ13]. **naphthalene-dione** [QJ13]. **naphthalene-dithione** [QJ13]. **naphthalimide** [QHS11]. **naphthofuranquinone** [MLC+11]. **naproxen** [YINM13]. **NaRb** [CHM+14, CHM+17]. **NaSc** [Kim13]. **NaTaO** [WCL+17]. **native** [YYI+12]. **Natta** [BAB+18]. **Natural** [GHP11, XHZXXZ10, CCA+12, CADSG18, LTdSJ+10, LdMCdA+12, LCZL11, Mit11a, MBSMJC18, NZ13, Pir13, PU14, TH13, WWL17]. **naturally** [SBEH11]. **Nature** [GI14, JEA13, ZQCJ10, ZMB+17, ACF+11, BHA19, Cys11, ETGLMJ+19, Kal18, KUS19, LQ13, LZD+11, MTR+19, MB15, NH18, RB11b, TC10, UDVD10, VVJ15, Wu11, YYI+13]. **natures** [She14]. **NaX** [DIOG12]. **Nb** [HDC+11, HLMO11, HSYM11, lLBqD+19, NMIP14]. **Nb-doped** [HLMO11]. **NBO** [DP16, GWZ+14b, NRHJ11, RJY+10, RJA+10, UDVD10]. **NC** [EMSB15, EMS16, LZZ+11]. **NCl** [OKR12]. **NCO** [PTS+11, DDF+12]. **NCS** [Qu13]. **ND** [ZH12, BB10]. **NdF** [SSW16]. **Near**

[MPB11, IAA15, KYS13, YWR+18, ZQCJ10, dARAV12]. **Near-exact** [MPB11]. **near-infrared** [YWR+18, dARAV12]. **near-IR** [ZQCJ10]. **near-resonance** [KYS13]. **neat** [AMMK11]. **need** [MR11]. **Negative** [DSC+11, yBZfC18, CDS+18, IAA15, Kry10, MMRRA10]. **negatively** [DCBB11, KWWH18]. **neglect** [HVR18]. **neglecting** [Fer19, Nas19]. **neopentyl** [MML+11a]. **nested** [Cal10]. **Net** [RLZ12]. **netted** [DW12]. **network** [Beh15, BGKK16, FCC11, MDC15, WZX15b, dAVdM17]. **network-based** [MDC15]. **networks** [CRA+11, CL08, LFF+10, LZZ19, MPD+15]. **Neural** [BGKK16, MDC15, Beh15, CRA+11, CL08, FCC11, LFF+10, WZX15b]. **neuraminidase** [PCF+18]. **neuraminidases** [YWY+12]. **neuropeptides** [dSSdSGA12]. **neurotransmitters** [RZG12]. **Neutral** [RFMC19, BCGC12, BGMD15, CAZ+11, DHYC19, EPS+16, FBRBR12, Gra11, MMRRA10, ONBP11, PSPS11, RTG+19, TCM+12, Val17, ZQCJ10]. **neutron** [CD15, Kar12c, Zag11]. **neutrons** [Kar15]. **newly** [VVY18]. **News** [BDF+16, BHH+13, CYC+15, DOE+14, FMPM+14, KRC+16, LCZL15, MML+16, MRS15, NKKN15, yOITn15, QSX+15, SDP+16, TY17, YAF+15, ZH15, ZWSF16]. **NEXAFS** [LRP+11]. **Next** [BAX+19, HMA+18, TXK+19, KRH13, LHX+19]. **Next-generation** [BAX+19, HMA+18, TXK+19, LHX+19]. **Ng** [SMC18]. **NH** [AM18, yBZfC18, EMSB15, MPRCEG12, WZM+13, XWCY11, XF19, CCL+13, CRSB12, CCL+10, LV12, LLG+12, MWH15, MPRCEG12, OKR12, RNB+10, SLZH12, SW12, XZL+12, RRVJ10, RB11b]. **NH-tautomeric** [CCL+10]. **NHC** [Pan16]. **NHS** [NRP+11]. **Ni** [AO12a, KYLC19, YL11, AAA12, BXR+13, FBD+13, GP13b, GZMC11, Kim18, LWX+14, MRT11, NKWT19, SFA19, SLC+18, SLZ+12, WJL+10, WRW+18]. **Ni-** [Kim18]. **Ni-based** [GZMC11]. **Ni-loaded** [LWX+14]. **niacin** [PDNC14]. **NiAl** [CJOOW11]. **Nickel** [ASD18, LSCMSFC19, DZO12a, SDR+13, VSMK13, TFA10, dCSDdMC13]. **Nickel-substituted** [ASD18]. **Nicolaides** [Ban12]. **Nicotinamide** [MDP12]. **nicotine** [SGKG12]. **NICS** [XWC10]. **Nikolai** [Pup11b]. **Nile** [FSBA12, MRÅ11]. **Nimrod** [Brä12]. **nine** [PMEP19]. **nitramines** [MOSK10, OB19]. **nitrate** [HM11, ZL10]. **nitrates** [HZZW11]. **nitration** [LLW+11]. **nitric** [BGMD15, MNE+13, ONBP11]. **nitride** [CJMC19, Che13, DHZS11, ES17, Esr18, FZX18, GWZ+14b, GAMM10, Ish14, TNT18, WG18]. **nitrile** [CMCN11, NAK+17, YNLD18]. **nitriles** [RFN+12]. **nitrites** [BL10]. **nitro** [CLY12, WGLX10, ZCC11]. **nitroaniline** [KC11]. **nitrobenzene** [SS18b]. **nitroethylene** [BBAL12]. **nitrogen** [BHMN19, BSO11, EAV16, EM19, GZ14, HZG12, HNBG15, KC19a, LZW+15, MS14b, PPDF11, PP19b, RD14, VKF+19, WLL19, YZZ16, ZKKR11]. **nitrogen-containing** [HZG12]. **nitrogen-doped** [EM19, HNBG15]. **nitrogen-heterocyclic** [GZ14]. **nitrogen/phosphorus** [BHMN19]. **nitrogenase** [CR18, VPOG19]. **nitrogens** [fXxBhD19]. **nitroguanidine** [DGR+16]. **nitrones** [ABM+19]. **nitropentaamminecobalt** [MMSC19].

nitropyridine [KC11]. **nitroso** [YRN+11]. **nitroso-oxime** [YRN+11]. **nitrosothiols** [XHZXXZ10]. **nitrosoureas** [CZJZ12]. **nitrostyrene** [JSLH14]. **nitrosyl** [ESS13, LLC+11]. **nitrosyls** [UMS13]. **nitrous** [Dau16, GC18, MZB+13, Rua10, SZ11, TSKN12]. **nitroxide** [BSM+15, ZLS+18]. **nitryl** [BL11]. **NL** [YFY17]. **NLi** [YLWrL12]. **NLO** [PCD14]. **NLO-X** [PCD14]. **NMR** [AM13a, BMF+14, ÇAS13, CCP18, CSP+10, CDT12, DSD18, EKN10, FBD+13, GSPR19, MC18a, OPP+14, ÖEDB11, Ped16, RRK16, RR19, SK10, TTM16, TKSK17]. **NO** [ESS13, LLC+11, SSAM13, STU19, ÁFV12, BAMA12, GMT18, Les12, MCV11, OG19, RNB+10, SK14, SSAM13, VLM+10]. **noble** [GI14, JEA13, KDOR17, MB15, PSK+16, SMC18, WLL19, XS18, XGH18a]. **nodal** [CSMZ10]. **NOF** [PM16]. **nomenclature** [Tch16]. **Non** [BPL13, Cor16, DKS11, Leh19c, SGL+16, Tob19, YLH+19, Brä12]. **non-** [DKS11]. **non-autoionizing** [Cor16]. **Non-Born** [BPL13]. **non-covalent** [YLH+19]. **non-dynamic** [Tob19]. **Non-Hermitean** [Brä12]. **non-interacting** [SGL+16]. **non-relativistic** [Leh19c]. **Nonadditive** [BW18, Cys11, RSN12]. **Nonadiabatic** [GW18, LKd+16, MNZPT19, MKD19, WDR+11, YT14, AC12, HKLW13, IHG10, PM12, SBL11, ZH12]. **nonadiabatically** [Kit14]. **nonadiabaticity** [GJ18]. **nonautoionizing** [DSSM18]. **nonbond** [BLWJ17]. **nonbonded** [ZFS+11]. **Nonbonding** [HL19]. **Nonclassical** [SSB19]. **noncollinear** [GEL18]. **noncompetitive** [AMMB+18]. **Noncovalent** [BMRM19, Wan11, BDG17, HMA+19, JNY17, MIKH19, MSNP18, MURR13, Sch15, YF16, YFY17, Zak13]. **nonempirically** [MIN13]. **nonequilibrium** [DKR10, DCZ17, Li15, Mar13, MMP11]. **nonframework** [SZ11]. **Nonharmonic** [RSM12]. **nonheme** [ASD14]. **Nonhydrodynamic** [BM10]. **nonidentity** [Buc11a]. **noninertial** [NF11]. **Noninnocence** [Joh17]. **noninnocent** [DG19]. **noninteger** [CG12, GE12b]. **noninteracting** [AST16, BEM12, RS13]. **Nonlinear** [SRMB15, YK11, Yak10, ABA11, BF11, BSM+15, BEPZ10b, CRA+11, CEV10, CKB18, DSRGD12, DB12, FSQ+11, HWL16, HWWW18, HSS18, IGMK11, JFDD10, KC11, KPL+17, KL11, LKDC11, LZW+15, LYL+12, MMF+13, MB12, NKF+13, PCD14, SKG11, SM17, SYQ+10, YLWrL12, YHLC15, ZSQ+10]. **nonlocal** [FMMD+10]. **nonlocality** [BSS16]. **nonmetal** [JHL+18, WCY+10]. **Nonorthogonal** [CC12, DCZ17]. **nonparametric** [GTSC+19]. **nonpolar** [KKT13, KKT14, SA18]. **Nonrelativistic** [ADB10, RZ17]. **Nonsingular** [Oht13]. **Nonstationarity** [Luz13]. **nonsteroidal** [MPE11, YINM13]. **nonstochastic** [MPMCM+11]. **norbornadiene** [TTD13]. **Normal** [DJ95, DJ12, HAX+18, Pan16]. **Normal-Mode** [DJ95, DJ12]. **normalized** [FZC14, LGL+19, LWY19, LZZ19]. **note** [RLER13a]. **notions** [KK14a]. **Novel** [KAG08, VRO+12, WCY+10, WZM+13, CMR13, DW12, DLM12, GfWlZ11, JWG+12, LZZ+11, LZZ+17, NVPCJ+13, Pop15, PL18b, RDM+11, SSTÖ11, TPdMB12, UJSJ13, XFW+14, XZ11, YZL+10, YSW11, ZZR+12]. **novo** [SBKJ18]. **NQR** [EA12]. **N —** [OK16]. **NTA** [MC17]. **NTChem**

[NKKN15]. **NTO** [LZZ+13]. **NTPA** [MC17]. **Nuclear** [GR10, MJ11, RLER14, STU19, BPL13, BJ12, CG12, Cyb11, DVDBM11, FKL+12, GJ18, JHSG18, MZB+13, Mam14, MVC13, MNZPT19, NS10b, NB17, SPSA11, TMC18, ZPM10, ZP16]. **nucleic** [Kuv10, TBST10, YDW13, ZDZO10]. **nucleobase** [ZKWZ17]. **nucleobases** [CAO18, Cys11, DSVP15, KZA+17, LCH14, TD19, WG18]. **nucleophilic** [Buc10, Buc11b, HLJZ11, Pli18]. **nucleoside** [HHYC+18, VFCSC17]. **nucleosides** [BS14]. **nucleotide** [Lak10]. **nucleotides** [LQZZ12]. **nucleus** [FAFR12, SL13]. **number** [Bib13, GGJD13, Kon11, LSW19, LZZ19, MK10a]. **numbers** [MHHPR+17, MKM11]. **Numerical** [FKBG19, HV11, JW18, AEÖ12, BKM15, CLC10, HYZS12, HYZS19, Jør18, Leh19a, Leh19b, Leh19c, MM10, PUGSFM18, RZSZ18, Sit15, TD11, Zak13, RW11]. **numerically** [GfWlZ11]. **nutshell** [BW13a, BW13b, Rup15b]. **Nylon** [BWB+18]. **nystatin** [VGS10].

O [AM18, BPG+10, BZZ15, BJ17, BSPK11, CS17, Con10, Den13, DZO11, FBRBR12, FTB11, GC18, GCD13, HLMO11, HSYM11, Kal18, KLK13, KSSK16, Kim19, KSST12, KLZQ15, KRG+13, LFP+19, MLY+16, MFK+12, MMC+19, MBA+13, MPD+10, MGD11, MGP16, NTNL10, OPP+14, PL18b, QSLY10, RFEGPP+16, RNB+10, RGR12, SB18, SYK+12, SK14, SA11b, SL11, SSP14, SZZZ11, SM17, SW12, VPFD10, WSML16, XF19, YYI+13, YIY+13, YSK+12, YC13, ZLY+14, dHLdS12, ACMRN10, BAMA12, BXZ+19, CdAFS+12, CJMC19, CTW12, Con10, DMG10, DCHC11, EML+11, Esr18, Fuk12, dDGNB10, HSYM11, LLL16, MMC+19, MKW11, MOH+12, PWL+10, PC16, PRPU+13, PL18b, RSL10, ŞBAT16, SMEH15, STL12, SLZH12, STU19, TSL11, WZC+12, XDM+10, XCL+18, YY18a, ZCG+17, ZPB12, ZSHL16, dOdCMUdALR11]. **O-loss** [DCHC11]. **O.** [SG14]. **O1s** [LdBF+12]. **O2** [KS18]. **Obituary** [DEPP11]. **observed** [WWC17]. **obtain** [FRGC10, SRASZ16]. **obtained** [CDSK12, LTdSJ+10, LSR+13, MPM15, Mas10, OK16, UV18a, ZZZ+18]. **Obtaining** [SY10]. **occasion** [RA10b]. **occupation** [AO12a]. **Occurrence** [DKR10]. **occurring** [FRNM12, SBEH11]. **OCS** [DCHC11, NKWT19]. **octa** [WLS+19]. **octa-2** [WLS+19]. **octagonal** [LZZ19, TNT18]. **octagonal-quadrilateral** [LZZ19]. **octanes** [VOK+18]. **octupolar** [BF11]. **Odd** [LW18, Var14, She12]. **Odd-hydrogen** [Var14]. **OEC** [YIY+13]. **OEt** [DPDR11]. **Off** [CN12, MSNP18]. **Off-center** [CN12, MSNP18]. **OH** [EMSB15, EMS16, FRNM12, KLZQ15, LZZ+11, MBA+13, dMOB12, RWW+19, SW12, VV18, VLK+11, YIY+13, YSK+12, ZCG+17, lAyL14, ACMRN10, BAMA12, BZZ15, CAAI12, CRSB12, DS12, DSZB18, HWHZ11, KZZ13b, LIK15, MXC18, MK11, MMCN+11, NP18, NL11, dMOB12, PGG12, RGR12, Sch12a, SMEH15, SD12, SKM11, SM16, SZL+15, TIN13, TBHL11, WXZ+11, EKN10, RRVJ10, dSNBG08]. **OH/C** [VLK+11]. **ol** [HNH+12]. **OLED** [OAA19]. **olefin** [ZLY+14]. **olefins** [DPDR11, Iku17]. **OLi** [YLWrL12, SM17]. **oligoacene** [Kim16]. **oligoisothianaphthenes**

[GHGF12]. **oligomer** [KFS13, MM13]. **oligomeric** [TDOD17]. **oligomers** [CZLD17, SMA11]. **oligonucleotides** [ACF+11]. **oligopeptide** [MM10]. **oligopyrroles** [DCBB11]. **oligosilane** [ZYZ+11]. **oligothiophene** [TZ11]. **Olof** [Pyy11]. **Olson** [BSS16, MSBF18]. **OMC** [WCY+10]. **On-site** [DLJT14]. **on-the-fly** [UTTn13]. **One** [Ber13a, CG12, Dum12, LCH14, Bud12, CAZ+11, CM15, CLY12, CYK17, FCS13a, FCS13b, GTR11, GI11e, GAMM10, GS10, HZS14, Kri13, LW15, Luz11a, MSC10, MBBT+12, PVS12, RZSZ18, SC12b, SZZ+19, SWS+14, TAY11, VBC+12a, VBC+12b, WWC17, WLZ+12b, YF16, ZZZ+18, TC12]. **One-** [CG12, WLZ+12b]. **one-center** [HZS14]. **one-dimensional** [CYK17, MSC10, RZSZ18, VBC+12a, VBC+12b]. **One-electron** [Ber13a, Dum12, LCH14, CM15, GTR11, GS10, Kri13]. **one-mode** [PVS12]. **one-parameter** [FCS13a, FCS13b, YF16]. **one-photon** [Bud12]. **one-pot** [LW15]. **one-to-one** [WWC17]. **One-two** [TC12]. **ones** [HMA+19, LW13]. **Onicescu** [OH19]. **ONIOM** [EFO11, EO11, KYH+13b, MTL+12, ŚKB18]. **ONO** [XX12]. **onset** [LB14a]. **onto** [CA17, CAO18, SFW12, SRS+17, Sta10]. **OO** [SBSD18, SSK+12]. **OOH** [NP18, PGG12]. **OPAL** [CwCW+11]. **Open** [CP16, DSM+19b, Gan14, GCK+17, GHP11, HNH+12, JEA13, JE10, MAT19, NSN17, NNSN17, QSX+15, RAMB18, Sha18, YMY+13, dGR14, GXZ+14]. **open-close** [HNH+12]. **Open-shell** [CP16, JEA13, NSN17, NNSN17, YMY+13, dGR14, GXZ+14]. **open-source** [DSM+19b, GCK+17, QSX+15, RAMB18]. **Opening** [TFBG14, AMMB+18, BAX+19, KMS+11, MBSMJC18, QB15, TXK+19]. **openings** [KUTS10]. **OpenMP** [WMK+19]. **Operator** [DJ95, CD18, DJ12, IM15, Mys12, Yos20]. **OPh** [DPDR11]. **Oppenheimer** [BPL13, GVPCK10, RSM12, RAN18, SK17a, Sut12, VVN+16]. **opportunities** [FAK19]. **OPPS** [ZPM10]. **opsin** [TU10]. **optic** [Zen11]. **Optical** [LRKM10, YBMK12, AMK10, ABA11, BF11, BSM+15, BSO16, CPL15, CZLD17, DWX+16, FSQ+11, FZX18, FBU+11, GAPK+19b, GDM+10, GKGM18, GRCATG19, Hat13, HWL16, HWWW18, HSS18, IGMK11, JdOS16, JFDD10, KC11, KPL+17, KL11, KMU+13, LYW11, LZW+15, LYL+12, MPC10, MNP19, Mas14, MPJ12, MFZ+18, MA11a, MMF+13, NKF+13, NMHPVG12, OGvSG18, RKM12, RRRV19, ŞBAT16, SSKS12, SLS+14, SM17, SYQ+10, WLZ+12a, YK11, YLWrL12, YHLC15, ZSQ+10]. **optics** [DSRGD12, LKDC11]. **Optimal** [FT15, GSPR19, NVI10, NB19, TCG17, YWR+18]. **optimally** [NTGC19, ZZ18]. **Optimization** [CL08, FCC11, HJ13, KYH+13b, Kub12, Lu15, MHT+08, SGH10, SPM+15, WWL17]. **optimizations** [YIY+13]. **optimized** [ANC+15, KPH+12, SXH18]. **Optoelectronic** [AFA13, JR19, BHAH+18, KA13, MANP17, OAA19]. **orbit** [Ash18, Ber13b, BDR12, CYL+18, KV19, LWL+12, MLK17, MC18b, RS12a]. **Orbital** [BT15, Kon10, MMM20, AOT+18, AK17, Ash18, ABA11, Bar11, CPF+11, Cin20, DVDBM11, Fin17, FA17, FMPM+14, FC19, GR10, Hog10,

HVR18, IKN13, IK18, JH15, KK14a, KLK13, KCK14, Kit17, KKT13, KKT14, KPH+12, KUY16, LB18, MSNP18, MMM16, MAF19, MFLP12, MSY+12, MMA10, Mur12, Nag15, OT14, OAT+13, Pir13, PU14, PNC19, RMC19, SIM14, Tal11, TD11, Tsu15, XHZXXZ10, YPDW14, BT17]. **orbital-free** [AK17, Fin17, FA17, Nag15]. **Orbital-Specific** [MMM20, Cin20, MMM16]. **Orbitals** [GZSMFN16, ABS11, ABS13, Boe12, CCL+16, CFV18, CC12, DZO11, EBR11, FK18, Fuk12, GZF14, GW13, GE12b, LSR+10a, LSR+11, Mat02, Mat10, May14, Mit11a, NZ13, Nik11, NB19, RMG+19, RRCO11, RLZ12, SOM10, TH13, Tsu15, WWL17, YZZH15]. **Order** [AF16, ABA11, BR10, BR16, BVA+14, DAC12, DCHC11, Dun15, EG10, FSQ+11, Gin10, HSS18, KC11, KK13, KM12c, LKDC11, LCL+10b, LPG+12, LYL+12, LG12, Luz08, MSNP18, MMF+13, NKF+13, PDR+14, Per10b, RL12, RS09, RS11a, SN15, TH13, UV18b, VRO+12, WLZ+12a, ZSQ+10]. **order-disorder** [PDR+14]. **ordered** [CPL15, HW12]. **Ordering** [GA19, AM10, GE12a]. **orders** [KK14a]. **Organic** [SA11b, WTW+15, BF11, BDG17, BWE16, CKL16, FM16, GNM+12, GRCATG19, HKZZ15, JPPA10, KMK+16, KSO19, LSR+10a, LSR+11, LV19, LYS+19, MXC18, MPMCM+11, MUNZVR12, MAP+10, MCL11, MLW16, NZAVR10, OPAVM18, PFdM13, PWY+18, PETB18, Puz17, RdPW+12, SFL+10, SB16, SAHAA16, TCA10, Val17, WWB+14, ZB18]. **organic-inorganic** [KSO19]. **organic-metal** [SFL+10]. **organization** [Brä11a, Chr10, Kuv10, RAK10]. **organoaluminum** [ALK18]. **organocatalytic** [TFZ+15]. **organochlorides** [BPT12]. **organocuprates** [GGZZ16]. **Organolithium** [IKC18]. **organometallic** [ED16, GZMC11, KWC10, TD11, YZW15b]. **organophosphine** [ZQW+17]. **organophosphine-catalyzed** [ZQW+17]. **organophosphor** [JNY17]. **organophosphorus** [CRB+12, HYZ13, PH12]. **Orientation** [SCTW10, WWL+11]. **orientations** [MK11, WML11]. **oriented** [LPM+11]. **origin** [GFB12a, GI11b, GI11c, MC17, MNS11, NJA+12, OB19, TIKN11, WLZ18, ZQW+17]. **Origins** [Zha15, AGG+18, Mur12, MB13]. **Ornstein** [CSTA16]. **orthogonal** [GN19, RPBB11, TKN13, Yur13, Yur15]. **orthogonalization** [JH15]. **orthonormal** [GS10]. **orthosilicates** [DCDD10]. **oscillating** [SRPD16]. **oscillator** [AAHN16, ACL12, Haj18, HRT12, KBG17, MR18a, PVS12, PABSK16, Roy14, Sta10]. **oscillators** [Tou11a]. **osmium** [ADR+18]. **other** [Ném14, SG19]. **outbreak** [KRH13]. **outer** [LLZ+14]. **outer-expanded** [LLZ+14]. **outgoing** [CW13b]. **Outstanding** [Ng12, Pie11]. **outward** [MB13]. **overestimated** [Zho18]. **overlap** [AEÖ12, HVR18, MML11b]. **overtone** [CK13, VV12, VV13]. **overview** [BBB16, DSL15, Li15]. **oxadiazole** [MUNZVR12]. **oxalate** [DdG+11]. **oxaziridines** [VGGPdL19]. **oxazol** [LW13]. **oxazoline** [MCC13b]. **oxicams** [FPRGMHGB12]. **oxidase** [TSKN12]. **Oxidation** [Ali19a, SFA19, BD14, CGIAI12, EM19, GMT16, GB18, GSB10, Jan10, KBF+13, LLW+12, MKM11, POLV12, SSP14, SR18, SM14b, TBHL11, XMZ+12, XGH+18b, ZSHL16, ZCW16, ZJC+13]. **oxidative**

[CAPGAIG18, FMP+17, GAI19, NTNL10]. **oxide** [Ali14, ASW13, BGMD15, Dau16, DLJT14, DWGX12, FSK+11, GC18, Hog13, KC11, LWX+14, LCH+11, MSK11, MGP16, ONBP11, Oni10, SZ11, TSKN12, WCY+10, XGH18a, YNLD18, YHL+13, YC13, ZDF13, ZRGE+19]. **oxides** [IKC18, Kan18, NAK+17, PSK+16, RGST12, RKCK19, VGGPdL19, VKF+19]. **oxidized** [FTB11, RRB12]. **oxidoreductase** [SR11a]. **oxime** [QCW+12, XZ11, YRN+11]. **oximes** [ZYSW17]. **oxirane** [BAX+19]. **oxo** [ZSAP11]. **oxo-titanium** [ZSAP11]. **oxoacids** [CK17]. **oxoanions** [HNBS18]. **oxocarbon** [JFDD10]. **oxodithioesters** [GCZ+14]. **oxoguanine** [YM12]. **Oxygen** [GLT13, SDY16, AGOP18, CAZ+11, dDGNB10, JAB12, KCK14, LSR+13, Mor12, MLW16, PMH+16, dSMPRSF18, SCZG12, SBSD18, VS19, WWHZ13, YYS15, YSS+10, YYI+13, YSK+12, YZZ16, dOdCMUdALR11, OD12, YYI+12]. **oxygen-evolving** [LSR+13]. **oxygen-oxygen** [SBSD18]. **oxygen/nitrogen** [YZZ16]. **oxygenated** [TYN13]. **oxyluciferin** [SR11b, dSdS13a]. **oxypentadienyl** [VGGPdL19]. **ozone** [ASK15, MKD19, Var14, WWX+11]. **ozonolysis** [AEAS+19].

P [ACMRN10, CdAFS+12, CD12, GWZ+14a, GWJ12, KLZQ15, PP14, SB18, TW10, VV18, XCL+18, ZCG+17, ZPB12, AGOP18, ED16, OD12, RPBB11, RRCO11, WFS13, XZYS10, DQZF12]. **P.** [SG14]. **P.-O.** [SG14]. **P218** [AB16b]. **p300** [DPRK12]. **P450** [SIS+08]. **P6** [UV18a, UV18b]. **Pa** [OM13b]. **package** [CwCW+11, NKKN15]. **packet** [Bae16, Cho19, GKT+12, HDÖS12, NTGC19, RW11, SSAM13, YLYC18, ZCG+17]. **packets** [OHDA13]. **packing** [PETB18]. **Padé** [DB13a, ZE18]. **PAH** [CM17]. **Pair** [TH13, BKM15, CCL+16, CFV18, HMH10b, LJK+18, LRMAA19, MT11, NMS+10, OM13b, RS12b, RS11b, SSP+17a, SLG11, TRZ+19, Var11, WH12, ZBK15]. **paired** [RLZ12]. **pairing** [ACF+11, EMS16, PS10a, SM13, VBC+12a, VBC+12b, ZKWZ17]. **pairs** [BTH18, BMB16, HL19, KME+18, KUS19, Lad14, SMR14, XSLF12, XTLA13, XTLA14]. **pairwise** [Dob14, KKL+16, PSC15]. **palladium** [KSG+12, LSCMSFC19, LW15, PW10, SDY16]. **palladium-catalyzed** [LW15]. **PAN** [ZL10, VUC13]. **pancreatic** [PCML08]. **Pandora** [TFBG14]. **Papers** [RA10b]. **para** [Kle11, NG11]. **para-Fermionics** [Kle11]. **para-hydrogen** [NG11]. **paradigm** [SLS+19]. **parallel** [CLKD15, Lya19, yOITn15, PCV19, SRPD16]. **Parallelization** [ZWSF16, MAF19]. **parallelized** [SPSA11, YAF+15]. **parameter** [FCS13a, FCS13b, IKN13, SZZ+19, SX15, WFS13, YF16]. **parameter-free** [SX15]. **parameterization** [HSS+11, PABSK16, PSPS11, SOF+10]. **parameters** [AGPDZ13, AK11, BMF+14, EKN10, FV11, FCC11, GSPR19, IIS+17, KAR12a, LJSS12, MGM11, MPM15, MOY13, Roy16, SPO+11, SR11b, SWS12, WDJ+17, YŞÖ12, dCSDdMC13, dOdCMUdALR11]. **Parametric** [BH19, LdMCdA+12, RSCS10, SOF+10]. **parametrizations** [WR15]. **parametrized** [Oht13]. **parent** [MR11, PGG12]. **Parr** [LSC+18].

Part
[Ban12, GI11b, Jør18, Mor13, BR08, BR12a, For12, GI11c, RB08, RB11a].
Partial [MCKD11]. **partially** [AA11]. **Participants**
[Ano12r, Ano10a, Ano10b, Ano10c, Ano10d, Ano11d, Ano11e]. **particle**
[ATPRV11, BPL13, DTF$^+$11, FMPM$^+$14, Kon11, MGM11, RMC19, SK17b,
VATPR11, VAT12]. **particles** [SKLC19, ZJS13]. **particular** [MT10].
Partition [GORW19, FC19, Tou11a, ZZZ$^+$18]. **Partitioning**
[Vyb08, MBSMJC18, Ols11b]. **partner** [MPB11]. **partners** [KB12]. **Passage**
[Zak16, Sat11a]. **passing** [LW18]. **passion** [Pup11b]. **passivated**
[GMT16, SS18b]. **passivation** [MSVMCI10, TCCI10]. **Path** [RCGLV$^+$14,
YK13, HFBC19, KSST12, Mak15, NKWT19, SGC13, WB17, ZLR15].
path-integral [ZLR15]. **pathogenic** [KRH13]. **pathway**
[KRG$^+$13, ZJC$^+$13]. **pathways**
[ASD14, JL12b, MJ16a, PP14, RBZ15, SYK$^+$12, TKS11, VC13]. **pattern**
[BS14, CD12, GPM$^+$15]. **patterns**
[DTFK15, LBdV16, MK12, MC18a, SM13, ZPR10]. **Pauli**
[CM15, CM16, Fin15, Fin16b, FDA16, LSC$^+$18, Nag10, PM16]. **Pb**
[NFQ$^+$11, Per10b]. **PBEint** [FCS13a, FCS13b]. **PBEP86** [YFY17]. **PbI**
[VVY18]. **PCM** [AMMK11, PS10a, VSN$^+$11, XX12]. **PCMSolver**
[DSM$^+$19b]. **Pd** [Bal16, BDFM10, BGMD15, DZ11a, HLZ$^+$14, IK18,
PRPU$^+$13, RK14, YS18, ZRR$^+$11]. **Pd-catalyzed** [YS18]. **PdCl** [Pan16].
PdH [NS19, ZRR$^+$11]. **PdO** [SM14d]. **peak** [HYH$^+$10]. **Peculiarities**
[OPS10, Tch16]. **penetrable** [RBVAG18]. **penetrating** [KMT$^+$12].
penicillamine [MVG18]. **penta** [BMX$^+$19]. **penta-2** [BMX$^+$19].
pentaaqua [dCSDdMC13]. **pentacene** [MIN13, IMS$^+$13]. **pentacene/C**
[MIN13, IMS$^+$13]. **pentacoordinate** [XCL$^+$18, Yam10]. **Pentagon**
[KK11b, LYW$^+$19]. **pentagonal** [SALK19, WZ10b, Yam10]. **pentahalogeno**
[ZFC12]. **pentalene** [RALK18]. **pentapeptide** [MRT11]. **Pentapnictogen**
[CYL$^+$19]. **pentazolides** [XZZ$^+$10]. **pentoxide** [Den13]. **peptide**
[CF17, FMKJ14, KMT$^+$12, MAW$^+$18, QZH13, QTCL10, SSK11, Sch10b].
peptides [KyH13a, MAD12, MLB$^+$10, SW12]. **perfect** [UDS19b].
perfluorobenzene [LZD$^+$11]. **Performance**
[DCDD10, KME$^+$18, LORR$^+$12, LDZG16, RAMB18, Zak13, AF19a, AM13b,
BSSS19, BHH$^+$13, CKB$^+$19, DCFD10, DGA$^+$13, FV11, FB17, cLqFtW$^+$14,
LZZ$^+$13, Lya19, Mar12, NKKN15, dSMPRSF18, dSdS13a]. **performances**
[ADR$^+$18, TCA10]. **perhalogenated** [YZZ16]. **perhydroxyl** [YM13].
Pericondensed [BR08, BR12a]. **Periodic**
[BCHN16, DMBJ15, Fuk12, Gar08, GMT16, GI10, KBGC12, Kut10, LPO$^+$12,
MMA10, NL11, RDB19, SW10, Tan13, TGRP19]. **periodically** [Xu16].
Periodicity [IKS08, HST13, IKS10]. **periodinane** [TM19]. **permeability**
[Pit12]. **permutation** [Fer19, Nas19]. **perniciosa** [PTD$^+$12]. **perovskite**
[Oni10, Oni12, OH12, OH13, VVY18, WTP$^+$19]. **perovskites**
[Kan17, KSO19]. **peroxidase** [ZST$^+$10]. **peroxide**
[FMCA11, NEEV15, SSP14]. **peroxides** [LdMCdA$^+$12]. **peroxotungstates**

[ZLY+14]. **peroxy** [BCS+12]. **peroxyacetyl** [ZL10]. **peroxynitrite** [ASD14]. **Persilacyclacenes** [KAG08]. **persistent** [LMC19, SMR14]. **Perspective** [Ale13, AST16, CM17, GEL18, GRD11, Jen13, KJ15, Lev16, Mag14, Mas14, MGP16, PU14, Pop15, Puz16, Puz17, Sha11b, Sic16, Sko16, Sto18, BMX+19, DPK18, GE12a, JNY17, JMX+15, Jia15, KJ16a, KJ16b, LSCMSFC19, NKWT19, Ols11a, Per18, PP14, Pul11, Tap15, TBB+19, XXJ+16, ZSZ14]. **Perspectives** [Blo15, BT15, Dob14, HJK14, IAK13, Jan13, JNZ+14, KO14, Kaw15, KJ16b, KJ14, Liu14, LG15, Mak15, MGN14, May14, Men15, MSM16, Nal15, Ném14, NTCK13, Nic14, PK16, RP16, RNC+14, Rus14, SN15, SX15, Sza13, TFBG14, Tok16, Wag14, WYM15, ZLR15, ZLWY13, Zil14]. **perturbation** [BDPT12, CEFMK12, DK13, DB11, DB13a, DCHC11, JHSG18, JNZ+14, Kry12a, LCL+10b, LPG+12, Lin14, NS13, PBB15, RMG+19, RS09, RS11a, Var11]. **perturbations** [DB12]. **perturbative** [PCV19]. **Perturbed** [NH18, Cal10, PVS12]. **perylene** [Cas15, HSS18, JR19, MANP17, WKE17]. **perylene-based** [MANP17, WKE17]. **PES** [QB15]. **pesticide** [HYZ13]. **PH** [AM18, EMSB15, MZLM17, DPDR11, GWM11, Pan16, XCL+18, MPJ12, OAC17, OG19, PJP10, SSP14]. **pH-rate** [SSP14]. **pH-responsive** [OAC17]. **pH-sensitive** [MPJ12, PJP10]. **Phase** [MS12, Nal15, RF10, AEAS+19, BGBV12, Boe12, BCNR18, BLM+12, CFOC+10, CRSB12, Che12, CF17, DMAB12, DD17, DZ11a, DMBL16, DCOC+19, EHKD11, FBRBR12, FMKJ14, FDMR11, GV19, GCK+17, GMT18, HDC+11, HDQ+13, HN12, Jen13, JWJ+12, KS11, Kim19, KZZ13b, LKOS17, LNGW14, LGZC15, LGW11, LdAA+11, Mak15, MCC12, MOSK10, MML+11a, MLB+12, MMM+12, NKWT19, NZLG15, Per18, PB10, RP16, RCM10, Riv11, RNE10, SDS19, SDS20, SF13, Ser11a, Ser11b, SK12a, SSdS17, TWR15, VF13a, VV18, VVN+16, WXZ+11, WZX11, WLG+11, WWLZ17, YC13, ZL10, MJ11]. **phase-space** [HN12]. **Phase/current** [Nal15]. **phases** [DM12, KMU+13, MB14, Sjö15, TFB11, dSdSPG11]. **PhCOCOCH** [SKS10]. **phenalenyl** [NKF+13]. **phenalenyl-based** [NKF+13]. **phenanthridine** [BZBZ13]. **phenanthroline** [YZW+15a]. **phenol** [COdF+11, HZW18, YY18a]. **phenolate** [ZSQ+10]. **phenolate-pyridyl** [ZSQ+10]. **phenols** [WGLX10, dSNBG08]. **phenomena** [EMED+12, TMC18, ZB18]. **phenomenon** [Bon17, LBdV16]. **phenoxy** [BAMA12]. **Phenyl** [IK14, Bon17, DDÇY12, DPRK12, HZW18, LD17, LVP12b, MXC18, SC12a, SC12b, SHW+13, TAY11, TT10, YWJ+11]. **phenyl-3** [TT10]. **phenyl-based** [MXC18]. **phenyl-methyl-benzimidazolyl** [SHW+13]. **phenylalanine** [TBHL11]. **phenylamino** [KAOB11]. **phenylazoaniline** [NVPCJ+13]. **phenylene** [LGL+19]. **phenylenes** [LWY19, MMF+13]. **phenylethyl** [MOH+12]. **phenylimino** [KAOB11]. **phenylphenol** [NVPCJ+13]. **phenylpropyl** [DFK16]. **phloroglucinol** [MK10b]. **phonon** [DLM12, Lar10]. **phosphate** [Owe17, Pat15, RNdA+10, Rud12]. **phosphatidylcholine** [MKSG13, TTM16]. **phosphazene** [KFS13]. **phosphide** [Kar12b, MM11].

phosphine [GWM11, JLZ+17, LFTL18, XZG+18]. **phosphine-boranes** [GWM11]. **phosphine-catalyzed** [LFTL18, XZG+18]. **phosphines** [SAG13]. **phosphinidene** [AKC10]. **phosphinoalkylidene** [XCD18]. **phosphinyl** [Wit18]. **phospholipid** [MP12, MDP12]. **phosphonate** [Owe17]. **phosphonic** [SPPT15]. **phosphonium** [AG10a]. **phosphor** [YBMK12]. **phosphoresce** [ZQJW13]. **phosphorescence** [AMMK11]. **phosphorescent** [MSRn+11, SLS+14, ZLLS10]. **phosphoric** [LFS+11, SCS15]. **phosphorous** [LC12]. **Phosphorus** [KLE+19, BHMN19, Buc10, Mor12, RMP+14, SZL+15]. **phosphoryl** [BGJSM+18, dCSDdMC13]. **Photoabsorption** [LdBF+12, BDF+18]. **photoassociation** [CZCW19]. **photocatalysis** [WCL+17]. **photochemical** [BAX+19, GGZZ16, MMSC19, SR11a]. **photochemistry** [BAA+18, KGVG11]. **photochromes** [LZZ+17]. **photochromic** [LWJL10, YWJ+11]. **photochromism** [YXM+18]. **photocyclization** [BO11, Bud12]. **photocycloaddition** [MBS+18]. **photodegradation** [KK19, MPE11]. **photodetached** [AA11]. **Photodetachment** [IAA15]. **Photodissociation** [HZW18, MOY13, DCHC11, LA11, LSL+08, XZCH11]. **photodissociations** [Bae16]. **photodynamics** [BS16]. **photoelectrochemical** [CWB+13, JK12, LGS+16]. **photoelectron** [CHH+19, HYH+10, OVT+16, SVPTM+10]. **photoemissive** [Ném14]. **photofragment** [GV19]. **photoionization** [CW13b]. **photoisomerization** [Bud12, GW18, MSH13]. **photoluminescence** [GMP+11]. **photolysis** [BGFD14]. **Photomagnetic** [BSM+15]. **photon** [Bud12, WLZ+12b, YWR+18, ZWLC12]. **photonic** [Tap15]. **Photophysical** [OAA19, ZKWZ17, BH10b, JWG+12, TPT19, YZW+15a, ZZR+12]. **photosensing** [NTCK13]. **photosensitizing** [CJSNLM11]. **photoswitching** [DP16]. **photosystem** [LSR+13, YYI+13, YSK+12]. **photovoltaic** [BSSS19, IIS+17, MNP19]. **photovoltaics** [GRCATG19]. **PhSiF** [XCL+18]. **phthalimide** [dLRR11]. **phthalocyanine** [DZO12a, SKY+13, WWC17, ZSAP11]. **phyllosilicates** [PDR+14]. **phylogeny** [WZ10a]. **Physical** [ÁIGVZW12, FSST16, GI11a, KBGC12, PS10b, PS14, RW12, Sha11a, She14, VUC13, Wan13, WYM15]. **physically** [RVO+14, VRO+12]. **physicochemical** [SMGZ13]. **physics** [Brä13, CRA+11, Lun13a, Lun13b, MC14, Rom10, SBD+16, Tou13, Brä14, NYA+13]. **physisorption** [KK19]. **pi** [DAC11, FC19, Tra19]. **picolinamide** [MDP12]. **picolinate** [SHW+13, DdG+11]. **picture** [BPT12, GdLT12, OS10b]. **pigment** [COdF+11]. **pioneer** [Mam14]. **pitfalls** [Swa13]. **pK** [BMK+14, COCF+14, ÇT14, GCDNGS12, KSS12, RZG12]. **pKa** [SN12]. **planar** [WCS+13, Yam10, YD17]. **Planarity** [NIK19]. **planarization** [WWD+15]. **plane** [AST19, IK18, RW11]. **planes** [THL+15]. **plasma** [LKJ13, MGK+11]. **plasmas** [SMV11]. **Plasmon** [ZY13, Mas14, MML11b, MJM19, YZ12]. **plasmon-enhanced** [Mas14]. **plasmon-induced** [ZY13]. **plasmon-molecule** [MJM19]. **plasmonics** [BDF+16]. **plastic** [IBA+11]. **plasticizer** [LL17]. **plastocyanin** [ZSZ14].

plateau [KLZQ15]. **platforms** [PCV19]. **platinum** [LPOP12, MM13, PEA+12, PP10, XZ11, ZCX+16, OAA19]. **plausible** [VFCSC17]. **Plesset** [BVA+14, EG10, NMIP14, RS09, RS11a, TH13]. **plot** [MAW+18]. **plus** [PS10a, PSGK17]. **PM3** [PI13]. **PMe** [BAA+18]. **pnicogen** [JLZ+17, Sch13]. **pnicogen-bonds** [JLZ+17]. **pnictogen** [EMSB15]. **pocket** [WTH+11]. **point** [BMRM19, BLdV19, Chu12, KC19a, Kuz19, MFR10, QB15, WH18]. **points** [KMNSP19, LA11]. **poisoning** [BvWG14]. **polar** [ATS+11, FBD+13, LL19, RRVJ10, SA18]. **polaraizabilities** [Ven12]. **polarity** [GA19, HFL+17, RMTG11]. **Polarizabilities** [EBR11, AM13b, FKL+12, KP11, KA11, LKN13, LKJ13, MNS11, OMÐ13a, SN11, LXW+12]. **Polarizability** [KWWH18, Ali14, BEM12, CCEGK12, COP16, KWLS15, KYS13, Mar11, Mar12, MA11b, XWCY11, dSSF16b, dSSF16a, SKL10]. **Polarizable** [HJK14, WYM15, Cal10, Cam10, Cam12, Cap16, Car19, DZO12c, GMA+19, LSKM19, PCR+11, SRN+19, SV11, WML11]. **polarization** [Ang10, AMMC19, GC19, IAA15, KK14a, MFB11, MOY13, Mit11b, OS10b, PWP13, RLZ12, TH12]. **Polarized** [SFM13, BŁ16, GIO12, HITU16]. **Polarized-unpolarized** [SFM13]. **polaron** [SGG+10]. **polarons** [TIKL13]. **pollutants** [MXC18]. **Poly** [XLGA12, BMR+13, IBA+11, JLS13, OCB+10, OCB+10, XLGA12]. **polyacetylene** [CFGC11]. **polyalanine** [Ire12]. **polyatomic** [Bae16, DK13, HKLW13, KP12, Sut12, Tou11a]. **polybasic** [KRH13, SGB11]. **polycyclic** [BRS10, Bla15, CA17, DI18, GMT18, LVP12b, RNV+12, SFM13]. **polyene** [GNM+12, NIK19]. **polyenes** [MMWA11]. **polyethylene** [YZZH15]. **polyfunctional** [NA12]. **polyhedra** [ALK18]. **polyhedral** [Pup11a, TDOD17]. **polyhedrons** [LGHL11]. **polyhex** [LSW19]. **polyhydroxybenzenes** [MK11]. **polymer** [DI15, FZH+18, JHSG18, MM13, PETB18, SPPT15, Wan11, YT14]. **polymerization** [AMAC12, CL08, LSG+14, LKZ+16]. **polymorphism** [GP13a, PAD+10]. **polymorphs** [Gao12, VVS+18]. **polynitrodiazoles** [RGTS11]. **polynitrogen** [THL+15]. **polynitrotetraazaoctahydroanthracenes** [ZL12]. **polynomials** [Rom10, RA10a, SMOD11]. **polynuclear** [OPF11]. **polynucleotide** [Yak10]. **polyoxides** [MCARL11]. **polyoxometalate** [MLY+16, TPCJ+12]. **polyoxometalates** [CB10]. **polypeptide** [MCE11, NRI15, PCML08]. **polypeptides** [YSG10]. **polyphosphate** [BGJSM+18]. **polyproline** [Ire12, MLB+10]. **polyprotic** [BMK+14]. **polypyridine** [SG19]. **polypyrrolic** [ZQXP17]. **polysulfides** [YSA+11]. **polyyne** [JB18, MM13]. **polyynes** [IA13]. **Pons** [Yos20]. **poor** [ALK18, NCMC+18]. **Pople** [HH18]. **POPOP** [IBA+11]. **Popular** [Li15, LORR+12]. **population** [DFV+12, MKD19, PM12, VGS10, dA12]. **populations** [GFRdG11]. **pore** [LS19]. **porous** [GZ14]. **porphine** [Joh17]. **porphyrazine** [HM10a]. **porphyrazines** [ZSAP11]. **porphyrin** [CJBMMAPR19, HSS18, MY17, VSN+11, ZSASS13]. **porphyrin-**

[CJBMMAPR19]. **porphyrin-based** [CJBMMAPR19]. **porphyrins** [CMR13, CJSNLM11, GLPA10, MSOV13, QJ13, TTD13, VC13, Yam11]. **portable** [Lya19]. **portisin** [COdF+11]. **Pöschl** [HR12, HFZ12, JZP17]. **posed** [BMB12]. **Position** [YOS15, ALRA10, KPL+17]. **positions** [MAT19, SY10]. **Positive** [FBRBR12, MMRRA10]. **positron** [KKT13, KKT14, OT14, SSA18]. **positronic** [GS11, NGS11, ZS11]. **Possibility** [MGB18, Sat11a, DMBL16, EM19, ZCX+16]. **Possible** [MFM18, POLV12, SYK+12, BMF13, KKC14, Kar15, LDZG16]. **Post** [SZ11, MSNP18, SYY16]. **Post-Hartree** [SZ11]. **post-HF** [SYY16]. **post-second-order** [MSNP18]. **pot** [LW15]. **potassium** [Ish14, MMV+19]. **potassium-iodide** [MMV+19]. **potency** [DKZ+10]. **Potential** [BAP12, Ber13c, DHZS11, FKBG19, LDADB+15, McC13a, MMM20, SB16, XZZ+10, ZLR15, AB16a, AAHN16, AC19, Agb12, AOLB12, ART08, AST19, AY15, BPVDB11, BP13, CDSK12, CJBMMAPR19, CNBPR+11, CSS16, CYL+18, CB19, DTVP+12, DB12, EMK14, Fin15, Fin16b, FA17, FB17, FMMD+10, FBU+11, FNIT16, Fuk12, GSZ10, Glu13, GORW19, Haj18, HDÖS12, HR12, HYZS12, HYZS19, HJRO13, HNBG15, HFZ12, IIH16, IOO18, JZP17, KC18, KMRG13, KMNSP19, KMM16, KRG+13, LFF+10, LV12, LKJ13, LL18, LDZG16, MPD+15, MDC15, MCP10, MOE+11, MOLF11, MGD11, MPRCEG12, MPT11, MPTZ13, Nag10, NTCG18, NMIP14, NMHPVG12, OOI+19, PGGRMP10, PML+11, PVS11, PM16, PKK+16, PSGK17, QD10, RSL10, RCP14, RDM+11, Roy14, Roy15, Roy16, RS13, SAS+12, SCLCPB12, SMOD11, SMV11, ST15, SXH18]. **potential** [SRS+17, Sik18, Sil14, SZ15, SDL+15, SZY17, TNN16, TG16, TSL11, TGRP19, TPdMB12, VOAH18, VPA11, Vik11b, WKE17, WZX+15a, WC14, YOS15, YW11b, YLC17, YLYC18, ZSAP11, ZLJ11, ZHF12, ZWL18, ZZZ+18, ZRLV10, Bud12, Yak11]. **potentially** [CWL+13, FDG18]. **potentials** [AGJ12, BW18, BC15, BC16, Beh15, BBA+16, Cal10, Cin20, EI11, ESS13, GMGRMP12, GH11, JH13, KH12, KWWH18, Kry12a, KGK13, LP10b, LLH15, MMM16, MZST16, MPB11, PDR+14, PMGMGR12, PGMGRM15, PM16, Roy13, SZZ+19, TH12, Tug13, VLG12]. **power** [LSC+18, CKB+19]. **ppy** [ZQJW13]. **PR** [DPDR11, GWM11, OPP+14, WLG+11]. **practical** [Pon19, RAMB18, SIM14, SLS+19]. **prebiotic** [KS19, VFCSC17]. **precision** [Kin13]. **precondition** [LW18]. **precursor** [SSTÖ11]. **predict** [KSO19, TFA10]. **predicted** [Jeo18]. **Predicting** [ABKJ18, BPK19, DWX+16, KRK+17, PO15, AMMB+18, CFOC+10, DE18, GAI19, TWR15]. **Prediction** [DFV+12, LC12, SGB11, SSP14, Ali19b, BBB16, BBA+16, CPL15, DGA+13, GB18, LCL+10b, LPG+12, PCD14, PWY+18, RMLPGGGH16, SLC+18, SRASZ16, SBKJ18, VPFD10, VRO+12, WZX15b, XYL+18, YC13, ZYSW17, ZW15, dOLdlV13, MGD11]. **predictions** [Bou11, Bou12a, KKH18, TKSK17, WLL19]. **Preface** [ACL10, ABC12, Ano13-49, BSS14, DC10, DBMPB11, HLSD14, HB18, NYA+13, NT15, Rei15, RSV10, Rup15a, RA10b]. **preference** [EAH13, JN13]. **preferences** [KM12b, LB18, MAW+18, NRS+11, NJA+12].

preliminary [CC12]. **Prelude** [AS19]. **preparation** [CS18]. **presence** [DPK18, DB15, EBR11, FRNM12, KSC15, Lae14, LB14b, Pit12]. **Present** [TSvL+16]. **Presentation** [EMK14]. **pressure** [KMU+13, Mil12, SIT+12]. **prevention** [Bal16]. **primary** [ABKJ18, MOSK10, NGS11]. **principle** [AFA13, CM15, DWX+16, GI11f, KLK13, Oht13, RD14, SMGZF19, SGC13, TCCI10, VDG13]. **principles** [AGG+18, BXR+13, Bon17, CC11a, CWW+16, CJOOW11, FTB11, Fra17, GNM+12, HMA+19, Jia15, Kan17, KSS12, Kim13, LLM13, LLL16, lLBqD+19, LIK15, LBdV16, LSCMSFC19, MBKH19, MJM19, Pan19, PP19a, Per10b, RZG12, RJLPGH+13, RRB12, TZ11, TWR15, Wan13, WLH+19, WZC+12, XCD18, YHL+13, ZWLC12, vL13]. **prion** [MRT11, MM10]. **priori** [LG10]. **prismanes** [GKGM18]. **Pristine** [BSS15]. **proapoptotic** [GTSC+19]. **Probability** [dA12, MNZPT19, MAPS18, NTCG18, YW16]. **Probable** [KRH13, GI10]. **probe** [BAB+18, LYS+19, LGS+16, RDB18, RDB19]. **probed** [LSR+10a, LSR+11]. **probes** [GSPR19]. **Probing** [GXZ+14, MVA19, RMY+13, SRA+11, TWHZ14, TG13]. **Problem** [DJ95, BW18, BMB12, Brä11b, DJ12, DB12, DVP18, Gru17, Ign11, Ign12, JW18, Mit11c, PJ19, RGPZD13, Rit12b, TPCJ+12, UYN+13]. **Problems** [LDZG16, Blo15, FRGC10, Kar09, Kar10, Mar12, RMG+19, SW10, Sha18]. **procedure** [GTR11, KMNSP19, NS10b, Sha11a, ZS11]. **procedures** [OKR12]. **Proceedings** [DC12, DC10]. **process** [AGB19, AGRI+12, CRB+12, CL08, DWPK14, GI11a, KK19, KTI+12, LYS+19, MJ16a, MNC12, SR18, TCG17, WZX+15a]. **processes** [BM10, CPAT11, KUS19, MWH15, Mar13, Mas14, PD11, RLW+13, RSL10, Tap15, TBHL11, TPT19, VKF+19, XZL+12, ZLWY13]. **processing** [LSKM19, ZH15]. **processors** [Lya19]. **prochiral** [WTZ+11]. **produced** [LdAA+11]. **Product** [Les12, SWS+14, SPM+15, TKN13, TSL11, Tri14]. **production** [MCRS16, PD11]. **products** [BO11, CADSG18, POLV12, Tal11]. **Professor** [LJ16]. **proficiency** [JXX+15]. **profile** [SIT+12, SSP14, STU19]. **profiles** [dHLdS12]. **program** [BHH+13, CYC+15, DOE+14, DCOC+19, LCZL15, MPZWD10, YAF+15, ZHF12, ZH15, ZWSF16]. **programmable** [CKB+19]. **programmed** [ÁFV12]. **programming** [Lya19]. **progress** [HDÖS12]. **progression** [Ish14]. **project** [TY17]. **projected** [KSN+10]. **projection** [KYH+13b, Pon19, Yos20]. **Projector** [KRC+16]. **prolate** [Kar12b]. **proline** [SHL+13, YZZ15]. **proline-catalyzed** [SHL+13]. **Prominent** [WLC+17]. **promiscuous** [RNdA+10]. **Promising** [LPO+12, SG19, Esr18, EM19, KM12b, LYS+19, MVG18]. **promoted** [LJK+18, LCM+11, Pli18, QCW+12, WTZ+11]. **promoting** [RNdA+10]. **promotion** [CAPGAIG18]. **propagation** [Bae16, EM16, KFS13, KUY16]. **propagator** [DZO12c, DZO12a, FMMD+10, POLV12, SM12, ZDZO10]. **propagators** [AMMC19]. **propane** [NTNL10]. **propen** [HNH+12]. **propene** [DPDR11, ZPW16]. **propensity** [PSKV19]. **propenylamine** [RJA+10]. **Proper** [SD13b, Fin15]. **Properties** [GLT13, GH11, IA13, KBF+13, KKT13, MOY13, McC13a, ONK+13, OA13, TBRIS12, TSS+15, AGCVG15, AFA13,

AFM+10, AMK10, AMAM18, ABA11, BŁ16, BHAH+18, BSM+15, BGKK16, Bon17, Bou12b, BH10b, Cap16, COdF+11, CGM12, CdLdSC18, CWB+13, CWW+16, CZLD17, CKB18, CB19, CSMZ10, Cor16, CADSG18, CHV14, DKS11, DCFD10, DAE+12, DWX+16, DHYC19, DWGX12, FZX18, FZC14, FPRGMHGB12, FBU+11, GAPK+19b, GLF+12, GWZ+14a, GMT16, GMR18, GB13, GKGM18, GRCATG19, GMM+18, HWL16, HWWW18, IGMK11, JA12, Jac12, JL12a, JWG+12, JR19, Jou13, JFDD10, KBGC12, KA13, KV19, KRK+17, KMF+11, KCK14, KJ15, KSSK16, KPL+17, KL11, KYLC19, KSY+11, KP12, KLZQ15, KMU+13, KK11d, KM19, Kuz19, LRKM10, Laz14, LZ12, LVdSdM14, LCH14, LZB10, LJW+11, LXW+14, LZW+15, LC16, LL19, LZZ+13, LLZ+14, LZZ+17, DVMC19, LHL+15].
properties
[MLY+16, MMP+18a, MCCGM+19, MBKH19, MSG16, MZB+13, MLC+11, MANP17, MNP19, MPTR12, MPMCM+11, MFZ+18, MG12, Mil12, MS17, MHHPR+17, MA11a, MA11b, MLDP10, MBA+19, MMF+13, MW15, MSRn+11, MC18b, NBL+14, NBI+10, NMHPVG12, NB19, NDM+12, OAA19, OGvSG18, OCB+10, OK19, OMĐ13a, Pan19, PP19a, PK13a, PCD14, PFdM13, Pit12, Pog12, PAKA15, PMAP12, PSK+13, QHS11, QJ13, QCB+10, RMLPGGGH16, RRRV19, RGTS11, RZC13, RC11, RSCS10, RBLZ15, SD13a, SMOD11, SSKS12, SLS+14, SB16, SXS+12, SLS+12, SLSZ13, SR13, SSTÖ11, SBB16, SM14b, SM14d, SM17, SRN+19, SYQ+10, TIKN11, TZ11, Tas14, TD11, TBRIS10, TBRIS11, TFMC19, THVP14, TFB11, TRZ+19, TCG13, TPdMB12, UTTn13, VOAH18, VMC11, VRO+12, VBO+15, WGLX10, WXB+11, WLZ+12a, WLZ+12b, Wan13, WDS19, Wu11, XLZ+19].
properties
[YK11, Yam11, YZL+10, YZL+11, YLWrL12, YZW+15a, YBMK12, YZW15b, ZZX10, ZLLS10, ZZR+12, ZQJW13, ZKWZ17, ZSQ+10, ZL12, ZCG+16, ZS12, ZCP11, dSdSPG11, dSMT+18, dOLdlV13, vL13, vLRRK15].
properties/activities [MPMCM+11]. **property**
[BXR+13, CWL+13, CJSNLM11, FSQ+11, GI11e, GMP+11, MY17, MCL11, MMP11, Nic11, Pea11, RGST12, ZYZ+11]. **property-specific** [Nic11]. **proportions** [Lu15]. **proposed** [TCA10]. **propyl** [CMCN11]. **propylene** [LS19, WML10]. **protease** [VHTEG15, dAGNJT12]. **proteases** [SKS10]. **protected** [MC18b]. **Protection** [CAPGAIG18, BSS15, GAI19]. **Protein** [PT13, AGRI+12, CR18, CHSO13, CSVCB12, DFF+13, GSR12, HXDY16, KFY+12, KKG12, LLZaH14, MYZ+10, MRT11, MRS15, MSK+12, Pop15, TYN13, TCM+12, TBHL11, YSW11, ZPM10, ZWLC12, ZTC11, dA12, TBST10]. **protein-coupled** [CSVCB12]. **Protein-nucleic** [TBST10].
proteins
[LDKB15, LKd+16, NTCK13, QZH13, RP16, RAK10, Sch10b, TCS10, YSG10].
protic [HFL+17]. **ProtNA** [TBST10]. **ProtNA-ASA** [TBST10].
protochlorophylide [SR11a]. **protocol** [BDF+18, CwCW+11, SCBP17].
protocols [COCF+14]. **Proton** [SCS15, DLCB15, DLM12, DSZB18, FDMR11, IKS08, IKS10, KAOB11, Kry11b, Kry12b, LZZ12, LYL+12,

MPE15, MNC12, MGP16, NMS+10, RY12, SPPT15, SYK+12, Sat11a, Tav11, Tav12, TH12, VF13a, Wan13, WJ11, XDM+10, YY18a, ZZ18].
proton-coupled [XDM+10]. **proton-electron** [LYL+12]. **proton-molecule** [TH12]. **proton-transfer** [NMS+10]. **protonated** [BH10a, MSH13, MURR13, NC11, dAVdM17]. **Protonation** [MLY+16, SF13, Kry11b, Kry12b, SGB11, dSTH17]. **protonic** [PUGSFM18]. **protons** [Coo12, HITU16, Kar15]. **prototautomerism** [YB11]. **provide** [WWC17]. **provides** [AB18]. **proximate** [RD14]. **PS** [YIY+13]. **PSB3** [BMX+19]. **Pseudo** [GFB12a, QZH13, WLZ18, Mit11a, Szc18, VDG13, ZZL+11, ZFC12]. **pseudo-** [Szc18, ZZL+11]. **pseudo-10-fold** [VDG13]. **pseudo-Jahn** [ZFC12]. **pseudo-natural** [Mit11a]. **pseudobond** [Exn11]. **Pseudodiradical** [MB13]. **pseudoharmonic** [YOS15]. **pseudopotential** [Ber13a]. **pseudopotentials** [PNC19]. **pseudorotation** [ZFC12]. **pseudospectral** [KPCV18]. **PSII** [SYK+12]. **Pt** [Bou12b, GAPK+19b, ÁFV12, KF17, LLL16, MMBK12, PP10, PRPU+13, YZL+10, ZLLS10, ZCW16]. **PtAu** [CTW12]. **pterin** [JCC10]. **PtPd** [XGH+18b]. **Pu** [PKK14, RMY+13]. **puckering** [WDSL14]. **pull** [DSRGD12, MNP19]. **pulse** [NWQX11]. **pulses** [DLCB15, GRLA18, HYH+10, SVPTM+10]. **pure** [HDQ+13, LZW+18, SHMR11, TÁ10]. **purely** [FT15]. **purification** [KJ16a, KJ16b]. **purine** [KZA+17, LLZ+14, XZ11, ZWZK19]. **purines** [CAPGAIG18]. **purpose** [YAF+15]. **push** [DSRGD12, MNP19]. **push-pull** [MNP19]. **pV5Z** [SLS+11]. **PVP** [SS18b]. **pyramidal** [SH18a]. **pyramidalization** [LGHL11]. **pyrazinamide** [SD13a]. **pyrazine** [NBL12]. **pyrazol** [TAY11]. **pyrazole** [SJZL12]. **pyrazolone** [LWJL10, PGG12, YWJ+11]. **pyrazolyl** [LXW+14]. **pyrene** [SYY16, YZL+11]. **pyridin** [PGG12, SC12a]. **Pyridine** [GP13b, CLXZ12, CCS13, LXW+14, SPIL14, ZS12, ZBBB17, dARAV12, YB11]. **pyridone** [HHCA10, MCC12]. **pyridyl** [YLW+13, ZSQ+10]. **pyrimidine** [CW16, HS11b, KZA+17, XFW+14, YDW13]. **pyrimidines** [KS19]. **pyrolysis** [WGLX10]. **pyrones** [CM12]. **pyrrol** [LYW11]. **pyrrol-2-ylmethyleneamine** [LYW11]. **pyrrole** [BS16, CCS13, CZLD17, MMP+18a, PPK+13]. **pyrroles** [IUMVB10]. **Pyrrolidine** [PMAP12, KDÇ12]. **Pyrrolidine-based** [PMAP12]. **Pyrrolidinium** [AVG19a, AVG19b]. **Pyrrolidinium-based** [AVG19a, AVG19b]. **pyrrolopyrimidines** [dOdONM12]. **pyruvic** [VF13b]. **pz** [HHL12a, HHL14].

Q [VF13a, WB17]. **QB3** [CFOC+10]. **QC** [MFLP12]. **QC-DMRG** [MFLP12]. **QC-simulated** [Eil14]. **QCTFF** [Pop15]. **QED** [IFT13]. **QM** [RNC+14, AHC+18, AMMK11, BTH18, Cap16, DMG10, Exn11, GFRdG11, KI15, MFB11, MOLF11, Men15, MG10, SDP+16, SD16a, SD16b, ST15, SLA12, STU19, TIKN11, UYN+13, VHTEG15, ZKW17, dAGNJT12]. **QM-cluster** [AHC+18]. **QM/Classical** [Men15]. **QM/MM**

[AHC+18, AMMK11, DMG10, Exn11, GFRdG11, MOLF11, MG10, SD16a, SD16b, ST15, SLA12, TIKN11, UYN+13, VHTEG15, ZKW17, dAGNJT12]. **QM/MM-ER** [TIKN11]. **QM/MM/MD** [AHC+18]. **QM/polarizable** [Cap16]. **QM/QTAIM** [BTH18]. **QMMM** [HCH+18]. **QR** [BB10, Bou12b]. **QR-SCMEH-MO** [BB10]. **QSAR** [KKM+12, MPMCM+11, PH12, XFW+14, ZFW+13]. **QSPR** [CD18, MPMCM+11, SN12, TFA10]. **QSPR/QSAR** [MPMCM+11]. **QSTR** [PI13]. **QTAIM** [BTH18, DP16, MAW+18, NH18, Sha11a, VHTEG15, XXJ+16, XWP+18, YXM+18, ZLZ+14]. **quadratic** [FYhC11, OPAVM18, RSN12]. **quadratically** [ISRK12]. **quadratric** [ZST+10]. **quadricyclane** [TTD13]. **quadrilateral** [LZZ19]. **quadruple** [MPT11, NZ13]. **Quadrupole** [MdAdCS12, AC11, BJ12]. **quality** [OKR12]. **Quantal** [SIB+13, SHKS15]. **Quantification** [SP19, Gru17, ORJ18, Rus14]. **Quantifying** [Mar12, MML11b]. **Quantitative** [CJSNLM11, HSN+11, Zha17, MY17, MBTVR12]. **quantities** [FSST16]. **quantization** [HKLW13, Kle11, SD13b]. **quantized** [Tou11b]. **Quantum** [Bal16, BSS16, BL10, BR16, Bra19, Brä13, CJBMMAPR19, Cav13, CKL16, Cho16, Cho19, COP16, DKZ+10, DLCB15, DFK16, DLM+11, DC14b, EAK+10b, EML+11, EMEPD15, Ezz10, FMKJ14, For17b, GbZA10, GGZZ16, HGB08, HS15, Hog13, HB14, Hop15, IFT13, IAK13, IOO18, IK14, Jen13, JXX+15, KWC10, KYS13, KMK+16, KYH+13b, KUTS10, LB14a, LZZ12, Luz11b, Mak15, Man16, MMP+18b, MNE+13, MBTVR12, NTCK13, Nic14, OWD18, ÖEDB11, PH12, PWY+18, PETB18, PKK+16, PSGK17, Puz17, Qu13, RGTS11, Rit11, RMP+14, SAG13, Shi13, SR13, SG14, ŚKB18, SBKJ18, SZY17, SSB+12b, Tap15, TFSRM11, UJSJ13, VVN+16, VBJK18, Wag14, WDSL14, WYWL13, WZX+15a, WWX+11, WCM14, WLD+10, XS18, XZJ+16, Xu16, YM12, YW11b, YZ12, YB11, ZCC11, ZJS13, dFR15a, dFR15b, dSMT+18, ASMP15, ABG12]. **quantum** [ANC+15, ASK15, BF11, Ban12, BAX+19, Blo15, BGL+16, BHH+13, BT15, BT17, BM16, BBB+12b, Bra10, Brä12, Buc12a, BN11, CD18, CKB+19, CM16, CSK12, CSG14, CW13b, Cho15, CYK17, Coo12, CPAT11, CN12, Dau16, DPK18, DSL15, DPRK12, Dil13, DMBL16, DSFT17, EAH13, FLCHL10, FBO+11, FNIT16, FSST16, Gag11, Gan14, GWZ+14a, GRCGRRHT19, GB10, GS11, GR10, HR13, HS11a, HITU16, HS11c, HEVMSA+19, HM12, Hor13, HMA+18, IFT14, Ish14, JN13, JHSG18, JMX+15, Kap12, KB12, KCDC15, KC18, Kar09, Kar10, Kha16, KCC13, Kit14, Kit15, Kle11, KN15, KK11d, LS17, LSS19, LV19, LSR+13, LCZL15, LHX+19, Lin14, Liu15b, Liu16, LSKM19, LEU+11, Luz11a, Ma14, MC11a, MR12, Mam14, MDC15, MPE15, Mar13, MSC10, MMŁ+16, MPD+10, MQG13, MPL+11, MBBT+12]. **quantum** [Mor13, MLDP10, MB12, MGP16, NC11, NKKN15, NS10b, NGS11, NBZG16, Ném14, Nic11, NVPCJ+13, NMSR14, NRP+11, NJA+12, Nym14, OPS10, OK19, OM13b, OSJ+12, PABSK16, PTH11, PMGMGR12, PMHM19, Pup11b, RP11a, RP11b, RL12, Rei15, RDM+11, RNE10, RNB+10, Rup15a, Rup15b,

SDS19, SDS20, SOF+10, SBEH11, SKHN13, SC12a, SPSA11, SN15, SK17b, SKLC19, SD13b, Sha18, She13, SIB+13, SHKS15, SKM11, SSA18, SGC13, Sjö15, SS19b, SFY12, SRA+11, STU19, SZ15, SCBP17, SPM+15, Tch13, TBB+19, TK16b, TH12, TXK+19, TFA10, Tri14, TB15, UTTn13, UV18b, VPFD10, VMR11, VVVB10, Vik11a, VOK+18, VO12, WYM15, WR14b, YNLD18, YÇÖ11, YZ13, YW11a, YS13, YH14a, YW16, YLC17, YLYC18, ZS11, ZX12, ZGSM15, ZH15, ZWSF16, ZZC12, ZWE12, ZRLV10, dHLdS12].
quantum
[dSTH17, vLRRK15, AGNS14, BMRM19, DMS+10, GP13a, SP19, ZBK15].
Quantum-chemical [DLM+11, ÖEDB11, Qu13, BF11, DMBL16, DSFT17, MGP16, Ném14, NVPCJ+13, SN15, VOK+18, YNLD18, DMS+10].
Quantum-chemical-aided [GbZA10]. **Quantum-classical**
[Cho16, Cho19, Mak15, SPSA11]. **Quantum-matter** [Tap15].
quantum-mechanical [LV19, VPFD10]. **quantum/classical** [CP11].
Quantumness [CD15]. **quartet** [HK11, SCZG12, ZCG10]. **Quartic**
[VBC+12b, FT15, dAB17]. **quartz** [LLM13]. **Quasi**
[XLLZ10, YZ10, BDPT12, Hog13, KUY16, MPM15]. **Quasi-classical**
[XLLZ10, YZ10]. **quasi-degenerate** [BDPT12]. **quasi-diabatic** [KUY16].
quasi-exact [Hog13]. **quasi-stable** [MPM15]. **quasiparticle** [MS12]. **qubit**
[MR12]. **quenching** [SAHG11, SAHA12]. **quest** [GI11d, GI11e, GI11f, LL18].
questions [Ng12, VATPR11]. **quinacridone** [Gao12]. **quinoline**
[MLPT10, MAN15]. **quinoline-derived** [MAN15]. **quinolinecarbonitriles**
[ZFW+13]. **Quinone** [XWP+18, KSAK17]. **Quinone-based** [XWP+18].
quintuple [SZS+10, SLZ+11c]. **quotient** [Tra19].

R [DPDR11, DQZF12, GWM11, NBL12, Pan16, CPL15, ESS13, GWM11, LL17, PCR+11, ZSHL14]. **R-** [PCR+11]. **racemase** [LZZ12]. **radial**
[IG11, Kha16, RZ17, SPO+11, vLRRK15]. **radiation** [TK16a]. **radiative**
[Ber13a, CCM08, SCZG12]. **radical**
[BLL+13, BAMA12, BRS10, BCS+12, CWZ+10, GAI19, GK12, HWHZ11, IUMVB10, JB11, JAB12, KAR12a, KZA+17, KI12, KZZ13b, LCG12, Les12, LLP+13, LSG+14, LVP12b, MMMM12, OKR12, dMOB12, PM17, RCM+19, SSI+10, SK14, SS18a, SPSA11, Sch12a, SB16, SLZ+11b, SLZ+11c, SLS+12, SKM11, SWS+14, WLWL14, XNL+14, YM12, YY18a, YSS+10, Zha14, Zha15, ZBK15, ZLWZ16, ZJC+13]. **Radicals**
[TWHZ14, lAyL14, Buc12b, CGIAI12, DI11, DFK16, HXX15, KK14a, KDA+11, LCL+11, LVP12b, MXC18, NP18, RLW+13, RMG+19, SZL+15, TIN13, TCA10, Wit18, YM13, YL10]. **radii** [GI10, SV11, TMC+13]. **radius**
[Bar11]. **Radu** [Tou13]. **rain** [PL18b]. **Ramachandran** [MAW+18]. **Raman**
[CK13, VV13, ÇAS13, KV11, LMZY15, PM12, TFSRM11, TSBSM12, VPFD10, VVS+18, VV12, YJ17]. **Ramos** [COP16]. **Randić** [AD17, DZ11b].
random [HFBC19, PR10a, Per18, Pog12, SSB12a]. **randomly** [GB10].
Range [BPG+10, AM10, Dun15, GW13, Haj18, IKN13, KAR12a, MJ16b, MIN13, MC18a, RR19, SSK11, SKY+13, ZZ18]. **range-determining**

[IKN13]. **range-separated** [ZZ18]. **Rapid** [AA15, NE11]. **rare** [BAP12, BGL+16, DLG12, JEA13, JMPP19, LWL19, MURR13, SZZ+19, TMC18, YJ17, ZQCJ10]. **rare-gas** [SZZ+19]. **Rashba** [KV19, SBD+16]. **Ratchet** [BEPZ10b]. **Rate** [WZHZ13, AFM+10, Buc12a, CAAI12, CGIAI12, DCOC+19, FLCHL10, FBM+10, MVC13, MIKH19, NZLG15, dMOB12, ZLWL16, ZXY13, SSP14]. **rates** [AC11, CCM08, RFEGPP+16, YK13]. **Rational** [LLZ+14, WR14b]. **rationale** [JWJ+12]. **rationalization** [ZXY13]. **ratios** [MOY13, TSL11]. **Rauhut** [LD17]. **ray** [FBO+11, ORJ18, ÖEDB11, SYK+12, SCL19]. **Rayleigh** [BDPT12, MB12, dSCC12]. **Rb** [ČFČ11, DIOG12, MLW10, RBTL19]. **RbH** [KHH10]. **RbSi** [LHL+15]. **RCOOH** [DQZF12, NBL12]. **RDC** [PT13]. **RDM** [KK14a]. **RDX** [Jeo18, MJ11, TJS17]. **RDX-** [Jeo18]. **Re** [BDR12, HFBC19, PP19a, ZLY+14]. **Re-weighted** [HFBC19]. **reach** [ADR+18]. **Reaching** [MAN15]. **reacting** [Gin10]. **Reaction** [BvWG14, Kaw15, LNGW14, NZLG15, SKS10, SR18, VPGC12, WWLZ17, ZSHL16, ZPW16, ABM+19, AGOP18, lAyL14, AG10a, AG10b, AASU+17, AEAS+19, AGNS14, AFM+10, ASD14, BPT12, BAMA12, BZZ15, BLWJ17, BXZ+19, Buc12a, CLXD15, DS12, DAA16, DPDR11, DZ11a, DSZB18, EHKD11, EKD12, EM17, FBM+10, Fra17, FUE+12, GWZ+14a, GZF13, GKT+12, HSN+11, HXX15, HHL+12b, HhGqZZ17, Iku17, IK14, JWJ+12, JAB12, KAR12a, KI15, KI12, LGM+18, LKOS17, Les12, LZZ12, LZFZ13, LLP+13, LWWZ13, LD17, LZW+18, LFTL18, LS19, LLC+11, LCCH11, LWC+10, LKLW11, LCZL11, LCS+11a, LCH+11, LCS+11b, LXLL11, MGM11, MHO+15, Met11, MEEA+13, MPRCEG12, MML+11a, MLB+12, MB13, Mor11, MKW11, MOH+12, NMS+10, NKWT19, NWQX11, Nym14, PTS+11, PDNC14, PWH+12, PL18b, RY12, RSL10, RMP+14, SYK+12, SSK+12, SAG13, SK14, SKS11, SD12, Sic16, SR11a, STL12]. **reaction** [SLZH12, STU19, SWS+14, SZ15, SZY17, SHMR11, TM13, TSL11, Tsu15, TGA+11, WXZ+11, WWHZ13, WWX+11, WJ11, XGH18a, XZL+12, XDM+10, YM12, YNLD18, YY18a, YK13, YGL+11, YZ10, YLC17, YLYC18, ZRGE+19, ZZW11, ZH12, Zha14, ZLWL16, ZCG+17, ZYSW17, ZWL18, ZPB12, ZXY13, ZSS+13, ZJC+13, Zil14, dHLdS12]. **reaction-field** [SHMR11]. **Reactions** [KKH+13, LLM13, MNE+13, OD12, TIN13, TM13, ACMRN10, AMMB+18, BRS10, BS14, BAX+19, Buc11b, CdAFS+12, CM12, Chr10, CJGTL12, DWJZ11, DAA16, DFK16, EMED+12, EMEPD15, FRNM12, FDMR11, GGZZ16, GB18, HDC+11, HLJZ11, HB14, Hop15, HXX15, HCL13, Kan11, KZZ13b, KMM16, LJK+18, LW11, LLF17, LGW11, LSG+14, MXC18, MIKH19, MAP+10, MBSMJC18, NKWT19, NAK+17, dMOB12, RLW+13, Sch12a, SHS+13, SKM11, SWS+14, TFZ+15, Var14, WLG+11, WLWT12, WZHZ13, WLWL14, XLLZ10, YSS+10, YS18, ZGSM15, ZXY13, ZQXP17]. **reactivated** [MG10]. **reactive** [Cho15, dDGNB10, RCM+19, RL12, Ser11b, XCD18]. **Reactivities**

[YM13, LLZZ10, MDNDO+16]. **Reactivity** [JS18, KSC15, OPF11, PMH+16, TWHZ14, TV13, BVRM10, Cha11, DVC14, DNCKCS+12, ESBVJY12, GFPAV19, GTSC+19, GGP13, HMA+19, HR19, Hog13, JWJ+12, KP10, KO14, MMMM12, MUNZVR12, MAP+10, MBA+13, MBBT+12, MBSMJC18, MCRS16, NAK+17, NE11, NZAVR10, OPAVM18, RGS+13, RBLZ15, RBTL19, SMGZF19, Ser11a, SC10b, TM19, WJ11, YSK+12, YXM+18, RdA11]. **reagent** [BPT12, LWWZ13]. **reagents** [VOK+18]. **Real** [GKT+12, HR13, Fin14a, FNIT16, GI11b, GI11c, PI16, RLER13b, SHKS15]. **Real-time** [HR13, FNIT16, PI16, SHKS15]. **realistic** [SPSA11]. **reality** [LG10, SDP+16]. **Realization** [PM12]. **really** [SMR14]. **rearrangement** [SKS11, WTH+11, YY18b, ZAE10]. **rearrangements** [WCGD12]. **rearranges** [MG10]. **reason** [PWP+18]. **ReaxFF** [BGKK16]. **recently** [JPPA10, TCA10]. **Receptor** [KKM+12, CRSB12, CSVCB12, MSY+12, SSP+17a, SK11, ŚKB18, WTH+11]. **receptors** [PRG+10]. **recipe** [STM18]. **recognition** [AGRI+12, JNY17, PvS10]. **recognitions** [YWY+12]. **Recognizing** [Cav17]. **recombination** [BMF13, dMOB12]. **reconstructed** [dLdOdAD12]. **Reconstructing** [YS13]. **reconstruction** [AST19, GD11]. **reconverge** [SWS+14]. **rectangular** [Lun13a, Lun13b, MPD+15, Tou13, YMY+13]. **recurrence** [HSN18]. **Recursion** [LWY13]. **recursive** [SGH10]. **red** [FSBA12, Kry10, MRÅ11]. **red-** [Kry10]. **Redox** [MLY+16, AC19, AGJ12, BBA+16, ESS13, KB13, KRK+17, LCH14, VLG12]. **reduced** [ABLT11, CM15, KK13, Lat13, MPE11, Per18, dCGAMV12]. **reductase** [SDM12, SLS+10, TSKN12]. **reduction** [AGOP18, Esr18, KGK13, QCW+12, SBSD18, VPOG19, WTZ+11, YHL+13]. **reductions** [Sri18]. **reevaluation** [GI14]. **reference** [NS13, NF11, SBKJ18]. **refined** [SYK+12]. **reflecting** [AA11]. **reformulation** [Lev10]. **refractive** [SHMR11]. **Regina** [HS15]. **regio** [CM12, GHCMCMQ17]. **regio-** [CM12]. **regio-selectivity** [GHCMCMQ17]. **region** [EMED+12, KYS13, OVT+16]. **regional** [NGS11]. **regions** [LdBF+12]. **regioselective** [Iku17, LKZ+16]. **regioselectivity** [DPDR11, DMWY11, NAK+17, YNLD18, Zha15]. **regression** [VSL+15]. **regular** [PR10a, Pal10]. **regulated** [MBA+19]. **rehybridization** [Sch15]. **REIN** [MRS15]. **Reinvestigation** [NRHJ11]. **relafen** [YINM13]. **related** [Buc12b, HNH+12, Kal18, Luz13, MSAB19, RALK18, RLW+13, SSI+10, TD11, TFMC19, UMS13, VLG12, WLWL14]. **Relation** [PM16, HSN18, KM12c, RBGGM18]. **relations** [AEÖ12, DB13a, GZSMFN16, LWY13, OOI+19, RS13]. **Relationship** [CZJZ12, DNCKCS+12, GXZ+14, Gra08, Gra11, LBdV16, MY17, RGST12]. **Relationships** [NBI+10, CJSNLM11, EKN10]. **Relative** [SFW12, BMX+19, LNV+18, MC17, Pan16, PSKV19, ZSZ14]. **relatives** [Fin14a]. **Relativistic** [BCK19, Fri12, Liu14, MM19, RLTAT19, SH18a, CSG14, DAC12, FSST16, GAPK+19b, Leh19c, MCCGM+19, MPTZ13, MZST16, NSN17, NNSN17,

OCGM+19, RR19, RTT10, SN15, SS12, ZE18, ZKKR11, ZQXP17]. **relaxation** [BMF+14, EBR11, FKL+12, GSPR19, Kit17, Ng12, RMJ11, SIM14, YT14, ZP16]. **relaxed** [RSL10]. **relaxivity** [GSPR19]. **release** [SYK+12]. **released** [MAPS18]. **releases** [Han19]. **Relevance** [Eng16]. **relevant** [ASHF13, KSD10, MPTR12, Wag14]. **reliable** [AB18, TKSK17]. **reliably** [Kuz19]. **reloaded** [Cav13]. **Remarks** [LF15]. **remediation** [RdPW+12]. **remembrance** [Mer11]. **Removal** [ASW13, HNBS18, ZZC12]. **Renner** [DMAB12, GFB12a, HV11]. **renormalization** [YKM+15]. **Rényi** [HN12, OH19]. **reorganization** [Gin10, MB13]. **repair** [ZTC11]. **Replica** [MRS15]. **Replica-exchange** [MRS15]. **Reply** [HYZS19, Lun13a, MMM20, PS13b, VV13, XTLA14, dFR15a]. **Report** [HDÖS12]. **representation** [AMMB+18, BAP12, BMB10, BH19, CLC10, CPAT11, HXDY16, HZW18, HFZ12, HW12, HAX+18, KUY16, Lai11, LQZZ12, LLZaH14, LLLT12, Liu15a, Luz08, MJ11, Mys12, PML+11, TCG17, WH12, YSW11]. **representation/classical** [Liu15a]. **Representations** [DJ95, FLvLA15, RSL10, DJ12]. **representative** [MK10a]. **representing** [ABS13, Gin10]. **reproducing** [PNC19]. **repulsion** [ALRA10, BWE16, Dil13, HSN18]. **repulsive** [DB13b, GWHH17]. **requirements** [WLL+13]. **research** [CJBMMAPR19, IAK13, dGR14]. **researching** [LYS+19]. **Residue** [DMG10, MG10]. **residues** [KRH13, PCML08, TK16a]. **resin** [NFD+10]. **resin-divalent** [NFD+10]. **resins** [NFQ+11]. **resistance** [yBZfC18, Cin11a]. **resistances** [CEM14]. **resolution** [DSFT17, JXX+15, Man16, MBSAG16a, MBSAG16b, SYK+12]. **resolved** [AT18, LMZY15]. **Resonance** [TTD13, AK11, BVP13, BRBRS11, BH10a, DSSM19, JH13, KH10, KYS13, LDKB15, MZB+13, PCMG12, SBMM11, YJ17, ZPM10, ZP16]. **resonances** [CL18, IROW10, LA11, SY10, SSAM13, WB17, YZ12, ZY13]. **resonant** [MVC13]. **Resonating** [ASK15, BCP10]. **respect** [MBTVR12]. **Response** [MBSAG16b, SRN+19, dSSF16a, AMAM18, BSO16, Cam12, FZC14, GMR18, GC19, HSS18, ISN13, IN15, KG17, KL11, KFJ+18, Laz14, MM19, TPT19, UYN+13, Yam11, YPDW14]. **responses** [LYL+12, YLWrL12]. **responsive** [OAC17]. **Resta** [AT18]. **restricted** [ABLT11, GZF14, GRD11, KYH+13b, NNSN17, UJSJ13]. **restrictive** [HMH10b]. **result** [SS10]. **resulting** [GPM+15]. **results** [CSSK+12, FLCHL10, JdOS16, KSG+12, Sit15]. **retarded** [FNIT16]. **retention** [KMS+11]. **retinal** [LCB10]. **Retraction** [GWJ12]. **retrieves** [ABM+19]. **revealed** [GSPR19, LYW+19, MJM19, RDB19, SYK+12, SM14b, WW11, YYI+12, YIY+13]. **reversal** [NSN17, NNSN17]. **reverse** [SKHN13, TFZ+15, WLWL14]. **Review** [Ban12, Brä12, CD15, CSG14, CLXD15, DVC14, DSL15, DC14b, Dun15, FZC14, For17b, HJ13, HFdGC14, IN15, LJ13, Lin14, Mai14, MC14, Nym14, PM16, RNP13, SMMT13, SBD+16, Tay12, Val13, WR14b, WCM14, ZP16, dGR14, AHC+18, Beh15, CJBMMAPR19, LFF+10, Leh19c, Li11, Lin12,

Liu15b, LC19, MWH15, Mor13, RMC19, RF10, Sch10a, TRZ+19, YZ13, YKM+15, Kry11a, Mas11, Mue12, Liu16]. **Reviewers** [Cav17]. **Reviews** [AB16a, AGNS14, AMAM18, Bae16, BW18, BC15, Beh15, BBB16, BM16, BBA+16, BSO16, BW13b, Cap16, COCF+14, CM15, CSS16, CKL16, DMBL16, D'y16, FFPD16, GGZZ16, HKZZ15, Hop15, HXX15, JW18, Jia15, KCC13, KKL+16, Laz14, Li15, LGZC15, LSP+16, LMZY15, Liu15a, Liu15b, LKd+16, MHO+15, MMG15, MDC15, MWH15, MW16, MMÅ13, Mos14, MZST16, NBZG16, OWD18, PDR+14, Ped16, PSMD16, Per18, PETB18, PI16, Rup15b, SFC16, Sch13, SB16, SHKS15, SG14, Sjö15, SCB+14, SZ15, SPM+15, TTD13, TSvL+16, Tch16, TK16b, TB15, Tsu15, Var14, WZX15b, YZ13, YKM+15, YZW15b, YH14b, YHLC15, ZF15, ZPZ15, ZBK15, ZB18, vL13, SGJ10]. **revisited** [DVDBM11, OPC17]. **Revisiting** [DHYC19, GGP13, MJ16a, NS10b, Sha18, VVJ15, VPOG19]. **Rg** [LL18, BPG+10]. **Rh** [PP19a, BTH18, BLRdA+10, MMRRA10, PRPU+13, RYW+15, SBB16]. **Rh-doped** [RYW+15]. **rhenium** [DG19, YZW+15a]. **rhodamines** [Zho18]. **rhodanine** [EAK+10b]. **rhodium** [DSH+13, LYR+17, MMRRA10, SH18b, WML10, ZZC15]. **rhodium-catalyzed** [SH18b, WML10]. **rhodopsin** [GLOGM+11]. **rhombic** [LFP+19]. **rhubarb** [JB11]. **ribbon** [WWL+11]. **ribbons** [SPD+18]. **ribose** [ZKWZ17]. **rice** [WHS+13]. **rich** [NCMC+18, TCSD12, WG18, YNLD18]. **Ricotta** [HS15]. **ridge** [VSL+15]. **rigged** [IFT13]. **right** [KBJ17]. **rigorous** [Mak15, vL13]. **Ring** [BR08, RB08, AKR12, AMMB+18, BAX+19, CLXZ12, DLLA10, GZ14, HZW18, KMS+11, KUTS10, LL18, LFP+19, LWJL10, LW18, LLLB13, MSK11, MBSMJC18, NHG+12, PCK19, QB15, RLTAT19, Sat11a, TXK+19, WDSL14, WCY+10, YY18b, YTY19, Yam10, YZ12, YT14, Zha14, BR12a, RB11a]. **ring-opening** [AMMB+18, BAX+19, MBSMJC18, TXK+19]. **ring-polymer** [YT14]. **rings** [ABTW14, BR08, BR12a, BBKO16, MMM19, RB08, RB11a, RNV+12, TKS11, VC13, WvRSW+11, WWD+15]. **rippling** [MFM18]. **RISM** [KSS12]. **Ritz** [DSSM18, MB12, SBM16]. **rival** [PC16]. **Rn** [KDOR17, LL18, SMC18]. **RNA** [BS14, CLL+11, CAO18, DSVP15, KZA+17, LLLT12, MYZ+10, MMR+10, TD19, ZKWZ17]. **Ro** [Roy14]. **Ro-vibrational** [Roy14]. **road** [HJK14, PP16]. **Robust** [AAAM12, LYW+19]. **robustness** [Fin14a]. **Roby** [ABKJ18]. **roentgenium** [DR18]. **Role** [BHAH+18, BR12b, CAPGAIG18, CM16, HSYM11, PCML08, WLS+19, AM13b, BLWJ17, CG12, CHSO13, DS11, EMK14, ETGLMJ+19, EMSB15, FNBK17, GbZA10, GLOGM+11, JNY17, KGVG11, KKG12, LSR+10a, LSR+11, LV19, LQ13, MIKH19, MAW+18, MSOV13, MMSC19, Per10a, PWH+12, RMJ11, SFL+10, SHL+13, SSP14, SC11, SC18, Var14, WCGD12, ZQW+17, ZWE12, dAVdM17, LWL+12, MB12]. **roles** [JLG+12]. **room** [LL19, TD11]. **room-temperature** [LL19]. **Roos** [Pyy11, SA11b, Sha11b, SL11]. **Rosa** [dGR14]. **Rosen** [PSGK17, Tou11a, ZHF12]. **rosiglitazone** [HSS+11]. **rotamer** [COdF+11].

rotamers [HNH+12]. **rotary** [OWD18]. **rotating** [HRT12, KBG17, Sta10]. **rotation** [AÖ12b, CPL15, DDF+12, HK11, HRT12, KBG17, QD10, Sut12]. **rotation-vibration** [HRT12, QD10]. **rotational** [AEÖ12, CCBR+12, DCR10, Puz17, RMJ11, SPO+11, VLM+10]. **rotations** [JdOS16, KMS+11]. **rotovibrational** [PBB15]. **route** [BMF13, HGB08, SRS+17]. **routes** [VPGC12]. **Rovibrational** [LLP17, AM12, FT15, VLFG12]. **rovibrationally** [Dau16]. **row** [BZBZ13, KWC11, MKM11, ZFC+17]. **RPA** [LZ10]. **RRKM** [DS12, STL12]. **RS** [ESS13]. **RT** [KKG12]. **Ru** [PP19a, MJ16a, OG19, SG19, YYI+12, ZPW16]. **Ru-catalyzed** [ZPW16]. **rubidium** [LHL+15, MMR+10]. **rubidium-doped** [LHL+15]. **RuCl** [CCL+10]. **rule** [DMWY11, JL12a, KT12a, MHT+08, MC18a, SD13b, XWC10, YLZ+17, KK11b]. **rules** [RBGGM18]. **Rung** [Jan13]. **Russian** [Tch16]. **ruthenium** [ADR+18, CWB+13, LYL+12, SLS+15, LGS+16]. **rutile** [EFO11, GP13a, HCL13, ZLWY13]. **rWC** [BTH18]. **Rydberg** [Ali19b, DLRMFY10, DTPC17, GV11]. **Rydberg-like** [DTPC17].

S [AM18, BAP12, BHA19, BGFD14, BMX+19, CCL+10, EMS16, FRNM12, GCD13, HJRO13, KA13, SBMM11, SB18, SK14, TOSN12, TSKN12, WSML16, YLZ+17, ZCG+17, ZLWZ16, XCL+18, ARG11, BPG+10, BAP12, BMX+19, CMCN11, DSFT17, EHKD11, EKD12, GWZ+14a, KMMS17, Kin13, LJK+18, MEEA+13, OD12, PCK19, PBR18, TCSD12, Tan13, TL15, WYWL13, XHZXXZ10, XXJ+16, YXM+18, Zha14]. **S-adenosylmethionine-dependent** [WYWL13]. **S-doped** [OGvSG18]. **S-nitrosothiols** [XHZXXZ10]. **S2p** [LdBF+12]. **S2s** [LdBF+12]. **saddle** [QB15]. **safety** [FUE+12]. **Sahni** [VUC13]. **salen** [TMM+14]. **salicilydenemethylfurylamine** [GW18]. **salt** [CLMY12, RMTG11]. **salt-bridge** [CLMY12]. **salts** [Bon17, BM10, LG15, LMCZ11]. **salts-catalyzed** [LMCZ11]. **same** [GI11e, VOK+18]. **sample** [Nic11]. **sampling** [BBB+12b, SKV12]. **samplings** [BS16]. **Sanderson** [SMGZF19]. **sandwich** [DZO12b, LXD13, WCY+10, YZW15b]. **sandwich-like** [WCY+10]. **sandwiches** [SSB19]. **Sanibel** [ÖS12b]. **Santos** [HS15, dFR15a]. **SAPO** [SACA18]. **SAPO-11** [GSB10, SACA18]. **SAPT** [JNY17]. **sarin** [XZCH11]. **satisfaction** [PSMD16]. **saturated** [CGIAI12, VF13a]. **SBO** [GZSMFN16, GZSMFN16]. **SBO-3G** [GZSMFN16]. **scaffold** [OSJ+12, ST15]. **scaffolds** [TFZ+15]. **scalability** [CKYR18]. **scalable** [CKB+19]. **scalar** [HEVMSA+19]. **Scale** [Lya14, CKYR18, DFF+13, RAMB18, SN15, SKV12, ZLWY13, MBTVR12]. **Scale-adaptive** [Lya14]. **scaled** [YF16]. **scales** [DP11]. **scaling** [DB13a, DVP18, JH13, KJ16a, KJ16b, Kri13, LCZL15, QSX+15, RCP14]. **SCAN** [KME+18]. **scandium** [BBYZ18, GGJD13, XCD18, OH13]. **scandium-based** [BBYZ18]. **Scanning** [ZLWY13]. **scarce** [SG19]. **Scarf** [QD10]. **Scattering** [IIH16, AY15, CD15, Cho15, CYK17, Cho19, Kar12c, Kar15, NA14, RL12, RW11, SY10, SSA18, TSBSM12, Zag11, ZH15, dSCC12].

scavenger [GAI19]. **scavengers** [MVG18]. **scavenging** [JB11, LCG12, PGG12, PM17, RCM+19]. **scenario** [CSS16]. **scènes** [Kry10]. **SCF** [KSS12, Nal13]. **ScFeO** [LL19]. **scheme** [DTVP+12, Gan14, KUY16, MA10, RZSZ18, SA18, SN15, Tav12, dAB17]. **schemes** [KF19, MGK+12]. **Schiff** [CPF12, MSH13, ZSQ+10]. **Schmidt** [EM17]. **Schrödinger** [FKBG19, HYZS19, KC16, BDPT12, CW11, CW13b, GMGRMP12, HYZS12, Kha16, Kri13, MNZPT19, PGGRMP10, PVS11, PVS12, PGMGRM15, WC14, ZLJ11]. **Schuster** [WCGD12]. **Science** [IMS+13, MMF+13, NKF+13, OH13, She13, YMY+13]. **sciences** [BHH+13]. **scintillation** [IBA+11]. **scission** [LSG+14]. **SCMEH** [BB10, Bou12b]. **SCR** [MWH15]. **screened** [ĆW13a, GH11, HZZW11, IOO18, JH13, KH10, KH12, KWWH18, LLH15, Roy13, Roy16, SDS19, SDS20]. **screening** [CCA+12, CRFR11, KWLS15, ST15, SLS+19, YŞÖ12]. **screw** [Lad14, XTLA13, XTLA14]. **SCRF** [TMC+13]. **scrutinization** [PMEP19]. **Sc** — [XCD18]. **SDWP** [TCG17]. **Se** [AM18, BHA19, EMS16, HJRO13, WSML16, KMMS17]. **Se-substituted** [KMMS17]. **Search** [LTdSJ+10, Lev10, MHO+15, MCP10, NKWT19]. **searching** [KYLC19]. **Second** [LYL+12, NKF+13, UV18b, ABA11, BHMN19, BR10, BR16, BVA+14, DCHC11, EG10, FSQ+11, HSS18, JMPP19, KC11, KK13, Kar12b, Kle11, LKDC11, LCL+10b, LPG+12, MSNP18, Per10b, TH13, VRO+12, YMY+13, ZFC+17, ZSQ+10]. **second-hyperpolarizability** [BHMN19]. **Second-order** [LYL+12, UV18b, ABA11, BR10, BR16, BVA+14, DCHC11, EG10, FSQ+11, HSS18, KC11, KK13, LKDC11, LCL+10b, LPG+12, Per10b, TH13, VRO+12, ZSQ+10]. **second-row** [ZFC+17]. **second-shell** [JMPP19]. **secondary** [CLL+11, LLLT12, PCML08]. **sections** [CK13, MGK+11, NA14, VV12, VV13]. **SEDD** [KSS12]. **segment** [MYZ+10]. **Segregation** [ALK19, GE12a]. **SeHCl** [MZLM17]. **select** [AC11, VMR11]. **selected** [CCA+12, CC19, EMED+12, EMEPD15, KM12a, Kin13, MMWA11, MLB+12, Sic16]. **selection** [YKN13]. **Selective** [CZCW19, SSP+17a, GRLA18, SLS+15]. **selectivities** [ZRGE+19]. **Selectivity** [IUMVB10, GHCMCMQ17, MAP+10, MPE11, SH18b, TFA10, VBJK18, ZPW16]. **selenide** [MA11b]. **selenium** [DLLA10, ESDO16, KM19, RR19]. **selenium-** [RR19]. **selenium-containing** [DLLA10]. **selenocyanate** [KMS+11]. **selenopeptides** [Dum12]. **selenylsulfide** [Dum12]. **Self** [Chr10, ISN13, Brä11a, FFF10, Fin15, GRD11, KKH+13, LYW11, QTCL10, RAK10, SIM14, SY10, SHMR11, VFCSC17, WDJ+17, ZZW11]. **self-assembled** [KKH+13, QTCL10]. **self-assembly** [FFF10, LYW11, VFCSC17]. **Self-consistent** [ISN13, Fin15, SY10, SHMR11, WDJ+17]. **self-consistent-field** [GRD11]. **self-energy** [SIM14]. **Self-organization** [Chr10, Brä11a, RAK10]. **self-reaction** [ZZW11]. **Semi** [RPVM10, BVP14, Eng16, Hat13, MFLK11]. **semi-biorthogonal** [BVP14]. **semi-core-valence** [Eng16]. **semi-empirical** [Hat13]. **semi-infinite** [MFLK11]. **Semi-local** [RPVM10]. **semicarbazone**

[YWJ+11]. **semicircles** [LQZZ12]. **semiclassic** [CPAT11]. **semiclassical** [EM16, FLCHL10, LBW11, Liu15a, NTCG18, RBD+10, SÁBA+12]. **semiconductor** [DLJT14, Fer11, KP11, Kar12b, SAHG11, VVY18]. **semiconductors** [BWE16, Eng16, HKZZ15, WDS19, YHL+13]. **semidirect** [Tri14]. **Semiempirical** [Bou11, GI10, HVR18, VS19, BO11, KDÇ12, MSVMCI10, dSMPRSF18, RS11b, SM14a, WKE17]. **Semilocal** [PSMD16, SFC16]. **Semiquantal** [OHDA13]. **semirandom** [Pog12]. **semiregular** [Bib13]. **Sensing** [NEEV15, IKC18, Man16, MBSAG16a, MBSAG16b, dSMT+18]. **sensitive** [CC11a, MPJ12, PJP10]. **sensitivity** [Bon17, OB19, ORJ18, YZ13]. **sensitized** [AGJ12, BDG17, FM16, cLqFtW+14, MY17, MANP17, PMAP12, QJ13, SG19, SSS15, WWB+14, Zha17]. **sensitizers** [CWB+13, LGS+16, SG19, SSS15]. **sensor** [HNBG15]. **sensors** [FBU+11]. **SeO** [ZLY+14]. **separated** [LJK+18, ZZ18]. **Separation** [Nal13, BLKB11, MPD+15, PETB18, SSP+17a, WH18]. **separations** [PWP13]. **Sequence** [NMS+10, CLC10, HW12, YSW11]. **Sequence-dependent** [NMS+10]. **sequences** [Gar08, GfWlZ11, HXDY16, KA11, Lad14, LQZZ12, LLZaH14, XTLA13, XTLA14]. **sequencing** [Che13]. **Sequential** [MMBK12, KB12, MFB11]. **Ser** [ScBsR+10, TK16a]. **Ser-His-Glu** [TK16a]. **series** [BDPT12, CWS15, CYK17, DSRGD12, DB13a, HFBC19, LSC+18, MBBT+12, MBSMJC18, MSRn+11, RZSZ18, SUL+11, SK12b, SZL+14, XFW+14, YZL+10, ZQJW13, vLRRK15]. **serine** [CLMY12]. **serine-** [CLMY12]. **serotonin** [CSVCB12, CSSK+12]. **Serrano** [Mer11]. **Serrano-Andrés** [Mer11]. **SERS** [TSBSM12]. **serve** [Fin14b]. **serving** [DSRGD12]. **set** [Ali14, BVCAP12, CHH+19, CC19, Chu12, DCZ17, Fuk12, HZG12, JA12, JH15, KRC+16, KME+18, KYS13, KB19, LV12, LWL+12, MG12, NDM+12, PWP13, Rud12, SKTI15, SXH18, SZS+10, SLZ+11c, SLZ+11a, SLS+11, TPdMB12, TWR15, VPA11, VSS11, YFY17]. **sets** [ANC+15, ABA11, BŁ16, GS10, HH18, Hil13, MSNP18, PCD14, RLER14, RVO+14, UGWL18, UV18b, VRO+12, Zak13, ZF15]. **seven** [BR08, BR12a, RB08, RB11a, RNV+12]. **Seventh** [NYA+13]. **Several** [Tch16, MMM+12, SLSZ13, XZYS10, YIY+13]. **sextet** [AM12, RB18]. **sextuple** [SLZ+11a]. **SGSA** [SOF+10]. **SH** [BDF+16, BXZ+19, CdAFS+12, dSNBG08]. **shallow** [CN12, Fuk12]. **Sham** [BW18, Bar11, Gan14, KdSM+10, KFJ+18]. **Shannon** [DBTA19, JZZH17, Nag15, NTCG18, Sit15, SDL+15]. **Shape** [CL18, NMV+14, BXR+13, BVP13, KP11, LKN13, SSAM13, XWCY11]. **shape-** [LKN13]. **shaped** [BN11, KKH+13]. **shapes** [IROW10]. **sharing** [BBKO16]. **SHCl** [MZLM17]. **sheet** [BHAH+18, SJW13]. **shell** [CP16, Fin14a, Fin15, GBS17, GXZ+14, JEA13, JMPP19, KK13, DVMC19, LSC+18, MSRn+11, NSN17, NNSN17, PJ19, STM18, SDY16, XS18, YMY+13, dSdS13b, dGR14]. **shell-confined** [PJ19]. **shell-inducing** [LSC+18]. **shells** [GHP11, PUH+11]. **shielding** [Cyb11, MGK+11, NB17, RRK16, SS12]. **shift** [Bou11, Bou12a, LCB10,

MFB11, Rit12a, Rit12b, SCB+14, SK10, TKSK17, XGH18a]. **shifted** [AAHN16, Kry10, Roy14]. **shifting** [dOR10]. **shifts** [CRSB12, CFGC11, FBD+13, RR19, Tap15]. **SHN** [NRP+11, SS11]. **short** [Dum12, GST11, NWQX11, RMC19, SB16, WWL+11, XCD18]. **short-living** [SB16]. **short-loop** [Dum12]. **shortcomings** [MGN14]. **should** [She13]. **showing** [DSD18]. **shuttle** [Ali19a, FDMR11]. **SHX** [EMSB15]. **Si** [GLF+12, JL12a, MGD11, TW10, TFB11, UKF+11, VPFD10, XCL+18, ZHL+19, CN12, ENV15, Esr18, GKGM18, LKN13, LBY+14, LW18, LLLB13, MCP10, MBA+13, MSVMCI10, OD16, PWL+10, WLWL14, ZCX+16]. **Si-** [ZCX+16]. **Si-doped** [ENV15]. **SiC** [LXLL11, TCCI10]. **SiCH** [FT15]. **SiCNT** [SD16a]. **side** [DSCO+13, MPE11, NHG+12]. **side-chain** [DSCO+13]. **sieve** [SACA18]. **SiF** [KMM16, KMM16, SLS+12]. **SiGe** [LLLB13]. **Sigma** [DAC11, FC19]. **sigma/pi** [FC19]. **signal** [GSPR19, QZH13]. **signature** [GDM+10]. **signatures** [BR08, BR12a, RB08, RB11a, SCL19, ZR13]. **signed** [SK17b, SKLC19]. **Significance** [Chu12, ELC08, Kut10]. **SiH** [HCL13, RLW+13]. **sila** [FC19]. **silapolycyclic** [TYL10]. **silica** [CRSB12, SFNC+18]. **silicate** [Ped16]. **silicene** [WLH+19]. **silico** [DAA16, ST15]. **Silicon** [Cza18, GKGM18, AMK10, CSK12, DHYC19, JLS13, KAG08, KMM16, LRKM10, LHL+15, MSK11, NEEV15, RK14, RKM12, XCL+18, dSMT+18]. **silsesquioxanes** [TDOD17]. **Silva** [COP16, HS15]. **silver** [AMK10, Boe12, BPK19, RFMC19, SS18b, YJ17]. **silver-ligand** [BPK19]. **silylene** [LCH+11, LXLL11]. **SIMD** [WMK+19]. **similar** [Pup11a]. **similarities** [BB16, MK10a]. **similarity** [ART08, Luz11b, MBTVR12, MBBT+12, Sat11b]. **Simple** [QBRA18, BM16, DCR10, Fin15, FB17, KV11, Lev10, LPM+11, MA12, MT10, SAS+12, SGL+16, SGKG12, STM18, SLS+19, Szc18, TLC+17, TC12, VSL+15, YZZ16, ZT13, ZDF13]. **Simplification** [CFOC+10]. **Simplified** [GZF14, GZSMFN16]. **simulant** [HYZ13]. **simulate** [SKLC19, SKV12]. **Simulated** [TCG17, VVS+18, AM13a, Eil14, JPP+11, MOE+11, VVN+16]. **Simulating** [DMBJ15, GMA+19, MRS15]. **Simulation** [LPM+11, CwCW+11, CSK12, CS17, CTDOLA10, DKZ+10, DGR+16, DLZ11, FFF10, Fra17, FNIT16, GW18, Hog13, IFT13, IFT14, Kim19, KSST12, LCT14, LL17, Mas14, MPD+10, MPZWD10, MG12, NKKN15, Net12, NDM+12, PP10, PMH+16, SLS+10, Tan13, UTTn13, YAF+15, YT14, YINM13, ZWSF16]. **Simulations** [Hor13, MSH13, Mar13, OHDA13, SIB+13, SHS+13, UYN+13, UTTn13, YK13, ÁFV12, AF19b, ATS15, BMF+14, BM10, CLKD15, CKYR18, GVPCK10, GSR12, GSPR19, HFBC19, IKC18, Kit15, KKH+13, KFS13, LFS+11, MGN14, MM10, MMT+13, MBS+18, PDR+14, Pha19, PIS18, PPK+13, QSX+15, RP16, RNC+14, SHKS15, SBL11, TGRP19, TSH17, TPdMB12, UV18a, ZWLC12, Zha17]. **sinc** [KRC+16]. **sine** [dAB17]. **Single** [Esr18, Sri18, Bar11, Bas11, DI10, DCZ17, ETGLMJ+19, EM19, Fra17, HNBG15, KG08, LZZ+11, DVMC19, MR12, MSOV13, RLZ12, SD13a, SD16a, SVPTM+10, SWS+14, TKS11, TC10, XGH18a, YW16]. **Single-**

[Sri18, DVMC19]. **single-electron** [LZZ+11]. **single-molecule** [Fra17]. **single-qubit** [MR12]. **single-wall** [SD13a, TC10]. **single-walled** [Bas11, HNBG15, MSOV13]. **singles** [HFD11, PCV19]. **Singlet** [RRVJ10, Kim16, PCK19, RMJ11, YSS+10, ZFS+11]. **singly** [SBM16]. **singularities** [SKG11]. **SiO** [DCDD10]. **Siroheme** [SDM12]. **Siroheme-containing** [SDM12]. **site** [AO12a, BGFD14, DLJT14, DPRK12, KRH13, KSY+11, MS10, OH13, PK13a, ŚKB18, SZ11, TOSN12, TSKN12, TYN13, WH18, XCD18, dCDC+11]. **sites** [ATL+14, BSO11, LKd+16, OPF11, QZH13, RDB18, RDB19, Ser11a, Ser11b, SACA18]. **situation** [CPF12]. **Six** [Nes10, BBKO16]. **six-membered** [BBKO16]. **Size** [MW15, BHAH+18, BGL+16, GWZ+14b, GI10, Kar12b, LKN13, MPMCM+11, WLZ+12a, ZRY+13, RS09, RS11a]. **size-** [LKN13]. **size-expanded** [ZRY+13]. **Size-extensivity** [RS09, RS11a]. **sized** [Puz16]. **skeletal** [SALK19]. **skeleton** [QJ13, YD17]. **slabs** [RKM12]. **Slater** [FB17, GZF14, GW13, Hog10, JH15, RLER14, RVO+14, RRCO11]. **Slater-type** [GZF14, GW13, Hog10, JH15, RVO+14]. **slit** [YS13]. **Sm** [FMKJ14]. **Small** [CHL+19, FBD+13, LMC19, Pop19, AGB19, BMK+14, BLRdA+10, Cha11, CS13, DVDBM11, FZC14, FC19, GR11, GP13b, GHP11, HFA+19, IIS+17, KKH18, KSS+19, KSG+12, LHL+15, MSG16, MPMCM+11, MM19, MCL11, MJ14, MMV+19, MJSC18, MMRRA10, NG11, OCGM+19, PL11, Puz16, RWW+19, Riv11, SD16b, SFM13, SGG+10, SBB16, TWR15, WJL+11, WWD+15, WR14a, YZ12, dSCC12]. **small-** [Puz16]. **small-medium** [MPMCM+11]. **small-molecule** [KKH18, WR14a]. **smaller** [MC18a]. **smallest** [CWL+13, WSL+11]. **smearing** [Bas11, BG11a]. **Smirnov** [BdTG11]. **Sn** [XCL+18, XZL+12, RK14, ZCX+16]. **Sn-doped** [ZCX+16]. **SnAlO** [KG17]. **SnC** [SD16b]. **SnCl** [Bou12b]. **SnCNT** [SD16a]. **SOA** [KZZ13b]. **sobering** [KKH18]. **Society** [Brä14, NYA+13]. **sodium** [AKHS13, CAPL12, FUE+12, LZZ+11, Oni12]. **sodium-sulfur** [Oni12]. **sodium-water** [FUE+12]. **Soft** [AGRI+12]. **softness** [PC13]. **Software** [BDF+16, BHH+13, CYC+15, DOE+14, FMPM+14, KRC+16, LCZL15, MMŁ+16, MRS15, NKKN15, yOITn15, QSX+15, SDP+16, TY17, YAF+15, ZH15, ZWSF16, ZPM10]. **soil** [ATS+11]. **solar** [AGJ12, BDG17, FM16, cLqFtW+14, LYS+19, MY17, MANP17, PMAP12, QJ13, SG19, SSS15, TZ11, WWB+14, WTP+19, ZSAP11, Zha17]. **solectrons** [CEV10]. **solely** [Fuk12]. **solid** [Bon17, Fuk12, HB14, MMC+19, MSM16, MML11b, Ped16, RMLPGGGH16, RLER13b, STM17]. **solid-state** [Bon17, MMC+19, Ped16]. **solids** [DLM12, DOE+14, FB17, Jen13, KKL+16]. **soliton** [SGG+10, VBC+12b]. **soliton-like** [VBC+12b]. **Solitonic** [GNM+12]. **solitons** [BEPZ10a, BEPZ10b, CEV10, Lak10, SPD+18]. **solubility** [RGS+13]. **soluble** [GLPA10]. **solute** [Cap16, MFB11]. **solutes** [Cam10, RTG+19]. **Solution** [KC16, AMMK11, ATPRV11, BKM15, Bra10, BCF+11, Cam12, DE18, DCOC+19, FPRGMHGB12, GCDNGS12, HS11a, HR12, HFZ12, ILBS10, KS11, Kha16, LLP+13, LGZC15, Lu10, MSH13, MK10b, MPE15, MB14, QSX+15, RZSZ18, RZG12, RP16, RCM10, RW12,

Rit12b, SL10, SM10b, WXB+11, Zag11, ZKWZ17, ZI19, DM12]. **Solutions** [FKBG19, AEÖ12, EI11, HYZS12, HYZS19, LDZG16, LEU+11, PS10a, PVS11, PVS12, PT13, PGMGRM15, RMLPGGGH16, SMV11, SCL19, TIKN11, ZLJ11, ZHF12, ZPZ15]. **solvable** [GMGRMP12, Kub12, PGGRMP10, PMGMGR12]. **solvated** [CLMY12, GMA+19, HFBC19, LCCH11, LSKM19]. **Solvation** [GLPA10, MSK+12, RTG+19, AM18, BH10a, Car19, DSM+19b, FAK19, JCC10, Li15, Owe17, PCR+11, RFN+12, SL10, SLS+19]. **solvation-layer** [RTG+19]. **Solvatochromic** [LCB10, MFB11]. **solvatochromism** [Men15, MRÅ11]. **Solvatofluorochromism** [FSBA12]. **solve** [Blo15, CRA+11, Ign11, Ign12, Kri13]. **solved** [SW10]. **Solvent** [CCC19, EKD12, HR19, RdA11, RMTG11, dAVdM17, AGOP18, BS11, Cap16, CYLL11, CS17, DLO16, DFF+13, GZF13, HFL+17, IGMK11, IK14, JN13, KI15, LJK+18, LWL+12, LLC+11, LWJL10, LDW+11, LLZ+12, MG12, MKHM11, QHS11, SN12, TC10, WLD+10, XX12, XWC11b]. **solvent-separated** [LJK+18]. **solvents** [COCF+14, HFL+17, KP10, MIKH19]. **Some** [Brä11b, Jou13, Luz12, SW10, Sha18, Sut12, VATPR11, ZYL+14, AF16, AMAM18, ALB18, BCGC12, DCR10, EAK+10b, EAK+10a, EI11, For12, GCDNGS12, GB10, GI11b, GI11c, HS11b, KCC13, Kin13, MANP17, MIKH19, MAP+10, PL11, Pie12, Roy13, SGL+16, Tch16, TCA10, VO11, XHZXXZ10, ZCC11, ZLZ+14, ZZC12, Sic16]. **SOS** [RNC+14]. **SOS/QM/MM** [RNC+14]. **soundness** [Sha11a]. **source** [DSM+19b, GCK+17, Hor13, QSX+15, RAMB18]. **sources** [LTdSJ+10]. **sp** [She13, MCK17]. **space** [BVP13, BGBV12, CDT12, Fin14a, GRD11, HN12, KPH+12, MSNP18, MFLK11, MQA17, Nal12, Nal13, PC16, RW12, SH19, SKTI15, SBL11, VMR11, WWL17, ZE18, vL13]. **spacers** [LYW11]. **spaces** [ALRAE11, KK14a]. **spacetime** [RW12]. **spanning** [Bib13, LSW19, LWY19, LZZ19, PL18a]. **sparkle** [FS11]. **spatial** [ABP13, CDS+18, GKGM18, Pit12, RBTL19, SR12]. **Spatially** [AT18, CKB18, GZF14]. **Special** [AH19, ÁIGVZW12, For17a, LV16, NYA+13, NT15, ÖS12b, Rei15, Rup15a]. **speciation** [HFL+17, RDB18]. **species** [GAPK+19a, GS11, HJRO13, Kal18, MGD11, RFMC19, SSI+10, SM14b, SM14c, SM14d, SM16, SBSD18, YHLC15, dHLdS12]. **Specific** [MMM20, Cin20, LZD+11, Lya19, MMM16, MSY+12, Nic11]. **specificity** [PS10a]. **Spectra** [MLY+16, AEKGZ12, AFC+10, ÁFV12, AEM+12, Ban12, BBB+12a, BS11, Ber13b, BBB16, BBAL12, BPK19, CP10, CFP+10, CHH+19, CS17, CML+16, CLMY12, DSH+13, Eil14, FBO+11, For12, GIO12, GKGM18, ILBS10, IHG10, JPPA10, JPP+11, KV11, KBMM10, LYW11, LWL+12, LMZY15, LLP17, MC11a, MPJ12, MSK11, MMÅ13, Mor13, NBI+10, OVT+16, ORJ18, PR10a, PCR+11, PJP10, RNC+14, ŞBAT16, SB10a, SPO+11, SZZZ11, TZ11, TFSRM11, TT10, TG13, VPFD10, VVS+18, VSN+11, Zen11, ZQCJ10,

ZWLC12, ZLE17, ZSZ14, ZQXP17, ZI19, dARAV12]. **Spectral** [LLH15, Mys12, CdLdSC18, FBU+11, KP12, KM19, LYR+17, SMGZ13, XLZ+19]. **spectral-luminescent** [KP12]. **Spectral/structural** [LLH15]. **spectrometry** [ABKJ18]. **Spectroscopic** [BH10b, Jac12, Mag14, NC11, NVPCJ+13, SZS+10, SLZ+11c, SLZ+11a, SLS+11, SXS+12, SLS+12, WFS13, BD12, CHM+14, CWB+13, CJOOW11, DAE+12, GFB12a, KSSK16, LJSS12, LZZ+17, MG12, MPTZ13, QHS11, RNdA+10, Sch10b, SYL+18, SLSZ13, SWS12, Tas14, VLG12, VLFG12, VBO+15, WXB+11, YZL+10, YZL+11, ZLLS10, ZR13, dSdSPG11]. **Spectroscopical** [MSBF18]. **Spectroscopies** [KKT13, MOY13, McC13a, OA13]. **spectroscopy** [Ber13a, BDR12, BWB+18, For17b, GFB12b, LdBF+12, Mas10, MML11b, ORJ18, Ped16, Puz17, SA11b, UTTn13, YJ17, ZPZ15, RdA11]. **spectrum** [AA11, BS16, BDF+18, BBB+12b, Bou12b, CWF11, CRSB12, DSD18, DHZS11, DWGX12, HHCA10, HRT12, HMH+13, HYH+10, JCC10, KBG17, NDM+12, QD10, RS12a, SBKJ18, WWC17, Zha17]. **Speculation** [KRH13]. **spent** [HB14]. **spermine** [SGB11]. **Spherical** [Kit15, PML+11, Roy15, CH17, CB19, CN12, GAPK+19b, Nik11, OHDA13, RLER13b, RAFR18a, RAFR18b, Roy16]. **Spherical-harmonics** [Kit15]. **spherically** [JZZH17, Nag16b]. **spheroconal** [MFLK10]. **spheroidal** [OPC17]. **Spin** [BDR12, DCdG10, JR12, Kle11, Luz11a, MLK17, NKWT19, SAHG11, SAHA12, Swa13, YYI+12, ATL+14, Ash18, Ber13b, Bla15, Bra10, CR18, CCP18, CYL+18, CFGC11, CSP+10, CDT12, DS11, DM16, FSST16, GXZ+14, GLXL18, GFRdG11, Joh17, Kap12, KK14a, KV19, KSN+10, KYH+13b, LVdSdM14, LWL+12, LB19, Luz12, MR12, MPRB+10, Mos14, MC18b, NSN17, NNSN17, OS10b, PBR18, Pon19, Qu13, RS12a, RLZ12, SR12, SRASZ16, SSP+17b, SBD+16, TÁ10, TD11, WH12, Yos20, Yur13, Yur15, ZSQ+10]. **spin-dependent** [DM16, NSN17, NNSN17]. **Spin-free** [Kle11, Luz11a, Luz12]. **spin-Hamiltonian** [TD11]. **Spin-inversion** [NKWT19]. **Spin-orbit** [MLK17, Ash18, CYL+18, KV19, MC18b, RS12a]. **spin-projection** [KYH+13b]. **spin-restricted** [KYH+13b]. **spin-spin** [CCP18, CFGC11]. **spinless** [NF11]. **spiro** [LLLB13]. **spiro-heterocyclic** [LLLB13]. **spiroborate** [QCW+12, WTZ+11]. **spiroiminodihydantoin** [SM13]. **spline** [HZS14]. **split** [GRD11, WLS+19]. **split-graph** [GRD11]. **splitting** [GWM11, HYH+10, SYK+12, SSK+12, Tan13, WTP+19, YYI+12]. **Spontaneous** [CCM08]. **spread** [BEM12]. **square** [LGHL11]. **squaric** [DLM+11]. **squeezed** [PSGK17]. **SR** [MC18b, MPD+15, MGP16, Oni10]. **Sr-doped** [Oni10]. **SrBi** [HLMO11]. **Src** [ZFW+13]. **SrH** [HMI+15]. **SrTiO** [OH13, WCL+17, OH12]. **SS** [SZZ+12]. **SSH** [DTFK15]. **stabilities** [AF16, MS17, SFW12, SUL+11, SM14c, ZYL+13, dAVdM17]. **Stability** [GV11, KZA+17, Kry11b, LWL19, MC12, PMEP19, TLC+17, USL+13, BMX+19, Boe12, CCC19, CYL+19, CWSZ13, DVC14, FBRBR12, GJ18, GB13, GAMM10, GWJ12, HLB19, Ire12, KK11b, Kry12b, LGHL11, LCZ15, LGS+16,

MNV+17, MC17, MCARL11, MMW19, MJ14, MMV+19, MM10, MS14b, MHHPR+17, Ng12, NRI15, ONK+13, Owe17, Pat15, PP19b, RSN12, SDS19, SDS20, SFNC+18, WJL+11, WCS+13, WJL+10, YZ13, ZBBB17, GCD13]. **Stabilization** [YZZ15, HR19, JdL08, MK11, OKR12, SBMM11, YD17]. **stabilized** [KUS19, LW18, XGH18a]. **stabilizer** [OKK10]. **Stabilizing** [GAPK+19a, MK12, PCML08]. **Stable** [Sat11b, BMF13, MPM15, MAN15, PAPCMM+16, fXxBhD19, ZCG+16]. **stacked** [NMS+10]. **stacking** [ACF+11, DB15, FSB16, KdPNNS16, LB18, MHZ18, ZS12]. **stacks** [FV11]. **stage** [Kap12, KYLC19, SZ15]. **stages** [LJ16]. **Stagnation** [PL11]. **standard** [KGK13, PJP08, Tug13]. **State** [HXX15, NBZG16, Nic11, ACF+11, Ang10, BPVDB11, BMF13, Bon17, Cao17, CMCN11, Cha11, CJOOW11, DGA+13, EMEPD15, FRGC10, FSBA12, GBK18, GSaY11, GWZ+14a, GWHH17, GRLA18, GLXL18, Glu13, GLOGM+11, HM12, HhGqZZ17, Ign11, Ign12, IIH16, IGMK11, JA12, JWJ+12, KAR12a, KYLC19, KFY+12, Kri13, LSL+08, LV12, LJSS12, LdAA+11, LZ10, LKd+16, MMP+18a, MPC10, MMC+19, MPT11, MPTZ13, MM13, MML11b, NZ13, OH19, Ped16, PGMGRM15, Per10b, PMAP12, RMJ11, RAGM10, RRCO11, SY10, SFM13, SGC13, SM14b, SS12, SZY17, TXK+19, THVP14, TB15, UV18a, VPA11, WKE17, YÇÖ11, YXM+18, Zak13, ZST+10, ZZ18, PB10]. **State-** [Nic11]. **State-of-the** [NBZG16]. **State-of-the-art** [PB10]. **State-to-state** [HXX15]. **statement** [Brä14]. **states** [Agb12, AM12, Ali19b, ADB10, ARG11, ALA15, AY15, Ban12, BG11b, BG11c, Buc11a, Cam10, CR18, CHM+14, CM16, CHSO13, Coo12, Cor16, DM12, DS11, DAR+11, DLRMFY10, DTPC17, DG19, DCHC11, DSSM18, DSSM19, FSK+11, GFB12b, GFRdG11, HK11, HGB08, HFD11, HMA+18, JH13, KH10, KT12a, KMF+11, KK14b, Kim16, KGVG11, Kit15, KZZ13a, KHH10, KKT13, KKT14, Lad14, LVdSdM14, LV16, LCL+10a, LP10b, LCL+11, LGP+11, LGP+12, LGZC15, LDADB+15, MPM15, MMWA11, MT11, MSM16, MQG13, MKD19, MPRB+10, Mor13, MNS11, MB12, NS19, Nal15, NDP10, Nic11, PE11, PSGK17, PRPU+13, Pup11a, RS12a, RAN18, SBMM11, SBM16, SFW12, SGG+10, SYL+18, SXS+12, SLS+12, SLSZ13, SR11b, SZZ+12, SFY12, SK12b, SCZG12, Swa13, Sza13, TTT13, TÁ10, TBB+19, TD19, VLFG12, VO12, WFS13, WC14, WJL+10]. **states** [XTLA13, XTLA14, ZCG10, Zil14]. **Static** [CCEGK12, CEFMK12, KA11, MNS11, BŁ16, FKL+12, FSB16, GH11, IOO18, LXW+12, dWLC14, MA11b]. **Stationary** [TIKL13, KMNSP19]. **Statistical** [BW15, Lun13a, Lun13b, Tou13, MPE15]. **statistics** [GTSC+19]. **status** [TSvL+16]. **stealing** [NMSR14]. **steel** [EAK+10b, EAK+10a, EI11]. **steered** [NWQX11, TSH17]. **step** [Jan13, SR11a]. **Stepanov** [Pup11b]. **steps** [Cys11, SLS+19, VVAO12]. **Stepwise** [LLL16, Pat15, DP12, LCM+11]. **Stereo** [YGL+11]. **Stereo-dynamics** [YGL+11]. **stereochemistry** [KMS+11]. **stereodynamics** [Kan11, YZ10]. **stereoisomers** [HHYC+18]. **stereoselectivities** [LD17, LFTL18]. **Stereoselectivity**

[ZXY13, CM12, ZQW+17]. **Steric** [GWM11, Dil13, TV13]. **sterically** [SBEH11]. **stilbazolium** [IGMK11]. **STO##** [VRO+12]. **STO##-3G** [VRO+12]. **stochastic** [MPMCM+11, NTCG18]. **Stockmayer** [HFBC19]. **stoichiometric** [AGCVG15, ALA15]. **storage** [BCGC12, CHL+19, CTDOLA10, GZ14, GZMC11, Ném14, NMIP14, Pha19, UDS19b, ZDF13]. **stories** [Tch16]. **story** [Kut10]. **strain** [AKR12, DLLA10, MMM19]. **strained** [Iku17, KBJ17]. **strains** [KK12a]. **strategies** [GAI19, WR14b]. **strategy** [BBB+12b, CL08, She12, YZZH15]. **strength** [ACL12, BPG+10, CG12, Den19, RB11b, SACA18, WLC+17]. **strengths** [BHH+13, MS14c, RLTAT19, RBZ15, ZYL+14]. **Stress** [LHX+19, Fin14b, GAI19, JMX+15, MPV+11, NIT16, XXJ+16, XWP+18, YXM+18]. **stretch** [GPM+15]. **stretched** [HB14, MJ16b]. **stretching** [CLXZ12, ZZ15]. **strong** [CL11, CSS16, DR18, DLM12, IROW10, Kit14, RDB19, SRPD16, Sto18, Vik11a, Vik11b, Vik13]. **stronger** [DI15]. **strongly** [Cap16, DM12, Dun15, Jia15, TKN13, WH18]. **strontium** [HMI+15, MMR+10, MHOG18, SSP+17a]. **Structural** [AGCVG15, CWW+16, DKS11, LZW+15, MPM15, MPTR12, MFR10, MMCN+11, MMRRA10, QHS11, QCB+10, SBEH11, TCSD12, TCG13, YLWrL12, ZHI17, ZCTG18, ART08, AVG19b, CWB+13, DMBL16, DHYC19, EPS+16, GAPK+19a, GKGM18, GMP+11, IAK13, KG17, LLH15, LZ10, MB14, MSK+12, MA11a, MKHM11, MW15, ORJ18, Pan19, PP19a, PK13b, RJY+10, RNdA+10, TOSN12, TBST10, TFB11, VLG12, WTH+11, WLL+13, WWD+15, YD17, ZWLC12, dSdSPG11]. **Structurally** [fXxBhD19, DC14b]. **Structure** [AKHS13, Ber13a, BMBD10, Boc17, CM15, CYL+19, FBRBR12, KSG+12, KKT13, LYW11, MMMM12, MCARL11, MOY13, McC13a, MTS15, OA13, Owe17, PAKA15, SIT+12, TBA13, Wu11, YSK+12, AB16b, AEKGZ12, AO12a, Ale13, ATS15, BZBZ13, BL10, BBYZ18, BG11b, BG11c, Bou11, Bou12a, Bou12b, BA13, CLL+11, CZJZ12, CWL+13, CJSNLM11, Cas15, CSVCB12, CJOOW11, DCBB11, DIOG12, DVC14, DSD18, DDÇY12, DMBJ15, DD17, DG19, DGA+13, DZO12b, DSH+13, D'y16, ETGLMJ+19, ESLM19, FLvLA15, FBO+11, Fin14a, Fin15, FBU+11, GBS17, GSZ10, GZ14, GP13b, GEL18, GJ18, GRCATG19, HMI+15, HMA+19, HLMO11, HLB19, HJ13, IGMK11, IK18, JWG+12, KS11, KK11b, KA13, KK11c, KRK+17, KJ15, KJ16a, KJ16b, KSD10, Kle11, KSY+11, KAOB11, KP13, KS18, KO12, KM19, Leh19c, LJW+11, LS19, LLLT12, LZZ+13, Lya14]. **structure** [Ma14, MMP+18a, MC11a, MY17, MSG16, MSH13, MPD+15, May14, MBA+13, MPZWD10, MCL11, MGB18, MS14b, MKM11, MLB+10, MJ11, MCRS16, NDM+12, PCML08, PT13, PMMGL+11, Puz10, QTCL10, RFN+12, RS12b, RKM12, RGTS11, RGST12, RAFR18a, RAFR18b, RMTG11, Rus14, RMY+13, SMK+12, SC12b, SB16, SRS+17, SSTÖ11, ScBsR+10, SSW16, SBKJ18, SCL19, STU19, TNT18, TZD+19, TD11, TSH17, TG13, TPCJ+12, Var14, VLM+10, Ven12, VSS11, VBO+15, WCS+13, WSV10, Yak11, YLW+13, YRN+11, Zha10, dOLdlV13, GFB12b, GGD12, NA12]. **Structure-dependence** [KSG+12]. **structure-property** [RGST12].

structure-stability [DVC14]. **structured** [Kim18]. **Structures** [CdAFS+12, GLT13, GCD13, IA13, JL12a, KBF+13, LFP+19, LHL+15, MS17, ONK+13, SM16, YWH+12c, ACMRN10, ALK18, ALK19, BMB10, Brä11a, BSO16, DWGX12, DM16, GR11, GLF+12, GZ14, GWJ12, HWL16, HWWW18, HM10a, JMPP19, Kim13, KSSK16, KYLC19, KMM16, Lad14, LL11, LWL+12, MZB+13, MK10a, MLW10, MUNZVR12, MUPC10, MJSC18, MM13, NH18, NZAVR10, OCGM+19, Puz16, QJ13, SSK+12, SLS+14, SIS+08, SACA18, SZZZ11, SKY+13, SCZG12, TSKN12, TYN13, TBB+19, VSN+11, WGLX10, WDS19, WJL+10, XTLA13, XTLA14, XWC10, XF19, YYI+13, YZL+10, YZL+11, YZW+15a, YC13, ZLLS10, ZZR+12, ZL12, ZQXP17, dHLdS12]. **Structuring** [KRG+13]. **studied** [AMMK11, BL10, CK17, DCHC11, FBO+11, SJZ+18, TTM16, ZL10, dSdS13b]. **Studies** [PCF+18, Roy13, ACF+11, AMK10, AVG19b, BD12, Buc11b, CJBMMAPR19, CCA+12, ÇAS13, CYLL11, CTW12, CWB+13, CSVCB12, CSSK+12, DSWL11, DSZB18, DB15, EAK+10b, EAK+10a, EI11, For12, GGD12, GKT+12, GZBH18, HTM10, HNBG15, Hop15, HWL16, JL12b, KDÇ12, KMM+18, KA13, KSY+11, KAOB11, Les12, LWL+12, LSR+13, LBY+14, LGZC15, LWJL10, LKLW11, MANP17, MLPT10, MAP+10, MMM+12, MSAB19, NTCK13, ONBP11, ÖEDB11, PBM10, PTD+12, PETB18, PAPCMM+16, RJY+10, RJA+10, RGTS11, RNdA+10, Ril10, Riv11, RGS+13, RGR12, Roy14, SMK+12, SD16a, SC12a, SJZL12, SIS+08, SK12b, SZ15, SSB+12b, TIKN11, TOSN12, TYN13, TAY11, Tan12, TIN13, TXL10, THSR13, UJSJ13, VGGPdL19, VPOG19, WZX11, WTH+11, Wan13, WZM+13, WYWL13, WLH+19, WHM14, Wit18, WWGW18, XS18, XFW+14, YZL+10, YZW+15a, YB11, ZZL+11, ZZX10, ZYZ+11, ZQJW13, ZLWY13, ZLZ+14]. **studies** [ZWL18, ZSZ14, dAGNJT12, YWY+12]. **Study** [Bar11, BWB+18, CH17, CYL+18, IFT13, IFT14, SGL+16, SS19b, ZCP11, AC19, AFC+10, lAyL14, AM12, AASU+17, AEAS+19, ATM17, AKC10, ASW13, AVG19a, ASD14, AMAC12, AG19, BMK+14, BD14, BF11, BCGC12, BDF+16, BDF+18, Bas11, BAMA12, BLB+18, BLR12, BS11, BEM11, BZBZ13, Ber13a, BL11, BLRdA+10, BHAH+18, BS14, BSSS19, BZZ15, yBZfC18, BXZ+19, BDG17, BLdV19, BMF13, Bon17, BGJSM+18, BDR12, BCF+11, BPSM12, BLM+12, BJ17, BJdlMAV12, BTH18, Buc10, BO11, BVRM10, BCS+12, BB16, BSV12, BSPK11, CRB+12, CMR13, CAZ+11, CLXZ12, CCL+13, Cao17, CPL15, CPF12, CCBR+12, CHM+14, CHH+19, CG12, CW16, CM12, CCL+10, Che12, CCS13, CWW+16, CZLD17, CLY12, CS13, CWS15, CZCW19, CK13, CFGC11, CGIAI12, CAPL12, CPAT11, CJOOW11, CD12, CS18, DWJZ11, DCBB11, DIOG12]. **study** [DMAB12, DAR+11, DSD18, DKS11, DPK18, DS12, DCDD10, DSRGD12, DPRK12, DPDR11, DTEMK11, DZ11a, DLO16, DG19, DMS+10, DCdG10, DDF+12, DdG+11, DQZF12, DWGX12, DSH+13, DCR10, DSFT17, DFF+13, EG10, ESDO16, ELC08, EAH13, EFO11, EO11, ETGLMJ+19, EBH11, EA12, ENV15, ES17, Esr18, EM19, ESBVJY12, FSQ+11, FZX18, FFF10, FO10, FM16, FTB11, FRNM12, FDNR10, Fin14a, FT15, FPRGMHGB12, FBU+11,

Gag11, GBS17, GWM11, Gao12, GLF+12, GGJD13, GZW16, GHGF12, GK12, GLXL18, GIO12, GFB12b, GC18, GP13b, GMT16, GMT18, GS11, GLOGM+11, GHCMCMQ17, GB18, GWME18, GD11, GSB10, GT13, GTSC+19, GGP13, GLPA10, GCZ+14, HNH+12, HMA+19, HK11, HDC+11, HLJZ11, HLZ+14, HZZ+19, HFD11, HHL12a, HHL14, HM12, HM10a, HKLW13, HZZW11, HFL+17, HHL+12b, HhGqZZ17, IIW+11, Iku17, IGMK11]. **study**
[IM15, JPPA10, JN13, Jal10, Jan10, JB18, JS17, JCCZ12, JSLH14, JLZ+17, JB11, JWG+12, JFDD10, KM12a, KS11, KWC10, KWC11, KP11, KBF+13, KKM+12, KI15, KI12, KK14b, KSAK17, KZZ13a, KZZ13b, KUTS10, KKT13, KKT14, KG08, KO12, KMU+13, KK11d, KBMM10, Lan10, LLF+12, LGM+18, LLM13, LKOS17, LJK+18, LVdSdM14, LPOP12, LZB10, LCL+11, LJL+11, LW11, LJW+11, LYW11, LGP+11, LMZ+11, LGP+12, LLP+13, LWX+14, LLL16, LYR+17, LLF17, LD17, LZW+18, LTL18, LFTL18, LLW+11, LLC+11, LGW11, LCZ15, LL19, LCCH10, LLZZ10, LCCH11, LJSS12, LXW+12, LWZ+14, LL17, LLW+12, Lu10, LWC+10, LCS+11a, LCH+11, LCS+11b, LXLL11, LLLB13, LW13, DVMC19, LKZ+16, MYZ+10, MLW+14, Ma14, MY17, MAD12, MBKH19, MSG16, MZB+13, MFB11, MK10b, MK12, MLC+11, MCP10, MMR+10, MCC12, MVG18, MP12, MTL+12, MSC10, MMW19, MOY13, MMWA11, MMC+19, MUNZVR12]. **study** [MUPC10, MDNDO+16, Men10, MFZ+18, MCL11, MKSG13, MS17, MHHPR+17, MM11, MSK+12, MPL+11, MGD11, MTS15, MPRCEG12, MMRRA10, MML+11a, MLB+12, MBBT+12, Mor11, MM13, MG10, MMF+13, MSRn+11, MSOV13, MCRS16, MOH+12, ND11, NS10a, NHG+12, NDH10, NBL12, NAK+17, NTNL10, NL11, NFQ+11, NHB12, NRGS11, NRS+11, NRP+11, NRHJ11, NJA+12, NIT16, NZAVR10, NEEV15, OAC17, OPC17, OAA19, OH12, OH13, OCB+10, OPP+14, OMĐ13a, OM13b, OD12, OD16, POLV12, PS13a, PEA+12, PTS+11, PWP+18, PDNC14, PMH+16, PE11, PWL+10, PSKV19, PK13b, PKK14, PRG+10, PAD+10, PRPU+13, PM17, Puz10, QHS11, QCW+12, Qu13, RYM12, RFN+12, RGPZD13, RRVJ10, RS12b, RSN12, RSM12, RCM+19, RD14, RRRV19, RGST12, RDB19, RYW+15, RI19, RCM10, RJLPGH+13, RDM+11, RBVAG18, RNE10, RNB+10]. **study**
[RS11b, RRB12, SF13, SB18, SSB19, SIT+12, SK14, SD16b, SBEH11, SSK11, SVRGV12, SB10a, SKHN13, Sat11b, Sch12a, SK17b, Ser11a, Ser11b, SLS+14, SKS11, SHL+13, SLSZ13, SHE10, Shi13, Shi18, SL10, SKM11, SM13, SR13, SSTÖ11, SLA12, SK11, SR18, SSA18, SSP+17b, ŚKB18, SMA11, SZ11, SBB16, SZZZ11, SZZ+12, SLZH12, SHW+13, Sri18, SMGZ13, SK10, STU19, SYQ+10, SWS12, SWS+14, SZL+14, SZL+15, SGL19, SYY16, SCZH16, SS13, TK16a, TV13, Tav11, Tav12, TM13, TT10, TDOD17, TU10, TYL10, TSL11, TFZ+15, TJS17, TFA10, TSH17, TFB11, TCCI10, TGA+11, Tug13, TWR15, TPT+13, TPT19, UKF+11, UMS13, VF13b, VPGC12, VFCSC17, Var11, VHTEG15, VVN+16, VLM+10, Ven12, VSMK13, VSMK15, VV12, VV13, Vie17, Vik13, VKF+19, VDG13, VS19, VO11]. **study**

[VO12, WML10, WXZ+11, WJL+11, Wan11, WvRSW+11, WLL11, WLG+11, WLWT12, WLZ+12a, WLZ+12b, WWHZ13, WHS+13, WHY+14, WJY15, WTW+15, WDJ+17, WWQG17, WG18, WZZL10, WTZ+11, WWX+11, WLD+10, Wu11, WSL+11, WZC+12, WRW+18, XNL+14, XX12, XSLF12, XGH18a, XLLZ10, XZCH11, XZ11, XWC11b, XGH+18b, YM12, YM13, YNLD18, YYS15, YY18a, YY18b, YZL+11, YZZH15, YZ12, YZZ16, YLZ+17, YZ10, ZKKR11, ZSAP11, ZSASS13, ZAE10, ZLR15, ZRGE+19, ZWWY10, Zha10, ZLLS10, ZZW11, ZLZ+14, Zha14, Zha15, ZLWL16, ZCX+16, ZKWZ17, ZBG+19, ZSQ+10, ZRR+11, ZPB12, ZSS+13, ZLWZ16, ZTC11, ZQXP17, ZLY+14, ZPW16, ZBBB17, ZDZL11, dSdSPG11, dSdS13a, dLRR11, dOR10, dOdONM12, dlLIAI+12, BVP13, SW12]. **Sturmian** [FRGC10, SS12]. **styrene** [DPDR11, MCC13b]. **styryl** [TPT19]. **styryl-bodipy** [TPT19]. **styrylnaphthalene** [Bud12]. **styrylnaphthalenes** [BO11]. **styrylquinolines** [BO11]. **subcluster** [ALA15]. **subgroup** [BSPK11]. **subphthalocyanines** [PZ19]. **subsidiary** [LWY13]. **Subspace** [TG16]. **subspaces** [TLC+17]. **Substituent** [BHMN19, EHKD11, EEMSS14, MKHM11, RY12, YRN+11, dSNBG08, DWZZ15, EAV16, JNY17, Val17, XX12, ZBG+19, ZYL+13, ZBBB17]. **substituents** [AG10a, AMK10, KMM+18, LZZ+17, SN11, WDS19, WLC+17]. **substituted** [AAA12, ASD18, BG13, CLXZ12, EHKD11, EKD12, IGMK11, IUMVB10, JLL11, KMMS17, lLBqD+19, MXC18, NAK+17, NZAVR10, PS13a, PP19b, PSK+13, RLTAT19, SSKS12, SN12, SMGZ13, SZL+14, SC18, TT10, Tug13, VSN+11, ZLY+14]. **Substitution** [SPIL14, Buc10, Buc11a, Buc11b, EMS16, HLJZ11, JLG+12, ND10, RFN+12, Ril10, RB11b, dAB17]. **Substitutional** [BSO11, KSS+19]. **Substrates** [dSSdSGA12, FBD+13]. **subsystem** [MA10, NS10b, Sha11a, YKN13, ZS11]. **subsystems** [GHP11, HS11c]. **subunits** [Sch15]. **subvalence** [dCDC+11]. **Successes** [Swa13]. **successive** [SM14b]. **such** [Ser11a]. **sudden** [CLXD15]. **suddenly** [MAPS18]. **sufficiently** [MK10a]. **sugar** [BS14, SKM11]. **sulfate** [CAPL12, FMP+17]. **sulfate-methane** [CAPL12]. **sulfated** [MCRS16]. **sulfenate** [ZAE10]. **sulfide** [BAP13, DWJZ11, JAB12, MA11a, MTS15, SSP14, TCSD12, YGLL10, YLZ+17]. **sulfinyl** [SFW12]. **sulfite** [SDM12, SBSD18]. **sulfonamide** [TPdMB12]. **sulfoxide** [LdBF+12, ZAE10]. **sulfur** [CK17, DI11, DSFT17, GFRdG11, GCD13, KM19, LKd+16, NFD+10, NFQ+11, Oni12, SFW12, SCB+14, dLdOdAD12]. **sulfur-** [NFQ+11]. **sulfur-containing** [NFD+10]. **sulfur/selenium** [KM19]. **Sulfuric** [dLdOdAD12]. **sulphonamides** [EAK+10a]. **sulphuric** [SMRK18]. **sumanene** [ONK+13]. **Sup** [LJ16]. **super** [Man16, MBSAG16a, MBSAG16b]. **super-resolution** [Man16, MBSAG16a, MBSAG16b]. **Superacidity** [VV18]. **superacids** [CS18, Val17]. **superalkali** [TL15, WCY+10]. **superalkalis** [STM18, Sri18]. **superatom** [JHL+18, YLWrL12]. **Superatomic** [MCK17, GAPK+19b, MC18b, TFMC19]. **superatoms**

[GAPK+19b, TFMC19, TFB11]. **superbases** [ÇT14]. **supercomputers** [CLKD15]. **supercomputing** [GE12a]. **Superconductivity** [DB13b, Lar10, BCP10, Dun15, MC14, SM10a]. **superconductor** [HKIH13]. **superconductors** [GdLT12, PK13b]. **supercritical** [BBB+12b, Ma14]. **superfluidity** [ZLR15]. **Superhalogen** [SMC18, SR13, Sik18, SM14b, SM14d, SM14c]. **Superhalogen-supported** [SMC18]. **Supermolecular** [MSM16]. **superoxide** [CWZ+10, PM17]. **superpolyenes** [NKF+13]. **superposition** [MBBT+12, VSS11]. **supersymmetric** [KB12, MPB11]. **Supersymmetry** [DJ95, DJ12, MB12]. **support** [ZCX+16]. **supported** [BAB+18, BJdlMAV12, Esr18, GLT13, SMC18, ZCW16]. **supports** [SAHA12]. **suppression** [YYI+13]. **supramolecular** [BMRM19, BHA19, Den19]. **supramolecularly** [KMK+16]. **surface** [BPVDB11, BP13, Bud12, DWPK14, ESBVJY12, FSK+11, GB18, HJRO13, JdL08, JK12, KK19, Kim18, KF17, LV12, LLL16, LDZG16, LDADB+15, MMG15, MCP10, MFK+12, MTL+12, MMC+19, MOE+11, MOLF11, MSVMCI10, MNE+13, MGD11, MPRCEG12, NA12, NTNL10, OD16, PP10, PWL+10, RCP14, RJLPGH+13, RSCS10, SCLCPB12, SR19, SPD+18, SB16, SXH18, SYS14, SZ15, SZY17, TFSRM11, TNN16, TBRIS10, TBRIS11, TSBSM12, TSL11, TBST10, TCCI10, VDG13, WWQG17, WZC+12, XGH+18b, YLC17, YLYC18, ZWWY10, ZLWY13, ZWL18, ZRLV10, ZDZL11, dLdOdAD12, TBRIS12]. **Surfaces** [TBRIS12, AA11, ART08, ATS15, BWW10, BAP12, BM16, BH19, CNBPR+11, CSMZ10, FFF10, FDA16, HDÖS12, HLZ+14, Hog13, HB14, HCL13, IAA15, KMNSP19, KMM16, KJ14, LRKM10, LFF+10, LZFZ13, MDC15, McC13a, PML+11, RYW+15, RFMC19, SSAM13, SRS+17, TBRIS10, TBRIS11, VPA11, WKE17, ZK12]. **surfactant** [BMB12]. **surfactants** [THSR13]. **Surprises** [DB12]. **Surprising** [KSG+12]. **survey** [Mai14, ZJC+13]. **survival** [LS17, LRP+11]. **susceptibilities** [KC11]. **susceptibility** [RP11a, SC10a]. **swarm** [SRS+17]. **switch** [CHL+19, CHV14]. **switched** [Kit14]. **switches** [XWP+18]. **switching** [HGB08, KB12, LYL+12]. **SWNT** [Jal10]. **SWNT-amino** [Jal10]. **Sylvio** [Ano11a, RdA11]. **symbols** [Ols11b, RBD+10]. **symmetric** [FDG18, KC16, KC18, KS18, Mit11c, Nag16b, NTCG18, PBB15, VSN+11, WH12]. **symmetrical** [CG12, KSS+19, RSN12]. **symmetries** [Brä13]. **Symmetry** [GAPK+19b, RBGGM18, AEÖ12, Ale13, Ali19b, BMB16, CR18, DLCB15, Fer19, FDNR10, GFRdG11, GMP+11, Lad14, Luz11a, MK11, NSN17, NNSN17, Nas19, PL11, RS09, RS11a, SR12, SC10a, Tob19, TPCJ+12, WLZ18, XTLA13, XTLA14, YIY+13, YKN13, ZWE12, SSK+12]. **symposium** [DC12, DC10, ÖS12b]. **syn** [CCC19]. **syn/anti** [CCC19]. **Synergistic** [YKN13, OGvSG18]. **synthase** [PTD+12]. **Synthesis** [MPD+15, CLY12, CLH14, LCCH10, LCCH11, LL17, LW15, ZYSW17, ZBG+19]. **synthesised** [JPPA10]. **Synthesizing** [YW16]. **synthetase** [ST15]. **system** [AEKGZ12, Bae14, BPL13, BEM11, Ber13b, BKM15, CAPL12, DLM12, Gan14, GFRdG11, KB12, KPL+17, KO10, KMU+13,

LDKB15, LZZ+11, LCCH11, Lun13a, Lun13b, MR11, MFM18, NMIP14, QSX+15, RAN18, RNdA+10, SDS19, SDS20, SW10, Tou13, VLK+11, Xu16, Xu19, ZX12, ZWL18]. **Systematic** [KSS12, WR15]. **Systems** [GLT13, IA13, KBF+13, ONK+13, ARG11, ACT19, Bae16, BR08, BR12a, BBB+12a, Brä11a, BDPT12, BWE16, BBA+16, Cap16, CJBMMAPR19, CAPGAIG18, CH17, CS13, CP11, CP16, DMAB12, DLRMFY10, DBTA19, DCDD10, DI18, Dun15, DB15, Fer19, Fin16b, FSST16, GB10, HS11a, HITU16, HFdGC14, HKLW13, IFT14, JE10, KH12, KK13, Kha16, KCC13, KSD10, KSN+10, KYH+13b, Kon11, Kry11b, Kry12b, KM19, Lad14, LS17, LV16, LGZC15, LC19, LRMAA19, LZD+11, LNI12, MCCGM+19, MMM19, MANP17, MNP19, MC11b, MSAB19, Nag16b, NKF+13, NDH10, Nas19, NGS11, NYS+10, NMV+14, OPC17, Per10a, PBB15, QTCL10, RB08, RB11a, RAMB18, RAGM10, Roy15, RS13, SLG11, ŞBAT16, SSK11, SMV11, SK17b, SKLC19, SHKS15, Sko16, SKV12, SMMT13, SBSD18, Swa13, TFSRM11, Tok16, TRZ+19, TC12]. **systems** [VOAH18, WCM14, XTLA13, XTLA14, YYI+12, YWH12a, YWH12b, YFY17, Zak16, ZWE12, dGR14, dOR10]. **systems*** [Mam14]. **Szeged** [Tra19].

T [BL12, BTH18, CPF+11, SLS+11, ZHL+19, GWM11, BBM17, BTH18, SD13c, WLL+13, XLLZ10, YGLL10, dOR10]. **T-cell** [WLL+13]. **T-junction** [SD13c]. **T4** [DFF+13]. **table** [Gar08, GI10, Kut10]. **Tables** [Rus14]. **TACA** [Ser11a]. **tailored** [GbZA10]. **tailoring** [AV19, BHAH+18, MMA10]. **take** [PUGSFM18]. **tame** [DB13a]. **tardy** [FK18]. **target** [HM10b]. **targets** [PUH+11]. **tartaric** [LCZL11]. **tautomer** [dAVdM17]. **Tautomeric** [SOM10, CCL+10, JN13, LDW+11, NRS+11, NJA+12, TSH17]. **tautomerism** [HS11b, PS13a, VF13b]. **tautomerization** [JS17, YY18b]. **tautomerizations** [MPGGS19]. **tautomers** [KAOB11, LCH14, Tav11, Tav12, ZR13]. **Tayloring** [PJP08]. **TB** [ZCP11]. **tBu** [HHL12a, HHL14, PP14]. **Tc** [ZLY+14]. **TCDD** [WWX+11]. **TCNE** [TD11, KBMM10]. **TCNE-methylsubstituted** [KBMM10]. **TD** [AFC+10, BDR12, JPPA10, ACF+11, BVCAP12, FPRGMHGB12, KI15, LJ13, Mas10, dSM19a]. **TD-DFT** [KI15, LGS+16, dSM19a]. **TDDFT** [WKE17, BGFD14, BAA+18, BHAH+18, ESDO16, HKLW13, IHG10, LYW11, LZ10, MMWA11, PJP08, PSK+13, VSN+11, YZW+15a, ZSAP11]. **Te** [AM18, BHA19, WSML16, XWC11a]. **tea** [MKHM11]. **Technical** [MMP11]. **technique** [KdSM+10, LKJ13, MJSC18, SR12, SOF+10]. **techniques** [DW12, LSR+10a, LSR+11, MQG13, Ols11b, RW11, SKV12]. **technology** [YSA+11]. **Teller** [DMAB12, AGPDZ13, DMAB12, GFB12a, HR12, HFZ12, JZP17, RGPZD13, SBD+16, TPCJ+12, WLZ18, YYI+13, ZFC12]. **Teller/Renner** [DMAB12]. **telluride** [KG08, MW15]. **tellurium** [ESDO16, RR19]. **tellurium-containing** [RR19]. **temozolomide** [KdPNNS16, KMMS17]. **Temperature** [Buc12a, GFPAV19, KKH+13, MKSG13, PMMGL+11, Boe12, CAAI12, CS17, Dun15, KAR12a, lLBqD+19, LL19, MOH+12, Nag17, TD11,

WCGD12, ÁFV12]. **Temperature-dependent** [GFPAV19, lLBqD+19]. **Temperature-programmed** [ÁFV12]. **temperatures** [Chu12, STM17]. **tendencies** [SMP10]. **Tensor** [SPM+15, BL19, Fin14b, JMX+15, LHX+19, Lya14, NIT16, XXJ+16, XWP+18, YXM+18]. **Tensorial** [SD13c]. **tentative** [YFY17]. **terephthalate** [TIN13]. **term** [IIH16, Ols11b, ZLJ11]. **terminal** [SLS+15]. **terminated** [dLdOdAD12]. **Terms** [Gin10, Glu13, KL11, PE11]. **ternary** [KYLC19, MS14b, OGvSG18]. **tert** [AMAC12, Pli18]. **tertiary** [MMM+12, PCML08, SAG13]. **test** [DAA16, Mar12, PWP13]. **Testing** [FCS13b, KK14a, FCS13a]. **testosterone** [KKM+12]. **tetra** [QJ13, SSA18]. **tetraammine** [MGK19]. **tetraanions** [DZO12a]. **tetrabenzoporphyrin** [LGS+16]. **tetracarbide** [PKK14]. **tetracarbindane** [ALK19]. **tetracarbon** [ALK19]. **tetrachloride** [YSA+11, ZSZ14]. **tetracoordinate** [YD17]. **tetrad** [DKS11]. **tetrads** [DKS11, DKS11]. **tetrafluoroborate** [MFK+12]. **tetrafluoromethane** [VVJ15]. **tetrahedral** [GAPK+19a, IIW+11, MPRB+10, Pup11a, RFEGPP+16, TGA+11, WWQG17, YGLL10]. **tetrahydrofuran** [dSdSPG11]. **tetrakis** [ZSASS13]. **tetramer** [FRNM12]. **tetramers** [MFOH18]. **tetramethyltin** [DAE+12]. **tetranitride** [XXJ+16]. **tetranitrooctahydroimidazo** [CC11a]. **tetraphene** [ZLS+18]. **tetraphene-bridged** [ZLS+18]. **tetraphenylbutadiene** [VVS+18]. **tetraphenylimidodiphosphinate** [SLS+14]. **tetrapyrrole** [ZQCJ10]. **tetrasulfonate** [DZO12a]. **tetrasulfur** [XXJ+16]. **tetrazole** [PP19b]. **Tetrel** [XCL+18, WLC+17, ZHL+19]. **TH** [ZHL+19, dOR10, JLL+18, LNGW14, LYW+19, NZLG15]. **Th-based** [LYW+19]. **THDDP** [SSKS12]. **THDP** [SSKS12]. **Their** [She14, ALK19, ALB18, AM10, BPT12, Buc12b, BO11, BSO11, CJBMMAPR19, CCL+16, CFV18, CTW12, DSC+11, For12, GTR11, GWZ+14a, GI10, HS11b, LWY19, MMW19, MKM11, MMSC19, PR10a, PL11, PSKV19, RBD+10, RBZ15, RLER14, Rua10, SACA18, SM14c, VGGPdL19, WJ11, XSLF12, YZL+11, ZR13, ZGSM15, ZF15, ZYL+13]. **them** [WXB+11]. **Theobroma** [dAGNJT12]. **theorem** [GW13, Lev10, Nag10]. **theorems** [LB14b, Tch16, ZWE12]. **theoretic** [AB18, IOO18, YOS15]. **Theoretical** [lAyL14, AM12, Ali14, Ali19b, ÁIGVZW12, ACMRN10, AAA12, AMMC19, AMAC12, BD12, Bar16, BAMA12, BGMD15, BHA19, BS11, BZZ15, BXZ+19, Boe12, BMF13, Brä14, BLM+12, BWE16, CMR13, CWF11, CAZ+11, CPL15, Cas15, COCF+14, CNSK11, CWZ+10, CTW12, CWB+13, CWS15, CS18, DIOG12, DSCO+13, Den13, DSRGD12, DSWL11, DWGX12, DSH+13, EAK+10a, ESDO16, ETGLMJ+19, FM16, Gao12, GZW16, GK12, GCDNGS12, GIO12, GFB12b, GMT16, GMT18, GDM+10, GSB10, HTM10, HK11, HDC+11, HDQ+13, HLMO11, HMH+13, HLJZ11, HZG12, HHYC+18, HHL12a, HWL16, HM10a, HWHZ11, IIW+11, IGMK11, IROW10, JHSG18, JFT13, JSLH14, JLZ+17, JWG+12, JFDD10, KS11, KB13, KWC11, KA13, KI12, KSSK16, KSY+11, KZZ13a, KZZ13b, KHH10, KAOB11, LKDC11, LOHB13, LJ16, LCL+10b, LZB10, LGP+11, LMZ+11, LPG+12, LSR+13,

LXW+14, LGZC15, LD17, LLC+11, LWJL10]. **Theoretical** [LDW+11, LXW+12, LWZ+14, LZZ+17, LLW+12, LWH+12, Lu10, LWC+10, LMCZ11, LCZL11, LCS+11a, LCH+11, LCS+11b, LXLL11, LW13, LYD+18, MLW10, MWH15, Mas10, MOY13, MDNDO+16, Men10, MAP+10, MMCNV19, MSK11, MJ14, MMV+19, MHHPR+17, MGD11, MBBT+12, Mor11, NYA+13, NL11, NMIP14, NFD+10, NFQ+11, NH11, NHB12, NIT16, OT14, ONK+13, PEA+12, PWP+18, Pan16, PMEP19, PSKV19, PKK14, PMC11, RFN+12, RMLPGGGH16, RI19, RCM10, Riv11, RGS+13, SK12a, SRASZ16, SLS+14, SLSZ13, SSA18, SZZZ11, SLZH12, SM14d, SK12b, SK10, SLS+15, SZL+15, SCZH16, TYN13, TWHZ14, TM13, TYL10, TXL10, TSH17, TFB11, TGA+11, TPT+13, TPT19, UKF+11, VF13b, WXB+11, WLL11, WLG+11, WTH+11, WLZ+12b, WHS+13, WHY+14, WTW+15, WWQG17, WHM14, WZZL10, WLL19, WJ11, WSL+11, WWGW18, XGH18a, XZL+12, XWC11b, XXbX+13, XCY15, XLZ+19, YZ13, YZL+10, YJ17, YHLC15, YC13]. **Theoretical** [Zha10, ZZX10, ZLLS10, ZYZ+11, ZZR+12, ZSHL14, Zha14, ZQW+17, ZYSW17, ZSQ+10, ZFS+11, ZL12, ZSS+13, ZTC11, dSdSPG11, dARAV12, dOdONM12, AZD+11, ASD14, AG19, BLL+13, BLB+18, BLRdA+10, BG13, yBZfC18, BPSM12, Buc10, CZJZ12, Cao17, CHH+19, CG12, CYLL11, Che12, CLH14, CZCW19, CGIAI12, CPAT11, DDÇY12, DPRK12, DTEMK11, DZ11a, DQZF12, DC12, EI11, EMED+12, ENV15, FMP+17, Fri12, GLF+12, GHGF12, GLXL18, GT13, GGP13, HYZ13, HSS18, Iku17, Jal10, Jia15, KO14, Kim16, KC19b, KO12, LS17, Lan10, LRP+11, LL11, LS19, LCZ15, LMC19, LLZZ10, LXD13, LW15, LdAA+11, MNP19, MCP10, MMR+10, MPTR12, MLPT10, MUPC10, MEF+15, MEEA+13, MSRn+11, MSOV13, MMSC19, ND11, NHG+12, NBL12, Ném14, NRGS11, NRS+11, OKR12, OAA19, OH12, OH13, OMÐ13a, ORJ18, POLV12, PM17, Puz10, RGR12, SF13]. **theoretical** [SA18, SFL+10, SSK11, SC12b, SKS11, SSTÖ11, SACA18, SRA+11, SYQ+10, Tch16, TK16b, VATPR11, VFCSC17, VLM+10, VSMK13, VKF+19, VO11, WGLX10, Wan11, WLZ+12a, WZM+13, WWB+14, XF19, YM12, YZZH15, YLW+13, ZAE10, ZWWY10, ZR13, ZKWZ17, ZPB12, ZW15, ZLWZ16, ZMB+17, dLRR11, dOR10, dOdCMUdALR11, DJB10, DC10, HHL14, LEU+11, Sit15]. **theoretical/computational** [Ném14]. **theoretically** [Jeo18, VMC11]. **theories** [Cam10, JNZ+14, Li15, Luz08, ZT13]. **Theory** [Ano13-49, BHA19, Buc12b, DCZ17, HKLW13, ISN13, IKN13, Koc13b, Kri13, Kut13, LMZY15, MIN13, NS13, SSI+10, SSK+12, SIS+08, SKY+13, TKN13, TH13, YSS+10, YKN13, YH14b, AC19, ABM+19, AM13b, AGPDZ13, BVP13, BAX+19, BGBV12, BLKB11, BJdlMAV12, Cam12, CCL+13, Car19, CEFMK12, Cha11, CH17, CM12, CZLD17, CC19, CK17, CF14, CTDOLA10, CSTA16, DWJZ11, DCBB11, DKS11, DLRMFY10, DB11, DMWY11, DGR+16, DG19, DCHC11, DSZB18, FZX18, Fin17, FA17, FMMD+10, Fri12, FSST16, GFPAV19, GCK+17, GM11, GEL18, GS11, GCZ+14, HMA+19, HR19, HLZ+14, HZZ+19, HMH10a, HMH10b, HKIH13, HYD11, HMA+18, IN15, IROW10, JR12, JPP+11, JHSG18, JMX+15, JW18, KAR12a, KCDC15,

KC18, Kar13, KKL+16, KSAK17, Kit14, KM12c, KYLC19, KdSM+10, KJ14, KMU+13, KFJ+18, KLE+19, Lar12, Lat13]. **theory** [LPO+12, LCL+10b, LW11, LWL+12, LPG+12, LBY+14, LHX+19, LLW+11, Lin14, LDZG16, LLZ+12, Lya14, LKd+16, MYZ+10, MLW+14, MJ16a, Mam14, MLC+11, MFK+12, Mas14, MW16, MLK17, MLB+12, MBBT+12, Mor13, MJM19, MCRS16, Mur12, Nag15, Nag17, NSN17, NNSN17, Nal13, NS10b, NAK+17, NTNL10, NL11, NMIP14, OK16, OD16, PS10b, PS14, PK13a, PABSK16, PP16, Pat15, PTH11, PR10b, PBB15, PU14, PM16, PJP10, PMAP12, PI16, PC13, QBRA18, RGPZD13, RCM+19, RB18, RMG+19, RMC19, RAMB18, RS09, RS11a, Rud12, SVRGV12, SLC+18, SN15, SN12, Sha18, SZS+10, SLZ+11c, SLS+11, SHL+13, SJZ+18, SM12, Sto18, SK12b, SD13c, SS13, TFBG14, TIN13, Tan13, TTD13, TH12, TDOD17, TG16, TXK+19, TLC+17, UV18a, VPGC12, Var11, VUC13, VBO+15, WKE17, WJL+11, WW11, WJY15, WB17, WDJ+17, WTZ+11]. **theory** [Wit18, XNL+14, XGH+18b, YKM+15, YLH+19, YWH12a, YWH12b, ZS11, ZQCJ10, ZLWY13, ZCX+16, ZBG+19, ZMZ13, ZSZ14, ZZ18, Zho18, dCSDdMC13, dSTH17, BM10, SP19]. **theory-based** [KSAK17, WJY15]. **there** [GI11f, SMR14, TKSK17]. **Thermal** [CEV10, FBM+10, NG11, AFM+10, AMMB+18, Chu12, Liu15a, MVC13, MCC12, Mar13, MOSK10, MML+11a, MB13, PP19b, RRRV19, YZ13]. **thermalization** [Nes11]. **thermalized** [PFdM13]. **thermally** [GMM+18]. **Thermochemical** [Kim19, Rus14]. **Thermochemistry** [ABTW14, ŞBAT16, AK11, BYAT13, ÇT14, HZG12, Rus14, WZX15b]. **Thermodynamic** [JAB12, VOAH18, XNL+14, COCF+14, DWGX12, Kim13, LZZ+13, OSJ+12, Pan19, PP19a, RMLPGGGH16, Tav11, TSH17, dOLdlV13]. **Thermodynamical** [Nag17]. **Thermodynamics** [MLW16, PK16, BvWG14, Bra19, DP11, PD11, PRFR17, RTG+19, WSCL11]. **thermoelectric** [KG17]. **thermostats** [GVPCK10]. **these** [MMM19, Ril10]. **THF** [HHL12a, HHL14, AG10b, RTT10]. **thiadiazole** [VMC11]. **thiazol** [DDÇY12, SC12a, SC12b]. **thiazolidine** [MBBT+12]. **thiazoximic** [LBM11]. **thieno** [ZWZK19]. **thieno-expanded** [ZWZK19]. **thienyl** [WDS19]. **thietane** [HL19]. **thiirane** [HL19, LCS+11b]. **thin** [ATS15, JK12]. **thio** [LKOS17, SF13]. **thioamides** [RMP+14]. **thioaminoacrolein** [NRP+11]. **thiocarbonyl** [BH10a, PJP08, dCSDdMC13]. **Thiocyanate** [LGS+16]. **Thiocyanate-free** [LGS+16]. **thioethers** [HL19]. **Thioflavin** [BBM17]. **thioguanine** [SS18a]. **thioketones** [MMW19]. **thiol** [JS17, KV11, OD16]. **thiol-functionalized** [OD16]. **thiolate** [MC18b, OPF11, ZZC15]. **thiolate-protected** [MC18b]. **thiols** [KV11]. **thione** [JS17, KKG12]. **thionucleobases** [CL18]. **thiophene** [BSSS19, CZLD17, MSG16, WDS19, YWR+18]. **thiophene-vinyl-thiophene** [BSSS19]. **thiophenols** [dSNBG08]. **thiosemicarbazone** [LWH+12]. **thiourea** [LCM+11]. **third** [KWC11, MMF+13, NKF+13, RS09, RS11a, WLZ+12a]. **third-order** [MMF+13, NKF+13, WLZ+12a]. **third-row** [KWC11]. **Thoughts**

[KN15, Lev16]. **Threading** [WMK+19]. **Three** [DMS+10, FMMD+10, HYH+10, Kry10, LQZZ12, MPD+15, MMP+18b, RAN18, ARG11, Buc10, Buc11a, CG12, GSaY11, Hog13, KV19, LWY13, Mat02, Mat10, MUPC10, RZSZ18, RAGM10, SD13b, SYL+18, SKY+13, WvRSW+11, WLZ+12b, Zha14, JA12]. **Three-body** [RAN18, ARG11, Hog13, RAGM10]. **three-center** [Buc10, Buc11a]. **Three-dimensional** [DMS+10, MPD+15, RZSZ18, SD13b]. **three-electron** [Buc11a, CG12, LWY13]. **three-membered** [Zha14]. **Three-peak** [HYH+10]. **three-photon** [WLZ+12b]. **three-state** [GSaY11]. **Three-unit** [LQZZ12]. **threonine** [WJY15]. **threshold** [HMH+13]. **through-bridge** [KyH13a, Nal12, Nal13]. **through-space** [CDT12, Nal12, Nal13]. **throughput** [CRFR11, KG17]. **thymidine** [MB14]. **Thymine** [TWHZ14, HYD11, TSH17, XSLF12, YM13]. **Ti** [FTB11, HLMO11, JL12a, KYLC19, MLY+16, TFB11, ZLY+14, CAZ+11, NKWT19, OPP+14]. **TiCl** [BAB+18]. **Tietz** [KBG17, AAHN16, HRT12]. **tight** [BLB+18, LNI12, WDJ+17]. **tight-binding** [BLB+18, LNI12, WDJ+17]. **Time** [Bae14, BDF+18, CP10, CW13b, HS11a, HKZZ15, HB14, ILBS10, SSAM13, Sko16, ZLE17, Bae16, BDF+16, Brä13, CEFMK12, CW11, DCZ17, DP11, FNIT16, HR13, HHCA10, IFT13, IFT14, JPP+11, LMZY15, Luz13, MJM19, NSN17, NNSN17, NDP10, Oht13, PVS11, PVS12, PJP10, PMAP12, PI16, RBGGM18, SLC+18, SHKS15, SL13, SHW+13, SKV12, Vik11a, Vik11b, WKE17, Xu19, YLYC18, ZCG+17, ZSZ14, ZZ18, Zho18, ZQCJ10]. **Time-dependent** [Bae14, BDF+18, CW13b, HS11a, HKZZ15, ILBS10, Sko16, ZLE17, Bae16, BDF+16, CP10, CEFMK12, CW11, DCZ17, HHCA10, JPP+11, LMZY15, Luz13, NDP10, Oht13, PVS11, PVS12, PJP10, PMAP12, PI16, SL13, SHW+13, Vik11a, Vik11b, WKE17, YLYC18, ZCG+17, ZSZ14, ZZ18, Zho18, ZQCJ10]. **Time-independent** [CP10, ILBS10, ZSZ14]. **time-reversal** [NSN17, NNSN17]. **times** [PR11a]. **TiO** [MFZ+18, ATS15, ALA15, EFO11, EO11, GP13a, HCL13, OGvSG18, TFSRM11, XMZ+12, ZK12, ZLWY13, ZDZL11]. **TiSi** [DHYC19]. **TiSiO** [MBKH19]. **titania** [SFNC+18]. **Titanium** [YSA+11, ALA15, Che13, DHYC19, OH13, RALK18, WWLZ17, YHL+13, ZSAP11]. **titanium-doped** [DHYC19]. **titanocenyl** [Con10]. **Tl** [LXD13, MLW10]. **TM** [PP19a, WSL+11, YL11, BLdV19, WSL+11, YL11]. **TMZr** [PP19a]. **TO/H** [ZHL+19]. **tolerance** [Kan17]. **tomentosin** [ZRGE+19]. **tool** [May14, MML11b, Sic16, TRZ+19]. **tools** [VLG12]. **topo** [MBBT+12]. **topo-geometrical** [MBBT+12]. **Topography** [AS19, dOdCMUdALR11]. **Topography-driven** [AS19]. **Topological** [MSAB19, AOT+18, BL10, BLdV19, BCNR18, DM12, HYD11, JXX+15, LNGW14, MZB+13, MGB18, OAT+13, PH12, PL11, PO15, TM19, BF11]. **topologies** [ART08, YWH+12c]. **Topology** [AGNS14, BL10, FMKJ14, GRCGRRHT19, Jen13]. **tops** [PBB15]. **toroidal** [CTDOLA10]. **torquoselectivity** [AMMB+18, MB13, MBSMJC18]. **torsion**

[DSCO+13, GWME18]. **torsional** [CMCN11, MMCN+11, RA10a]. **Total** [NA14]. **Townes** [HYH+10]. **toxic** [SD16b]. **toxicity** [PI13]. **tpy** [LWL+12, ZQJW13]. **Tr** [CDL+19]. **tracking** [WLZ18]. **trail** [dGR14]. **trains** [SVPTM+10]. **traits** [LSC+18]. **trajectories** [Cho15, Cho16, YS13, YH14a]. **trajectory** [MMG15, SPSA11, XLLZ10, Xu16, YW16, YZ10]. **trans** [BSM+15, Bud12, CCL+10, FMKJ14, KZZ13b, MB13, XZ11, GLOGM+11, LCB10]. **trans-** [KZZ13b]. **trans-3** [MB13]. **trans-diarylethylenes** [Bud12]. **trans-isomers** [FMKJ14]. **trans-RuCl** [CCL+10]. **trans-to-cis** [Bud12]. **transcriptase** [SKHN13]. **transcription** [Nag17]. **transesterification** [GCZ+14, MCRS16]. **Transfer** [SS10, AKC10, ARH+13, BSS16, CS17, DS11, DAA16, FV11, FDMR11, FSBA12, GI11a, GHCMCMQ17, JdL08, KyH13a, KUS19, KAOB11, KT12b, KBMM10, LZZ12, LYS+19, LYL+12, LXW+12, Lu10, MANP17, MPE15, MHOG18, MNC12, NMS+10, NBZG16, OK19, QJ13, RY12, RS12a, SSK11, SMRK18, Sch15, SHS+13, SCS15, Tav11, Tav12, TCG13, WJ11, XDM+10, YH14b, Zen11, ZZ18, ZB18, dA12, dCDC+11]. **transfer/induction** [dCDC+11]. **Transferability** [GSR12, STM17, RLER10]. **transferred** [HSN18]. **transfers** [KyH13a, YYS15, YY18a]. **transform** [SFY12, YŞÖ12]. **transformation** [DMAB12, DM12, DK13, HHYC+18, IM15, Jør15, Jør18, Mam13, Rua10, SN15, TSS+15]. **transformed** [Hor13]. **transistors** [SAHAA16]. **Transition** [BLdV19, Pie11, ALK18, BEM11, BZBZ13, Ber13a, BVP14, BB10, BDR12, Buc11a, BN11, CWW+16, Cho16, Cho19, CP13, Dau16, DMS+10, DMBL16, EMED+12, EMEPD15, GRLA18, GFB12b, GM11, GZBH18, JHL+18, KWC11, Kin13, Kry12c, Lar12, LCB10, LKd+16, MKM11, NKWT19, NZ13, Qu13, RZC13, SDS19, SDS20, SFW12, SAHG11, TMC+13, TTD13, VSMK13, VO12, WWC17, WR15, ZK12, ZFC+17, ZHI17, ZSZ14, Zil14, KAR12a]. **transition-metal** [GZBH18, TTD13, WR15]. **transition-metal-doped** [RZC13]. **transition-metal-like** [JHL+18]. **transitions** [AC11, BCNR18, BTH18, CK13, GC19, lLBqD+19, LZ10, MS12, MLDP10, PJP08, SLC+18, VV12, VV13, Zen11]. **Translation** [RLER13b, Laz14]. **translational** [Lad14, Tou11b, XTLA13, XTLA14]. **translations** [Hog10]. **transmembrane** [KMT+12]. **Transmission** [RBGGM18, CDT12, NTCG18, NA12, SD13c]. **transmitted** [Cho15]. **Transport** [Yam11, DCZ17, DLZ11, ETGLMJ+19, Gao12, Jan10, JR19, KM12c, MSG16, MMP11, OH12, OH13, PFdM13, RBGGM18, RRRV19, SSKS12, SSB12a, WDS19, ZYZ+11, ZQJW13, ZY13, ZB18]. **transporting** [MCL11]. **Trap** [YZZH15]. **trapped** [TG13]. **Trapping** [PDNC14, LL18]. **treatment** [AEKGZ12, BHV+11, ISN13, Jør18, KL11, Kry12a, Mam13, MSNP18, PMGMGR12, SKG11, SSAM13, WJY15, AM13b]. **trees** [AD17, Bib13, DZ11b, Du12, LSW19, LWY19, LZZ19, PL18a]. **trends** [BCHN16, DMBJ15, MT10]. **tri** [AM18]. **tri-coordinated** [AM18]. **triacetate** [AKHS13]. **triacetin** [MCRS16]. **triad** [TK16a]. **triafulvenone** [ŞBAT16]. **Trial** [Hog13]. **triaminotrinitrobenzene** [BF11]. **Triangular**

[EMSB15]. **triatomic** [BCHN16, SA11a]. **triazides** [CWS15]. **triazine** [CLH14, MJ11, TJS17]. **triazol** [CLY12]. **triazole** [LLW+11, THSR13]. **triazolin** [IK14]. **tricarbon** [ZJC+13]. **tricarbonyl** [YZW+15a]. **trichelates** [LOHB13]. **trichloroacetyl** [SKS11]. **tricks** [SCB+14]. **tricyclic** [ZWZK19]. **tridiagonal** [HFZ12]. **tridiagonalization** [ZHF12]. **triel** [CDL+19]. **trifluoride** [DWGX12, For12, LQ13]. **trifluoroacetylacetone** [NRGS11]. **trifluoroethylene** [OCB+10]. **trifluoromethylphenyl** [SAHAA16]. **trifluromethyl** [DPRK12]. **trifluromethyl-phenyl** [DPRK12]. **trigonometric** [HR12]. **trihalomethanes** [MNV+17]. **triiodide** [VVY18]. **trimer** [PMMGL+11]. **trimers** [LJW+11, MZLM17]. **trimethyl** [Owe17]. **trimethylamine** [SC18]. **trimethylnaphthalenes** [OMÐ13a]. **trimethylxanthines** [SMGZ13]. **trinitrate** [LL17]. **trinitro** [CLH14, Men10, MJ11, TJS17]. **trioxide** [SQ10]. **tripeptide** [ScBsR+10]. **triphenylamine** [ZZR+12]. **triphenylphosphonium** [AG10b]. **triphosphate** [YTY19]. **triple** [ABG12, KKC14, KC16, KC18, MPT11, NZ13, Tob19]. **triples** [PCV19]. **triplet** [BMF13, GLOGM+11, Kim16, LSL+08, MGD11, RMJ11, YSS+10]. **triply** [GCD13]. **tris** [AC19, FO10]. **tRNA** [ST15]. **tropolone** [PS13a]. **Tropospheric** [dlLIAI+12]. **Tropsch** [MJ16a]. **TrR** [CDL+19]. **truncated** [MSNP18]. **Trypanosoma** [SLA12]. **tryptophan** [BSV12]. **Tsallis** [Gra08, OH19]. **TSSCDS** [KMNSP19]. **tuberculosis** [ST15]. **TUHC** [LSW19]. **Tunable** [ZX12]. **tuned** [MIN13, WDJ+17, ZZ18]. **tungsten** [Yam10]. **Tuning** [DWZZ15, GMT16, GMM+18]. **Tunneling** [HZW18, KC18, Xu19, CW13b, MVC13, TCG17, WZX+15a, XDM+10, XZJ+16, Xu16, ZLWY13]. **Tutorial** [AB16a, Bae16, BC15, Beh15, BBB16, BM16, BW13b, IN15, JW18, Laz14, LSP+16, Liu15b, LKd+16, MW16, Mos14, Nym14, OWD18, PSMD16, Per18, PI16, Rup15b, SMMT13, SBD+16, SPM+15, Val13, ZP16, vL13, AHC+18, BC16, Liu16, LC19]. **twinning** [GE12a]. **twisted** [FSBA12, LXW+12]. **Two** [Cho15, GSaY11, VOK+18, ART08, BKM15, BCF+11, CFP+10, ČW13a, CG12, CH17, CK17, CF17, DTF+11, Dw13, DSSM18, GW13, GI11e, GN19, HV11, JWJ+12, KWLS15, KYLC19, KAOB11, LMZ+11, LWJL10, Mam13, Mar12, MBA+13, MLDP10, MAN15, NZ13, Pir13, QB15, RP11a, RD14, RPVM10, RDB19, RNC+14, RAGM10, SDS19, SDS20, SBMM11, SBM16, SN15, SSAM13, TC12, WLZ+12b, Yak11, Yam11, YM14, YWR+18, ZWLC12, Zil14, ZJS13]. **Two-** [GSaY11, CG12, WLZ+12b]. **two-component** [SN15]. **Two-dimensional** [Cho15, ART08, Dw13, Mam13, MLDP10, RNC+14, SSAM13]. **two-dimensionally** [Yam11]. **two-electron** [BKM15, ČW13a, CH17, DSSM18, KWLS15, Pir13, RAGM10, SDS19, SDS20, SBM16, YM14, ZJS13]. **two-particle** [DTF+11]. **two-photon** [YWR+18]. **two-range** [GW13]. **two-stage** [KYLC19]. **two-state** [JWJ+12]. **Type** [TBRIS12, AGJ12, AY15, BPG+10, Boe12, GMGRMP12, GZF13, GZF14, GW13, GE12b, HITU16, Hog10, Hog13, IIS+17, JH15, LSS19, cLqFtW+14, Mat02, Mat10, Mit11c, PS10a, PP19a, PGMGRM15, RVO+14, TBRIS10,

TBRIS11, TFZ+15, XLGA12, YD17, ZZL+11]. **types** [LMZ+11, RDB19, SMMT13, SKY+13]. **typical** [ZZL+11]. **tyrosine** [TBHL11]. **tyrosyl** [ST15].

U [BB10, OGvSG18, WDJ+17]. **UB3LYP** [YSK+12]. **UBD** [NYS+10]. **UBHandHLYP** [YSK+12]. **UC** [LLZaH14]. **UC-Curve** [LLZaH14]. **UCC** [NYS+10]. **UFF** [JLL11]. **UiO** [MLW16]. **UiO-66** [MLW16]. **ULO** [NYS+10]. **ULO-MRCC** [NYS+10]. **ultra** [NWQX11]. **ultra-short** [NWQX11]. **ultrafast** [PETB18]. **ultrashort** [Vik13]. **Uncatalyzed** [CF17, DP12]. **Uncertainty** [ORJ18, Rus14, Coo12, OOI+19, RBGGM18]. **uncharged** [MP12]. **Uncontracted** [HH18, UGWL18]. **Unconventional** [SS11, MC14, ZYL+14]. **Understanding** [CRB+12, LSP+16, LG15, MIKH19, MB13, NAK+17, OGvSG18, VSL+15, XSLF12, YWY+12, ZJC+13, Kim16, LKN13, May14, PWH+12, SB16, TBHL11, XZCH11]. **uneasy** [fXxBhD19]. **Unexpected** [BTH18, Cor16]. **unicyclic** [DZ11b, GA19]. **Unified** [Mam13, PMGMGR12, DP11, GTR11, PD11]. **uniform** [LG12, RL12]. **unimolecular** [MLB+12, RLW+13, WLWL14]. **Unique** [GPM+15, MOLF11, YD17, AEKGZ12]. **uniqueness** [She14]. **unit** [CHL+19, LQZZ12, MYZ+10, Sch10b]. **Unitary** [NS13, GRD11, PBR18, SN15]. **united** [CC11b]. **units** [ALK19, BBKO16, LSKM19, MPD+15, ZH15]. **universal** [BVP14, CD18]. **unnatural** [OM13b]. **UNO-** [NYS+10]. **Unoccupied** [ALA15]. **Unpaired** [KK13, KK14a, BMB16, QCB+10]. **unpolarized** [SFM13]. **Unraveling** [AGNS14]. **unrestricted** [AHT12, NSN17, Tob19]. **unsaturated** [OPAVM18, SAG13, VF13a, ZYSW17]. **Unsaturation** [WLS+19]. **Unstable** [Ban12, Mor13]. **unsupported** [NZ13]. **unsymmetrical** [FDNR10]. **unusual** [MBSMJC18]. **unusually** [BMF13, XCD18]. **UO** [MTR+19]. **Update** [KRC+16]. **Updates** [BDF+16, BHH+13, CYC+15, DOE+14, FMPM+14, KRC+16, LCZL15, MMŁ+16, MRS15, NKKN15, yOITn15, QSX+15, SDP+16, TY17, YAF+15, ZH15, ZWSF16]. **upon** [CRSB12, MS14a]. **upper** [FDA16]. **uptake** [DLLA10]. **uracil** [KS18, MYZ+10, MZB+13, MR11, YPDW14, ILBS10]. **uracil-dimer** [KS18]. **Uranyl** [ZKKR11, KRK+17, Lu10, Lu10]. **urea** [EBH11, LWZ+14]. **urease** [BMB12]. **urils** [MGK19]. **Use** [GE12b, CP11, FT15, KJ14, MR11, SIM14, Sic16, SV11]. **used** [AGJ12, KDA+11, MUNZVR12, NZAVR10, PSPS11, Sza13]. **useful** [FDG18]. **uses** [ZF15]. **Using** [CRA+11, TWHZ14, AAHN16, AA11, Ale13, AC12, ABKJ18, AFM+10, ASW13, BLRdA+10, Boe12, BVA+14, BWB+18, CRFR11, CG12, CNSK11, CK17, CF14, CAPL12, DK13, DCHC11, DFV+12, DQZF12, ESDO16, EM19, Fuk12, FC19, GRLA18, GI10, GS10, HS11a, HSN18, HJ13, Ish14, KH10, KC18, KRK+17, KCK14, KPH+12, KFJ+18, KUY16, Lad14, LRP+11, LCL+10b, LPG+12, LKJ13, MdAdCS12, Mam13, MOLF11, MBA+13, MAW+18, MBBT+12, MMA10, NC11, NH18, NMIP14, OT14, OHDA13, OH19, OSJ+12, PDR+14, PT13, PK13a, PK16, PJP10,

RTG+19, RZSZ18, RFEGPP+16, RSCS10, RRCO11, SAS+12, SA18, SY10, SOF+10, SN12, SSAM13, SZS+10, SLZ+11c, SLZ+11a, SLS+11, SB10b, SM12, Sri18, SK12b, TNN16, TMC18, TG13, TWR15, Val17, WML10, WB17, WDJ+17, WH12, XTLA13, XTLA14, Xu19, ZWSF16, ZS12]. **using** [ZZ18, ZCP11, dAB17]. **uteroferrin** [KSY+11]. **utilizing** [KFS13, Tou11a]. **UV** [AFC+10, BSS15, Bou12b, ÇAS13, DSD18, FPRGMHGB12, MSBF18, PJP08, PJP10]. **UV-Vis** [DSD18]. **UV-visible** [Bou12b]. **UV/VIS** [PJP10, PJP08]. **uvarovite** [MPZWD10, VPFD10].

V [Lu10, Tch13, TFB11, ZLY+14, Ang10, AMK10, BN11, KWC10, lLBqD+19, LW18, NKWT19, NTNL10, SS13, TD11, XCL+18]. **V-shaped** [BN11]. **VA** [Eng16]. **vacancies** [MMC+19, VS19]. **Vacancy** [ABP13, ES17]. **vacuo** [MK10b]. **vacuum** [EPS+16]. **Vague** [Kry11b]. **vagueness** [Tch16]. **Valence** [ALHC18, YPDW14, Ali19b, ASK15, BCP10, BVP14, BB10, CYC+15, DG19, Eng16, FDNR10, FGD+19, KSY+11, NZ13, OVT+16, PCK19, RCP14, TPCJ+12, YIY+13, YSK+12, YD17]. **valence-bond** [BCP10]. **valent** [KO14, LXD13, SSW16, YYI+12]. **Validating** [KF19]. **Validation** [BDF+18]. **validities** [CLXD15]. **validity** [HMH10a, SXH18]. **value** [Liu15a, XWC10]. **valued** [HDÖS12, YW16]. **values** [ÇT14, Cin11a, GCDNGS12, HITU16, JZZH17, MC11b, RZG12]. **vanadium** [BBYZ18, RJLPGH+13]. **vanadium-and** [BBYZ18]. **vanadyl** [DdG+11]. **vancomycin** [LSR10b]. **vancomycin-group** [LSR10b]. **van't** [Buc10]. **vapor** [Chu12, LKOS17, TFBG14]. **variants** [RPBB11]. **variation** [JWG+12]. **Variational** [FAFR12, CDS+18, DSSM18, Kri13, NS10b, Oht13, dMOB12, SBM16, SSB12a, Sha11a, ZS11, MHT+08]. **variations** [KBGC12, MB12]. **variety** [AM10, TOSN12]. **Various** [MGK+12, ART08, HFL+17, KMT+12, PSK+13, SMMT13, STM17, YÇÖ11]. **VASP** [WMK+19]. **vdW** [KMNSP19]. **vdW-TSSCDS** [KMNSP19]. **vector** [AMMB+18, HEVMSA+19, HAX+18, JMX+15]. **vector-based** [AMMB+18, HAX+18, JMX+15]. **vegetable** [PWH+12]. **vegetable-aldehyde** [PWH+12]. **Velocity** [Yak10]. **verdazyl** [Shi18]. **versatile** [GAPK+19a]. **versatility** [MGP16]. **version** [CYC+15, NF11]. **versions** [ND10]. **Versus** [FKBG19, AM18, CAPGAIG18, CLMY12, DI15, DLP17, FLCHL10, GKGM18, HYZS12, HYZS19, KyH13a, Kut13, LJK+18, MMF+13, SALK19, SL10, VMC11]. **vertex** [FSQ+11, GAPK+19a, SALK19]. **Vertical** [ABG12, GMA+19, SLC+18, SOM10]. **vertices** [BBKO16]. **very** [QBRA18]. **VI** [Lu10]. **via** [BGL+16, BLKB11, CHH+19, CS17, Dw13, DMWY11, DWZZ15, Gan14, GLXL18, JHSG18, KZA+17, LCK+16, MB12, MCRS16, OPC17, Ols11b, PR10a, PM12, PM16, SGB11, SLC+18, SRA+11, TGRP19, YŞÖ12, Eng16]. **Viable** [fXxBhD19]. **vibration** [HK11, HRT12, KBG17, LZW+15, QD10, SPO+11]. **vibration-rotational** [SPO+11]. **Vibrational** [AC12, CTVA12, Cyb11, FKL+12, KKT13, KKT14, SD12, AF19a, AGCVG15, BBB+12a, BBB16, CP10, DK13, DCFD10,

DWGX12, For12, FKC12, dDGNB10, HH18, Ish14, KL11, LJW+11, LWWZ13, MC11a, MBKH19, MCE11, MB14, MMCN+11, NDM+12, PM12, PBB15, RPBB11, RSM12, RC11, Roy14, ŞBAT16, SA11a, SPO+11, SZZZ11, SZL+14, TU10, Tou11a, WHY+14, YWH+12c, ZGSM15, ZPZ15, ZQXP17]. **vibrationally** [LMZY15]. **vibrations** [CNBPR+11, CMCN11, Eil14, LBW11, NH18, ZZ15]. **Vibrio** [PI13]. **vibronic** [PETB18]. **view** [AY15, BMRM19, BLdV19, vL13]. **viewpoint** [LS19]. **Vignale** [PS13b]. **VII** [SIS+08]. **vinyl** [BSSS19, DP12, KI15, WZZL10]. **vinylallenes** [LW11]. **vinylation** [VLK+11]. **vinylboronates** [SLS+15]. **vinylcatechin** [BCF+11]. **vinylcyclopentadiene** [VV18]. **vinylidene** [OCB+10]. **vinylideneflouride** [OCB+10]. **vinylideneflouride-trifluoroethylene** [OCB+10]. **vinylpyranoanthocyanin** [COdF+11]. **vinylpyranoanthocyanin-phenol** [COdF+11]. **violation** [BR12b]. **Viraht** [VUC13]. **virial** [Nag10]. **Virtual** [KN15, CCA+12, CRFR11, KPH+12, LG10, Lya19, MSNP18, RMG+19, SDP+16, ST15]. **virtue** [FYhC11]. **viruses** [WZ10a]. **VIS** [PJP10, AFC+10, ÇAS13, DSD18, MSBF18, PJP08]. **Visible** [FPRGMHGB12, Bou12b, WCL+17, dARAV12]. **visual** [LLLT12]. **Visualization** [Val13, Ash18]. **visualizes** [ABM+19]. **Vitae** [Ano11a, Ano11c, KK12b]. **vitamin** [WTH+11, WLD+10]. **vitro** [CG12]. **Viver** [Yos20]. **VIVO** [MG12]. **Vleck** [Jør15, Jør18]. **VMD** [CRFR11]. **VO** [Che12]. **Volterra** [CYK17]. **Volume** [Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g, Ano12h, Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n, Ano13k, Ano13q, Ano13r, Ano13s, Ano13t, Ano13u, Ano13v, Ano13w, Ano13a, Ano13b, Ano13c, Ano13d, Ano13e, Ano13f, Ano13g, Ano13h, Ano13i, Ano13j, Ano13l, Ano13m, Ano13n, Ano13o, Ano13p, Ano13x, Ano13-35, Ano13-41, Ano13-42, Ano13-43, Ano13-44, Ano13-45, Ano13-46, Ano13-47, Ano13y, Ano13z, Ano13-27, Ano13-28, Ano13-29, Ano13-30, Ano13-31, Ano13-32, Ano13-33, Ano13-34, Ano13-36, Ano13-37, Ano13-38, Ano13-39, Ano13-40, Ano13-48, Ano14a, Ano14b, Ano14n, Ano14t, Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14z, Ano14c, Ano14d, Ano14e, Ano14f, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14o]. **Volume** [Ano14p, Ano14q, Ano14r, Ano14s, Ano14-27, Ano14-37, Ano14-43, Ano14-44, Ano14-45, Ano14-46, Ano14-47, Ano14-48, Ano14-28, Ano14-29, Ano14-30, Ano14-31, Ano14-32, Ano14-33, Ano14-34, Ano14-35, Ano14-36, Ano14-38, Ano14-39, Ano14-40, Ano14-41, Ano14-42, Ano15a, Ano15b, Ano15c, Ano15d, Ano15e, Ano15t, Ano15x, Ano15y, Ano15z, Ano15-27, Ano15-28, Ano15-29, Ano15-30, Ano15-31, Ano15-32, Ano15-33, Ano15-34, Ano15f, Ano15g, Ano15h, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n, Ano15o, Ano15p, Ano15q, Ano15r, Ano15s, Ano15u, Ano15v, Ano15w, Ano16a, Ano16s, Ano16t, Ano16n, Ano16u, Ano16v, Ano16w, Ano16x, Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16b, Ano16c, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m]. **Volume**

[Ano16o, Ano16p, Ano16q, Ano16r, Ano17a, Ano17b, Ano17m, Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x, Ano17y, Ano17z, Ano17c, Ano17d, Ano17e, Ano17f, Ano17g, Ano17h, Ano17i, Ano17j, Ano17k, Ano17l, Ano17o, Ano17p, Ano17q, Ano17r, Ano17s, Ano18a, Ano18r, Ano18s, Ano18t, Ano18b, Ano18o, Ano18u, Ano18v, Ano18w, Ano18x, Ano18y, Ano18z, Ano18-27, Ano18-28, Ano18-29, Ano18c, Ano18d, Ano18e, Ano18f, Ano18g, Ano18h, Ano18i, Ano18j, Ano18k, Ano18l, Ano18m, Ano18n, Ano18p, Ano18q, Ano19a, Ano19t, Ano19b, Ano19c, Ano19d, Ano19o, Ano19u, Ano19v, Ano19w, Ano19x, Ano19y, Ano19z, Ano19-27, Ano19e, Ano19f, Ano19g, Ano19h, Ano19i, Ano19j, Ano19k, Ano19l, Ano19m, Ano19n, Ano19p, Ano19q]. **Volume** [Ano19r, Ano19s, Ano12o]. **vortex** [GKS10]. **vorticity** [BL19, HMH10a]. **vs** [Ali19b, DG19, SP19, Yam10]. **VSc** [BBYZ18]. **V —** [LW18]. **vsLab** [CRFR11].

W [HNBS18, MLY+16, ZLY+14, GAPK+19b, SXS+12]. **W1BD** [VF13a]. **W2** [OK16]. **W2w** [OKR12]. **Waals** [BPG+10, BAP12, Ber13b, GRCATG19, KKL+16, NRI15, PABSK16, SZZ+19]. **waistline** [TMC+13]. **walks** [PR10a]. **wall** [DI10, SD13a, TC10]. **walled** [Bas11, ETGLMJ+19, HNBG15, KG08, MSOV13, SD16a]. **walls** [RBVAG18]. **Wannier** [PABSK16]. **warm** [DW12, Ng12]. **Watch** [ZLWY13]. **Water** [Kim18, RFEGPP+16, WW11, XMZ+12, AF16, ATS15, BBB+12b, BPSM12, BCS+12, Cha10, CNSK11, Chu12, CK17, CAPL12, DPK18, DE18, EFO11, EO11, FMCA11, FUE+12, GSZ10, GLPA10, HDQ+13, HS11b, KK11c, KV11, LLF+12, LLM13, LJW+11, LNGW14, LCB10, Ma14, MAD12, MFB11, MK10a, MK10b, MPE15, Mar12, MTL+12, MPV+11, MOE+11, MD11, MRÅ11, NS10a, OHDA13, OD12, PW10, PCMG12, QSLY10, RRVJ10, RAK10, SYK+12, SSK+12, SMEH15, SMEH16, SK12a, SJZ+18, SL10, SCL19, SW12, SJW13, SHMR11, TGRP19, Var14, WCGD12, WWD+15, WTP+19, WSV10, XS18, XGH18a, YY18a, YYI+12, YT14, ZKWZ17, Zak13]. **water-gas** [XGH18a]. **water-soluble** [GLPA10]. **Watson** [PS10a, SKG11]. **Wave** [AB16a, HDÖS12, Kut13, NS13, TKN13, TH13, YKN13, Bae16, BR12b, CW13b, Cho19, CSMZ10, D'y16, GBS17, Gao11, GKT+12, HR12, Hog13, IK18, KRC+16, KH10, Kar13, NTGC19, Oht13, OHDA13, OH19, RZ17, RW11, SSAM13, SGH10, Tob19, WC14, WH12, YLYC18, ZHF12, ZCG+17]. **Wave-function-based** [AB16a]. **wave-functions** [Hog13]. **wave-packet** [Bae16]. **wavefunction** [CH17, DAC11, GWHH17, ZWSF16]. **wavefunctions** [AC12, Lai11, Yur13, Yur15]. **wavelengths** [JdOS16]. **Wavelet** [SFY12, GSPR19]. **wavepacket** [GWZ+14a, HKZZ15, Han19]. **waves** [GNM+12]. **way** [GfWlZ11, SKLC19]. **WC** [BTH18]. **weak** [LMZ+11, LLZ+12, MAW+18, YJ17, ZFS+11]. **weaker** [MK12]. **weakest** [SRA+11]. **weakly** [Mit11a]. **weighted** [HFBC19, Tra19]. **Welcome** [Ano13-49]. **well** [DB12, Fuk12, HB14, KC16, KC18, NTCG18, SDL+15, WZX+15a, Xu16, Xu19]. **wells** [BN11]. **wet** [ZK12]. **Where** [GAI19, Dil13].

Whether [GI11e, GI11f]. **Which** [CB10, DI15]. **Whittaker** [RA10a]. **wide** [AM10]. **widely** [PSPS11]. **width** [LA11]. **widths** [CRSB12, SY10]. **Wiener** [Du12, GA19]. **Wigner** [ISRK12, Liu15a, Sta10, ZWE12]. **window** [YWR+18]. **wings** [BR12b]. **wire** [RP11b, SD13c]. **wires** [TFB11]. **withdrawing** [BSSS19, KPL+17]. **within** [BVP14, FS11, Gin10, IROW10, JMX+15, KG08, LZ10, MMM19, OGvSG18, PCR+11, SA18, SGC13, Sut12, VAT12, XXbX+13, dCDC+11]. **without** [DB11, Hog10, Kap12, LW18, MB12, PP16]. **Wittig** [AG10a, AG10b]. **WO** [ZLY+14]. **Wolfenstein** [BdTG11]. **Wolfsberg** [Koc13b]. **work** [HDÖS12, LFF+10, NMSR14, RF10]. **work-stealing** [NMSR14]. **working** [GI11b, GI11c, JA12]. **workloads** [Lya19]. **world** [GI11b, GI11c]. **written** [NF11].

X [BPG+10, CWS15, DIOG12, DVDBM11, EKN10, EMSB15, EMS16, GB13, HNBG15, KyH13a, LJL+11, LMZ+11, LLG+12, LC16, LGW11, LJSS12, LDADB+15, MZLM17, MPRB+10, MCK17, PCD14, RLTAT19, SPO+11, SKS10, SZS+10, SLZ+11b, SLZ+11c, SLZ+11a, SLS+11, SYQ+10, SZL+14, TW10, TL15, WZW17, XZL+12, YIY+13, YLC17, ZCG+17, BPG+10, CWS15, Dau16, DB15, EMSB15, FBO+11, KyH13a, LCL+10a, LWL19, MZLM17, MPRB+10, ORJ18, ÖEDB11, PCD14, SYK+12, SLS+12, SCL19, TW10, YLC17]. **X-ray** [FBO+11, ORJ18, ÖEDB11, SYK+12, SCL19]. **X1** [WZX15b]. **XBr** [EMSB15]. **XC** [LORR+12]. **XC-functionals** [LORR+12]. **XCCH** [RB11b, TL15]. **Xe** [KDOR17, EAV16]. **xenon** [BAP12]. **Xiamen** [CYC+15]. **Xiao** [VUC13]. **Xiao-Yin** [VUC13]. **XIV** [SSI+10]. **XMPH** [SYQ+10]. **XMVB** [CYC+15]. **XOClF** [LJL+11]. **XSClF** [LJL+11]. **XUV** [SVPTM+10]. **XV** [DC10, YSS+10]. **XVII** [SSK+12]. **XXXIV** [RA10b]. **XY** [SPIL14, LMZ+11, SPIL14]. **XY/HX** [SPIL14]. **xylene** [SR18].

Yb [MPT11]. **YCN** [GZW16, ZW15, ZCTG18]. **YHX** [EMS16]. **yielding** [Fin15, FA17]. **Yin** [VUC13]. **yl** [DDÇY12, PGG12, SC12a, SC12b, WLS+19]. **ylide** [AG10a, AG10b, SFW12]. **ylides** [DI10]. **ylmethyleneamine** [LYW11]. **YN** [RMLPGGGH16]. **ynone** [LFTL18]. **YO** [EMS16]. **Yoon** [LJ16]. **Young** [Yur13, Yur15]. **ytterbium** [LOHB13, TBB+19]. **yttrium** [DHZS11]. **Yukawa** [SMV11]. **yy** [ZR13]. **yy-G** [ZR13].

Z [lAyL14, KAOB11, Kuz19, EAV16, LBM11, SLS+15, ZPW16]. **Z-** [Kuz19]. **Z-selectivity** [ZPW16]. **Z-vinylboronates** [SLS+15]. **ZDO** [GZSMFN16]. **zeolite** [GSB10, LS19, NL11, SZ11]. **zeolites** [MWH15, PvS10, RDB18, RBLZ15, RBTL19, UMS13]. **Zernike** [CSTA16]. **Zero** [LA11, Boe12, KO14, WH18]. **zero-point** [WH18]. **zero-temperature** [Boe12]. **zero-valent** [KO14]. **Zero-width** [LA11]. **Ziegler** [BAB+18]. **zigzag** [BEPZ10a, FKL+12, LSW19, PPDF11, SD16a, SD16b, WWL+11]. **zigzag-edged** [WWL+11]. **Zinc** [MA11b, AG19, BPT12, CWZ+10, DLJT14, HSS18, MA11a, OPF11, dSMPRSF18, WWC17, Yam11]. **zinc-oxygen** [dSMPRSF18]. **zinc-thiolate** [OPF11]. **zinc-zinc**

[AG19]. **Zintl** [TZD+19]. **zirconia** [MCRS16]. **Zn** [ASHF13, DD17, JL12a, PAKA15, VO12, XZZ+10, XWC11a, YL11, Bal16, CRB+12, DSD18, MC17, MRT11, ZSASS13, dCDC+11]. **ZnO** [ESDO16, BRBRS11, KA13, LPO+12, MTL+12, RZC13]. **ZnO-based** [LPO+12]. **ZO** [EAV16]. **zone** [BG11a]. **Zr** [Bou11, Kim19, WJL+11]. **ZrF** [BLKB11]. **ZrN** [RMLPGGGH16]. **ZSM** [JLL11, SZ11]. **ZSM-5** [JLL11, SZ11]. **zündel** [MNC12]. **zwitterionic** [KRG+13, RFMC19, YZZ15, ZZ18].

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Anonymous:2013:CIIn

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Anonymous:2013:CIIo

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Anonymous:2013:CIIp

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Anonymous:2013:CIIr

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Anonymous:2013:CIIt

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Anonymous:2013:CIIu

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Anonymous:2013:CIIv

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Anonymous:2013:CIIb

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Anonymous:2014:CIIj

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Anonymous:2014:CIIn

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Anonymous:2014:CIId

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Anonymous:2014:CIIf

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Anonymous:2014:CIIg

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Anonymous:2014:CIIh

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Anonymous:2014:CIIi

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Anonymous:2014:CIVa

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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

[Ano14-39] Anonymous. Cover image, volume 114, issue 21. *International Journal of Quantum Chemistry*, 114(21):i–ii, November 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVt

[Ano14-40] Anonymous. Cover image, volume 114, issue 22. *International Journal of Quantum Chemistry*, 114(22):i–ii, November 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVu

[Ano14-41] Anonymous. Cover image, volume 114, issue 23. *International Journal of Quantum Chemistry*, 114(23):i–ii, December 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVv

[Ano14-42] Anonymous. Cover image, volume 114, issue 24. *International Journal of Quantum Chemistry*, 114(24):i–ii, December 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVc

[Ano14-43] Anonymous. Cover image, volume 114, issue 4. *International Journal of Quantum Chemistry*, 114(4):i–ii, February 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVd

[Ano14-44] Anonymous. Cover image, volume 114, issue 5. *International Journal of Quantum Chemistry*, 114(5):i–ii, March 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVe

[Ano14-45] Anonymous. Cover image, volume 114, issue 6. *International Journal of Quantum Chemistry*, 114(6):i–ii, March 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVf

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Anonymous:2014:CIVg

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Anonymous:2014:CIVh

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Anonymous:2015:CIIa

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Anonymous:2015:CIIb

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Anonymous:2015:CIIc

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Anonymous:2015:CIId

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Anonymous:2015:CIIe

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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

[Ano15j] Anonymous. Cover image, volume 115, issue 13. *International Journal of Quantum Chemistry*, 115(13):i–ii, July 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVo

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Anonymous:2015:CIVp

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Anonymous:2015:CIVq

[Ano15m] Anonymous. Cover image, volume 115, issue 16. *International Journal of Quantum Chemistry*, 115(16):i–ii, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVr

[Ano15n] Anonymous. Cover image, volume 115, issue 16. *International Journal of Quantum Chemistry*, 115(16):iii–iv, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVs

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Anonymous:2015:CIVt

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Anonymous:2015:CIVu

[Ano15q] Anonymous. Cover image, volume 115, issue 18. *International Journal of Quantum Chemistry*, 115(18):i–ii, September 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVv

[Ano15r] Anonymous. Cover image, volume 115, issue 19. *International Journal of Quantum Chemistry*, 115(19):i–ii, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVw

[Ano15s] Anonymous. Cover image, volume 115, issue 19. *International Journal of Quantum Chemistry*, 115(19):iii–iv, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVa

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Anonymous:2015:CIVx

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Anonymous:2015:CIVy

[Ano15v] Anonymous. Cover image, volume 115, issue 21. *International Journal of Quantum Chemistry*, 115(21):i–ii, November 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVz

[Ano15w] Anonymous. Cover image, volume 115, issue 22. *International Journal of Quantum Chemistry*, 115(22):i–ii, November 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVaa

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Anonymous:2015:CIVab

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Anonymous:2015:CIVac

[Ano15z] Anonymous. Cover image, volume 115, issue 24. *International Journal of Quantum Chemistry*, 115(24):i–ii, December 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVb

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Anonymous:2015:CIVc

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Anonymous:2015:CIVd

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Anonymous:2015:CIVe

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Anonymous:2015:CIVf

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Anonymous:2015:CIVg

[Ano15-32] Anonymous. Cover image, volume 115, issue 8. *International Journal of Quantum Chemistry*, 115(8):i–ii, April 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVh

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Anonymous:2015:CIVi

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Anonymous:2015:IIa

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Anonymous:2015:IIb

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Anonymous:2015:IIc

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Anonymous:2015:IId

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Anonymous:2015:IIe

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Anonymous:2015:IIf

[Ano15-40] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(6):v–viii, March 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIg

[Ano15-41] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(7):iii–vi, April 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIh

[Ano15-42] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(8):iii–vi, April 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIi

[Ano15-43] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(9):v–viii, May 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIj

[Ano15-44] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(10):v–viii, May 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIk

[Ano15-45] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(11):iii–vii, June 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIl

[Ano15-46] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(12):iii–vi, June 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIm

[Ano15-47] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(13):iii–vi, July 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIn

[Ano15-48] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(14):iii–vi, July 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIo

[Ano15-49] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(15):iii–vi, August 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIp

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Anonymous:2015:IIq

[Ano15-51] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(17):iii–vi, September 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIr

[Ano15-52] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(18):iii–vii, September 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIs

[Ano15-53] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(19):v–x, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIt

[Ano15-54] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(20):iii–vii, October 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIu

[Ano15-55] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(21):iii–vi, November 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIv

[Ano15-56] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(22):iii–vi, November 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIw

[Ano15-57] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(23):v–viii, December 5, 2015.

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Anonymous:2015:IIx

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Anonymous:2016:CIVa

[Ano16a] Anonymous. Cover image, volume 116, issue 1. *International Journal of Quantum Chemistry*, 116(1):i, January 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVk

[Ano16b] Anonymous. Cover image, volume 116, issue 10. *International Journal of Quantum Chemistry*, 116(10):i, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVl

[Ano16c] Anonymous. Cover image, volume 116, issue 10. *International Journal of Quantum Chemistry*, 116(10):i, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVm

[Ano16d] Anonymous. Cover image, volume 116, issue 11. *International Journal of Quantum Chemistry*, 116(11):i, June 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVn

[Ano16e] Anonymous. Cover image, volume 116, issue 12. *International Journal of Quantum Chemistry*, 116(12):i, June 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVo

[Ano16f] Anonymous. Cover image, volume 116, issue 12. *International Journal of Quantum Chemistry*, 116(12):ii, June

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Anonymous:2016:CIVp

[Ano16g] Anonymous. Cover image, volume 116, issue 13. *International Journal of Quantum Chemistry*, 116(13):i, July 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVq

[Ano16h] Anonymous. Cover image, volume 116, issue 14. *International Journal of Quantum Chemistry*, 116(14):i, July 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVr

[Ano16i] Anonymous. Cover image, volume 116, issue 15. *International Journal of Quantum Chemistry*, 116(15):i, August 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVs

[Ano16j] Anonymous. Cover image, volume 116, issue 16. *International Journal of Quantum Chemistry*, 116(16):i, August 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVt

[Ano16k] Anonymous. Cover image, volume 116, issue 17. *International Journal of Quantum Chemistry*, 116(17):i, September 05, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVu

[Ano16l] Anonymous. Cover image, volume 116, issue 18. *International Journal of Quantum Chemistry*, 116(18):i, September 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVv

[Ano16m] Anonymous. Cover image, volume 116, issue 19. *International Journal of Quantum Chemistry*, 116(19):i, October

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Anonymous:2016:CIVb

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Anonymous:2016:CIVw

[Ano16o] Anonymous. Cover image, volume 116, issue 20. *International Journal of Quantum Chemistry*, 116(20):i, October 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVx

[Ano16p] Anonymous. Cover image, volume 116, issue 21. *International Journal of Quantum Chemistry*, 116(21):i, November 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVy

[Ano16q] Anonymous. Cover image, volume 116, issue 22. *International Journal of Quantum Chemistry*, 116(22):i, November 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVz

[Ano16r] Anonymous. Cover image, volume 116, issue 23. *International Journal of Quantum Chemistry*, 116(23):i, December 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVaa

[Ano16s] Anonymous. Cover image, volume 116, issue 23. *International Journal of Quantum Chemistry*, 116(23):ii, December 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVab

[Ano16t] Anonymous. Cover image, volume 116, issue 24. *International Journal of Quantum Chemistry*, 116(24):i, December

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Anonymous:2016:CIVc

[Ano16u] Anonymous. Cover image, volume 116, issue 3. *International Journal of Quantum Chemistry*, 116(3):i, February 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVd

[Ano16v] Anonymous. Cover image, volume 116, issue 4. *International Journal of Quantum Chemistry*, 116(4):i, February 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVe

[Ano16w] Anonymous. Cover image, volume 116, issue 5. *International Journal of Quantum Chemistry*, 116(5):i, March 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVf

[Ano16x] Anonymous. Cover image, volume 116, issue 6. *International Journal of Quantum Chemistry*, 116(6):i, March 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVg

[Ano16y] Anonymous. Cover image, volume 116, issue 7. *International Journal of Quantum Chemistry*, 116(7):i, April 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVh

[Ano16z] Anonymous. Cover image, volume 116, issue 8. *International Journal of Quantum Chemistry*, 116(8):i, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVi

[Ano16-27] Anonymous. Cover image, volume 116, issue 8. *International Journal of Quantum Chemistry*, 116(8):ii, April 15,

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Anonymous:2016:CIVj

[Ano16-28] Anonymous. Cover image, volume 116, issue 9. *International Journal of Quantum Chemistry*, 116(9):i, May 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIa

[Ano16-29] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(1):ii–vi, January 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIb

[Ano16-30] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(2):61–66, January 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIc

[Ano16-31] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(3):131–136, February 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IId

[Ano16-32] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(4):253–257, February 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIe

[Ano16-33] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(5):333–337, March 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIf

[Ano16-34] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(6):405–409, March 15, 2016. CO-

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Anonymous:2016:IIg

[Ano16-35] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(7):483–488, April 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIh

[Ano16-36] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(8):555–560, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIi

[Ano16-37] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(9):657–662, May 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIj

[Ano16-38] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(10):731–736, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIk

[Ano16-39] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(10):731–736, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIl

[Ano16-40] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(11):795–800, June 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIm

[Ano16-41] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(12):891–896, June 15, 2016. CO-

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Anonymous:2016:IIn

[Ano16-42] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(13):973–978, July 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIo

[Ano16-43] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(14):1051–1056, July 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIp

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Anonymous:2016:IIq

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Anonymous:2016:IIr

[Ano16-46] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(17):1269–1273, September 05, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIs

[Ano16-47] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(18):1323–1327, September 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIt

[Ano16-48] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(19):1383–1387, October 5, 2016.

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Anonymous:2016:IIu

[Ano16-49] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(20):1437–1441, October 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIv

[Ano16-50] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(21):1493–1498, November 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIw

[Ano16-51] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(22):1613–1617, November 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIx

[Ano16-52] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(23):1747–1751, December 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIy

[Ano16-53] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(24):1823–1828, December 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVa

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Anonymous:2017:CIVb

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Anonymous:2017:CIVl

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Anonymous:2017:CIVm

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Anonymous:2017:CIVn

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Anonymous:2017:CIVo

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Anonymous:2017:CIVp

[Ano17g] Anonymous. Cover image, volume 117, issue 14. *International Journal of Quantum Chemistry*, 117(14):??, July 18, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVq

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Anonymous:2017:CIVr

[Ano17i] Anonymous. Cover image, volume 117, issue 16. *International Journal of Quantum Chemistry*, 117(16):??, August

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Anonymous:2017:CIVs

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Anonymous:2017:CIVt

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Anonymous:2017:CIVu

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Anonymous:2017:CIVc

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Anonymous:2017:CIVd

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Anonymous:2017:CIVv

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Anonymous:2017:CIVw

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Anonymous:2017:CIVx

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Anonymous:2017:CIVy

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Anonymous:2017:CIVz

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Anonymous:2017:CIVe

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Anonymous:2017:CIVf

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Anonymous:2017:CIVg

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Anonymous:2017:CIVh

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Anonymous:2017:CIVi

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Anonymous:2017:CIVj

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Anonymous:2017:CIVk

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Anonymous:2017:IIa

[Ano17-27] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(1):1–5, January 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIb

[Ano17-28] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(2):75–79, January 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIc

[Ano17-29] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(3):151–156, February 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IId

[Ano17-30] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(4):??, February 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIe

[Ano17-31] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(5):??, March 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIf

[Ano17-32] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(6):??, March 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIg

[Ano17-33] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(7):??, April 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIh

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Anonymous:2017:IIi

[Ano17-35] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(9):??, May 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIj

[Ano17-36] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(10):??, May 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIk

[Ano17-37] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(11):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIl

[Ano17-38] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(12):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIm

[Ano17-39] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(13):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIn

[Ano17-40] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(14):??, July 18, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIo

[Ano17-41] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(15):??, August 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIp

[Ano17-42] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(16):??, August 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIq

[Ano17-43] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(17):??, September 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIr

[Ano17-44] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(18):??, September 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIs

[Ano17-45] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(19):??, October 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIt

[Ano17-46] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(20):??, October 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIu

[Ano17-47] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(21):??, November 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIv

[Ano17-48] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(22):??, November 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIw

[Ano17-49] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(23):??, December 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIx

[Ano17-50] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(24):??, December 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVa

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Anonymous:2018:CIVb

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Anonymous:2018:CIVm

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Anonymous:2018:CIVn

[Ano18d] Anonymous. Cover image, volume 118, issue 11. *International Journal of Quantum Chemistry*, 118(11):e25642:1–e25642:??, June 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVo

[Ano18e] Anonymous. Cover image, volume 118, issue 12. *International Journal of Quantum Chemistry*, 118(12):e25652:1–e25652:??, June 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVp

[Ano18f] Anonymous. Cover image, volume 118, issue 13. *International Journal of Quantum Chemistry*, 118(13):e25668:1–e25668:??, July 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVq

[Ano18g] Anonymous. Cover image, volume 118, issue 14. *International Journal of Quantum Chemistry*, 118(14):e25701:1–e25701:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVr

[Ano18h] Anonymous. Cover image, volume 118, issue 15. *International Journal of Quantum Chemistry*, 118(15):e25702:1–e25702:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVs

[Ano18i] Anonymous. Cover image, volume 118, issue 16. *International Journal of Quantum Chemistry*, 118(16):e25790:1–e25790:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVt

[Ano18j] Anonymous. Cover image, volume 118, issue 16. *International Journal of Quantum Chemistry*, 118(16):e25803:1–e25803:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVu

[Ano18k] Anonymous. Cover image, volume 118, issue 17. *International Journal of Quantum Chemistry*, 118(17):e25804:1–e25804:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVv

[Ano18l] Anonymous. Cover image, volume 118, issue 18. *International Journal of Quantum Chemistry*, 118(18):e25805:1–e25805:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVw

[Ano18m] Anonymous. Cover image, volume 118, issue 18. *International Journal of Quantum Chemistry*, 118(18):e25810:1–e25810:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVx

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Anonymous:2018:CIVc

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Anonymous:2018:CIVy

[Ano18p] Anonymous. Cover image, volume 118, issue 20. *International Journal of Quantum Chemistry*, 118(20):e25828:1–e25828:??, October 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVz

[Ano18q] Anonymous. Cover image, volume 118, issue 21. *International Journal of Quantum Chemistry*, 118(21):e25829:1–e25829:??, November 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVaa

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Anonymous:2018:CIVab

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Anonymous:2018:CIVac

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Anonymous:2018:CIVd

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Anonymous:2018:CIVe

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Anonymous:2018:CIVf

[Ano18w] Anonymous. Cover image, volume 118, issue 5. *International Journal of Quantum Chemistry*, 118(5), March 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVg

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Anonymous:2018:CIVh

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Anonymous:2018:CIVi

[Ano18z] Anonymous. Cover image, volume 118, issue 9. *International Journal of Quantum Chemistry*, 118(9):e25628:1–e25628:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVj

[Ano18-27] Anonymous. Cover image, volume 118, issue 9. *International Journal of Quantum Chemistry*, 118(9):e25631:1–e25631:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVk

[Ano18-28] Anonymous. Cover image, volume 118, issue 9. *International Journal of Quantum Chemistry*, 118(9):e25632:1–e25632:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVl

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Anonymous:2018:E

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Anonymous:2018:IIa

[Ano18-31] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIb

[Ano18-32] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(2):??, January 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIc

[Ano18-33] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(3):??, February 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IId

[Ano18-34] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(4), February 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIe

[Ano18-35] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(5), March 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIf

[Ano18-36] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(6), March 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIg

[Ano18-37] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(7), April 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIh

[Ano18-38] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(9):e25471:1–e25471:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIi

[Ano18-39] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(10):e25472:1–e25472:??, May 16, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIj

[Ano18-40] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(11):e25473:1–e25473:??, June 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIk

[Ano18-41] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(12):e25474:1–e25474:??, June 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIl

[Ano18-42] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(13):e25475:1–e25475:??, July 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIm

[Ano18-43] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(14):e25476:1–e25476:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIn

[Ano18-44] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(15):e25477:1–e25477:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIo

[Ano18-45] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(16):e25478:1–e25478:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIp

[Ano18-46] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(17):e25479:1–e25479:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIq

[Ano18-47] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(18):e25480:1–e25480:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIr

[Ano18-48] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(19):e25481:1–e25481:??, October 05, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIs

[Ano18-49] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(20):e25482:1–e25482:??, October 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIt

[Ano18-50] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(21):e25483:1–e25483:??, November 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIu

[Ano18-51] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(22):e25484:1–e25484:??, November 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIv

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Anonymous:2018:IIw

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Anonymous:2019:CIVq

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Anonymous:2019:CIVt

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Anonymous:2019:CIVu

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Anonymous:2019:CIVi

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Anonymous:2019:IIl

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Anonymous:2019:IIn

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Anonymous:2019:IIo

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