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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

M

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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