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Nelson H. F. Beebe
University of Utah
Department of Mathematics, 110 LCB
155 S 1400 E RM 233
Salt Lake City, UT 84112-0090
USA

Tel: +1 801 581 5254
FAX: +1 801 581 4148

E-mail: beebe@math.utah.edu, beebe@acm.org, beebe@computer.org (Internet)
WWW URL: https://www.math.utah.edu/~beebe/

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Title word cross-reference

$(0.0 \leq x \leq 0.3)$ [WZ99]. (110) [Bre99]. $(4s)$ [KSW98]. $(5s)$ [KSW98]. (C_{2v}) [AFM99]. $(d+s)^3$ [Bec97a]. (Γ) [LMAK93]. $(J=0)$ [CB93b, CB94a]. $(n=0,1,2)$ [WMZ98]. $(n=1,2,,6)$ [HL93b]. $(n=1,2,4)$ [XKB+99]. $(n=1--3)$ [IBS95]. $(n=1--4)$ [ST97, WMD95]. $(n=1--6)$ [GFY+99]. $(n=2--12)$ [XSG97]. $(n=2--14)$ [Bou94]. $(n=2--4)$ [CCS99, SPR94]. $(n=4,5,6)$ [RT98]. $(x=2--16)$ [LXWZ99]. + [BA91, BYGA99, CR96b, CB93b, CB94a, DV91, HZ91b, MSM96, MLK94, Oku98, PGM95, RNS93, Ska92, SC95, XY95]. $0s$ [RLR90]. $1,4$ [SWD+99]. $1\,^1$ [BP93b]. $1\,^1B_u^+$ [NNH98]. $1\,^2$ [BP93b]. $1-x$ [GFRR94]. $1/2$ [BHX96]. $1/r_{ij}$ [PCO+94]. $1/Z$ [GLMP98]. $10D_q$ [MBA94]. **$187.00** [Kar96]. $1s$ [FAV92]. 2 [HGL99, LUU90, LCP+91, LSGS91, SSM+99]. $2\,^1A_g^-$ [NNH98]. $2\,^3$ [BP93b]. 20 [LS99]. **$208** [Ber96b]. 3 [Boe91, CB93b, CB94a, RT99]. $3n$ [Roo93b, RL97]. 4 [BT95, RT99]. $4n+2$ [OS95]. 5 [MMCC99]. 540 [MUL99].

6 [SSM+99]. **$60.00** [Mon93]. 7 [SSM+99]. **$79.00** [Str91]. =
[ANB94, Ali99, BCY95, BZQ95, GARC97, Kor90, NBS95, NG95, NL96a, PZTPMC99, STMR97, SG96b, SL97, SNH99, YZX96]. [2 + 2] [Fir94]. *
[BB94, JKK+92, LJ95]. +
[ANB94, BCMÖ97, BB95, Bou94, Bro95a, CWZ98b, CLOFR98, CDB90, Csa96, DS90, DSS90, FV96, Gao93, GS94, GPS90, JM93a, KSF91, KKWT99, KGv93, KA95a, LHL91, MCOS94, MMRSN92, NBS95, Pal94, PS93, PHH94, Pro94, Pro95, RNS93, SPS96b, SZ97b, SC95, STC96, TNSM99, TFSZ95, UJS90, WY99, WMD95, YD96, YSHD97]. $^{+(-)}$ [BCY95]. $\overset{+}{}_{2}$
[BK94b, ELMY96, UJS90, ZTC97]. −
[CLOFR98, CDB90, Csa96, HZ91b, KKWT99, KK93, KGv93, MTNF99, Oku98, Ort98a, PGM95, SKE92, SEKEB98, WYZ+92]. $\overset{-}{}_{2}$ [ZTC97]. $\overset{-}{}_{2g}$ [BČ95]. $\overset{-}{}_{3}$ [Kal90]. $\overset{-}{}_{I}$ [DM97b]. $\overset{-}{}_{II}$ [DM97b]. $\overset{-}{}_{II} \rightarrow$ [DM97b]. ^{0} [CBAM97]. ^{1}
[BČ95, BYGA99, CBT93a, CRsP93, GARC97, HMK96, LP99, LU92b, NÅJ91, NÅJ92, RNS93]. ^{119} [GARC97]. ^{13} [BZ92, GS97b, GARC97, KH96a, RN96]. ^{131} [SCL96]. ^{17} [KH96a]. ^{19} [GARC97]. $^{1}A_1$ [CCS98]. $^{1}A\prime$ [KA96]. $^{1}\Delta_g$ [FSW+91, MLK94]. $^{1}\Phi_g$ [Pet92]. $^{1}\Pi_u$ [Pet92]. $^{1}\Sigma$
[CWJ+99, FSW+91, SES93]. $^{1}\Sigma^{+}$ [BFV+93, PVČ+90, TGS99]. $^{1}\Sigma_g^{+}$ [RA96]. $^{1}\Sigma_g^{+}$ [BP93b, MLK94]. ^{2} [BRL92, BKL97, BLK97, ELMY96, KA95b, LU92b, LK94, Man99, PS93, Sel93, SZ97b, UJS90, WY99]. $^{2+}$
[BL99, BB95, BDH+97, CAJ95, CG97b, EJ93, FLLZ91, GS94, JM93a, KGv93, MMRSN92, Pro94, Pro95, TJ97, Wil90]. $^{2+/3+}$ [ZBL99]. ^{2,6} [XSA+92]. $^{2-}$ [BMG95]. $\overset{2-}{}_{4}$ [BADM97]. $\overset{2-}{}_{II}$ [DM97b]. ^{207} [GARC97]. ^{29} [GARC97]. $^{2}\Lambda$ [Pet92]. $^{2n-}$ [LRM93]. $^{2}\Pi_g$ [MM94]. $^{2}\Sigma^{+}$ [LBG97, Man95a, Man95b, RNS93]. ^{3} [BP93b, CBT93a, CRsP93, LU92b, NÅJ91, NÅJ92]. $^{3+}$
[BMG95, BDH+97, DDN95, MNC95]. $^{3-}$ [CJX+92, NG95]. ^{35} [GARC97]. ^{377} [TWK+92]. $^{3}\Pi_g$ [TGS99]. $^{3}\Sigma^{-}$ [FV96]. ^{4} [HMLK98, LU92b, SES93]. $^{4+}$ [ABCM93, SK99a]. $^{4-}$ [NMCK92]. ^{5} [LU92b]. $^{5+}$ [BMA90, Cze99, SK99a]. ^{6} [Tew94, Tew97]. $^{6+}$ [BMA90, SK99a]. $^{6-}$ [REU+91, XYC98]. $^{7+}$ [SK99a]. ^{9} [KP97]. ^{e} [BLK97]. $^{\infty}$ [KP97]. ^{M} [PAT93]. ^{N} [PAT93]. $^{n+}$ [WMZ98]. ^{o} [BKL97]. $^{\prime}$ [AS93, KJL96, LK90, UJS90, YZX96]. $_{0}$ [GS90b]. $_{0.4}$ [Li97]. $_{0.6}$ [Li97]. $_{0.8}$ [Min96]. $_{1}$
[DM98, ELMY96, GJOV97, GS90b, MW92, NÅJ91, NÅJ92, WP90]. $_{1-x}$ [SPFL93, WZ99]. $_{1.2}$ [Min96]. $_{10}$ [BKM90, REU+91, VR92]. $_{105}$ [RKPE95]. $_{111}$ [RKPE95]. $_{12}$ [CJX+92, Csa96, Eva97, TST+99]. $_{123}$ [RKPE95]. $_{13}$ [LMC97a]. $_{14}$ [LGT94]. $\overset{2}{}_{1}$ [DM99]. $_{1A}$ [PW97]. $_{2}$ [AS93, ARBB95, ANB94, ACHT95, Ali99, ABCM93, ABDM94, ADM98, BA91, BZMR92, BILA95, BUZ94, BDNT97, BBC+94, BP93c, BP93b, BHGC99, BML98, BB91, BBC92, BB94, BFRN90, BYE+97, BCY95, BDH+97, CWX93, Cai93, Cai94, CPBC95, CR96b, CGG96, CB93b, CB94a, CRK+91, CF93, CLGW95, CPD+98, CDP+99, Cun92, DSS90, DOPS91, DDN95, DZ97, DDC97, EBG95, FDC92, FSBS+95, FCVL98, FSW+91, FB90, FMD+96, GKKM96, GJPZ97, GPS90, Gin97, GV93, GJOV97, GZDZ97, GL96, GS90b, HMGP93, HSLL92, HBL99,

HP98, Hir92, HHPT91, IBS95, JMP99, JKK$^+$92, Jen94, JMD95, JJ97, Jur97e, KJ95, KA96, KP97, Kor90, LW92, Li93, LF95, LV97, Loh91, MSD95, MALT96, MLT98, MTP$^+$98, MHM95a, MECE97, MHY98, MK90, MLL99, MM94, MGNK95, MCA95a, MTD93, MTTS93, MLK94, MRST95]. $_2$ [Min94a, MZ95, MDM94, MD91, NM95, NBS95, NÅJ91, NÅJ92, NL96b, OTS$^+$95, Oku98, Ort98b, PGM95, Pal94, PBS99, PSBL98, PPSK96, PPK97, PGS97, RN96, RA91, RD97, RA96, RCWN94, RKH$^+$98, Roz97, RP98b, RS97b, RNS93, SE93b, SM96a, SDP$^+$95, SAB$^+$97, SCS98, SL93, SP92a, SRP$^+$98, SX96, SBAD90, SP92b, SZC97, SST93, STMR97, SCS94, Ska92, SZCO99, Sme92, SGGMGFS96, SES93, SG97, SGB98, Sta98b, SC95, STC96, SC99, SNH99, TJ97, TGS99, TMA97, TPR96, TFSZ95, TZCT97, TS92, TMD96, VH96, VÅJ$^+$92, VBN95a, VBN95b, VR92, VJ95, VJ97, WFS93, WY99, WI96, WDS97, WL99, WL92, WMD95, YNMT98, YNST99, YD96, YSHD97, YK97, ZC96, ZTC97, ZBL99, ZGPS97]. $_{20}$ [CXFP99]. $_{24}$ [WYW96]. $_{240}$ [CXFP99]. $_{26}$ [RG99]. $_{28}$ [LSC98, REU$^+$91]. $^+_2$ [Ata97a, BSHP97, CGG96, GSSD$^+$96, LA97, LBG97, MUMH97, RS97b, Sch97, SBOB97, Úle92]. $^-_2$ [CGG96, HZ91b, LBG97]. $_{2h}$ [BBC92]. $_{2n}$ [GFY$^+$99]. $_2 \to$ [XFF98]. $_3$ [AMC97, BUZ94, Boe91, BB91, BDD93, CCC$^+$95a, CLOFR98, CPN91, CEM$^+$96, DR92, Del92, DZ97, DM98, DLF99, FCVL98, Fra99, Gao93, GS94, GWB97, GARC97, Hag99a, JMP99, Jen94, KP96, Kal90, KS95a, KJ95, KLO$^+$98, KGv93, LJ95, LDGA96, Li93, LF95, Loh91, MCL95, MLT98, MGNK95, Moc99, MCCF95, Nag96, Oku98, Pal94, PZTPMC99, PCF94, PPSK96, PPK97, RN96, RA91, SL93, SRP$^+$98, SBAD90, SK91, SP91, SZC97, Ska92, SW95, SLL$^+$91, SL97, SC99, VX99, WY99, WL99, WMZ98, WZ99, XFF98, YK97]. $_{3-\delta}$ [Li97]. $_{3-x}$ [Min94a, YZX96]. $_{3-y}$ [Min98]. $_{32}$ [XYC98]. $^+_3$ [Hag99a, KLT97, TMA97, WSB94]. $^-_3$ [NG96]. $^2_3$ [DM99]. $_3 \to$ [YD96]. $_4$ [AS93, ABCM93, BL99, BILA95, BUZ94, BHGC99, BBC92, BB97a, BL98, DZ97, EMS92, FCVL98, GS94, GV93, Gut99b, HP98, JKK$^+$92, JKJ94, JG95, Jen94, KP96, KGv93, KC97, Loh91, LSC98, LCS98, MVS97, MHM95b, MNC95, NS91, PCF94, RKG96, SC99, VBN95a, VBN95b, WYW96, WY99, WI96]. $_{40}$ [CJX$^+$92, LCS98]. $^{+1}_4$ [MVS97]. $^{2-}_4$ [CCWCF96]. $_4 \to$ [YSHD97]. $_5$ [CCC$^+$95a, KS95a, KJ95, KGv93, NM95, NG95, NG96, OSS95, RA91, SG96b, SC98b, SC99]. $_{5+\delta}$ [Min96]. $^{2+}_5$ [DWB98]. $_6$ [BL99, BUZ94, BBC92, Bou96, BDH$^+$97, Csa96, Cze99, DN96, DDN95, JKK$^+$92, KBBK90, MLL99, RA91, RB93, RKG96, SDO91, Ska92, TJ97, WG94, ZBL99]. $_{60}$ [BBZ91, BSS$^+$97b, CCC$^+$95a, CC92c, DM98, DM99, FLWZ90, HRRBL97, HL93b, LRM93, LU92a, LL99, MCCF95, RRC94, SZCO99, TST$^+$99, TFSZ95, XY95, YZX96]. $^{2-}_{60}$ [HOF$^+$97]. $^{3-}_{60}$ [HOF$^+$97]. $_7$ [BB91, JH90, Li93, SBAD90, SG97, WL99]. $_{7+\delta}$ [Min94a]. $_{70}$ [BBZ91, LFS94, TZCT97]. $_{78}$ [AS99, RG99]. $_8$ [BUZ94, BB91, CG97b, Csa96, DDC97, Eva97, GSSD$^+$96, JG95, JH90, NMCK92, RA91]. $_{80}$ [CXFP99, SLA97]. $_{81}$ [REL$^+$90]. $_{86}$ [SLA97]. $_{87}$ [REL$^+$90]. $_{88}$ [SLA97]. $_9$ [BKM90, VR92, XYC98]. $_{93}$ [RKPE95]. $_a$ [MK95]. $_B$ [CMSF93]. $_C$

[JMS95, BB91, DMB97, Fri93a, Fri93b, KCP90, Li93, Mar94c, MS94]. $_{\text{cam}}$ [CL90]. $_{g}$ [BFRN90, ČDM91, LP99]. $_{I}$ [DM97b]. $_{II}\rightarrow$ [DM97b]. $_{\infty}$ [FMD+96]. $_{J}$ [Man99]. $_{k}$ [Zha91]. $_{m}$ [Kor90]. $_{n}$ [AS93, BAL95, Bou94, BDD93, Cas97, CCS99, FLLZ91, GFY+99, Ike99, IP93, IBS95, Kar90, Kor90, LDP93, LCP+91, MKRW99, NYKY98, ST97, SPR94, WMD95, XKB+99, XSG97]. $_{s}[\rho]$ [LBPL97]. $_{u}$ [LP99]. $_{x}$ [BSS+97b, GFRR94, LXWZ99, MW90b, Min94a, SPFL93, SZCO99, SL97, WZ99, YZX96]. $_{x}[\rho]$ [LBPL97]. $_{y}$ [LF95, MW90b, SZCO99]. $_{z}$ [KA95b]. A [SST93]. $\mathrm{A_2B_2}\leftarrow \mathrm{X^2A_1}$ [BJ98]. α [BKEMM94, FMS+99, HWB97a, JI95, Jon92a, KG98, LH94, NSS+95, NMCK92, Pal92b, PTKS+92, SCMF93, SWMB94, SST93, SST94, TWK+92, VABM94, WL92, Woo98]. $\alpha 2$ [VDD96]. α^2 [BSS97a]. α_N [ZLHZ94, ZLHZ94]. as [HHKM95]. B [PMN+92, SPH98, SST93, SH90b]. β [BH92, CFR96, FWZ97, For94, GKM90, HWB97b, HWB97a, LCP+91, LU92b, NMSJ99, Ram90, Suh91, TCB99]. β_1 [TWK+92, WD91, WTD+94]. β_2 [GHB+99]. $\mathcal{L}_N$ [FJR96]. $\mathcal{S}_N$ [FJRS97]. $\cdot$ [HZ91b, MLL99, MTTS93, SDP+95, SST94]. $\cdots$ [SST93]. $\chi^{(2)}$ [Mun92]. D [BK95, DBM99, HM95, Hos97, MK97a, BS91b, GFRR94, Mor96a, STM96b, SJ97, TV92, ZFZ92]. D_{2h} [Har97a]. δ [FS95a, Flo95, LTSL96, MGNK95, Ram90, SMM+90]. $\Delta^{-1/2}$ [NS95b]. $\delta E/\delta\rho$ [TŚPKM94]. e [Pai97, PL98, Pai99]. ϵ [Ram94]. η [DMB97]. η^5 [SC98b, SC99]. f [Boe96]. $f(r)$ [PZDM97, PZDM98]. f^6 [DDN95]. G [HZ99, LBG95, LG96]. γ [Bla99, BH92, Ram90, SRP+98]. $h-b-1$ [GT97, TG96]. I [TLC98]. I_h [TLC98]. j [Roo93b, RL97]. $J=0$ [VJ95]. K_a [PWL98]. $\kappa-\pi$ [CD93]. L^2 [CM96a, Hil98]. λ [KRRB99]. $\lambda,\mu,\nu\geq -2$ [LK93]. $\langle 1/r\rangle$ [Csa94, Csa95]. $\langle r^n\rangle$ [Csa93]. $\leftarrow$ [GS90b]. $\leftrightarrow$ [BA91, HZ91b]. $\longleftrightarrow$ [HB95]. m [BKWL97]. $m=0,1$ [Kor90]. μ [Gal98, PVU+93, SJ91]. μ_3 [BUZ94]. N [CC92a, CC92b, Flo97a, Flo97b, FJRS97, Fri93a, Har90, KSH94, KPR97, KLM91, KL92a, LB96a, McD97, MZ93, Mor93b, RPKM95, Sam97, SWD+99, SK99b, SFM94, TZ97a, Tew94, TT98, Val96, ZH99a, HL93b, LDJH92, LDHJ92, MHN98, MKRW99, MMCC99, MSM96, MK98b, PM95, PK99, RT98, RK92, SM96b, She90d, WGR+94, Yam97, RM96, Tew97]. $n=1,2$ [Kor90]. $n=1,5$ [SGB97]. $n=1,7$ [SGB97]. $n=45$ [MKRW99]. N^6 [SSM+99]. $\nabla^2 n/n$ [MHN98]. $\nabla n/n$ [MHN98]. nl^N [KS95b]. $n\leq 7$ [Cas97]. $\mathrm{NO_2}$ [BJ98]. $N\prime$ [SWD+99]. ν [KL92a]. ν_{17} [TWWC91]. O [LT99]. O_4 [Har97a]. O_h [LT99]. $O\supset C_4$ [FC99]. p [DM95, JDJP99, SMM+90]. P^o [HMLK98]. π [BSS+97b, BSP98, Dia99, FS99, GX98, GH96b, GH92, JM94, KMR92, KEG+97, LB93, LRM98, LL99, LB94, MD92b, MK99, PP92, PZWJC96, PB97a, Rep96, Tri98c, TDK+94, VDBPR97b, ZM95]. $\pi*\leftarrow n$ [DV96]. π^* [GH96b]. π^2 [ML99]. $\pi^2+\pi^2$ [RW92]. π^4 [ML99]. $\pi\rightarrow\pi$ [NNH98]. $\pi\rightarrow\pi*$ [LHNK99]. $\prime$ [CAM+97, DZB92a, Enc96, SWD+99, VVO98]. R [MBA94]. r_{12}^{-2} [LK92]. r_{12}^{-1} [Pan95]. $r_{23}^{\lambda}r_{13}^{\mu}r_{12}^{\nu}$ [LK93]. r_{ij} [Kin99]. $\rho(r)$ [PZDM97, PZDM98]. $\rightarrow$ [BRL92, BPVP92, BYGA99, CR96b, FSW+91, GS90b, Jur97e, LP99, LAM92, PPSK96, PPK97, RNS93, SES93, UJS90]. $\rightleftharpoons$ [XY95]. S

[Ort97, Boe96, FFD98, GJP91, HHKM95, SK99a, Wil96]. $S = 0, 1/2$ [LP97d]. S_1 [MJLL99]. Σ [MHS95, BAR94, JM94, KEG$^+$97, ŠG96a, TAY$^+$97]. $\Sigma^+ \leftarrow\!\!\!/\!\!\!\rightarrow \Sigma^-$ [Par99]. *sp* [Ell91]. t [RW92]. T_1 [TWK98]. T_c [DBM99]. $T_c[\rho]$ [LKLBD98]. $U(2n)$ [BG98b, BG98c, BG98d]. v [BYGA99, KLM91]. $v\prime$ [BYGA99]. $Y'' = F(X, Y)$ [Sim95]. Z [KSH94, Rey90]. $Z = 1--24$ [PZ91].

***** [FL95, NNH98].

-2 [CAM$^+$97]. **-acetylpropanamide** [ZH99a]. **-adrenergic** [GHB$^+$99]. **-adrenoceptor** [TWK$^+$92, WD91, WTD$^+$94]. **-Al** [SRP$^+$98]. **-alanine** [Ram90]. **-Alkane** [WGR$^+$94]. **-Alkanes** [MK98b]. **-allyl** [FS99]. **-aminobutyric** [Ram90]. **-aminohexanoic** [Ram94]. **-aminoimidazole** [HGL99]. **-aminopentane** [Ram90]. **-aminophenyl** [SWD$^+$99]. **-androstane** [PTKS$^+$92]. **-Argon** [PL98, Pai99]. **-Atom** [Pai97]. **-Atomic** [KS95b]. **-Azido-3prime-deoxythymidine** [DZB92a]. **-bend** [NMSJ99]. **-Benzohydroquinone** [DM95]. **-Bi** [MGNK95]. **-bipyridyl-3** [Enc96]. **-bis** [SWD$^+$99]. **-bithiophene** [VVO98]. **-Butane** [MSM96]. **-Butyl** [RW92]. **-Butylbenzene** [PK99]. **-butyrolactone** [BH92]. **-C** [SC98b, SC99]. **-Chemisorbed** [BDD93]. **-conjugated** [GX98, LB94]. **-Conjugation** [PB97a, LL99]. **-cristobalite** [GKM90]. **-cyclodextrin** [HWB97b, HWB97a]. **-cyclopropan** [CAM$^+$97]. **-D** [LUU90, CB93b, CB94a]. **-DCNQI** [Sta98b]. **-deoxyadenosine-5** [KJL96]. **-dianthryl** [LK90]. **-difluorobenzene** [JDJP99]. **-DIIS** [Sel93]. **-Dimensional** [Mor96a, TZ97a, CC92a, CC92b, Hos97]. **-diol** [Enc96]. **-doped** [FS95a, LTSL96, SMM$^+$90]. **-Electron** [PZWJC96, TDK$^+$94, GH92, LDJH92, LDHJ92, PP92, Rep96, ŠG96a, ZM95, Flo97a, Fri93a, KPR97, MK99, RPKM95, Val96, Flo97b, SK99b]. **-electronic** [Dia99]. **-Electrons** [GFRR94, TAY$^+$97]. **-elements** [ZFZ92]. **-Ethyl-Indole-3-Acetic** [RT98]. **-fluoropropane** [RK92]. **-fluorotoluene** [JDJP99]. **-Fold** [HL93b, PM95, SM96b, She90d]. **-Framework** [KEG$^+$97]. **-function** [Jon92a]. **-glycylcarbonyl** [Tew97, Tew94]. **-Halogenobenzoic** [BKWL97]. **-HD** [Voj96]. **-helical** [Pal92b]. **-helices** [TWK$^+$92, Woo98]. **-heptane-HZSM-** [MMCC99]. **-His** [GSSD$^+$96]. **-hydrido-bridged** [Gal98]. **-hydroxyketones** [FWZ97]. **-hydroxypentanoic** [Flo95]. **-Hydroxypropionic** [CFR96]. **-Hydroxytetronic** [BKEMM94]. **-Hydroxyurea** [LB96a]. **-Indacene** [HHKM95]. **-indole** [RT99]. **-ionone** [TCB99]. **-K** [ZLHZ94]. **-ketoenolyl** [For94]. **-Ketoesters** [SWMB94]. **-krypton** [Pai99]. **-layer** [Boe91]. **-manifold** [DDN95]. **-Membered** [BT95]. **-Methyl** [MZ93]. **-methyl-** [RT99]. **-methyl-derivatives** [SSM$^+$99]. **-Methylacetamide** [TT98]. **-Methylformamide** [TT98]. **-Methylpyridones** [RM96]. **-methylthio-** [SSM$^+$99]. **-MSH** [JI95]. [**?**]NaSaha:1999:LES. **-Neon** [PL98]. **-Ni** [BDD93]. **-one** [CAM$^+$97]. **-opioid** [PVU$^+$93]. **-Pairing** [DMB97]. **-phosphate** [KJL96]. **-pleated** [Suh91]. **-poly** [GT97]. **-polyazamacrocyclic** [HBGR99]. **-propiolactone** [BH92].

-protonation [SSM+99]. **-Pyridylacetic** [NSS+95]. **-quinonenediimine** [SWD+99]. **-reduced** [KG98]. **-related** [Nal92a]. **-Representability** [Mor93b, Sam97, Har90]. **-representable** [KLM91, KL92a, SFM94]. **-residue** [LS99]. **-S** [BUZ94]. **-separation** [MHS95]. **-Sextet** [KEG+97]. **-SiO** [WL92]. **-Spiral** [LCP+91, LU92b]. **-state** [TWK98]. **-subunit** [SCMF93]. **-tensor** [LG96]. **-Tensors** [LBG95]. **-Tetrasilane** [Yam97]. **-tetrazine** [Ort97]. **-Type** [FFD98, Wil96, Boe96, Ell91, SMM+90]. **-wave** [DBM99].

/1 [Boč90]. **/6** [FL95, Les92]. **/6-31** [FL95, Les92]. **/blood** [BPHB96]. [**?**]CSaha:1999:LES. **/Cu** [Eng92]. **/INDO** [KSIH92]. **/M** [BDH+97]. **/MC** [FZZ92]. **/MCLR** [NÅJ91]. **/Molecular** [BLBP97]. [**?**]NSaha:1999:LES. **/Q** [RSCP91].

0 [Ber96b, Brä95, Car96, Deu96, Kar96, Lin96a, Sjö96, Tri96]. **0-19-506643-X** [Deu96]. **0-19-508091-2** [Lin96a]. **0-19-508523-X** [Mic96a]. **0-19-509775-0** [Mic96a]. **0-19-855573-3** [Str93]. **0-387-57874-9** [Brä95]. **0-387-94376-5** [Sjö96]. **0-387-94380-3** [Car96]. **0-444-82171-6** [Tri96]. **0-7923-3264-4** [Ber96b]. **0-7923-3664-X** [Kar96].

1 [ARBB95, BRA+99, Brä96c, HRH99, JZ95b, KJ95, MAL93, Mav98, MCM98, DZB92b, RA91, SB98, SAL+94]. **1-Bisnitroxyphenylethylene** [TD96b]. **1-D** [MCM98, SB98]. **1-dimethyl** [MSRP90]. **1000-Tesla** [BMG+98]. **11-14** [JPP87]. **11-diene** [RGHH94]. **13-atom** [KJ97]. **13-Molecule** [PVLG93]. **13C** [Mon98, PRC98]. **155.00** [Ano92l]. **158** [DV91]. **18-crown-6** [Tho96]. **1980** [CD81]. **1984** [Cal90f]. **1986** [Cal90d]. **1987** [Cal90d, Cal90c, Cal90a, JPP87]. **1988** [Ågr90, Cal90g, Lun91]. **1989** [Cal90e, Cal90b, Lun91, Tay91]. **1990** [Ano90a, Ano90b, Ano92k]. **1991** [Ano91a, Ano91b, Ano93h, Bir94, Eri92, Lun92, Kar93]. **1992** [Ano92a, Ano92b, Ano93g, FMT93, Jør92, Kar93, Lin93]. **1993** [FR94, Mon94, Wha96]. **1994** [Ano94a, Ano94b]. **1995** [Ano95a, Kra96]. **1996** [Ano96a, Ano96b]. **1b** [FMS+99]. **1b-adrenergic** [FMS+99]. **1D** [LO93, TDK+94]. **1S** [JM95].

2 [BP93b, JZ95b, Jur98b, Lin96a, MTD93, MCM98, OSA+97, PVLG93, RK95, SB98, SP92b, Sta98b]. **2-** [AEHM91, MH98]. **2-alkenylfurans** [EVSN92]. **2-Aminoethanethiol** [Bue96]. **2-Aminoethanol** [Bue96]. **2-D** [MCM98, SB98]. **2-diazacyclobutadienes** [JZ95b]. **2-Dihydro-1** [JZ95b]. **2-dimethylcyclopropanone** [CAM+97]. **2-Dithietes** [MF96]. **2-electron** [DWB98]. **2-Hydroxypropanal** [OSA+97]. **2-Hydroxypyridine** [MTD93]. **2-isomer** [MZ91]. **2-Nitrophenylcyanate** [Mor96c]. **2-Nitrophenylthiocyanate** [Mor96c]. **2-Pyridone** [AL95, MTD93]. **2-substituted-1** [SLG+96]. **2-Trifluoromethylvinyl** [KH97]. **2/6** [Les92]. **2/6-31** [Les92]. **20-component** [BOL+90]. **202nd** [Bir94]. **21G** [LJ95]. **21st** [Kra96]. **23S** [Voj96]. **273K** [RBB+94]. **28H4** [LSC98]. **29-July** [CD81]. **2D**

[LO93]. **2e** [TN96]. **2N** [SES93]. **2nd** [Car96, Sta90, Str92]. **2NH** [XFF98].

3 [Brä96b, Brä96c, BHKK93, CBT93a, Car96, CFR96, Dun96b, LJ95, Maz98, MH98, MC95, PVLG93, RK95, SAL$^+$94, TD96b]. **3-21G** [LJ95]. **3-540-57801-3** [Brä96b]. **3-540-57962-1** [Brä96c]. **3-540-58703-9** [Dun96b]. **3-Aminopropionamide** [CFR96]. **3-calculated** [BHKK93]. **3-center** [DWB98]. **3-di-** [CAM$^+$97]. **3-dialkylnitroxybenzenes** [TD96b]. **3-Didehydroproline** [RK95]. **3-dienes** [SLG$^+$96]. **3-Diketopiperazine** [PVLG93]. **3-Dimensional** [VRR92]. **3-dimethylimidazol-2-ylidene** [Cio93]. **3-Dimethyluracil** [PIG94]. **3-Dipolar** [SAL$^+$94]. **3-Isothiazolones** [MC95]. **3-j** [Lai94]. **3-methyl** [SCJK90]. **3-pyridinecarboxylic** [KBM92]. **3-Pyridyl-** [MH98]. **3-substituted** [PHBB94]. **3-Triazole** [PGS97]. **31G** [AKCS91, LJ95]. **330** [Ano92j]. **3d** [Boe93, Nag96, RW98]. **3p** [MTTS93]. **3prime** [DZB92a]. **3S** [WD97].

4 [AAS93, Ber96b, TD96b]. **4-** [BBB$^+$95]. **4-31G** [AKCS91]. **4-aminobutanol** [KR93]. **4-chloro-indole-3-acetic** [RTKP96]. **4-Currents** [AAS93]. **4-dihydropyridines** [PHBB94]. **4-Diphenylpentane** [LV93]. **4-Nitro-1** [PGS97]. **4-phenylene** [Lah92]. **4-trioxane** [BJM$^+$94]. **4.2** [RBB$^+$94]. **45.00** [Cal93]. **48** [CAK$^+$96]. **4CuCl** [BBC92]. **4d** [MS93b]. **4th** [Brä95, Str92].

5 [HRH99, Maz98, PW97, Sjö96]. **5-** [MSS99a]. **5-C** [KJ95, RA91]. **5-Contracted** [Maz98]. **5-Fluorouracil** [MRT97]. **5-hexatriene** [HRH99]. **5-HT** [PW97]. **5-lipoxygenase** [ARBB95]. **5-Me** [Sta98b]. **5-tetranitroimidazole** [CP99b]. **5-trinitroimidazole** [CP99b]. **55A** [Lun91].

6 [LJ95, Tri96]. **6-31** [FL95, Les92]. **6-31G** [LJ95]. **6-benzyl** [Tew92]. **6-dihydronicotinic** [BBB$^+$95]. **6-Dimethoxy-1** [TD96b]. **6-furfuryl** [Tew92]. **6-j** [Lai94]. **6-thioguanine** [RBB$^+$94]. **60th** [Ano94-36].

7-cyclooctatetraene [PMS94].

8-tetrachlorodibenzo-p-dioxin [MEP90].

9 [Brä95, Dun96b]. **9-dimethylguanine** [YJL92]. **9-j** [Lai94].

= [BL99, Bou96, GARC97, IP93, JKK$^+$92, KSN93, Moc99, SM96a, SGB97, SGB98, SC99, TST$^+$99].

A/T [LSGS91]. **AA** [SST93]. **Ab-initio** [FR92, FR93a, RK91, SKRK90]. **Abacus** [Mon93, Sri97]. **able** [GV92]. **above** [CB96a]. **above-threshold** [CB96a]. **abrupt** [SLS91]. **Absolute** [RPB$^+$97, Sie93]. **Absorbed** [DP94].

Absorption [AEAO99, BJ98, BMG+98, Che96, CCZ97, GSSD+96, KLT97, SZ95, WDCA97, AHM97, BBS90, BFV92, GS90b, LA97, Lin91, SZ97b, YCML91]. **Abstraction** [BCS96, Jur97a, YNMT98, CMG92, TUK90]. **AC** [Moi97]. **Academic** [Ber96b, Cal90e, Cal90b, Kar93, Kar96]. **Acceleration** [Sel93, TMR99]. **accelerator** [Kin99]. **Accelerators** [Hom93]. **Acceptor** [Mor93a, Mor96b, AB99, EE91, FKR92, GBS99, MCT99]. **acceptors** [PC91]. **Account** [PTP95, MG93a]. **Accounts** [PB97b]. **ACCs** [BG98c]. **Accuracy** [JKRW98, JGR98, JMR98, LDP93, Núñ95b, UWB94, Lan95, LH94, MDM94, TNS96, Ber96b]. **Accurate** [A.95, Aqu95, BKL97, BLK97, DLV95, Dun96a, Dun97, EJ93, FR93b, IYFI99, JM99, Jur97a, KKT93, KLI92, KLLI97, LK94, NB93, Núñ94a, SGGC99, Sim98, SLD95, Taş93, Taş96a, BSS97a, BS95, FFD96, KE90, KD92, New97, SSC92, MHL94, NL96b]. **ACE** [Ish96]. **ACES** [SGW+92]. **Acetaldehyde** [ADPS98]. **Acetaldehyde/Vinyl** [ADPS98]. **Acetaldimine** [ADPS98]. **Acetaldimine/Vinylamine** [ADPS98]. **acetate** [BH92, STS95]. **Acetic** [FT95, FT96, FT97a, RTKP96, RT99, RT98]. **Acetone** [MR92b, PBB92, DV96]. **Acetonitrile** [MDD93]. **Acetyl** [RK95]. **Acetylene** [FF94a, Fou94, Jur99a, AD92, HMG+92]. **Acetyloxyl** [KVS98]. **acetylpropanamide** [ZH99a]. **ACh** [WJC+98]. **AChE** [WJC+98, WJC+99]. **AChE-catalyzed** [WJC+98, WJC+99]. **Achieving** [MVS97]. **Acid** [AP93, AP96, BAK97, CFR96, DM95, FT95, FY95, GJLA99, LX95, NSS+95, RFG99, RT98, SPG97, SHC+98, Tew94, YW92, BOL+90, BKEMM94, BS91c, BBB+95, CLR+93, FT96, FT97a, FHHE90, FR92, Flo95, HWB97a, KK99b, KE91, KBM92, LHNK99, Les92, PTM92, PHBB94, Ram90, Ram94, RTKP95, RTKP96, RT99, SSM+99, Tew97, TFR99, TBP99]. **Acid-Base** [SPG97]. **Acidic** [BKR97]. **Acidities** [BMP93, RPB+97, DDN99, MBP91]. **Acidity** [DLG95]. **Acids** [BDG96, BKWL97, MBP97, AHM97, ACC92, CLC90, HWB97b, KKM99, MKBP97, SJB90]. **ACPQ** [PTP95, PTP95]. **acrylonitrile** [HDY+91, MMA+92]. **action** [BP90, JGCJ96, WD91]. **Activated** [NP96b]. **Activating** [DBF+96]. **Activation** [CBSR+98, CC96, Jur97a, MÅ99b, MC94, PW97, RR94, Sak98, ST96b, BYE+97, Cun92, FMS+99, PBS99, PVU+93, RNS93, SC98b, SC99, TWK+92]. **Activation/Cyclization** [MC94]. **Active** [EBG95, HM99, KN99b, KW98, NK98, SBIP97b, VC92, BMDM90, BP93d, DFGB99, GK92, KK99a, KM90a, KN99a, KSK91, MHY98, SZCO99, TKK+90, WWFR99, TNS92]. **Active-site** [HM99, DFGB99, TNS92]. **Active-Space** [EBG95]. **Activity** [DZB92a, FT95, GJOV97, NHN97, PW97, Reg92, TBBE98, ZCT98, BTKVG99, Bha99, BBE95, CMA+99, FT96, FT97a, HB94, I'H90, Khu92, KBM92, Lev94, Pul90, RFM90, SM94, SC96]. **actual** [Tay91]. **Actually** [Sta98c]. **Acylation** [DDP96, WJC+98, SCA93]. **acylhydrazones** [DBR+96]. **ad** [And93b]. **Adams** [Brä96b]. **Adaptation** [PKJ99]. **Adapted** [CDDM96, Flo97a, JPJ95, JM99, KPR97, MPKR94, NU95, PRTV97, PTP95, RPKM95, VDBPR97a, CLZ99, Cio91, Flo97b, GLM91, JRS+99, LP93, LV97, MD99, PC99, VDBPR97b, ZWD98a, ZWD98b]. **Adatom** [SD98]. **adatoms**

[PTL90]. **Addendum** [Ano94c, Csa90a, Mey97]. **Addition** [AMKS93, ET97, HWS92, OSA+97, YTYS97, TFR99]. **additions** [DGMW90]. **Additive** [Lev97]. **additivity** [May92]. **Adducts** [FW92b, FW92c]. **Adenine** [LF90, MKM93b, Tew94, HB95, Tew97, SSM+99]. **Adiabatic** [KC98a, Nag95a, SB98, STMR97, CSG99, Gin91, GL95, II94, KLC98b, OKY+99, PY92]. **Adiabaticity** [Lef97]. **Adjoint** [KE93]. **Adler** [Deu96]. **admissibility** [HYS91]. **adrenergic** [FMS+99, GHB+99]. **adrenoceptor** [TWK+92, WD91, WTD+94]. **Adsorbate** [NNMH96, HS99]. **Adsorbates** [DDH+96, Hea97, Kun90, PBPN90, PSBL98]. **Adsorbed** [GMR+93, JAG95, LLZ98, KSH92, MVB92, PCB92, SM99]. **Adsorption** [JSG97, NTL96, Bre99, Cas92, CPD+98, GE92, HS99, MD91, SCS98]. **Advanced** [CD81, Kar93, Yur95]. **Advances** [KPD93, Rig92, Ano92j, Csi82]. **Advantages** [FFD98]. **Affinities** [CA97, GKKM96, Jur97g, NKUS97, PD93, STMR97, BHKK93, DS90, GW91, KCLI95, OS92, SPB90]. **Affinity** [BDG96, GJLA99, STC96, MMA+92, RB93, SP92a]. **aflatoxin** [WP90]. **AG** [SST94, ANB94, Ali99, CBAM97, SNH99, GE92, KSN93, NHN97, NKUS97]. **AgCl** [VABM94]. **agent** [BVV91]. **agents** [BHV96, DBR+96, WTD+94, WWFR99]. **AgF** [VABM94]. **Aggregate** [DP93, DS99, NYNY99]. **Aggregates** [NY98]. **Aggregation** [LL94a, MDD93, AD92, BMFPV92]. **Agonist** [VDD96, WD91, WTD+94]. **Agostic** [JKK+92]. **AGP** [Col97]. **Agreement** [TGDS97]. **AH** [BCY95, NBS95]. **Aib** [NSS92]. **Aid** [FSHC99, Jac97, Jac98]. **aims** [Cle92a]. **Al** [BCY95, BZQ95, Min94a, SRP+98, Bau98, DFL98, DLF99, HS99, KJ97, LMC97b, MVS97, Min94a, MBML91, RNS93, TIPM96, VG90]. **Al-doped** [Min94a]. **alanine** [Ram90]. **Alberte** [Ano99a]. **Alcohol** [ADPS98, CAK+96, Ryd94, KH97, RAM91]. **Alcohols** [BSP97, DDN99]. **alcoholysis** [TF92]. **Aldehyde** [SSMK93]. **Aldehydic** [VBUS99]. **Alder** [Bra97b, MV98a, SLG+96]. **Algebra** [Alt96, CP92, Jon92a, KS90, LP92, Löw92g]. **Algebraic** [Ada94, CXFP99, DlD99, FC99, For92b, GMI95, GYDY97, Iac92, IL95, IP93, KKT93, Lai94, PRSDS92, SM96c, AR92, Ano90g, ČPV90, GDYY97, Jør92, KS92, MPSLB91, Réa90, RSCP92, Sim99c, Brä96b, Lin96a]. **Algebrants** [Pos91, PK92b, LP97d]. **Algorithm** [Cul95, HO94, Ish96, SB98, Sel93, ST96a, TCM98, WWM+98, GP91a, HVS98, MV91, MVHV96, PS92c, SB92a, VM92, ZDO96]. **Algorithmic** [Lio92]. **Algorithms** [FGRS98, PR97, ZO95, Pos91, Rig92, Roo93b, ZO94, ZDO99]. **AlH** [RNS93, CWJ+99]. **alignment** [Ata97a]. **aliphatic** [CLC90, DDN99]. **Alkali** [BK94c, LRM97, MLR+98, Bat92, BRS95, CMB95, Csa94, KO91, KBBK90, LRM93, YZX96]. **Alkali-Doped** [LRM97, YZX96]. **alkali-earth** [CMB95]. **Alkaline** [DTA+96, KPTŚ94, Sta98c, CC92c, Csa94, LRM93, STS95, TSS95]. **Alkaline-Earth** [DTA+96]. **Alkaline-Earth-Intercalated** [Sta98c]. **alkaloids** [Bha99]. **Alkane** [CD90, WGR+94]. **Alkanes**

[Gin95, Gin96b, MK98b, BKM90]. **Alkenes** [ET99]. **alkenylfurans** [EVSN92]. **Alkoxo** [CdBKZ99]. **Alkoxo-Bridged** [CdBKZ99]. **Alkyl** [FLF96]. **alkylating** [BVV91, BHV96]. **Alkylation** [Cha95]. **Alkylidenes** [BC97a]. **Alkylperoxyl** [ET99]. **Alkynes** [Jay92]. **All-** [MI93]. **All-Electron** [SSO+97, SG93, BK97, MKRW99, SG92]. **All-trans** [KBT94, YAD92, CPA98]. **All-Valence** [RL92, MAAP90]. **Allene** [FF94b]. **Allinger** [Ano96-58]. **allotropic** [WTSN94]. **Allowed** [Pon97]. **alloy** [DLF99, KJ97, SPFL93]. **Alloys** [DFL98, FD96a, MLR+98]. **Allyl** [RML97, BT96, FS99]. **allyl-nickel** [BT96]. **Allylic** [PRB96, PBHB95]. **almost** [EMS92]. **AlO** [MCOS94]. **Along** [Pon97, AM90a, Art93, LV97, LAM91, LAM92, Pal92b]. **alpha** [AP93, JJ96, KSW98, HHPT91]. **alpha-Aminoisobutyric** [AP93]. **alpha-function** [JJ96]. **alpha-particles** [KSW98]. **Alternant** [BE95, BE98, HA93, KBGE97, TDK+94, TDO97, ZSK97, AH92a, Dia99, Hal93]. **Alternating** [Kup94]. **Alternation** [LP96, LN96, MD93c, TAY+97, CP99a]. **Alternative** [GR95b, GR96b, Gin96a, HKC96, JKJ95, MAPLB92, SB92b, ZYZ90, BT96, LU92a]. **Altmann** [Lin93]. **Alumina** [NMvB+98, SWMB94]. **Aluminum** [BPL97b, Tri97, BPL94, BBRT94, Kie97, LB94, VG90, BHL+99, GL92]. **AM** [MAL93, ARBB95, BH92]. **AM1** [PHM+91, PBHB95, BHPB93, BHPB95, BPHB96, GARC97, KK99b, KGVM97, MKK96, MALT96, MLT98, PIG94, PBB92, SBM97, SSMK93, BP92b, DE92, SBD+92]. **AM1-based** [BPHB96]. **am7** [HS92b]. **America** [Bir94]. **American** [Bir94]. **Amides** [BK94c, Mar97c, RBT99]. **Amine** [Sen96]. **Amino** [BDG96, DB94a, Jur98a, ŠH96, BOL+90, GL97, HGL99, KKM99, Les92, Tew92, TBP99]. **Amino-Nitro** [DB94a]. **Aminoalkylation** [MKK98]. **aminobutanol** [KR93]. **aminobutyric** [Ram90]. **Aminoethanethiol** [Bue96]. **Aminoethanol** [Bue96]. **aminohexanoic** [Ram94]. **aminoimidazole** [HGL99]. **Aminoisobutyric** [AP93]. **aminopentane** [Ram90]. **aminophenyl** [SWD+99]. **Aminopropionamide** [CFR96]. **Ammonia** [MSCS95, CBL95, HW91, WG99, ZY94]. **AMO** [PČe90]. **Among** [AMKS93, ZC95, Csa93, DM92]. **Amorphous** [TNM98, BJ92, Tos95]. **Amphipathic** [NAK95]. **Amplitude** [Day96, MSRSP93]. **Amplitudes** [Day95, MMD96, MMP95]. **Amsterdam** [Tay91, Tri96]. **Analgesic** [Reg92, RFM90]. **analog** [LUU90]. **analogous** [Tri98c]. **Analogs** [KGv93, LS92a, LBBE98, MC94, Sak98, SM98, WYW96, BBSS96, Les91, LU92b, RA91]. **analogues** [MEP90, WSTB90]. **Analyses** [CDDV93, CDM+94, NYKY98]. **Analysis** [AZAC97, AFTM95a, AFTM95b, AFO+97, AFTM98, AM90a, Art98, ADM98, BW99, Bue96, BP95, CB94a, CV99, Dia99, FS94, FS95b, Gho95, GARC97, HC91, IK94, Jac97, JKK+92, JBT+95, KT96, KJ93, LP97b, LL97, MI93, Mor96c, MT96, MSCP92, NK96a, Nal94, Nal95a, NM95, NS93b, NB97, OSA+97, PP95, PO97, PKM94, Par97, PV94, PGS97, PS94a, PB95c, PJ96, Pon97, RKN97, RT98, SLtM+94, SB95a, SM96b, Sch95b, SS91, SLDB91,

TMD96, VB94, WHF92, ZM96, Ali99, AYAZ95, AFZ+99, BE93, Bha99, BRV99, CB93b, CC91b, CDG04, FLHT90, GVV+90, HSES94, ITT+94, ISOA99, Jac98, Kin93, KRRB99, KC97, LLL91, LAM91, LM92, MESH93, Min90a, MEP90, MSRP90, Nal92d, Nal92b, NM92, PL91, PLBB99, PB99, RTKP95, RT99, RAM91, SCA93, Sch95a, SC96, Tac92]. **analysis** [Tac94, TYTY91, TWWC91, VX99, VES+99, ZPBC97, Ish92, YITY93]. **Analytic** [GKKA97, GC91, Loh96, MZM94, Sza95, TK92, CJM+91, DS92]. **Analytical** [BPL97b, CTC95, DDG93, DW90, GRK96, Gus98, HO94, IHG95, KKWT99, Mor96a, QS98, RDK97, SZL95, Tac96, BMA99, Hos97, WB93, RDK02]. **Analyticity** [RH96b]. **Analyze** [PÅS+97, SMO+96, BBSS96, LV97]. **Analyzing** [KC98a, KLC98a, KC98b, KLC98b]. **Ancillary** [CAK+96]. **and/or** [NMN+97]. **Andreas** [FMT93]. **androstane** [PTKS+92]. **androstanediones** [KPTVT+97]. **anesthetics** [DB97]. **angle** [STKK92]. **angles** [FCMB99, MEB91]. **Angular** [Can97, Ols96, Pal93b, TN96, YPC97]. **angularly** [DSW93]. **Anharmonic** [CB93a, MS97b, RDF98, Sch95b, BFV92, LC90, LF99, Réa90, Sch95a, WN90]. **Anharmonicity** [SB95a, Taş96b]. **anhydrase** [GK92]. **anhydride** [HMK99]. **Anion** [BSP97, CFDS90, ESP98, Jur99a, RML97, Yam97, CJX+92, Jur99c, Pro95, XYC98]. **Anionic** [FLRV97, GSJS97, KSN95, DS90, KSN93, KJL96]. **Anions** [BMP93, Can97, DBG92, DZO97, MKM93b, PZ95, YNMT98, Can94, KSSG95, MW90b, MRST95, MCB99, Pro94]. **Anisole** [DZOR98]. **Anisotropic** [BHX96, Bra97a, WG95, BMFPV92, DOPS91, MK90]. **Anisotropies** [Can97, RGT95]. **Anisotropy** [GARC97]. **Annealing** [BLRD92, MT96, BV93, IBS95, JH90, KI94, LS99]. **Annihilation** [LZ96]. **Announcement** [Ano90g, Ano90c, Ano90d, Ano90e, Ano90f, Ano91c, Ano91d, Ano91e, Ano92h, Ano92c, Ano92d, Ano92e, Ano92f, Ano92g, Ano93c, Ano93d, Ano93e, Ano93f, Ano94d, Ano94e, Ano94f, Ano94g, Ano94h, Ano95c, Ano95d, Ano95e, Ano96c, Ano96d, Ano96e, Ano96f, Ano96g, Löw94a, Par95a, Par95b, Par95c]. **Anomalous** [SWD+99, NMN+99]. **anomeric** [MT91]. **Ansatz** [GR95b, GR96b]. **ansätze** [SB92b]. **Antagonist** [MTP+98, WD91]. **Antagonists** [DBF+96, MTD93, ARBB95, WLB+94]. **Antalya** [Yur95]. **Antarafacial** [RW92]. **anthracene** [KL93a]. **anthraquinone** [HGP91]. **anti** [BD95b, TCZ91]. **anti-malarial** [TCZ91]. **Antiaromaticity** [MSP94, PMS94, ZH99b]. **antibiotic** [NSS92]. **antibiotics** [BS95]. **Antibound** [BR97]. **anticancer** [BS95, SC96]. **Anticonvulsant** [MAAP+98, TBBE98]. **Anticonvulsivant** [BBE95]. **antidepressant** [CMA+99]. **Antiferromagnetic** [SB95b, YITY93]. **antihydrogen** [AZ99]. **antileishmanial** [Bha99]. **antimalarial** [BJM+94, DBR+96]. **antioxidant** [BP90]. **antiparallel** [Xu99, Per93]. **Antiparallel-spin** [Per93]. **antisite** [CFDS90]. **Antisymmetry** [Pal95, VA90]. **Antitumor** [FT95, FT96, FT97a]. **Antiviral** [DZB92a]. **Any** [AB97, KJ95]. **Aperiodic** [ASI94b, IAN+94, BOL+90]. **Apoenzyme** [FVN98]. **Apomorphines**

[GJOV97]. **appearing** [PCO+94]. **Applicability** [Lef99, MHM95a, MUMH97, MHM95b, PS94b, SMPJ94, Sch93, ZP90, PL93, TNS96]. **Application** [ASP97, ABR95, ATI97, Bat92, BCMÖ97, BD94a, BG98a, BKLV94, CCM+96, CT96, CMFA93, CGMG92, CB94b, DDA92, DRBE96, DA91, Dun99, EBG95, FSVZ97, FFD98, GYDY97, GW98a, HKC96, Her98, IK94, JM95, JM96a, KFS92, KBT94, KKE+96, KL97b, KL97a, LTY90, MR92b, MD93c, Nic99, NV94b, NS93b, PM93, SCL96, SDW+98, SZL95, SZ97a, SPB90, SS99b, STY+98, SGGMGFS96, Ste96, SATP94, TNSM99, TMSI98, TC98b, VH96, BZMR92, CT95, Che92, CM99, DWM90, HC96b, HDB+95, LC90, MRC99, MK90, MM94, Ort97, Rom92, SN99, ŠG96a, SOK+98, Sim95, TGS99, WP91, WA94, Wil99b, BTKVG99, BD95a, Boe93, CCWCF96, CA92b, CTC95, GRB+93, Har94, KLC98b, KRZ91, KCLI95, LKM99, LV97, Lin91, LJS94, MFH91, Nag96, NYNY99, NV97a, PS92c, RVP92, SSM90]. **Application** [TC98c, VZ92, YB99, ZPBC97]. **Applications** [ADB96, Cal90b, CWZ98a, DQB97, Enk97, GP95, GG97b, GLBM96, Hom93, KBB+90, Kup98, LLC+94, LDJH92, MPR97, NS93a, O'C96, PEBS97, PG95, SM96b, SB96, TZ97a, Wil96, ZLHZ94, Ada94, Ave89, Bal90, CC92b, Ced90, Del92, Har91, Kha91, Löw92h, Nal95b, Sem96a, ZM95, ČVW91, CMB95, Csi77, KS90, LBL98, Ort98a, PK92b]. **Applied** [BLE96, BČ96b, CJH98, ČB96b, Dau94, KD98, KPTS97, Kra96, LCLO95, Muk92, PDT97, RDK97, Roz97, VJ95, VJ97, AZ99, CFMA95, Cze99, Ell91, FHHE90, FR98, HMK99, NPL90, RDK02, Ano93g, Sta93]. **Approach** [ÁC94, ATI97, AO93, ABLA97, BM96, CLZ95, CLSI94, CG96, DlD99, DFDK99, DC95, Del98, Dew92, FK94, Fer96, FFD98, FBKD97a, FBKD97b, FBKD97c, Flo97a, Fri93a, Fri93b, GJ95, GD94, GSD97, GGSA98, GYDY97, Har97b, Huz96, JPJ95, JZ95a, JZ95b, Jur96a, KSR95, KNA94, KPTŚ94, Kry98, Kup98, LY98, LP96, LD95, LBBE98, MKM93a, May98, MKM96, MPJ97, MPJ98, MSCP92, NY98, Nic96, NS93b, Pal97b, PPP97, PC95, RP96, SA96, SAR96, SM96c, SG94, SGGMGFS96, SLD95, SP94, XY95, Ada94, AM90b, BA91, Brä96b, VD90, CPA98, Csa90b, CK91, DM92, DB94b, EMP92, FMR91, Flo97b, FJR96, FDD95, GDYY97, GDB98, JK90, KSS92, KKS99, Kin99, KFK91, KPM+90, KLM91, KSW98, LF94, LLL91, LF99, LP92, MM99a, Mar99a, Min90b, MAPLB92, MSF91]. **approach** [MV92, MSC92, NYNY99, NM96, NS92, NMCK92, OKY+99, PBPN90, PA92, PY92, Pic92, PB95b, PS92b, PFK99, RTS91, RSCP92, Røe91, RK91, RMF90, SK99a, SGK99, SCP91, TD03, WLB+94, WG99, Wil99a, WP95, Yu95, YUSM99, ZYZ90, ZM90]. **Approaches** [BA97a, BBC+96a, BAK96a, Chr97, FGRS98, FWC+93, JOC97, NB97, PTP95, RZ96, RWT92, CGG96, Chr92, Hei95, HBGR99, Mat97, PP92, PČe90, RWT91, Sch92a]. **Appropriate** [Gin95, MYN+96]. **Approximants** [CG95, CB93a, LBPL97]. **Approximate** [AGH91, BMA99, CV94, Fer95, HHKM95, KS98, Mez97b, MYPL90, MP91, NP96a, Núñ95b, Ort98a, Ort99, OYL91, PTP95, SDW+98, CD92, ČPV90, JGP91, Rin96, RSCP92]. **Approximately** [SFM94]. **Approximating**

[BMDM90, TNI96]. **Approximation** [BKR97, BPE97, CM96a, Che93, CC97a, GVB97, Hag97, KS94a, Kir95, KLLI97, LLC+94, MJS93, MV99, NS95a, Ney95a, Ney95b, PP98a, SZ96, Sha95, STY+98, SBIP97b, VZ93, ZC95, AZ99, BZMR92, Bec94, BKL91, BDPS97, CFMA95, Gin91, GRB+93, KS90, KSIH92, Kün99, NM96, NI94, PRSDS92, RRC94, RK92, SNNY99, SS91, SS92e, TGS99, YB99, ZDO96]. **Approximations** [BAD99, DP97, GvLB96, LV98, LP94, Sah95a, HC96d, KPB99, SN90a, TP90, TK92]. **Aquatic** [ML97]. **Aqueous** [BMP93, JI95, SM98, AGAP98, AFM99, BHH92, CDB90, DV91, ESHP99, MBP91, NOY98, SWK90, WO92]. **Aquifer** [Har97b, Har98b]. **Ar-HCO** [DQB97]. **arbitrarily** [TTOY93]. **Arbitrary** [Kat98b, KPA95, LS93a, LDP93, PS96, BSS97a, DW90, GSM90, Geg91a, Geg91b]. **architectures** [KJD+93]. **Area** [Art98, KM99a]. **arginine** [SS90]. **Argon** [BOX94, LLC+94, Loh96, NG97, PL98, II94, Pai99]. **Arithmetic** [KL97b]. **Arnaut** [Ano93h]. **Arnold** [Mic92]. **Aromatic** [DD93, EMMK94, Jur98b, KEG+97, KN92, KGv93, LL92, ML97, RL94, SF96, AGM99, BLC95, GJDD97, KM90c, LBBK91, MEP90, PVN90, TKK+90, VRR92, Yu95]. **Aromaticity** [DV99, Hal91, Rin94, FF90, Jur99d]. **aromatics** [LYSL95]. **array** [YITY93]. **arsenide** [SP91]. **Artemisinin** [BJM+94]. **Artemisinin-like** [BJM+94]. **Arthur** [Deu98b]. **artifact** [CG97b]. **Aryl** [Mor98a]. **Arylamines** [Cha95]. **arylethylidene** [METHH94]. **arylidene** [METHH94]. **ASA** [MGNK95]. **ASADH** [HM99]. **ASADH-A** [HM99]. **ASED** [And94]. **ASED-Mo** [And94]. **ASI** [Ano92j, Ano93h, Eri92]. **Asp** [DV91]. **Asp-158** [DV91]. **aspartic** [TNS92]. **aspect** [Tit96]. **Aspects** [BS93, BF94, BMG+98, BK98, DS96, JY94, Löw97b, SC97, BSP98, CH91, KK92b, MG90, PBS99, RVL97, Sch92c, SBZ92a, TCA+91, Tay91]. **Assembly** [PÅS+97, SKZ96, Con92]. **Assessing** [MPR97, Núñ95b]. **Assessment** [Art93, KG97, KG98, TNS96]. **Assignment** [NV97b]. **Assignments** [FSHC99]. **Assisted** [BTTS97, Hag97, Hag94]. **Associated** [Löw93d, MSCS95, WT98, GS92b, SD91, TKO+92]. **Association** [ROSM96, NH90]. **associative** [MD91]. **Astronomy** [Rau02]. **Astronomy-inspired** [Rau02]. **Astrophysics** [Enk97]. **Asymmetric** [CS98, MM99a]. **Asymmetrical** [Taş96a]. **Asymmetries** [RGT95]. **Asymmetry** [PM93]. **Asymptotic** [BE98, GBRA94, HA93, HS93, Núñ96, QS98, KKWT99]. **Asymptotics** [BČ96b, San97]. **Atkins** [Str93]. **Atom** [AS96, Aqu95, BCL98, CLKMTA95, De 97, DC95, DD98a, DD98b, FF94a, Fou94, FD96b, GMR+93, GBJMA94, JR96, KUN+98, LKMC93, LKFF98, MK97a, Mor96a, Mor94, MMD96, MPJ98, Pai97, RS94, Roś96, ROSM96, SG98, SSD96, SGB97, TNM98, UWB94, WBD97, YLD97, A.95, AGNS92, BKL98, Cha92, DMR96, DD95, EKI94, Fer92, Hos97, Ish92, KSH92, KJ97, KSK+99, LCB98, LKVS97, LK94, MEB91, OB95, Pai91, RMF90, SCS94, TMR99, TG96, Whi99, ZA95, HW87a]. **Atom-** [HW87a]. **Atom-Atom** [ROSM96, MEB91]. **Atom-Symmetric** [YLD97]. **Atom-Vacancy** [FD96b].

Atomic [AC97, ABR95, AYDR96, AR99b, ÁC94, BP93a, BK96, BGS98, Can97, CC97b, CA97, CDDV93, DDD93, DZF93, ETV94, Fan97, FD93, GP95, GD94, GG97b, HW84, HW87a, HW87b, HSS+95, Ish90, KSH94, KS95b, KBL95, KT96, KS96, KN99b, KY93, LKBJ97, Lin97, Lin96b, LBKLC98, LK93, Mar97a, Mic94, MM98, Mon98, NK98, Pah98, Pen93, Pen96, RH95b, Roz97, SKN95a, SKN95b, TVP93, TSPK96, VBD+98, YD97, Zha96, ACAT92, AYAZ95, AR99a, Can94, Csa90a, Csa91, DM94a, Dav90, GL92, Har94, HFM91, Hos97, KKNY99, KE90, KN99a, KY92, LMV92, LM93, LO90, MFH91, Mon94, NWT92, PBPN90, Par99, PZ91, Rau02, RR95, SW92, SKRK90, TNI96, TBW90, UBA92, VA90, WSTB90, Yu95, ZYZ90, WS92]. **atomic-electron** [TNI96]. **Atomic-Molecular** [Fan97]. **Atomistic** [KJD+93]. **Atomization** [EPB97]. **Atoms** [ABR95, AM98a, AH97, Bad94, BOX94, BKM93, CBAM97, CC95, CV99, CGR+94, Dat95, DPP+94, GSD97, Gin96b, GLMP98, HWB05, HC96e, JOC97, JM99, KWT95, Koh95, LV98, Mar91, Mar97a, Mar98b, McD97, MÅ99b, MTL97, PCC93, Pie93, PDT97, PB97a, QS98, RPJZW96, Røe91, SMPJ94, Sch98, SD96a, SGK+95, SKZ96, She97, SS97b, SFGW96, ZWJP95, ASM91, BK95, BKL91, Boe97, Brä95, Brä98b, BGS97, Cal93, CCWCF96, Csa94, DD89, FR98, GL99, GW91, HW92, HW94, HW96, HW00, HBJ+92, HFM91, KM99b, LaF90, LBL98, MFH91, NM91, PY89, PZA92, PG95, PA99, SAB+97, Sco90, SB90, Sem94, SK99b, SKC99, TK92, Tit96, TC98c, VG90, ZP92b, ZB92, ZPBC97, Cal90e, Brä98a]. **Attachment** [MP93, AFM99]. **Attack** [DD93, Yu95]. **attacking** [Kry96]. **Attempts** [MMA+92, Zie96]. **Attraction** [HS91, SPH98, US97]. **Attractive** [HKC96]. **aufbau** [Dia99]. **Augmented** [AB97, KPA95, Pah98, DBF+92]. **August** [Bir94]. **AuPt** [CPD+98]. **Aurora** [SKC99]. **autocorrelation** [CÅ92a]. **Autodissociative** [CAJ95]. **Automata** [SSD96, SKC99]. **automatic** [Rig92]. **Auxiliary** [FS97, GOAY98, LDP93, WT98, FS09]. **Auxin** [RT98, RTKP95, RT99]. **auxins** [RTKP96]. **Average** [JM93b, KPR97, MR92b, MSPS90, PAAM98, SGK+95, MRD92]. **Averaged** [CJA94, CJH98, KS95b, BBS91, SAW97, SZ97b]. **Averages** [Pop98, Val96, Ort93]. **Avery** [Cal90b]. **Avian** [NK96a]. **avoid** [TS92]. **avoided** [TGS99]. **avoiding** [CE90]. **AX** [IP93]. **Axial** [DL92, HC96e, JBS97]. **azabenzenes** [SLS91]. **azaborines** [MZ91]. **Azabutadienes** [Mor96b]. **Azasilatranes** [DS96]. **Azide** [YK97, SK91]. **Azido** [DZB92a]. **Azines** [DT96]. **aziridines** [PWL95]. **Azo** [Shu96]. **Azotobacter** [SZ98]. **azulene** [GS90a, GS90b].

B [Cal90d, Cal90c, KJ95, Kor90, NÅJ91, NÅJ92, RA91, Sta90, FSW+91, BS91b, Bau98, Bou94, DBLV94, GK90a, JM93a, LGT94, LP99, Mar97b, SST94, WP90, MLK94]. **B-DNA** [BS91b]. **B-spline** [DBLV94]. **B.C.C** [PTL90]. **B.V** [Ågr90]. **B3** [Csa96]. **B3LYP** [Bau98]. **Ba** [BSS+97b, DDN95, Li97]. **Bacillus** [HB94]. **Back** [Hos97]. **Back-of-envelope** [Hos97]. **Backbone** [FWT+96, LV93, PFMC97]. **Backbone/Side** [LV93]. **Backbone/Side-Group** [LV93]. **backbones**

[BV93]. **Background** [SIM93a]. **bacterial** [HM99]. **bacteriophage** [KRRB99]. **Bacteriorhodopsin** [Woo98, SHF94]. **Balance** [HM97c, MC91a, MC91b, VAVN91]. **Balanced** [MHY98]. **Band** [ÅGL97, Ara94, CL97, CCC+95a, CM94, FFD98, GSSD+96, Gin95, Lad97b, Min94a, Min98, MAD98, NC95, SK91, Spr96, TDK+94, And90, BBS90, Boe93, EC96, Fau92, FFD96, For92b, KPM+90, LO93, MW92, SBAD90, SS92g, TWWC91, VCMLL90, Yam90, YYLB90, BRS96]. **Band-Structure** [CM94]. **Bands** [FDF97, Gin97, SBM97, BADM97, Loh91]. **barbituric** [KK99b]. **Bare** [AM98a, BDD93, CB99]. **Bargmann** [MSRSP93]. **barrelene** [FKR92]. **barrelene-based** [FKR92]. **Barrier** [ADPS98, Che97, LP97c, MPV94, Sak98, ALS+91, CMG92, HZ93, Hag99b, WFS93, WSB94, ZBL99]. **Barriers** [ART94a, BW99, Bue96, HMGP93, Jur97a, JK90, LS92b, RBT99]. **Barry** [Brä96b]. **Base** [Brä93b, CD93, FW92b, SPG97, ŠH96, Tew94, ZL98, BHV96, FL95, LJS94, PS99, TCB99, Tew97, YNO92, FW92c]. **Base-Pair** [FW92b, FW92c]. **Based** [BDG96, BPL94, CDDM96, DMFR93, GLBM96, GSM98, JM95, JBT+95, KSY97, Kon94, MS97b, Mos98, MV99, RB95, RABZ94, RWT92, SZL95, SZ96, SZ97a, SDE94, SL98, Wen98, ZLHZ94, BJM+94, BBLK94, BFRN90, BPHB96, CKB91, CB99, EKI94, FKR92, FF90, GSKC99, Jac92, JM96a, KRZ91, KSIH92, LP98, MM99a, Min90a, PLBB99, RWT91, SGGC99, SSC92, Suh93, TYY91, TGS99, TD03, DGMW90]. **Bases** [AP96, BNLF96, JBS97, SM98, CXFP99, DBL+90, DS90, FHHE90, GT97, Les92, MBP91, SSM+99, WS92, YJL92]. **Basic** [BKR97, Chr89, Tay91, Dun96b, Jac92, LM95, Bud92, HC96a, NM92, Str91]. **Basicity** [BK94c, PZTPMC99]. **Basis** [AHI96, AMKS93, AHWA96, BC96a, BR94, BEJ98, Bro96, BDH+97, CM96a, ČHM95a, ČHM95b, ČHMA95, CSS93, Dat95, DLV95, Fer96, FFD98, FR93a, Flo97a, Gin95, GT93, HH97, Hil98, HS91, HS92f, HS92e, JM99, Jur98a, Jur98b, KSR95, KKT97, KL97a, Kru92, Kut94, LJ95, LTP96, MSD95, NNMH96, PG94, Pah98, PVLG93, PHH94, Pen93, Pen96, PMN+92, PDT97, RPJZW96, Sad97, SPOAS97, SA96, Sur94, TZ97a, Taş97, Ter97, TJ95, US97, UBA92, Wil96, AM92, AH92b, Bla99, BC97b, Boe96, BSP98, BGS97, BG98b, BG98c, BG98d, Cul91, CB91, DBLV94, DWM90, DBF+92, Flo97b, FR98, Geg91b, HBJ+92, ISOA99, Ish91, Ish92, JRS+99, JEB92, Jug90b, KH96a, KH95, KYW95, Les91, LP92, LO90, Lon99, MHS95, MFH91, MS92, NE95, PCO+94, PKJ99, PB99]. **basis** [Qui02, RAI99, RLR90, REU+91, Sme92, SS92f, Sta98d, SBZ92b, Tal93, TKSH93, Tit92, VCCM92, VAVN91, WBP91, WSW96, Wil99a, YNO94, vMVvLvD97, HBJ+92]. **Basis-Set** [ČHMA95, PHH94, AM92, MFH91, PB99, WSW96]. **BaTiO** [AMC97]. **bay** [KL93a, VS95]. **bay-** [KL93a]. **bcc** [MESH93]. **BCS** [Aon98, PC95]. **Be** [JM95, TST+99, CL94, CDDV93, Löw94c, Sta98c, BSHP97, BKL98, JM93a, JM96a, KP97, LBG97, RA96, REL+90, RKPE95, FMD+96]. **BeC** [DTA+96]. **Becke** [Jur97a]. **become** [Klo90]. **BeFH** [ASP97]. **beginnings** [Brä96c, LF94]. **BeH** [CAJ95, SL93, SGGMGFS96]. **Behave** [ATP+96]. **Behavior** [BE98, BHX96, DS93, GBRA94, LTSL96, Núñ96, PČP92, PV98,

TKMA92, WSW98, GS90b, PAC90, YUSM99]. **behind** [Kry96]. **being** [Klo90]. **Beings** [Fuk95]. **BEM** [DV91]. **Benchmark** [Jon93, Tri97, REU+91]. **bend** [NMSJ99]. **Bending** [Sen96, LSGS91]. **Benoxaprofen** [BD95b]. **Bent** [OCK99, DV99]. **Bent-bond** [OCK99]. **benz** [KL93a]. **Benzaldehydes** [SSMK93]. **Benzene** [CCZ97, Oli99, ČPV90, DV99, GZSvD99, MZ91, OTG91, SLS91, VDBPR97b, Vin92, YNO94, Cio94]. **Benzene-Tetracyanoethylene** [Cio94]. **BenzeneAr** [VH96]. **Benzenes** [Cha97, MG93b]. **Benzenoid** [GRK96, Ran97, GH92, Gut99a, HGP+92, RG99]. **benzenoids** [Hal93]. **benzo** [KL93a, WP92]. **Benzocyclobutadiene** [KGC+96]. **Benzocyclobutadienes** [KEMM93]. **Benzocyclobutenes** [KEMM93]. **benzodiazepine** [GVV+90, VL91]. **benzofuran** [PHM+91]. **Benzohydroquinone** [DM95]. **benzoic** [HWB97b, HWB97a]. **Benzoyloxyl** [KVS98]. **benzyl** [Tew92]. **benzylidene** [METHH94]. **Benzylimidazole** [VDD96]. **Bergman** [BS95]. **Berlin** [Brä95, Brä96b, Brä96c, Dun96b]. **Bernard** [Ano99a, Ano99e]. **Berry** [BKL92]. **Beryllium** [MFP96, Mor94, PZ95, Boe95, REKP92, ZA95, LBL98, MV90]. **Bessel** [TZ97a, TZ97b]. **Bethe** [BJMK92, Por97, Por98, Por99, PR97]. **Between** [Aon98, BBC+96a, BLBP97, BP93c, BTN98, BPL97b, BL92b, Bra97b, Coo94, Del96, FF94a, FF94b, GM93, GG97a, Gin97, HP97, Iga95, JTZ+96, JBT+95, Jur98a, KBA96, Löw95e, Löw99, Mar97a, ML97, Mon98, MPJ98, MBP97, NYY96, NK96a, OHSF97, Pie93, PS94a, Reg92, RML97, RRS97, RW92, SF95b, Sch99b, Scu95, WGR+94, YW92, Ågr91, AGM99, AMH+92, BBTU97, BP93b, BCD91, BHV96, CZ94a, CWJ+99, CE90, DFGB99, DBF+92, For92b, GDYY97, JKGM99, KDB90, Kün99, LB94, Luk92, LSGS91, MS91, Mar94c, MD99, NNH98, Pro95, RPT90, Sch92c, Sco90]. **Beyer** [Brä98c]. **Beyond** [BJLK98, BPE97, Sha95, SV95, Kun90]. **BH** [GR95a, Jas94, LV97, SL93, VDBPR97a]. **Bi** [MGNK95, MM94]. **bi-orthogonal** [MM94]. **Bibliography** [Ano99b]. **bicyclo** [CAM+97]. **Bicyclobutane** [Gal96]. **bifurcated** [DS93, MRBM91]. **big** [RF94]. **bilayer** [CPGC99]. **Bilirubin** [SRS92, AGAP98]. **Binary** [VV95]. **Binding** [AR93, Bér97, BBC+96a, BSP97, BRA+99, CLR+93, DPP+94, Gho94, JTZ+96, KPTŚ94, LRM96, Mar94d, MHÅ98, MAD98, RP98a, TVP93, TR94, WP93, Wan94, AMH+92, BRV99, Cas97, CL90, CML92, Csa90a, Csa91, EC96, GVK99, GL92, HGP91, Kap99, KL93a, KÅ99, KRRB99, Mar90, Pro95, RKH+98, SM92a, STKK92, SJB90]. **Binney** [Kum93b]. **Binomial** [GİA96]. **Binuclear** [CdBKZ99, SBIP97a, FWS97]. **BiO** [Li97]. **Biochemical** [Bir94, OLC+96, CH91, RCB+99]. **Biochemistry** [JPP87, Cal90c]. **Bioctahedral** [CF96]. **Biographical** [Ano90h, Ano91f, Ano92i, Ano94i, Ano99c]. **bioligand** [CPGC99]. **biological** [CMA+99, Kha91, Kov98b, LBBK91, LB93, PMO90, RF94, RD90, WK90, WMW92]. **Biologically** [MKM96, RL94, SZCO99, KM90a, TKK+90]. **biology** [Ano90i, KWZ98, Löw91a, Löw91b, Löw91c, Löw91d, Löw92b, Löw92c, Löw92d, Löw92a, Löw93a, Löw93b, Löw94b, Löw95c, Löw95f,

Löw95d, Löw95b, Löw96a, Löw96b, WA94, Löw90c]. **biomembranes** [KO91]. **biomimetic** [RC99]. **Biomolecular** [CDD+99, EB97, Mic97, Bir94, Jak93]. **Biomolecules** [MFAT98, MGK99, Ano96-31, Pul90]. **Bioorganic** [Sta96a]. **biopolymers** [FG96, FM92a]. **Biorthogonal** [KSR95]. **biosynthetic** [HM99]. **Biosystems** [MVL96, TMM97, MVL98]. **bipolaron** [Mat96]. **bipyridyl** [Enc96]. **Biradical** [KMVÅ95, OS90]. **Birge** [Mic97]. **birthday** [Ano94-36]. **Bis** [TD96b, BB94, SWD+99]. **Bis-** [TD96b]. **bisbenzylisoquinoline** [Bha99]. **Bisected** [Lah92]. **bisector** [TS92]. **Bisnitroxyphenylethylene** [TD96b]. **Bistability** [GMMH97]. **bitetrahedryl** [XSA+92]. **bithiophene** [VVO98]. **Biuret** [LS92a]. **BK** [GK90b]. **Blackwell** [Kra96]. **Blanchard** [MPP+97]. **Bloch** [MS97a, MS97b, OK96, Por97, Por98, Por99]. **Block** [Gin98]. **Blockade** [Pec93]. **Blocks** [Mar94b, PÅS+97]. **blood** [BPHB96]. **Blue** [SC98a]. **Blueshifts** [Her93a, Her93b]. **BN** [SPR94, BMG95, MPSF97, SPR94]. **Bob** [Par94a]. **Boc** [NSS92]. **bodies** [Mez94b]. **Body** [BD94a, BD94b, CN99, FS95c, FS97, IK97, JOC97, KFS92, KBT94, KZVGB97, Kon94, Lin96b, LFD94, MHM95b, NB97, PPP97, Pie93, Sta93, SPL97, SKS98, VVS94, WD95, WD97, Ano93g, BD95a, Cim96, FS09, HC96a, HC96b, HC96c, HC96d, Ish92, KSF91, KE90, MHM95a, MUMH97, MVHV96, Muk92, Mur90, SH90a, SKE92, VCMLL90, YKN+99, ZC99, ZP90]. **Bohm** [Dun99]. **Boltzmann** [LP97a, PWL98]. **Bonchev** [Mon93]. **Bond** [Amo96, AH96, BvL96, CWZ98a, CDD+99, CP99a, CD93, CXL97, Cul95, GLBM96, Har97a, HH92, Her97, HP97, JM96c, Jur97b, KJ95, KGC+96, KZVGB97, LP96, LTP96, LN96, Mar94d, NFVM94, ÖOD96, PRC98, RG94, RK96, RC97, Rin94, SBD+92, Sut96, TAY+97, TC98b, WWM+98, AS99, BBTU97, CR96b, CRK+91, DA91, DS93, EMS92, For92b, GT97, ISOA99, Jur99c, KE90, KT95, Kry96, LP92, MVHV96, McW90, McW99, MSRP90, NL96a, OCK99, RPT90, Rin96, RD97, RK92, SM96a, SY91, SCJK90, SG92, SLDB91, SC98b, SC99, TG96, VES+99, WG99, WZ99, Zha91, Boe96, Brä93b, HMG+92]. **Bond-Breaking-Bond-Forming** [NFVM94]. **Bond-centered** [Boe96]. **Bond-Cleavage** [RC97]. **Bond-Formation** [RC97]. **bond-forming** [CR96b]. **Bond-Polarizable** [PRC98]. **bond-rupturing** [CR96b]. **Bonded** [AK97, BA97b, KS94a, KS94b, Kry98, VBV92, BCLS94, CS99, Cul91, Kar90, RFG99, SES93, VM92, WG99, WBS99]. **Bonding** [BC97a, BTN98, CAK+96, CKM91, CCG+96, DE92, Del98, FT95, Fou94, KY93, MTD96, NG96, Oli99, PB97b, RKG96, SM98, SSP98, SRW96, SG93, SS92c, SC95, Suh94, TT98, VB94, WS94a, XLW+99, Ali99, CWZ98b, CP99b, Del92, EZ92, FT96, FT97a, Flo95, KH97, LJS94, PBPN90, PCB92, PZTPMC99, PTL90, Ram90, RC92a, Ram94, SLG+96, TMD96]. **Bonds** [BF95, BL92b, DDH+96, FSF96, Gin96b, Pon98, Sur94, Sur95, YDFS98, CP99b, DWB98, DS93, DSW93, Ert90, Kor90, Li92, Mar97c, PCD99, RA91, Røe91, YOTY93]. **Book** [Ågr90, Ano92l, Ano92k, Ano92j, Ano93g, Ano93h, Ber96b, Brä95, Brä96b, Brä96c, Brä98b, Brä98a, Brä98c, Cal90g, Cal90d, Cal90f, Cal90c, Cal90e,

Cal90b, Cal90a, Cal93, Car96, Deu96, Deu98a, Deu98b, Deu99, Dun96b, Eri92, Gre98, Jen99, Jør92, Kar93, Kar96, Kla93, Kra96, Kum93b, Kum93a, Lin93, Lin96a, Lun91, Lun92, Mat97, Mic96a, Mic99, Mic97, Mon93, Mon94, Mon99a, Mon99b, Pau99, Deu97, RKS99, Sjö96, Sta90, Sta93, Str91, Str92, Str93, Tay91, Tri96, Tri99, Wha96, Zer99b, Zer99a, BD95c]. **Books** [Ano98a, Zer98a]. **Boolean** [Löw92g]. **Borabenzene** [KEG+97]. **Borane** [BP92b]. **boranes** [MAC96]. **borazine** [MZ91]. **borealis** [SKC99]. **Born** [AZ99, CW97, CFB97, KLM91, RL98, STY+98, SNNY99, Suk95, Sut99a, TN96]. **Born-von** [CW97]. **Boron** [BF96, Bou94, WYW96, BFV+93, LMV92, LFD99, VCMLL90, ZSK97]. **boron-like** [LMV92]. **Boron-Nitrogen** [WYW96]. **Boronlike** [VIK98]. **borrowing** [McH91]. **Bose** [MVL98]. **Boson** [MS97b]. **Bosonic** [Oht98]. **Boston** [Cal90e, Cal90b]. **Both** [Gin95, RP98a, BA90, DO90]. **bottlenecks** [Ran93]. **Bound** [BGS98, CB99, Csa96, FKK99, FS95c, GSJS97, HMLK98, VJ95, VJ97, EE91, KD92, LS99, NI94, Roc99, WTD+94]. **Boundaries** [CLKMTA95, TSPK97]. **Boundary** [AM97, BE95, LKMC93, LCLO95, PTH+97, LKVS97, YNNR97]. **Bounded** [Núñ94b]. **Bounds** [AR99b, Fer91, TVP93, Taş96a, Žit94, AR99a, Csa94, Csa95, Fer90, LK94, PG95, PFK99, TP90]. **Box** [LLL97, LKMCVT95, LKMCVT96, OKI98, Whi99]. **Boxes** [Aqu95, LKFF98, A.95]. **Boys** [Pri98]. **BPh** [BUZ94]. **Br** [DKM97]. **Bragg** [Jac92]. **brain** [BPHB96]. **Branch** [RG96]. **branched** [Art94b]. **branching** [CDG04]. **Brandt** [Car96]. **Breach** [Mon93]. **Breaking** [DDH+96, GS94, NFVM94, ÖOD96, SW97, CGG96, CRK+91]. **breaks** [CH91]. **breakthrough** [BBCL92]. **Breathing** [AMD+97]. **Breit** [EKI94, FM92b, Ish90, Ish91, Moh92]. **Brewer** [Brä95]. **bridge** [AB99]. **Bridged** [BAD99, CdBKZ99, DBG92, FWS97, Gal98]. **Bridges** [Shu96]. **Brillouin** [DMFR93, GLM91, KS90, LV97, Wen98]. **Britain** [Kra96]. **Broken** [CC98, Coo92, Nob99, Oza92, YO92, RVP92, Ran93]. **Broken-symmetry** [Nob99]. **bromide** [TBP99]. **bromine** [CB91]. **Brownian** [NH90]. **Brueckner** [ASI94a, KKJ94, MHN98, Ort98a, Ort99, Scu95, WB94]. **Brueckner-Coupled-Cluster** [Scu95]. **BSSE** [FGRS98, GRT96, HVS98, MV91, MVHV96, May98, VM92]. **BSSE-Free** [FGRS98, HVS98, MV91, MVHV96, VM92]. **buckminsterfullerene** [FLLZ91, TMH94, FLWZ90]. **Building** [Emc97, Mar94b, PFMC97, PÅS+97]. **Built** [GVC96, LDJH92, LDHJ92]. **Bulk** [OLC+96, RHC96, Tri97, LXWZ99]. **bupivacaine** [DB97]. **Butadiene** [DC97, BT96, PČe90]. **Butane** [MSM96]. **Butenolide** [MM95]. **Butyl** [RW92]. **Butylbenzene** [PK99]. **butylcyclopropanone** [CAM+97]. **butyrolactone** [BH92].

C [Ågr90, Ano92j, Ano93h, BL99, BSS+97b, Brä95, Brä98b, Cal90f, CCC+95a, CMF+98, Eva97, GFY+99, GARC97, JKK+92, Jen99, KJ95, Kor90, MCCF95, RA91, SC98b, SC99, Wha96, XY95, YZX96, AS99, BZ92,

BBZ91, BSS+97b, BKM90, CCC+95a, CD93, CXFP99, CL92, CC92c, DR92, DM98, DM99, EDF+98, FLWZ90, FLLZ91, GV93, GS97b, HMG+92, HRRBL97, HZ94, HOF+97, HL93b, JM93a, KP96, KH96a, LRM93, LU92a, LFS94, LL99, LSC98, LCS98, MLL99, RG99, RN96, RRC94, RA91, RK92, SK99a, SCA93, SDO91, Sel93, Ska92, SLA97, SZCO99, TST+99, TPR96, TFSZ95, TZCT97, TMD96, WYW96, XY95, YZX96, JTZ+96, MPSF97]. **C-** [SCA93]. **c-BN** [MPSF97]. **C-H** [HZ94]. **c-Myb** [JTZ+96]. **C-NMR** [BZ92]. **CA** [SST94, BC97b, FLLZ91, CCC+95a, HBJ+92, Pro95, YDDP92, WZ99]. **CaC** [DTA+96]. **cadmium** [LMMK93]. **CaF** [LW92]. **cage** [BBZ91]. **cages** [FLWZ90, FLLZ91, ZSK97]. **Calais** [Löw96d, Pau97]. **Calcium** [BPL97b, WLB+94]. **Calculate** [ZLHZ94, CE90, MMA+92, MIW91, RSCP92]. **Calculated** [ČHMA95, CGR+94, DE92, Dat95, HS95, KD95, LV98, YLLJ96, BHKK93, FR93a, GFS92, LH94, RRC94, SNH99]. **Calculating** [ACAT92, CZ94b, Coh97, DZO97, HZ99, JM96b, RSCP91, SF94, Val96, CB96a, Har94, NZ92, Roo93b]. **Calculation** [ASP97, AL98, ALRP96, BZ92, BLB95, BB97b, BL92b, CJA94, CÅ92a, CCZ97, Csa91, DDG93, DV98, DZ96b, ETV94, FCVL98, GSD97, GMI95, Har97b, HU94, Iga95, Jas94, JR96, Jon97, JM96c, KMR92, KKNN97, KSY97, KPTŚ94, KLT97, Lev94, LTP96, LD94, LR94, LS92b, MHÅ98, MHS95, MBA97, Mez94a, MVV+97, MAD98, Mor96b, PSAUS90, PVLG93, Pen93, Pen96, PMN+92, RN96, RPB+97, RLR90, RL97, SM96b, SBM97, SSO+97, SZ96, SZ97a, SCP91, Sem96b, SSMK93, Sme92, SATP94, VDCK97, WD97, WR96, WZ99, YYLB90, YLD97, ZW96b, BDK90, BP90, BKL98, CMG92, CS96a, Csa90a, CB91, DDN99, DD97b, DDA92, DOPS91, DKTZ94, DB94b, EMP92, FGM90, HZF+91, KPW+95, KNN96b, KE90, KD92, KCLI95, KSK91, KSIH92, Kur90, LRR92, LLB99, MRC99, MGLBP95, MPP92]. **calculation** [MD93b, MD92c, OS91, Rey95, RH92, REU+91, SAW97, SS92a, SN99, Sch92a, SPB90, SSC92, TTM99, Tit96, TŚPKM94, VZ92, Wen93, WL92, WKP+95, YBZ92, ZZW94, Kov90b, Mun92]. **Calculations** [AHI96, AH97, BBZ91, Bér97, BNLF96, Boe92, BEJ98, BPL94, BS94, BJLK98, BL98, CM96a, CMF+98, ČHM95a, ČHM95b, ČHMA95, CCC93, CFB97, CM94, CLKMTA95, Cul95, DHL+94, DREW98, DRBE96, Dun96a, Dun97, EP98, EMMS94, Fer96, GKKM96, GDID98, GMS97, GRT96, GT93, GPD94, Gre94, GP97, HMGP93, HLS94, HBL99, HNB92, HMLK98, HC96e, HZ94, IAN+94, IK97, Jac97, JCÁ96, Jen94, JL91, JAG95, JSG97, Jur96a, KLLB98, Kar98, KS98, KBL95, Kol97, KA95a, KL97b, KL97a, LMC97a, LP97a, LRM96, LBM94, LY98, LFS94, Lin96b, LCLO95, LL92, MYN+96, MSD95, MF96, Mar95c, MAI95, MSCS95, Mor93a, Mor97b, MRD92, NV94a, NV94b, Núñ97, NV97b, Oku98, Ort98b, PCE95, Pah98, Pra97, RML97, RSD97, Ryd94, SB95a, SO94, SNMB97, SPF96, SRS92, SG93, SST93]. **Calculations** [SR96, SBIP97b, SLA97, SBD+92, SAL+94, ŠH96, Sta96a, SL97, SDG97, TJ95, Tri97, VV95, VIK98, WD95, WZW96, Wil96, YNY99, ZO95, ZC95, Ågr90, AEHM91, AMC97, AM92, BK97, Ber96b, BMDM90,

Bla99, BT96, Boe95, Boe97, BJA99, BB91, BBC92, BB94, BB95, Bou96, BB97a, BW90, BS92, BCY95, CD92, CZ94a, CA90a, CMA93, CRK+91, CKB91, CMB95, Csi76, DVJ93, DV96, DBF+92, DO90, Egu96, ELMY96, EJ93, FAV92, FLLZ91, FWS97, FFD96, För92a, For94, FGS92, FS92, GKM90, Gur99, HMG+92, HSLL92, HR99, HBJ+92, HFM91, HS99, HE90, HZ92, HS92d, HW91, Hua92, Ish90, IGK+92, Jac98, JWG95, JH90, JC90, KSSG95, KLO+98, KH96a, KKNY99, Kir92, KKL90, KF96, KK93, Kov90a, Kov90b, KYW95, LGBL94, LMC97b]. **calculations** [Lan95, LMMK93, Les91, LHL91, LW92, Lin92, LFD99, Loh91, LBL98, LXWZ99, Man95a, Man95b, MKRW99, MW92, MVS97, MZ91, MECE97, MD92b, MGNK95, MLK94, MAAP90, MNC95, MSS99b, NPL90, NV97a, Ort98a, Ort99, PWL98, PVČ+90, PA92, PTKS+92, PSBL98, PZA92, PNB94, RC92a, RTKP95, ROL+90, RC92b, REU+91, RK92, RP98b, Sae92, STKN90, SDO91, SCMF93, SHF94, SGGC99, SBAD90, SB90, SKE92, SEKEB98, SG92, SST94, Sta95, Sta96b, Sta98d, Sta98e, SZ97b, Sut99b, SPR94, SJ91, SJR91, Tal93, Tos95, VABM94, Van96, VR92, VM92, VAVN91, Was91, WB94, WL90, Wen96b, WP90, WN90, YNO92, YNO94, YAD92, ZO94, ZDO99, ZWD98a, ZWD98b, Bro95a, HHPT91, SJ97, Wen96a, WGP99, vMVvLvD97]. **Calculus** [Kin96, Ney95b]. **Call** [Ano90g, Ano90i, Ano98b, Ano98c, Ano98d, Ano98e, Ano98f, Ano98g, Ano98h, Ano98i, Ano98j, Ano98k, Ano98l, Ano98m, LZ91]. **Callaway** [Tri95]. **Cambridge** [Kra96]. **camphor** [CL90]. **Can** [Bau98, GVK99]. **Cancer** [Lad97a, Brä96c, LF94]. **cancérisation** [GK90b, GK90a]. **cancérogène** [GK90b]. **Cannabinoid** [Reg92, RFM90]. **cannabinoids** [PBHB95]. **Canonical** [FK94, KFK91, PVN90]. **capacities** [NOY98]. **capacity** [MCA95a, Pal93a]. **Capping** [ZLWES99]. **Capture** [BMA93, BF96, BMA90, KSW98, SK99a]. **Car** [Kry93]. **Carbanions** [OKI98]. **Carbene** [Sak98, Cio93, DR92]. **Carbenes** [SG97, SGB98, EVSN92]. **carbide** [KPW+95]. **Carbides** [SGB97]. **Carbó** [Tay91]. **carboanion** [CKB91]. **carbocation** [CKB91]. **Carbon** [AMRT94, AMKS93, BKS96, BF95, MR92b, TAY+97, VDCK97, XR94, CC92c, DI95, FLWZ90, KTK+90, KL94, Suh93, TFT+91, WTSN94]. **carbon-** [Suh93]. **Carbon-Carbon** [BF95]. **Carbonic** [BAK97, GK92]. **Carbonyl** [ET97, VBUS99, GS97b, XSA+92]. **Carbonyls** [SZL95, SG97, SGB98, MSMR99, SG96b, Van96]. **Carborane** [RA91]. **Carborane-hydrocarbon** [RA91]. **Carboxyl** [KVS98]. **Carboxylic** [MBP97, MKBP97]. **carbyne** [DM98, DM99]. **carcinogen** [WP90]. **Carcinogens** [LP97b]. **Cardiac** [MBV+98]. **cardiotonics** [KBM92]. **Career** [Kas99]. **Carlo** [ACB+99, ACAT92, ACHT95, BRL92, BBMM99, BBC+94, BBC+96b, BRA+99, BRV99, CDC98, KNN96b, KKNN97, KI94, Kid99, Mar97c, MB97b, MR92a, Rey90, Rot96, Rot97, UBA92, VBD+98]. **Carotenoids** [TCM98]. **carriers** [LTSL96]. **Cartesian** [BRV90, KA95b, Le 97, Sch92b, SF95b, Sta91]. **CAS** [BP93d, PPP97, YNY99]. **CAS-SCF** [YNY99]. **case** [BA91, BBMM99, CT95, For92b, Geg91b, LB96b, LAM92, MVS97, Pal91,

PDO92, PCD99, RRC94, SC99, TMA97, Whi99, CLGW95]. **cases** [hJH97, Löw92h]. **Casimir** [Mon94, LM93]. **CASMP2** [YTYS97]. **CASPT2** [BBC+96a]. **CASSCF** [BBOR96, BBC+96a, GMMH97, JK90, KP92, LHNK99, MCOS94, Pra97, SG93, XLW+99, YTYS97]. **CASVB** [CTG97, TC98b]. **Catacondensed** [Ran97]. **Catalysis** [FB96, MÅ96, SNMB97, SPG97, Tch96b, KÅ99]. **Catalysts** [SDE94, EZ93]. **Catalytic** [HBH98, NHN97, Ryd94, CJX+92, CDG04, DD99, EZ92, FNSV99, GWB97, Nov92, PB95b, TCA+91, XYC98]. **catalyzed** [BT96, KKS99, PHBB94, SJ91, WJC+98, WJC+99]. **catastrophe** [DD90a]. **catecholamine** [GJPMML91]. **cathodic** [HDY+91]. **Cation** [AKD96, GKKM96, GMS97, Jur99a, Yam97, BLC95, Gal98, YNNR97]. **Cationic** [Bou94, FW92b, FW92c]. **Cations** [BSHP97, MKM93b, Bro95a, HDB+95, KO91, Kha92, LE92, MRST95, Pro95]. **Cauchy** [BOX94]. **Caused** [TMDB98, Fan90]. **causing** [Hag99b]. **Cavities** [RPJZW96, ZWJP95, PB95b]. **Cavity** [CDD+99]. **CBC** [KJ95]. **CC** [GR95a]. **CCCH** [CMF+98]. **CCD** [PTP95, PTP95]. **CCSD** [PTP95, PPP97, PTP95, VDL95]. **CCSDT** [HKC96]. **CD** [RN96, CRsP93, GFRR94, IK97]. **CdS** [ZLWES99]. **CECAM** [Ano96-31, FG96]. **CECAM-NSF** [FG96]. **Cell** [HM97a, Lad97a, Wil96, LF94, SMH92, WM92, Brä96c]. **Cell-Shedding** [HM97a]. **Cells** [NV94a, NV94b, KPM+90]. **Cellular** [SSD96, SKC99]. **Cellulose** [GZ98, SSK+92]. **Center** [BR94, BF94, GY95, HO94, HS91, HS92e, IY99, KJ95, LR94, MBA97, MS93b, Pan95, SPH98, SKTN97, SN98, VC92, Bud92, BFW92, Cio90b, CMSF93, DWB98, DW90, EC96, JGP91, Jon92b, Jon93, MTNF99, MT90b, MS92, MGLBP95, RA91, STKN90, SP90, Whi99, ZFZ92]. **Centered** [Boč96, MV98a, Boe96, VCCM92]. **Centers** [BP96c, KZ99, KTK+90, TTM99]. **central** [BS91b, MPSLB91, MGLBP95, NSS92]. **centricity** [BBLK94]. **Century** [Kra96]. **CEQ** [JC90]. **cerium** [KRZ91]. **Certain** [AFTM95a, AFTM95b, AFO+97, AFTM98, PMM97, AFZ+99, BCD91]. **CF** [FAV92, GS94]. **CFHH** [BD94b, BD95a]. **CFPHGLF** [WD97]. **CG** [PC99]. **CGA** [GJDD97]. **CGCGTTAACGCG** [BS91b]. **CH** [KBGE97, PZTPMC99, SG97, SC99, TFSZ95, TZCT97, BDD93, Cai94, Del92, ELMY96, FCVL98, Fra99, Gin97, KSF91, KLO+98, LJ95, Oku98, RN96, SLL+91, TMA97, WY99, YSHD97, SC98b, SC99, YSHD97]. **Chain** [BSB94, CAÖ96, DWR99, DZ96b, FDF97, GV93, PFMC97, RM99, ST93, CLC90, FC99, FMD+94, FMD+96, GL96, HZ91a, LTY90, MD93b, PK90, PC99, TTOY93, TBW90, VZ92]. **Chain-Length-Dependent** [ST93]. **chainlike** [FFD96]. **Chains** [CMFA93, Jac97, Sta97, AGM99, BOL+90, CA90a, CMA93, CPA98, CP99a, FDAC90, FADC91, HGP91, Jac92, JGCJ96, Jac98, LO93, MFCA94, MCA95b, NYKY98, RR95, Rep96, TBP99, YAD92]. **Chairman** [Ber96a]. **Chalcogenides** [DREW98]. **challenge** [GZ97, GZ06, Deu98b]. **Challenges** [KPD93]. **Challenging** [BA97a].

Chalmers [Gre98]. **Change** [KS98, RD90, TTOY93]. **Changes** [FW92b, FW92c, AM90a, FL95, Hag96, Pal93a]. **Changing** [SB97a]. **channel** [FKK99, KO91]. **channeling** [NST94]. **Chaos** [GBJMA94, CPW92, Kar93]. **Character** [Bor94, CLSI94, Her97, KM92, PB97b, PGH95, FJR96, NNH98, TG96]. **Characteristic** [PM95, YD97, ZW96b, DM97a]. **Characteristics** [KZ99, RW92, SN99, VH96, Voj96, EZ93, GS91, TP94]. **Characterization** [DTA$^+$96, HS99, JI95, KC98b, PV94, RK97, CPD$^+$98, KJL96, KLC98b, LM92, Ran95, RK99, WM92, AKCS91, SCMF93]. **Characterizations** [BPL94]. **Characters** [WFK97]. **Charge** [AYDR96, ÁC94, ATI97, BK96, BLBP97, BK95, BAD99, CLSI94, CM94, Del96, HP98, HSS$^+$95, KO95, KMM95, Kup94, KKM99, LK90, Lon99, MK99, MKM96, MKM97, MM98, Mon98, MM95, NMN$^+$97, NMN$^+$98, Nal94, Nal95a, NM95, Nal97, PC91, SBM97, SBAD90, SG94, SR96, SMO$^+$96, SHC$^+$98, Sta98a, Sur95, Sur97, WPB98, YDFS98, ASM91, BADM97, CMB95, Cul91, DM94a, GZSvD99, GBS99, HE90, HSES94, LKM99, MESH93, MCA95a, Nal92d, Nal92b, NM92, Nal98, Sta98b, SN90b, HE90]. **Charge-** [NMN$^+$97]. **Charge-Conjugation** [Kup94]. **Charge-dependent** [Lon99]. **Charge-Exchange** [KO95]. **Charge-Mediated** [NMN$^+$98]. **Charge-Transfer** [ATI97, CLSI94, SBM97, Sta98a, WPB98, PC91, GZSvD99, LKM99, Sta98b]. **Charged** [Brä98c, GH96a, HL93b, NBS95, PCC93, VBF95, WA94, Woo99, BKS97, GW91, HFM91, MFH91, NYKY98, TIA$^+$92, VFBP96]. **Charges** [ÁC94, BKM93, CV99, CDDV93, LV98, Mon98, Roz97, SK99b]. **CHD** [RN96]. **Chebyshev** [NS95b]. **chelates** [HBGR99]. **Chemical** [ADB96, AR96, AFTM95a, AFTM95b, AFO$^+$97, AFTM98, AK97, AH96, Bir94, BSHP97, BPL97b, BK98, CN94, CXL97, CCE$^+$93, CL95, CCG$^+$96, DP94, Dun98, ESP98, ETV94, FSF96, Gho94, Gin95, Gin96b, GJPMML91, GJLA99, Gre94, GWCT97, GKS99, IK94, KSKJ94, KZ94, LP97b, LL94b, Löw94c, MB97a, May98, Mon98, MTD96, MM95, NOYY94, NN94, Nal92a, Nal95a, Nal97, NS95a, NS95b, Ney95a, Ney95b, NV94a, NV94b, PRC98, PZ95, PS94a, Pon97, Pon98, PCD99, Ryd94, RKG96, SKJ98, Sch93, SRW96, SDE94, Sur94, Sur95, Sut96, SFGW96, TKNI96, VdV96, VB94, VBV92, WS94a, Wen96a, YDFS98, ZCT98, ZZZY96, AKS$^+$90, ABSW95, Ano92k, AFZ$^+$99, BZ92, BA91, Ber96b, Bha99, BS91c, VD90, CMG92, CRK$^+$91, DVJ93, Deu98a, DO90, EVSN92, FLWZ90, FLLZ91, FL95]. **chemical** [FS99, GKM90, GS97b, GB90, HZ91b, Kar96, Kha91, Kry96, Lad94, Lan95, MUL99, MD94, MD95, MCA92, MCT99, ML99, MV92, NOYF92, Nag96, NOY98, NM96, NE95, NV97a, OYNY98, PTL90, RT99, RD90, STKK92, SG92, TIA$^+$92, TP92, TNSM99, TLTL92, TMA97, TŚPKM94, TCM99, TMD96, WJC$^+$98, Wen96b, WZ99, WZ96, YOTY93, Yur95, Mon93]. **Chemical/Molecular** [VBV92]. **chemically** [SES93]. **Chemisorbed** [BDD93]. **Chemisorption** [FWBT94, NM95, SFGW96, FL91, LaF90, MtPC$^+$96, NF92, SW92].

Chemistry
[All94, AAS93, Bad95, BG98a, BR94, BPL97b, Cal96b, CCC93, CC98, Cle92a, DN96, Dew92, Enk97, GZ98, HPSC97, JPP87, KPD93, Kir95, Kor95, Löw90c, LZ92, LZ94, Löw95f, MDS98, Mos98, Nic99, Ryd94, SS97a, WSM+94, Ano90g, Ano90i, Ano91g, Ano92j, Ano96-58, BAF+95, Brä98b, BBE95, Cal90c, CDB99, ČVW91, Coo05, Csi77, CD81, DS99, ESTM95, FS99, Gur99, HW04, Hei95, Hei90, Hin88, Kel97, Ken93, KWZ98, KH95, KH96c, Kra96, LGT94, LZ91, Löw91a, Löw91b, Löw91c, Löw91d, Löw91e, Löw92b, Löw92c, Löw92d, Löw92a, Löw93a, Löw93b, Löw94b, Löw95c, Löw95d, Löw95b, Löw96a, Löw96b, Mat96, Mat97, NSÁS+90, Pár98, Pau95, Qui02, RS00, SR93, SR02, SPS96a, SHB+96, SP95, SN97, Smi96, Str92, Tay91, Tet93, Tri96, UBA92, WA94]. **chemistry** [WP95, Löw91a, Löw91b, Löw91e, Löw92b, Löw92c, Löw92d, Löw93a, Löw93b, Löw94b, Löw95c, Löw95d, Löw95b, Löw96a, Löw96b, FCA91, Jen99, Tri96, Zer99b, Ano93h, Cal90g, Str92, Wha96]. **Chemists** [Mon99c]. **Chichester** [Cal90g, Cal90d]. **chimeric** [ITT+94]. **chiral** [RVP92]. **Chirality** [FWC+93]. **Chiroptical** [RF94]. **Chirped** [MY99]. **Chloride** [BSP97, TBP99]. **chlorinated** [AKS+90, BTKVG99]. **chlorine** [AFM99, FEE+98]. **chlorine-oxygen** [FEE+98]. **chloro** [RTKP96]. **Chlorophyll** [SKTN97, STKN90]. **chlorpromazine** [BD95b]. **CHO** [MZ95, SLG+96, Mar97c]. **Choice** [JKRW98, JGR98, JMR98, PDT97]. **choices** [MHY98]. **Christoffersen** [Str91]. **chromophore** [SCMF93]. **Chromophores** [Che96, KMR92]. **Chymotrypsin** [NK96a]. **CI** [BBC92, BFRN90, BMG95, BKL98, CC91a, CRK+91, CKB91, CB99, CSZ97, DN96, DLV95, Del90, Ert90, FV96, FBKD97a, FBKD97b, FBKD97c, Flo97a, Flo97b, GR95a, GR95b, GR96b, HKC96, HMLK98, KL93b, KBL95, KRZ91, Kün99, LD95, LH90, LG96, NS91, PCO+94, PPSK96, PR97, SS92d, SBIP97b, SKRK90, Was91, WZW96, YNO92, YNO94]. **CI-based** [CB99]. **Cinchonidine** [SWMB94]. **Circle** [RH95a]. **circuit** [KRBT94]. **Circuits** [GRK96]. **circulants** [LLSY92]. **CIS** [SWD+99, JZ95a, MRB+96, MZ95, MGK99, Suh92, IHG95, SE97, Fir94]. **cis}-** [JZ95a]. **cis}-Cycloadducts** [Fir94]. **cis}-Stilbene** [MGK99, MRB+96]. **CISD** [CMCR96]. **Cl** [BZQ95, DDC97, GARC97, NL96a, STMR97, BCS96, JC90, LJ95, Moc99, NL96b, Oku98, RN96, TIPM96]. **Claredon** [Kum93a]. **Clarendon** [Cal90f, Kum93b]. **Class** [KP93, Kat93, Kat97, Kat98a, Kat98b, Kat91, NWG+99, PK92a]. **Class-sum** [Kat98a]. **Class-Sums** [KP93, Kat93, Kat98b, PK92a]. **Classes** [FJRS97]. **Classical** [CN99, FLHT90, GLBM96, GBJMA94, HM97c, JCÁ96, KLW92, KC93, MLT+96, NP96b, PS94a, Pri95, RZ96, Ryl99, VdV96, DV96, FG96, GL96, McW99, MEB91, RW99, REU+91, SHB+96]. **Classification** [JM94, PV99, Was96, WT98]. **Claude** [Mic96a]. **Cleavage** [RC97, BBTU97]. **Clementi** [And93b, Ano92m, Ano92-46, KK92b]. **Clifford** [Alt96, LP92]. **Cliffs** [Str92]. **Clifs** [Wha96]. **ClO** [BYGA99, FEE+98, Fra99]. **Cloppa** [GARC97]. **Close** [Hed95]. **Closed** [AM98a, BMA93, BEG94, HT97, Pal97a,

PKM93, MC91a, MC91b, Moh92, MCB99, VDL95]. **Closed-** [BMA93]. **Closed-Shell** [AM98a, BEG94, PKM93, MC91a, MC91b, Moh92, MCB99, VDL95]. **Closure** [BO93]. **Clothing** [DM96]. **cloud** [VDBPR97b]. **Cluster** [ASI94a, AT99, BRS96, BXZ95, BDD93, CLSI94, CDDM96, CS98, EDF+98, FP96, HK95b, JM93a, JKJ94, JM95, JKJ95, JG95, JKRW98, JGR98, JMR98, JM93b, JPJ95, KD98, KKJ94, Kry98, Kun90, LMC97a, LCLO95, LSC98, MI93, Mar97b, MALT96, MCM98, MAI95, NU95, NS93a, NS93b, PVLG93, PHH94, PTP95, Scu95, SST93, Sur95, SFGW96, Sza95, TJ95, UWB94, VR95, AMC97, Ada91a, BUZ94, BDK90, BX94, BB91, BBC92, BB97a, Bre99, CGG96, CS99, ČPV90, CC92c, EKI94, För92a, Har99, HC91, HS99, II94, JM96a, JKGM99, Jur99d, Kal90, KSSG95, KB92, LP93, LP98, LCS98, MMP95, MB93, NS92, PBPN90, PCB92, Pal92a, PP92, PP91, PČP92, PB95b, PNB94, RK91, SRP+98, SB90, SST94, SB92b, Vin92, WB93, WB94, WL90, YNNR97]. **Cluster-Series** [MI93]. **Cluster-Size** [BDD93]. **cluster-type** [CS99]. **Clustering** [Mar95c, Ike99]. **Clusters** [AML+95, AMD+97, ABR95, Boč96, Bou94, BDD93, DDH+96, DRBE96, GD96, HLS94, HU94, Jur98b, KSN95, Loh96, MMP+94, MDJ98, MLR+98, NM95, NG97, NC95, NS97a, NS97b, PTP95, Roś96, RKPE95, SPF96, VDCK97, VBF95, ARDP92, ACB+99, AGNS92, AD92, BGS99, BUZ94, BMDM90, BAL95, BFP93, BYE+97, Cas91, Cas97, CS96a, CBL95, CCS99, ČPV90, CPD+98, EZ92, FLWZ90, FB90, GKM90, GFY+99, GWB97, GRB+93, Gur99, HCRR94, HSLL92, IBS95, KSN93, Kap99, Kar90, KI94, KS94c, KF96, KBBK90, KJ97, LP98, LXWZ99, MD92a, MKRW99, MAL93, MNC95, Mur90, RRC94, REL+90, SCP93, SKE92, VG90, VFBP96, WI96, WMZ98, XSG97, YNNR97]. **CN** [JMP99, NG95, NG96, Bau97, Del92, JMP99]. **CNDO** [Boč90, DDG93, KSIH92]. **CO** [Bou96, BL98, SC98b, SC99, VR92, Ano93g, NG95, Cas92, CLGW95, EZ92, hJH97, LD95, MLT98, NL96b, PCB92, RKH+98, SM96a, SDP+95, SCS94, SG96b, SG97, YBM97, Jur99c]. **CoAl** [DDC97]. **Cobalt** [GK92, SFGW96, WWFR99]. **Cocatalysis** [Sak97]. **CoCl** [CCWCF96]. **coefficient** [Kin94, Xu99]. **Coefficients** [BK94a, BP93c, De 97, GİA96, MK98a, PAT93, RWT92, ZW96b, BP93b, CBT93b, Kat91, Kat98a, Luk92, PC99, PZA92, RWT91, SDO91, SMH92, Wen93]. **Coenzyme** [FVN98]. **Cofactors** [DV98]. **cognition** [TD03]. **Coherence** [CDB90, GH99]. **Coherent** [BS93, Ike99, MVL96, BCD91, TC98c]. **coherent-dissipative** [BCD91]. **coiled** [SKM99]. **coils** [SKM99]. **Coinage** [LLZ98]. **cold** [Mar90]. **Coleman** [Cal90a]. **Collaborator** [Par94a]. **Collapse** [RM99]. **Colle** [FGM90, Mor93b]. **collective** [BAL95]. **college** [Str93]. **collinear** [GDYY97]. **Collision** [DD98b, FSW+91, MLK94, Voj96]. **Collision-Induced** [MLK94, FSW+91]. **Collisional** [HHHP99]. **Collisions** [BF96, GBS93b, GH96a, Mic94, BMA90, DMR96, FMR91, GDYY97, KSK+99, Par99, Réa90, RMF90, SK99a, TMR99]. **collocation** [KH96c]. **color** [KŽ90]. **color-pairing** [KŽ90]. **colorful** [Bal90]. **COLUMBUS** [She91]. **Combination** [AS96, KEG+97, PMN+92, BJA99, TNI96].

Combinatorial [ZCT98, Kat98a]. **Combine** [VdV96]. **Combined** [BLBP97, EC96, VBV92, Ano96-31, DV96]. **combining** [Rig92]. **CoMFA** [VES+99]. **Comformational** [RWT92]. **Commack** [Ano92k]. **comment** [MEB91]. **Comments** [Brä93b, CSS93, CC92c, Löw96c, PDC96, LLL92]. **Common** [HH97, LSS96, Van96]. **Commutator** [MV98b]. **Como** [FR94]. **Companions** [Par94b]. **Comparability** [BKM90]. **Comparative** [ADPS98, BLE96, GJDD97, IGK+92, KGVM97, KG99, PHH94, RTKP96, RK95, Roz97, SP91, SEKEB98, SR96, ANB94, MKK96, MEP90, RKH+98, Sta98b, VES+99, WB94, CWZ98b]. **compared** [Hag92, hJH97, Sin92]. **comparing** [OS92, GS97b]. **Comparison** [AOH96, BBTU97, BBC+96a, CLGW95, CL92, Csa95, DS90, DZO97, GL92, JMS95, Jur96b, KLC98a, LJ95, LP94, LS93b, MPJ98, MR94, PČe90, PB96, PAAM98, Pra97, RL94, RRS97, STZ96, Sza95, Tri97, ZON+96, ZC95, CGG96, KF96, LG96, Ort93, Par92b, Sch92b, Suh93, CZ94a, PČP92, RTKP95, SB92b]. **Comparisons** [CS96a, MM99a, Sem94, TFSZ95, DBF+92]. **Compensation** [ST96b]. **Competition** [KM92]. **Complementarities** [NK96a]. **Complementary** [KZ99]. **Complete** [EBG95, IY99, Jur98a, Jur98b, MHY98, PCO+94, vMVvLvD97]. **Completeness** [Hil98, JBS97]. **Complex** [AMRT94, BPL94, Cio94, CCE+93, DP94, GS92a, GS92b, HPSC97, KW98, KB93, KE93, MKM93a, PM93, PV94, PV98, SWF93, SL93, SDW+98, SSD96, VH96, And93a, BS91b, CPN91, GZSvD99, GZDZ97, MLL99, MLK94, NL96b, Sch92c, SC99, WM92, WFS93, ZBL99]. **Complexation** [XY95]. **Complexes** [ATI97, BKWL97, Bér97, BCRL94, CdBKZ99, CC96, DL92, GL97, JKK+92, KS94b, MSCS95, MBA94, MBP97, NG95, RKG96, SBM97, SZ97a, SBIP97a, STM96a, Sta98a, TMSI98, TSS97, XY98, BCLS94, BDPS97, Bro96, CC92c, Cun92, DSS90, Del92, EE91, FZZ92, FWS97, FS99, HRRBL97, HWB97b, HWB97a, ITT+94, Kar90, MAC96, NL96a, OSS95, PC91, ROL+90, RCWN94, SC96, STM96b, VABM94, VM92, WG99, WMD95, WWFR99, YZX96]. **Complexity** [Art94b]. **Component** [CJH98, HBL99, LX95, LKLBD98, MBV+98, SS97b, vvBS96, BOL+90, BSS97a, KBKT93, Zho93]. **Components** [GVB97, QS98, Luk92]. **composite** [BG98b]. **Compound** [DL92, LEG+94, GC91]. **Compounds** [BLE96, BHPB95, CF96, DZB92a, Dau94, DD93, ET97, EMMS97, FT95, GKKM96, GARC97, KJ93, LL92, NN94, PD93, RGHH94, SR96, SBIP97b, Sta98a, TB95, VV95, VDD96, BJM+94, BHH92, CMA+99, FT96, FT97a, FEE+98, JF92, Khu92, Kin94, LRM93, LRR92, LC93, Loh91, Lun91, MUL99, MKK96, RC92b, SJ97]. **Comprehensive** [ÁC94, Jon97]. **Compressed** [Art97]. **compression** [VFBP96]. **Compton** [AYAZ95, MRL99, RGT95, SAW97]. **Computation** [BE93, CV98, CMCR96, DVL+91, GOAY98, Hea97, HO94, Jur97b, Jur97c, Jur97e, Jur97d, Lai94, LDP93, McD97, MS92, MS93b, Nic99, NB93, Núñ94a, Núñ94b, Núñ95a, Núñ96, Pie93, PDC96, RH96b, Rin96, Taş93, ČVW91, Hop90, MFCA93, SWD+99, Suh91]. **Computational** [BJM+94, BPL97b, GBL97, HPSC97, HBGR99, Hin88, Jay92, Jur98b,

Jur99b, Jur99a, KPD93, KÅ99, KRRB99, Kry93, LSS96, MZ93, MPOG99, Mos98, NSÁS$^+$90, NGM$^+$95, PMO90, PW97, PM95, PTM92, Qui02, RC92b, Sza95, TNS92, VRR92, WG99, Wen96a, Ano90i, Ano91g, Ano93h, BAF$^+$95, CL92, Coo05, CF99, FCA91, FADC91, KK92b, MSRP90, PAC90, PACO90, Pos91, SCP93, Tri96, Wen96b, CD81, Ano92k, Ano92j, Cal90g].
computationally [BS95, TSS95]. **Computations** [FGRS98, Löw90c, Ryc94, Sim98, LS99, Löw91a, Löw91b, Löw91c, Löw91d, Löw92b, Löw92c, Löw92d, Löw92a, Löw93a, Löw93b, Löw94b, Löw95c, Löw95f, Löw95d, Löw95b, Löw96a, Löw96b, MRST95, MSC92, Sin92, SZCO99]. **Compute** [BR94, MKM96, RL94]. **Computed** [HH92, Jur97g, SBD$^+$92, KSF91, MR97, MSPS90, Nes94]. **Computer** [BPL97a, BRA$^+$99, GMI95, Har99, SKZ96, ACB$^+$99, Jon92a, Löw92g]. **computers** [Cle92a, FKHD97, Har91, Ken93]. **Computing** [DB99, RWT92, ST96a, Sim97, TNM97, WPB98, BDPS97, Con92, Jur99d, Ken93, LGBL94, OS90, PS92c, RWT91]. **Concentration** [SR96, BPHB96]. **concept** [VD90, KLC98b]. **Concepts** [Nal95a, Nal95b, Atk91, LM95, Nal92d, NM92, TD03, Dun96b, Str93]. **Concerning** [GŁ94, HM95, Ney95b]. **Concerted** [Pon97]. **Concluding** [Löw90d]. **condensate** [DBM99]. **Condensation** [TMM97, MVL98, PL93]. **Condensed** [ACPR98, Cab96, Chr94, CCZ97, Her98, Löw90c, Mar94b, Mar97a, Mar97b, BCD91, CDB90, Chr92, Lei99, Löw91a, Löw91b, Löw91c, Löw91d, Löw92b, Löw92c, Löw92d, Löw92a, Löw93a, Löw93b, Löw94b, Löw95c, Löw95f, Löw95d, Löw95b, Löw96a, Löw96b, Lun92]. **Condensed-Phase** [Her98, Mar97b, Cab96]. **Condition** [BA93, Pon98, PCD99]. **conditioned** [JK92b, SBZ92c]. **Conditions** [AM97, BE95, LP94, YO92, HYS91, NST94, YNNR97, ZP92b]. **Condon** [AD97, LKMCVT95, LKMCVT96, PRSDS92, PSM94, Pal97a, PLS99, RSCP92, VV91]. **conductance** [CDB90]. **conducting** [AMH93, Sta98e]. **conduction** [EC96]. **conductive** [TYY91, TYTY91]. **Conductivity** [BMK96, LRM96, LRM97, RML97, jYL94]. **conductor** [TNS96]. **conductor-like** [TNS96]. **conductors** [Sta98b, Yam90]. **conduisant** [GK90b]. **cone** [BR92, KH95]. **conference** [Ano91g, Fuk90, Löw90d]. **Configuration** [BEG94, BLG95, BL98, DM94b, EBG95, Huz96, JCM$^+$92, KSR95, MHG95, MR92b, PS96, Pen96, PAT93, SWF93, YJL92, BE93, CC91a, CGG96, DM92, Duc90, HC91, IHG95, MM93, RTS91, SWD$^+$99, SG90, SBZ92d]. **configuration-interaction** [CC91a]. **Configuration-Interaction-Oriented** [SWF93]. **Configurations** [CC97a, CDC98, HM97a, FW92a, WM92]. **Confined** [CLKMTA95, PZWJC96, WGR$^+$94, ZWPJ94, SR99]. **Confinement** [RM99, ZWJP95, Art96]. **confinements** [PKJ99]. **Confirmation** [Tri98c]. **conformal** [CSH99]. **Conformation** [MVV$^+$97, SKJ98, SRS92, Csi82, FT97a, WTD$^+$94, Luo95]. **Conformation-Transitional** [Luo95]. **Conformational** [Bue96, CDDV93,

CDM+94, DZOR98, GSSD+96, HS92b, Jac97, LS99, LVCP91, MSM96, MT96, MPIP99, NSS92, NAK95, NMSJ99, NP96b, PLV92, RL95, RKN97, RT98, RGHH94, RK95, Tew92, Tew94, VDD96, WHF92, Cab96, ITT+94, JGCJ96, MG90, MT91, RTKP95, RTKP96, RT99, SDP+95, SSM+99, Jac98]. **Conformationally** [AV92]. **Conformations** [BRA+99, FT95, SST93, FT96, LCP+91, LU92b, LE92, Pal94, Ran95, SST94]. **Conformers** [PK99, AGAP98, HRH99]. **Congress** [Bir94, MDS98, Lad94]. **Conjecture** [Csa96]. **conjectured** [TP90]. **Conjoint** [GR96a]. **Conjugacy** [Pal95]. **conjugate** [MBP91]. **Conjugated** [JCA97, Kan93, KBT94, GFS92, GX98, HZ91a, Kir92, KRBT94, LB94, MB92, PVN90, SPB90, YB99, YAD92, GRK96]. **Conjugation** [DB94a, Kup94, OKI98, PB97a, Kor90, LL99]. **Connect** [VdV96]. **Connected** [JM93b, MZM94, LP98]. **Connecting** [Pal97a]. **Connection** [Löw95e, Löw96c, Löw99, Nag95a, BCD91, GL95, KDB90, Mat90]. **Connections** [Ino96, Scu95]. **Connectivity** [RD98]. **Conquer** [GGSA98, Zho93]. **Conrotatory** [JZ95b]. **conscious** [Cha96, Gre98]. **Consequences** [Suk95, BSS+97b]. **Conservation** [FSVZ97]. **Consideration** [Zap95]. **Considerations** [ECBH96, BSP98, MKRW99]. **Considered** [AS96]. **Considering** [BAK96a]. **Consistency** [DTM96, SM96c, vDvLR99]. **Consistent** [AGNS92, CV94, CM94, DMFR93, Fer96, Fri93a, Huz96, JK92a, Kol97, MB98, Pan93, PM97, Sch95c, SG98, Ste96, TKMA92, VVS94, VdV96, BBS91, BZMR92, DM94a, FCMB99, FNSV99, FDD95, GRTR96, Ish90, KKNY99, KL92a, MHN98, MRT95, MC91a, MC91b, Moh92, NSTFC94, ZWD98b]. **Constant** [EPB97, FGRS98, FF94a, LC90, Sta91, TFT+91]. **Constants** [AST93, Bec97a, DM95, LP97a, SB97b, Sch93, SS92c, CWZ98b, FV96, For94, GR95a, MRST95, PVČ+90]. **Constrained** [IK94, Sad97, TKMA92, Val94, Cul91, KDB90, MK90, WW97, ZP92b]. **Constraints** [BDT96, GGHP94, KKWT99, MYPL90, MP91]. **constructed** [Ell92]. **Construction** [Ban91, Bro93, CWZ98a, ČHM95a, Her97, MD93a, Mey94, Mey97, DM97a, ZWD98a]. **Contact** [HNB92, PV91]. **Containing** [AHI96, CV98, JM96c, RD98, US96, BOL+90, DA91, Kin99, LC93, LK93, NMSJ99, OS92, Sem94, VRR92]. **Contemporary** [KPD93]. **Content** [Min96, Li97, LV97]. **Contents** [Ano95-47, Ano96-59, Ano96-60, Ano96-61, Ano96-62, Ano97p, Ano97q, Ano97r, Ano97s, Ano98q, Ano98r, Ano98s, Ano98t, Ano98u, Ano99q, Ano99r]. **context** [LBL98, Røe91]. **continued** [MM91]. **Continuous** [AB97, Nic99, BRV90, Rod91, Sme92, Tom91]. **Continuum** [DBLV94, PTH+97, WR96, CT95, DVJ93, FM92a, GJPMML91, MCT99, RVP92, TCM99, BFP93]. **Contour** [Ort95]. **Contracted** [CV94, PDT97, CB91, SS92d, TKSH93, VAVN91, Maz98]. **Contracting** [Val96]. **contraction** [Ish91, SS92d]. **Contribution** [LZ96, WL99, GS90b, VÅJ+92]. **Contributions** [Ano98b, Ano98c, Ano98d, Ano98e, Ano98f, Ano98g, Ano98h, Ano98i, Ano98j,

Ano98k, Ano98l, Ano98m, BK96, Ano90g, Ano90i, BPVP92, CDB99, Cim96, GSKC99, KK92b, LZ91, PBPN90, Per93]. **Control** [DDH+96, Jos97, MY99, TC98c]. **Controlling** [BRZY97]. **Conventional** [FGRS98, Nic99]. **converged** [FADC91]. **Convergence** [BF94, BDD93, Csa94, DP96, Hom93, KZ99, Kin99, Kol97, LXWZ99, Núñ97, Sel93, WBD97, CFMA95, GR95a]. **Convergent** [TM93]. **Conversion** [ML99, GS90a]. **Converters** [KB93]. **convolution** [PLS99]. **Cooper** [AS95, Tac94]. **Cooperative** [DD99]. **Cooperativity** [SS92c, Suh94]. **Coordinate** [KZ99, MD93a, Nag95a, NM95, PM93, PDT97, SWF93, BA92, WI98]. **coordinated** [ASM91]. **Coordinates** [CN99, DZF93, DZ94, LB97, LKBJ97, MBA97, Zha96, BRV90, CTF92, GS92b, Sch92b, ST91, TFYY91]. **Coordination** [Dau94, Ryd94, TD03]. **copacking** [WP91]. **Copenhagen** [Kar93]. **coplanar** [Les92]. **copolymers** [BL92a]. **Copper** [Bér97, ETV94, Fou94, LBM94, PM93, KCP90, Yam90]. **Core** [Coo95, CL95, Fer96, FDF97, LEA+94, MTL97, SZ96, See97, SGK+95, SR96, Ågr91, ÅC92, AMH+92, BCLS94, BC97b, FAV92, HBJ+92, KLO+98, MM99b, PO91, PW91, Sir99, TM99, Van96, VG90, WBP91, YBZ92]. **Core-Level** [See97, VG90]. **core-optimized** [MM99b]. **Core-Valency** [SGK+95]. **Coriolis** [Man95a, Man95b]. **Coronene** [ROSM96]. **Coronene-Coronene** [ROSM96]. **Correct** [GBRA94, San97]. **Corrected** [EMMS97, Lad97b, PB96, RRS97, BDPS97, CLGW95, LO93, Per93, SS98]. **Correction** [CSS93, CS98, DD93, GR96a, Kry95, IHG95, KF96, MRD92, PO91, Sut99a, TC98c]. **Corrections** [AZ99, Del98, EMMS94, KS94a, Lev97, LTP96, PPP97, PP98b, Sie93, BLG95, LP98, WS92]. **Correctly** [Bau98]. **corrector** [Sim95]. **Correlated** [CZ94b, CSS93, GKKA97, Hoo94, JBS97, Kin96, KP97, KLT97, Kup94, Mar95c, NWG+99, PBB94, PK96, Ryc94, SE92, SO94, SN98, BBMM99, Che92, FW92a, KM99b, KA95b, Lev99, Mar94c, MB93, PP91, PČP92, PA99, ZA95, PCD99]. **Correlation** [AL98, ABR95, BP93e, BP95, BCL98, CBT93a, Can97, CGLP96, CC97b, CGR+94, CA97, DW97, DC97, FT97b, FR93b, FS93a, FS94, FS95b, Fue94, FS92, GS94, GJPZ97, GSD97, GGSA98, GLMP98, GVB97, GSKC99, Hed95, HP97, HM97b, JCA97, JMD95, JJ97, KNA94, Kin94, KM97, KBL95, KH96b, LO93, Lad97b, LRM93, LMR94, LP94, LG95a, Lev97, Lin94, LKLBD98, LBLKC98, Löw95a, Luk92, MSD95, Mar95b, MK96, MK97b, MK98a, MPJ97, MPJ98, Muk96, NKUS97, NB97, PKM93, PC95, PP98b, PR97, PSS97, QS98, RS98, Roś96, SMPJ94, SBM97, SA96, SFG+98, SW97, SS97b, SM95, Suh94, SKS98, WSW98, Xu96, YNNY99, YDFS98, Zie95, Ada91a, ADB95, AC95, Bec94, BMDM90, BKL91, Bro96, Bud92, BFW92, CBT93b, Can94, CGG96, CLGW95, Csa91, Dav90]. **correlation** [DSS90, DDN95, EKI94, FGM90, För92a, GNF90, GL95, GVB96, HC96d, Ish92, Iva96, Iva97, KBKT93, KKK90, KL93b, KKL90, KCLI95, LCB98, LS92b, MHN98, MK95, MSF91, MD92c, NOS94, PGM95, PP92, Per93, PS92b, PRVS95, RH92, Røe90, Sæb90, Sae92, STKK92, SS91, Suh91, Suh92,

Suh93, SS98, WI98, XSA+92, Xu99, HC96c]. **Correlation-Corrected** [Lad97b]. **Correlation-Energy** [Fue94, Csa91, WI98]. **Correlation-Factor** [Fue94]. **Correlation-Kinetic** [QS98, SS97b]. **Correlations** [Ara94, BA90, BXZ95, Bor94, BPL97a, CD93, FUI97, Krü97, TN96, Ukr94, SS99a, SGK99]. **Correspondence** [JKGM99, RW99]. **Corresponding** [Bro93]. **corrugation** [Eng92]. **Costs** [Sza95]. **Could** [Sta98c]. **Coulomb** [EKI94, AM98a, BCC99, CB99, CH94, DHPC95, DKBB97, FT97b, FADC91, GSM98, GY95, HO94, Jon93, KC93, KMP94, KS95b, KH96c, LBMR95, NYLBNSB97, Núñ94a, NI94, PA92, PS94b, QS98, SPS96a, Sie93, WS95, Xu99]. **Coulomb-Hole** [CH94]. **Coulomb-Hole-Hartree** [DHPC95]. **Coulombic** [Cio90b, Löw90d]. **Count** [GRK96, GH92]. **counterexample** [Gin91]. **Counterion** [LP97a, PL93]. **counterions** [TBP99]. **Counterpoise** [CSS93, LTP96]. **Coupled** [ASI94a, AB97, BXZ95, CJA94, Cha97, CDDM96, CPTR96, CS98, DP97, FK94, GVC96, HK95b, JM93a, JKJ94, JM95, JKJ95, JG95, JKRW98, JGR98, JMR98, JM93b, JPJ95, KKJ94, Kru92, KB92, LLC+94, Lef97, MCM98, NY98, NU95, NS92, NS93a, NS93b, NP96b, Oli99, PHH94, Pen93, Pen96, PTP95, RSGC96, Ryl99, Scu95, Sur95, Sza95, UWB94, WB94, Ada91a, BX94, CMA93, CGG96, ČPV90, CPGC99, DS92, EKI94, FKK99, Fan90, För92a, GL99, Har99, HC91, JM96a, JKGM99, Kal90, LP93, LP98, MMP95, MM99b, MB93, MD93b, NYNY99, OCK99, Pal92a, PP91, PČP92, PNB94, RFG99, RBT99, SB90, Sir99, SB92b, TGS99, TFR99, Vin92, WB93, Wil99b, XSA+92, YOTY93, ZZW94, PP92]. **coupled-channel** [FKK99]. **Coupled-Cluster** [ASI94a, BXZ95, CDDM96, CS98, HK95b, JM93a, JKJ94, JM95, JKJ95, JG95, JKRW98, JGR98, JMR98, JM93b, NU95, PHH94, PTP95, Sza95, UWB94, KB92, WB94, Ada91a, Har99, JM96a, JKGM99, Kal90, LP98, MB93, Pal92a, PP91, SB92b, WB93]. **Coupled-Cluster-Type** [Sur95]. **Coupled-Pair** [CJA94, TGS99]. **Couples** [BDH+97]. **Coupling** [BS93, Bar90, BL92b, EEL97, EPB97, GARC97, KMVÅ95, Lah92, Nal97, PSD97, PBB92, PAT93, RL92, YPC97, BZ90, BBCL92, CTF92, Cze99, DM94a, FWS97, FV96, For94, GSPSM93, GS90b, JRS+99, KCP90, McH91, MNC95, PVČ+90, PZA92, RGO94, SBZ92b, TLTL92, TGS99, VPŠ+90]. **Coupling-Constant** [EPB97]. **Couplings** [AO93, Suk95, DRGC90, GPS90]. **Covalent** [KM92, PBPN90, GRTR96, KL93a, NSTFC94]. **Coverage** [AMT+99]. **CP** [PM95, BB94, JKK+92]. **Cp*** [BB95]. **CPHF** [DBF+92, SE95b, SE97]. **Cr** [SAB+97, VÅJ+92]. **Cracow** [Nal95b]. **CrC** [SG92]. **CrCO** [hJH97]. **Created** [SKTN97]. **Creation** [GDID98]. **Crick** [FL95, ZL98]. **cristobalite** [GKM90]. **Criteria** [JBS97, Nal97, Núñ95b, CLC90, FF90, MM93]. **Criterion** [FSVZ97, Zha91]. **Critical** [BHX96, BHKK93, DE92, HK95a, MC94, SK99b, Kum93b, Kum93a, Mez90, ZJ89, ZJ93, ZJ96, ZJ02]. **Critically** [MPR97]. **CrO** [WZ99]. **Cross** [CM96a, ČHMA95, JGCJ96, RH96b, SLD95, WS94b, CCS98, KSW98, SK99a, WM92]. **Crossing** [BKLV94, BKLv95, KMVÅ95, BL91, BFL91, Rin96, TGS99]. **crown** [Tho96].

Cryolite [BPL97b]. **Crystal** [AOH96, DM96, DTM96, KD98, KPTŚ94, MSS99a, Pan93, PVLG93, RK95, STM96a, Sta96a, Sta97, Sta98a, TSPK97, AS93, BILA95, CRK$^+$91, DO90, GGHP94, PS99, PS92c, RK91, SKRK90, SJ97, Sta95, Sta96b, Sta98b, Sta98d, Sta98e, WL90]. **Crystal-Field** [STM96a]. **crystal-orbital** [Sta98d, Sta98e, WL90]. **Crystalline** [CCC$^+$95a, ETV94, GT97, Sta97, AST95, Boe96, BJA99, CRK$^+$91, HMK99, NWT92, PAC90, PACO90, PDO92, TNS92, WSTB90, ZWD98a, ZWD98b]. **Crystallization** [IP94]. **crystallography** [HMK99, MHK95]. **crystallohydrates** [Sta95, Sta96b, Sta98d]. **Crystals** [ATI97, KSKJ94, KPTS97, OK96, Sta96a, SL97, TD96a, VR95, BRS96, Lev94, RK91, SKRK90, SZ97b]. **Cs** [KWT95, KKWT99]. **CSe** [LHL91]. **CSF** [TGS99]. **CSF-based** [TGS99]. **Csizmadia** [Ano92j, Ano93h]. **CT** [SST94]. **Cu** [BB91, Cas92, Eng92, Li93, LF95, Min94a, SM96a, SBAD90, SG96b, SGB97, SNH99, WL99, EDF$^+$98, FWBT94, HS99, MLB92, NKUS97, TJ97]. **Cu-C** [EDF$^+$98]. **Cu-like** [MLB92]. **cubane** [CKB91]. **Cubic** [ČHM95a, ČHM95b, ČHMA95, OK96, SB97b, KPW$^+$95, LL99, PTL90]. **Cubic-Grid** [ČHM95a, ČHM95b, ČHMA95]. **cuboctahedron** [RK96]. **cubylcubane** [XSA$^+$92]. **CuCl** [BBC92, BADM97]. **CuH** [Rot96, Rot97]. **Cumulant** [KF98]. **cumulants** [SF94]. **Cumulative** [SKRK90, KY92]. **CuO** [AS93, VBN95a, VBN95b, Min96]. **Cuprate** [DMB97, DBM99, Mat96]. **Current** [BK96, LZ96, Löw94c, MBV$^+$98, RVP92, AB99, Hei95, Kha91, Löw91e, Mat97]. **Currents** [ACPR98, SF96, LK99, AAS93]. **Curriculum** [Ano91z, Ano91-27, Cle92b]. **Curvature** [Oku98, LL99]. **Curve** [BKLV94, BKLv95, Ran94, BL91, BFL91, Hir92, Rin96, VÅJ$^+$92]. **Curve-Crossing** [BKLv95, BFL91, Rin96]. **Curve-fitting** [Ran94]. **Curves** [Jas94, CCS98, MCOS94, SES93]. **cusp** [KKWT99, ZP92b]. **Cutoff** [Mez94a]. **Cuts** [RG96]. **Cvitanović** [Kar93]. **cyanate** [Pro94]. **Cyanide** [LLZ98, MSCS95]. **Cyano** [UWB94]. **Cyanoacetylene** [AST93]. **Cyanoketine** [RW92]. **Cycle** [KP93, PK92a]. **Cyclic** [BEG94, BE95, BE98, BČ95, BČ96b, KBGE97, LP96, TBČP95, Che92, ITK91, Kar90, LRM98, MBP91, PP92, PP91, PČP92]. **cyclicity** [BBLK94, BBLK94]. **Cyclization** [MC94]. **Cycloaddition** [FF94b, Fir94, RW92, FF92, FF96]. **Cycloadditions** [RR94, SAL$^+$94]. **Cycloadducts** [Fir94]. **cyclobutadiene** [ČDM91]. **Cyclobutene** [JZ95b]. **cyclodecyl** [Gal98]. **cyclodextrin** [HWB97b, HWB97a]. **Cyclododecapeptide** [LUU90]. **cyclooctatetraene** [PMS94, Tri98c]. **Cyclopenta** [RL94, VRR92]. **Cyclopenta-Polycyclic** [RL94]. **Cyclopentadiene** [Bra97b, SL98]. **Cyclopentadiene-Based** [SL98]. **cyclopentaldienyl** [BB94]. **cyclopropabenzene** [EMMHP92]. **cyclopropan** [CAM$^+$97]. **cyclopropanone** [CAM$^+$97]. **cyclotrimer** [MZ91]. **Cysteine** [BBD97]. **cytochrome** [CLR$^+$93, CL92, KKS99, LC93]. **Cytosine** [GL98, PCE95, ZL98, BHV96, FL95, PWL98, TG96].

D [Ano93g, BBC92, Brä95, BYGA99, Cal90c, Cal90a, Dun96b, Lin96a, LUU90, LCP+91, LSGS91, Mat97, Mon93, Mon94, Sta93, PAT93, SST93, SST94, CBT93a, CB93b, CB94a, GJOV97, HP98, IHG95, MCM98, SPH98, SB98, SST93]. **d'activation** [GK90b]. **Dahmen** [Car96]. **DAN** [Mun92]. **Dancoff** [DP97, VZ93]. **dans** [GK90b]. **Data** [BMG+98, HL93a, HPSC97, Jur96b]. **Dative** [SL93]. **David** [Gre98, Jør92]. **Davidson** [JGP91]. **Davydov** [För97]. **Day** [Dav98]. **dC** [GT97]. **DCl** [RN96]. **DCNQI** [Sta98b]. **DCS** [Pai91, Pai97, PL98, Pai99]. **deactivation** [GS90a]. **deacylation** [WJC+99]. **deaminations** [HDB+95]. **deaminoarginine** [SS90]. **Debye** [ZW96a]. **decane** [Lu99]. **Decarboxylation** [FB96, NSS+95]. **Decay** [ABB93, VBF95, Ale95, GZDZ97, SLS91]. **Decomplexation** [XY95]. **Decomposition** [BAK96a, BAK96b, Jur99a, Pec93, PÅS+97, PGS97, PSCZ97, YPC97, AKCS91, CRK+91, RK92]. **Decompositions** [AT93, MR94]. **decoupled** [Nal91, Nal92c]. **Decoupling** [BJLK98]. **decsilane** [Lu99]. **Dedication** [Ano92m]. **Deduced** [MPJ97, MSF91, Sin92]. **Deep** [BP96c]. **Defect** [LBM94, LMMK93, MKDL93, Mar99b]. **Defects** [Kry98, MI93, MPSF97, CFDS90, GKM90, Kun90, LW92, MGNK95, SX96]. **Deficiency** [Mez97a]. **Define** [Bad94]. **Defined** [Mor96a]. **defining** [BP93d]. **Definite** [KS95b, Ols96]. **Definition** [Ada99, BKLv95, ČHM95a, GR94, Mon98]. **Deformation** [Pec93]. **Deformations** [BG98a]. **deformed** [DSW93]. **Defranceschi** [Cal90e, Enk97]. **Degeneracy** [BP96a]. **Degenerate** [CJA94, JG95, LD94, Pal98, RDF98, AI99, KSF91, MHM95a, MHM95b, MRD92, YG90]. **degenerated** [HOF+97]. **degree** [Art94b]. **Degrees** [NP96b]. **Dehydration** [BAK97]. **dehydroalanine** [NMSJ99]. **Dehydrogenase** [CAK+96, Ryd94, GVK99, RAM91]. **del** [BG98b]. **del-operator** [BG98b]. **Delayed** [MBV+98]. **Delhalle** [Cal90e]. **Delocalization** [CD93, KM92]. **Delocalized** [SBIP97a]. **delta** [SBL+94]. **delta-doped** [SBL+94]. **Deltafunction** [LB95]. **Denmark** [Kar93]. **Dennis** [Ano92k]. **denominator** [LC90]. **dense** [KH96a, Mar90, MAK+91]. **Densities** [AZAC97, CC95, CM94, DBB94, DMFR93, FUI97, HSS+95, KKT93, Kup94, Mar96, Mic94, Núñ95b, Núñ96, OHSF97, PV97, PS94a, PB95c, PJ96, SRM98, SP94, CCWCF96, CMB95, KM99b, MS91, MAC96, PA99, VES+99, YKN+99]. **Density** [AMRT94, ART94a, AL95, ASP97, ABR95, AM98a, And94, AYDR96, ÁC94, ASI94b, ADM98, Bad95, BDG96, BAR94, BIM97, Bér97, BM96, BDK90, BCRL94, BG98a, BAL95, Bra97b, BS94, BYE+97, BCL98, CdBKZ99, CG97a, CZ94a, Cha98, CGLP96, CSP98, Cio94, Coh97, CPA95, CA97, CB94b, Dau94, DPP+94, DZ94, DD98b, DZ96a, DI95, Dob98, DKBB97, Dun96a, Dun97, Eng95, EMMS94, EMMS97, FEE+98, FP94, FT97b, FWC+93, GMS97, GR94, GR96a, GG97a, Gho94, GD94, GSD97, GD96, GWB97, GBRA94, Gör98, GPD94, GG97b, Gre94, GWCT97, GLBM96, GK91, GDF92, HMGP93, Hag97, HHKM95, HM95, HM97b, HBH98, Jac97, JBT+95,

JH90, Jou97, JZ95a, JZ95b, JM96c, Jur96a, Jur96b, Jur97a, Jur97b, Jur97c, Jur97e, Jur97d, Jur97f, Jur97g, Jur98a, KLLB98, KBGE97, KBWJ96].
Density [KVB97, KS94a, KSSG95, KBA96, KD98, KS94b, KVS98, Koh95, KMM96, KL97c, LZ96, LY98, LP94, Lev97, LLZ98, LKLBD98, Lu99, LLBM$^+$95, LAS$^+$95, MG97, Mar94b, Mar94d, Mar95a, Mar95b, Mar98b, Mar98a, MRT97, MFP96, MSMR99, Maz98, MB98, Mez97b, Mic96b, MDJ98, Mor93b, MCA95b, MNC95, MSCP92, Nag94, Nag98a, NV97b, OHSF97, PCE95, PY89, PP98a, PMDM97, PZDM97, Per98, PB96, PEBS97, PRTV97, PAC90, PACO90, PGS97, PSCZ97, PAAM98, PK96, PS94b, RL95, RPKM95, RHC96, Rey95, RPB$^+$97, RDK97, RP98a, RSD97, RRS97, SPH98, Sam97, SPOAS97, SDW$^+$98, SSO$^+$97, SF95a, SD97, SPC96, SZL95, SZ96, SZ97a, Scu95, SCP93, Sha95, STY$^+$98, SNNY99, STMR97, SR96, SFM94, SMO$^+$96, SAL$^+$94, SG97, ŠH96, SLD95, SDG97, SC99, SATP94, Suk94, Suk95, Sur97].
Density [TKNI96, Tac96, TC98a, Tet93, TG95, The97, TSPK96, TSPK97, TB95, TCM98, Tri97, Val94, VB94, Wło95, WR96, YNY99, YNNR97, ZC96, Zap95, ZC95, ZPBC97, Ali99, AC95, ABSW95, Ano92l, BOL$^+$90, BOA95, BMDM90, BCD91, BDPS97, BS92, Cal90a, CCS98, Cha92, CLGW95, CP99b, CMA$^+$99, CES87, CA91, CEM$^+$96, Csa90a, Csa90b, CK91, Csa92, Cze99, DA91, DDC97, EDH$^+$92, GJPF92, GRBA92, GNF90, GW91, GSKC99, HCRR94, HMG$^+$92, Har94, HK95a, HLJ96, Hol98, Hud99, Jac98, JWG95, Jur99d, Jur99c, KK99a, KC97, KL90, KLM91, KL92a, KK92b, KPB99, LCB98, LBL98, Mar92b, MHN98, Mar99a, MVS97, MECE97, MLL99, MESH93, MRT95, MRST95, MR97, Min90b, MYPL90, MP91, MSF91, NYKY98, NM94, Nal95b, OGK90, PSAUS90, PMDM98, PP90, Per93].
density [PG96, PNB94, PG95, RVP92, RDK02, REKP92, SH90a, SN99, ŠG96a, SCP91, SP92b, SP95, Sem96a, SPM$^+$96, SSC92, SCS94, SS91, SG96b, Spr93, SD91, SNH99, TNSM99, TP90, The94, TC98c, TGDS97, Tri96, Van96, VVO98, WW97, WS92, WGP99, WMZ98, YB99, Yor95, ZTC97, ZY94, Zie96, CES87, Mar99a, PMDM98, PZDM98, Cal90a, Cal93]. **Density-Dependent** [KLLB98, Scu95]. **Density-Functional** [Dun97, Gör98, Hag97, PSCZ97, SPOAS97, SCP93, CZ94a, GK91, MG97, MNC95, PY89, Tet93, CCS98, Csa90a, Csa90b, CK91, EDH$^+$92, GNF90, GW91, HCRR94, Har94, HK95a, SH90a, SS91, Spr93, The94, TC98c, Yor95, Cal93]. **Density-gradient** [ZPBC97]. **density-gradient-expansion** [SS91].
Density-Matrix-Response [TCM98]. **deoxyadenosine** [KJL96].
Deoxymyoglobin [GSSD$^+$96]. **deoxythymidine** [DZB92a]. **depedence** [GH92]. **Dependence** [CR93, EPB97, FP96, FMD$^+$94, FDAC90, GLLY94, KSH94, MPV94, MBA94, SC98a, SG90, AM92, FV96, FR93a, HSWS95, LP99, MJLL99, MPIP99, PB99, SLS91]. **Dependencies** [YNNY99, Boe92, vMVvLvD97]. **Dependent** [ASI94a, AV92, AM97, CT96, CSP98, DFDK99, DD98b, FBKD97c, Gör98, JR96, KLLB98, KSY97, LG95b, Mor96b, RB95, RW98, SB95a, Scu95, ST93, TC98a, TCM98, Tri97, Bec94, BDP$^+$92, BFL91, BMA99, CT95, CCS98, DD95, FMR91, GBS99, KCLI95, Lon99, PG96, RH92, Rod91, RMF90, TC98c, YB99, SB92a]. **Depleting**

[DP93]. **depletion** [BH99]. **Depopulation** [KSK+99]. **Deposition** [CL95, AST95, CH91]. **depositions** [WTSN94]. **depth** [MCB99]. **Depths** [PB95a]. **Derivation** [HWS92, KC98a, Sah95a, Bro95b, HC96a, Hos97, MD99, Vin92]. **Derivative** [KSY97, MK97a, CJM+91, EMP92, Sem96b, Tho96, TŚPKM94]. **Derivatives** [AST93, Bra97b, CCM+96, GBVM93, GKKA97, GJLA99, Jou97, Kin96, LSC98, Lu99, MS98, MH98, MV99, SSK+92, Sza95, TBBE97, TBBE98, TSRP99, VDD96, BBB+95, BBE95, CJM+91, CTC95, DB93, HDY+91, IGK+92, LB94, LCS98, MZ91, MSRP90, RAM91, SZCO99, SSM+99, WB93]. **Derived** [HPSC97, JBT+95, KY93, Roz97, FF90, KKL90, KY92, PLBB99]. **dermal** [MK96]. **descent** [BA92]. **Describe** [Bau98]. **Described** [DZF93, GSM90, Löw91e, Røe90]. **Describing** [Sza95, BA90, DCK92, Sch92c]. **Description** [Hed95, KGC+96, KMM96, MKM97, NP96b, Per98, PA99, Ryl99, Sch99b, Tom91, BUZ94, BFRN90, Cio91, DDC95, DBM99, KK90, Nal98, TYY91, VPŠ+90, YNNR97, GVV+90]. **Descriptions** [Cio94, Loh96, Mar95c, TC98b, VdV96]. **descriptor** [Kin93]. **Descriptors** [Art98, BDG96, KRB+97, RD98, MRB+96]. **Design** [ARBB95, Ott94, San97, ZCT98, Jug90b, KPM+90, RC92b, SHB+96, WWFR99, BL92a]. **designing** [AI99, Sla92]. **desorption** [MD91]. **Destabilization** [MSP94]. **Detachment** [DZO97, RB93]. **Detailed** [TYTY91]. **Determinantal** [Csa93, TM93, Csa95]. **Determinants** [Iga95, For92b, PVU+93, PK92b, RTS91, WB94]. **Determination** [BK96, BFH96, CA92b, CMFA93, CL94, DM95, DDD93, DZ94, Her97, KCI98, MTNF99, MS97a, PNB94, Sch93, VJ95, VJ97, BRL92, Cal90e, DD89, DS90, GL92, KK99a, PL91, ZP90, BOL+90]. **Determine** [Hag98, Su93, Tos95]. **Determined** [BDNT97, PSO90]. **Determining** [Maz98, PRVS95, XY98, BP90, HZ93]. **Detour** [TNM97]. **developed** [Bir94]. **Development** [Fau92, GSM98, Her98, Löw95a, Löw97b, MBV+98, MPOG99, SSO+97, ST96b, Sut96, BAF+95]. **Developments** [Jon94, LJN+98, Ott94, Sem96a]. **Deviation** [Gui98]. **devices** [Sla92]. **Devoted** [Löw90c, Löw91a, Löw91b, Löw91c, Löw91d, Löw92b, Löw92c, Löw92d, Löw92a, Löw93a, Löw93b, Löw94b, Löw95c, Löw95f, Löw95d, Löw95b, Löw96a, Löw96b]. **DEWAR** [DD90b, Ano92-45, Ano92-44]. **DEWAR-PI** [DD90b]. **Dexanabinol** [PB97b]. **DF** [GGSA98]. **DFT** [SPF96, AOH96, AHI96, BBTU97, BLE96, BBC+96a, BT96, Boe97, BTN98, Bro95a, CCS99, Dav98, GFY+99, GS97b, GL95, GJDD97, Gut99b, hJH97, Kün99, MB97b, MPJ98, NL96b, Pra97, SC96, ST97, SW95, SGB97, SGB98, TŚP97, VV95, ZC95]. **DFT-evaluated** [SC96]. **DFT-LDA** [MB97b]. **dG** [GT97]. **Di-** [MK98a]. **Diabatic** [KO95]. **Diacetylene** [CMF+98]. **Diagnosing** [NM95]. **Diagonal** [DMB97, Sam97, Lás93]. **Diagonalization** [Gin98, Ter97]. **Diagram** [FD96b]. **Diagrammatic** [NS93b, ZC99, Jør92, MM91]. **diagrams** [Rin96, Zho94]. **dialane** [MHL94]. **dialkylnitroxybenzenes** [TD96b]. **Diamagnetic** [KM97]. **Diamond**

[BKS96]. **Diamondlike** [KPTS97]. **dianthryl** [LK90]. **Diatomic** [AZAC97, BEJ98, BZQ95, DlD99, Gra97a, Kru92, Kup94, LKMCVT95, LKMCVT96, LTP96, MRL99, MP93, NS95a, NS95b, Ney95a, Ney95b, PP98a, Suz99, YDFS98, BL91, BLG95, Cal90e, DD89, GDYY97, JY94, NSTFC94, NE95, Par99, Ran93, RSCP92, VA90, VPŠ+90, Wil99a, NE95]. **Diatomics** [NBS95, PPK97, CKM91]. **Diatomics-in-Molecules** [PPK97]. **diazacyclobutadienes** [JZ95b]. **dibenzotricyclic** [WLB+94]. **Diborane** [MHL94]. **dibucaine** [DB97]. **dication** [DWB98]. **Dications** [MFP96, PS93, BL99]. **Dicretization** [TS92]. **Didehydroproline** [RK95]. **Dielectric** [Dun99, JSKC95, LP97a, PTH+97, Sim99a, DVJ93, GC91, Sim99b]. **dielectrica** [VD95]. **Dielectrics** [MO98]. **Diels** [Bra97b, MV98a, SLG+96]. **diene** [RGHH94]. **dienes** [SLG+96]. **Dienophiles** [MV98a]. **Dieter** [Car96]. **difference** [NM96, RPT90]. **Differences** [HH92, OHSF97, DFGB99, GVK99, MT91]. **Different** [BW97, BMK96, JSKC95, KZ99, MB98, MD92c, Roz97, RRS97, SKN95a, SKN95b, Sta98a, WBD97, ZLWES99, BOL+90, NPL90, SE92]. **Differentiability** [YG90]. **Differential** [CM96a, Kin96, Mar98b, NS95a, NS95b, NE95, Ney95a, Ney95b, ZM97, ACZ91, BZ92, EZ92, NSTFC94, SN99]. **Difficult** [UWB94]. **Difficulties** [VVO98]. **Diffraction** [PM93, Eng92]. **Diffractionally** [GYDY97]. **diffuse** [DBF+92, LMV92]. **Diffusion** [BMK96, DM96, LL94a, TNM98]. **Diffusion-Limited** [LL94a]. **Difluoride** [ALRP96]. **Difluoroacetylene** [Jur97f]. **difluorobenzene** [JDJP99]. **Difluorodiazete** [Jur96a]. **Difluorovinylidene** [Jur97f]. **digallane** [MHL94]. **Dihedral** [HT97, TL98]. **Dihydrated** [GL97]. **Dihydro** [JZ95b]. **dihydronicotinic** [BBB+95]. **dihydropyridines** [PHBB94]. **dihydroxynaphthalenes** [Kha92]. **DIIS** [Sel93]. **diisopropylaminoethylmethylphosphonothiolate** [HJ94]. **Diketopiperazine** [PVLG93]. **dilated** [MM94]. **Dilations** [KE93]. **dilayer** [WSTB90]. **diluted** [GSPSM93]. **Dimension** [BP96a, KSH94, NB93, PP92]. **Dimensional** [Art98, BBC+94, DM96, DTM96, Eid99, FWT+96, Gin96a, Har98a, Her96, KPR97, KK91, Kup94, Lad97b, LS93a, NV94b, NB97, Núñ95a, Núñ97, RPKM95, SB97b, SSD96, Spr96, Sta96a, TBČP95, TE96, TZ97a, Ukr94, VBUS99, WG95, YO92, ZYY95, BL92a, BS91a, Ber96c, CC92a, CC92b, DS99, DB94b, GDF92, HR99, Hos97, KG92, LLL91, LL99, LM92, MD93b, MSC92, NYKY98, NV97a, RSCP91, SB95b, Spr93, Sta95, Sta96b, Sta98b, Sta98d, Sta98e, Tac92, TKO+92, TTOY93, Mor96a, VRR92]. **Dimensionality** [DQB97, See97]. **Dimensionally** [Val94]. **Dimensions** [HM95, IP94, MK97a, NYLBNSB97, TZ97b, PZ91, WDS97]. **Dimer** [AKD96, AOH96, CMF+98, CCB+97, Fou94, LB95, NG97, PIG94, SKTN97, SST93, CCC+95b, MRBM91, STKN90, SDP+95, SST94, ZY94, vMVvLvD97]. **Dimer-Units** [SST93]. **Dimerization** [GP97, Mor97a, PB97b, GHB+99, LTY92]. **Dimers** [CBSR+98, JZ95a, YY96, Cul91]. **Dimethoxy** [TD96b]. **Dimethyl**

[Sen96, Jur99c, MSRP90]. **Dimethyl-Amine** [Sen96]. **dimethylcyclopropanone** [CAM+97]. **dimethylguanine** [YJL92]. **dimethylimidazol** [Cio93]. **dimethylnitramine** [CRK+91]. **Dimethyluracil** [PIG94]. **dinaphthonorbornadiene** [SCC91]. **Dinuclear** [Bér97]. **diol** [Enc96, KM90c, WP92]. **Dioxide** [AMRT94, AMKS93, XR94, GKM90, SLG+96, TFT+91]. **dioxin** [MEP90]. **dioxodihalides** [TGDS97]. **Dioxygen** [Bér97, BBC+96a]. **Diphenylacetylenes** [DB94a]. **Diphenylpentane** [LV93]. **diphenylpolyenes** [LB94]. **Diphosphate** [FVN98]. **dipolar** [MK90, SAL+94]. **Dipole** [BP93c, BP93b, Can97, CJA94, GSJS97, KSF91, MS98, Mon98, SPS96b, SC98a, Sut99b, DOPS91, KY91a, KY91b, KM90c, MK90, Par92b, SDO91, SSC92]. **Dipole-Bound** [GSJS97]. **Dipole-Moment** [MS98]. **Dipole-Octupole** [BP93c]. **Dipositronium** [PK96]. **Diprotonated** [Sta95]. **dipyridyl** [AEHM91]. **Dirac** [DJ12, Csa92, DJ95, Dat95, DN96, EKI94, GC91, Ish90, MHN98, MC91a, MC91b, Moh92, VIK98, ZP92b]. **Direct** [AL98, BTTS97, BD94a, BD94b, BD95a, CMB95, DRBE96, FGRS98, FP94, GVB97, KBGE97, VdV96, VHFL93, ZDO96, SO97, VR90]. **directional** [BMP92]. **Directly** [BDNT97, Sin92]. **Dirichlet** [Núñ95a, Núñ97]. **discovery** [Kha91]. **Discrete** [HR95, OLC+96, VJ95, VJ97, Ale95, Geg91b, Ish92]. **discretized** [CGMG92]. **Discrimination** [Reg92]. **disk** [Brä96b]. **Diskette** [Ano95f, Ano95g, Ano95h, Ano95i, Ano95j, Ano95k, Ano95l, Ano95m, Ano95n, Ano95o, Ano95p, Ano95q, Ano96h, Ano96i, Ano96j, Ano96k, Ano96l, Ano96m, Ano96n, Ano96o, Ano96p, Ano96q, Ano96r, Ano96s, Ano96t, Ano96u, Ano96v, Ano96w, Ano96x, Ano96y, Ano96z, Ano96-27, Ano96-28, Ano97a, Ano97b, Ano97c, Mic96a]. **disorder** [Lás93]. **Disordered** [DFL98, LRM96, SLtM+94, BCD91, CDB90, LO93, PK90]. **dispersed** [EZ93]. **Dispersion** [BP93c, HP98, MJS93, ADB95, BP92a, CPA98, MK90, BP93b]. **Dispersion-Energy** [BP93c, BP93b]. **Displaced** [Coo94]. **Displacement** [KMM95, MK99, MKM96, MKM97, MM98, KKM99]. **displacements** [MTNF99]. **Dissimilarity** [Mez97a]. **Dissipationless** [MVL96]. **Dissipative** [ATP+96, BS93, KMM96, O'C96, Sch99b, BCD91, Sch90, Sch94]. **Dissociation** [Ata97b, DM95, Jos97, JM96c, Jur97b, LTP96, Mar95b, Moi97, Rot96, Ata97a, CLOFR98, CKB91, HMG+92, JY94, Jur99c, Rot97, SP92b, VES+99, ZGPS97]. **Dissociative** [CFB97, MD91]. **Dissociative-ionization** [CFB97]. **Distance** [GM93, HSS+95, LNT99, MC94, MBA94, HSWS95]. **Distances** [GR95b, GR96b, HP97, BBLK94, BDPS97]. **Distortion** [Kup94, WTD+94, WG95]. **distortions** [Cas97]. **Distributed** [ÁC94, FFD98, Wil96, Wil99a, LGBL94]. **Distribution** [And94, KBWJ96, ML97, MK98a, MV99, Ols96, RPKM95, SHC+98, TSPK96, ASM91, DOPS91, GSM+92, HE90, MYPL90, MIW91, Nal92d, SBAD90, WN90]. **Distributions** [BK96, CYY95, HA93, LP97a, MFAT98, PV94, PV98, SPC96, SMO+96,

WS94a, HSES94, Jac92, KKM99, LO93, TNI96, Tom91]. **Disubstituted** [Cha97]. **Disulfides** [Jur97b]. **Dithietes** [MF96]. **dithionite** [PBBH93]. **Divalent** [MBP97]. **divergence** [BW90]. **divergence-free** [BW90]. **divergent** [ČVW91]. **Divide** [GGSA98, Zho93]. **Divide-and-Conquer** [GGSA98, Zho93]. **Division** [Bir94]. **DM** [Brä95, Brä96b, Brä96c, Car96]. **DNA** [BS91b, BDP+92, Bor94, BPL97a, Brä93b, CH91, CD93, GBS99, JTZ+96, JDB99, KL93a, LP97a, LF90, LSGS91, PWL95, PWL98, PBR96, RBB+94, SM98, SST93, SST94, ŠH96, Tob99, TG96, WP90, YDDP92]. **Do** [ATP+96, JCM+92, DLF99]. **Doctoral** [Ano99n]. **dodecamer** [BS91b]. **dodecylsulfate** [SWK90]. **Does** [Far97, MSP94, WI96, LADV92]. **Domain** [JTZ+96, Krü97, KDHW90, KRRB99, PRVS95]. **Domains** [NK96a]. **dominant** [JDB99]. **Donor** [Kov98a, Mor93a, Mor96b, AB99, EC96, EE91, FKR92, GBS99, GDF92, MCT99]. **Donor-Acceptor** [Mor93a, Mor96b, FKR92]. **donor-bridge-acceptor** [AB99]. **donor-DNA-acceptor** [GBS99]. **donor-pair** [GDF92]. **Dopamine** [GJOV97]. **Doped** [DD97a, DP93, DM96, DTM96, Dun99, LRM97, LF95, Yam97, AMC97, BRS95, DYD96, DS99, DD90a, FS95a, LTSL96, Min94a, SMM+90, SBL+94, TTOY93, YZX96, YYLB90]. **doping** [AKS+90, ABCM93, CEZ+99, MS94, SAB+97]. **Dordrecht** [Ano92l, Ano93h, Ber96b, Cal90c, Cal90e, Cal90b, Cal90a, Eri92, Kar93, Lun91, Lun92]. **dot** [EC96]. **Double** [BL92b, CDDM96, Gra97a, KBL95, Kor90, Mey94, Mey97, Par97, PB95a, TKSH93, Ert90, FCMB99, MTNF99, NL96a, PBR96, Sta98b, BKL98]. **double-helix-mediated** [PBR96]. **Double-Ionization** [Par97]. **Double-Linked** [KBL95, BKL98]. **Double-Point** [Mey94, Mey97]. **double-stack** [Sta98b]. **Doubles** [HKC96, WB94]. **Doublet** [Jur99b, HZ99, VX99]. **Doubly** [NBS95, Pal98]. **Douglas** [Boe97]. **Dowrick** [Kum93b]. **Dressed** [PLA98, xLTY92]. **DRF** [DV91]. **Driven** [GW98a, Mic96b]. **Drude** [Amo96]. **Drugs** [MAAP+98, BD95b, TCZ91]. **dry** [MG91]. **Dual** [JM96b, Wło95, ARBB95, Wło94]. **due** [GDF92, MT91, RD90, XSA+92]. **d'unification** [GK90a, GK90b]. **duplex** [YDDP92]. **duration** [Hag94]. **During** [YBM97, Dun96b, LM95]. **Duschinsky** [PSD97]. **dushinsky** [GS90b]. **DV** [LH94, SST93, SST94]. **DV-X** [LH94, SST93]. **DVR** [BJ98]. **Dy** [Li93]. **Dye** [Shu96, BDZ94]. **Dyes** [Che96, BBS90]. **Dykstra** [Ågr90]. **Dynamic** [ALRP96, BA97b, CAÖ96, GBS93b, MFP96, PP95, SAS99, TFOY92, WSW98, Art93, BCX92, BP92a, Chr92, LO93, LTY92, SDO91]. **Dynamical** [AT93, FWBT94, Her98, SSM90, FLHT90, KPW+95, TD03]. **Dynamics** [ABB93, ADB96, Ata97b, BS93, BTTS97, BM96, BCMÖ97, BSHP97, Brä93b, CN94, CD93, CFB97, CCT98, DHL+94, DD98a, DD98b, DKBB97, Dun98, FWT+96, GBS+93a, GH99, GLBM96, GW98a, HGC93, HL93a, Hop90, KMM96, LLC+94, LM95, MHÅ98, MY99, MK98b, Mon94, NY98, Nic96, OMTS97, ÖOD96, Oku98, PTC94, PPSK96, PPK97, PP98b, RB95, SB95a, SB97a, SB97b, SNMB97, SD96b, SM92b, The94, TBW90, WGR+94, WZ96,

ZZCSE94, AEJ91, Ata94, Ata97a, BZ90, BA91, BJ92, BFL91, BFV+93, BMFPV92, Cor92, DD95, DÖ94, ESHP99, EE91, GVK99, GGHP94, HM99, Hag99a, JO94, KDHW90, KYW95, KJ97, Kry96, LADV92, LUU90, MD92a, MCB99, MJLL99, Nag96, PY92, RC99, SHF94, Sch92c, SCP95, SKC99, TW90, TW92, TCB99, Tho96, TMR99, TD03]. **dynamics** [Tul91, WLB+94, WGP99, Yur95, Kar96, Deu98a, Dun96b]. **Dyson** [SS98, TMD96]. **Dyson-corrected** [SS98]. **DZP** [JG95].

EA [Bau98]. **Early** [SL93, Cle92a]. **Earth** [DTA+96, Sta98c, CMB95, Csa94, LRM93]. **easier** [BAF+95]. **Eckart** [Ell92]. **Eclipsed** [Pal94]. **ed** [Car96, Sta90, Str92]. **Ed.** [Mic97]. **EDA** [SBM97]. **Edge** [BSS96, CF96, ML99]. **Edge-** [CF96]. **edge-to-loop** [ML99]. **Edited** [Ano92k, Ano92j, Ano93g, Ano93h, Cal90c, Cal90e, Cal90a, Enk97, Eri92, Kar93, Lun91, Lun92, Mon93, Sta93, Tay91, Ber96b, Kar96, Mon94, Tri96]. **edition** [Brä95, Str93]. **Editions** [Str92]. **Editor** [Cal90d, Mat97]. **Editorial** [Löw90b, Löw90c, Löw91c, Löw91d, Löw91a, Löw91b, Löw92b, Löw92c, Löw92d, Löw93a, Löw93b, Löw94b, Löw95c, Löw95f, Löw95d, Löw96b]. **Editors** [Dun96b]. **Eds** [Kra96]. **Effect** [AMKS93, ABDM94, BSS96, Bau97, Bre99, ČHMA95, CEZ+99, CL90, DB94a, DZ96b, FLF96, GFS92, GMS97, GH99, HGP91, KUN+98, KEMM93, MV98a, NK96a, PSD97, PRC98, PM93, SKJ98, SY91, SIM93a, SS92c, Sri97, ST96b, TG96, Wan94, WBD97, Xu96, ZLWES99, Aon99, BLG95, EMMHP92, EC96, EMS90, EBMS92, Gao93, GSPSM93, GS90b, HZ91a, ISOA99, KA96, LaF90, MT91, Pet92, ŠG96a, SLG+96, VS95, WW97]. **Effective** [Ara94, BCLS94, Coo95, CPTR96, CL94, CL95, FD96a, Gin97, GG97b, GvLB96, KFS92, KPTŚ94, KA95a, MTL97, PG94, Pai97, PL98, Pai99, Sch99b, SR96, STM96a, SJ97, BAR94, BC97b, CB99, DP96, Ell91, ERC91, FDD95, HS93, KDB90, KLO+98, PO91, RCB+99, STM96b, SBZ92d, TM99, Tom91, TC98c, Van96, WBP91, YBZ92]. **effectiveness** [WK90]. **Effects** [AL95, Ata97b, Boe98, BKLv95, CBT93a, Can97, CAK+96, CV99, CPA95, CCZ97, CDC98, CC96, DLG95, DP94, DC97, DZOR98, EMS92, EMMS94, FT95, FDF97, GJOV97, Gra97b, Hag94, HBL99, Ish91, JCA97, Jay92, KM92, Kar98, Ken97, Ken98, KZ94, KY93, KN92, KMM95, LFD94, MSD95, MB97a, MKM96, NONY97, NKUS97, NG96, NB97, Oku98, PCE95, PKM93, PVLG93, RPB+97, SB95a, SRW96, See97, SAFK97, SFG+98, SM92b, SM95, Suh94, SKS98, WSW98, ZWJP95, ADB95, BDZ94, Ata94, BMDM90, Boč90, BBRT94, BFP93, Bro96, Cab96, Can94, Cas91, CP99a, CA90b, Cul91, Dia99, DDN95, FT96, FT97a, FKR92, GJPMML91, Gur99, Jug90a, KTK+90, KL93a, KKL90, LM91, Les91, LL99, LF90, xLTY92, LE92, MG90, MRB+96, MAK+91, MCA92, MCT99]. **effects** [MRT95, MR97, PGM95, PZTPMC99, PHBB94, PK94, RCB+99, RH92, SCA93, SLDB91, Suh92, TLTL92, TMR99, TUK90, TCM99, VX99, WGP99, XKB+99, YJL92, STKK92, TBP99, XSA+92]. **Efficiency** [KKT97]. **Efficient** [CZ94b, Hag95, Hag96, Hag98, LP97d, MFCA93, SPH98,

WWM+98, BS95, Sim99c, TSS95]. **Efforts** [Sha95]. **Eigenchannels** [Fan97]. **Eigenfunctions** [Kru92, LP97c, Mor96a, NB93, Núñ94a, Mar99a, PVN90]. **Eigenproblems** [Ada99]. **Eigenspectra** [SB98]. **Eigenstates** [PB95a, XY98]. **Eigenvalue** [HA93, Sad97, FKK99, JK92b]. **Eigenvalues** [Aqu95, FK94, GW98b, KBWJ96, KP93, MS97a, Mor96a, PK92a, Sie93, ST96a, Sim97, TE96, A.95, Egu96, Fer90, LLL91, LLSY92, She90b]. **Eigenvector** [LLSY92]. **Eigenvectors** [Wul94, NZ92]. **eight** [YAD92]. **Eighth** [Sim98]. **Eighth-Order** [Sim98]. **eikonal** [CF93]. **Einführung** [HW87a]. **Einstein** [MVL98]. **Einstein-like** [MVL98]. **ejection** [BJ92]. **El-Sayed** [Kra96]. **Elastic** [Sim98, KFK91]. **elastin** [LUU90]. **elastomeric** [LCP+91, LU92b]. **Electric** [ABB93, ABDM94, Bau97, CJA94, Gus98, HC96e, Kar98, KBM92, MKM93b, NY98, NG95, OK96, SKZ96, ZZ93, ASM91, CT95, Can94, DB94b, Fer92, KA96, Kie97, KY91a, KY91b, Mar91, PNB94, SM94, SBAD90, LF90, MCT99]. **Electric-Field** [HC96e, MKM93b, NG95, KBM92]. **electroactive** [GJDD97]. **Electrochemical** [CGS+94, YUSM99]. **Electrode** [WR96, LRR92, Rey95]. **Electrodeposition** [SLtM+94]. **Electrodes** [LLZ98, KPM+90]. **electrodynamics** [KH95, RW99, Woo99]. **Electroluminescent** [PB97a]. **Electromagnetic** [CV98, OS95]. **Electron** [AM98a, And94, Ara94, BMA93, BF96, Bad95, BK96, BS93, BCMÖ97, BGS98, CBT93a, Can97, ČHM95a, ČHM95b, ČHMA95, Che93, CA97, CL94, Day95, Day96, De 97, Del96, DP97, DDN95, DÖ94, DZO97, DZOR98, Flo97a, FS93b, Fri93a, Fue98, FUI97, Hag99a, Hed95, Ish96, IP94, JCA97, JMD95, JJ97, Jur97g, KM92, KPR97, KNN96a, KBA96, KS96, KD95, KV96, LO90, LBLKC98, Löw95a, LBG97, MM91, MSD95, Mar92b, Mar94b, Mar94d, Mar96, Mar98b, MB98, MB93, MBA97, MRL99, MCM98, Mik94, MK99, MP93, Muk96, NMM97, NKUS97, Nes94, NMKP94, Núñ96, Oht98, Ols96, OHSF97, Ort98b, Pai91, PGM95, PP92, PV97, PV98, PZWJC96, PTC94, PS92b, Pon97, Pon98, RPKM95, RML97, Røe90, RDK97, Roś96, SS99a, SA96, SAR96, SSO+97]. **Electron** [SF95a, SD96a, SN98, SG93, STMR97, SR96, SW97, SM95, Suh94, Suk95, TN96, TC98a, TM93, TSPK96, TSPK97, TDK+94, US97, Ukr94, Val96, WS94b, WS94a, WZW96, Wil96, Xu96, YNNY99, YAD95, ZO95, ZON+96, ZH99b, Ågr91, ÅC92, ACHT95, Ano92l, AMH+92, AH92a, BMA90, BBCL92, BK97, BKY99, BMDM90, BSP98, BCY95, Bud92, BFW92, Cam92, CBT93b, Can94, CGG96, CB99, CB96a, Che92, Cio90b, Csa92, DM97b, Dav90, DWB98, DWM90, FMR91, Flo97b, FR98, GP91a, GJP91, GVB96, GW91, GSKC99, GH92, HSES94, JM94, KMR92, KG92, Kin99, KKL90, KM99b, KTCN93, KCP90, KCLI95, KL90, Kry96, KSK91, KSW98, LBBK91, LB93, LM91, LDJH92, LDHJ92, LS92b, MMA+92, MG91, Mar94c, Mar99a, MKRW99, MBG90, MKDL93, MHS95, MHY98, MAC96]. **electron** [MM94, MAAP90, MFCA93, NNY+96, NM96, Ort91, Ort92, Ort93, Ort95, Ort98a, Ort99, Pic92, PVN90, PKJ99, PA99, Pos91, PK92b, PBR96, Rep96, RH92, RB93, Røe91, RDK02, RMF90, Sæb90, Sae92, SK99a, SP92a, STKK92, ŠG96a, SB95b, SPB90, SK99b, SG92, SH90b, Suh91, Suh92, Suh93,

SD91, SS98, SBZ92b, SBZ92d, SB92b, TST+99, TNI96, VES+99, WDS97, WW97, XSA+92, Xu99, YKN+99, YJL92, ZM95, ZO94, ZDO99, ZP92a, ZBL99, ADB95, LRR92, RB93]. **Electron-Electron** [SF95a, GVB96]. **Electron-Hole** [KM92]. **Electron-Pair** [KM92, WS94a, ZH99b, Røe91]. **Electron-Phonon** [BS93]. **Electron-Repulsion** [Ish96, MFCA93]. **Electron-Rich** [WZW96]. **Electron-spin** [LBG97]. **electron-transfer** [BCY95, ZBL99]. **Electron-withdrawing** [LRR92]. **electronegativities** [GW91]. **Electronegativity** [All94, CN94, DLG95, GJ95, Gho94, KN92, Nal91, Nal92a, Nal92c, Yor95]. **Electronic** [AEAO99, AHM97, ARDP92, AH97, AMKS93, Ano93i, Ano93j, Ano97d, Ano97e, Ano97f, Ano97g, Ano97h, Ano97i, Ano97j, Ano97k, Ano97l, BL92a, BUZ94, BBS+97, BXZ95, BKM93, BFH96, BS94, BJLK98, CWX93, Cai93, Cai94, CMCR96, CLSI94, CR96a, Cha97, CXL97, CAJ95, CCT98, Cio94, CSZ97, CF96, DJF98, DB94a, DZ96a, DL92, EZ93, FDC92, FS95a, GBRA94, HAEMA92, IAN+94, Ino96, JCÁ96, JBT+95, Kan93, KGC+96, KEG+97, KPD93, KT95, Kru92, KGVM97, KG97, KG99, LMC97a, LBBK91, LZ96, LY98, Li93, LF95, LEG+94, Löw99, MI93, MCL95, MHM95b, MRL99, MB92, MVV+97, Mic94, MTD93, Mik94, MAI95, MH98, MK97b, MC95, Mor96c, Mor97b, Mor98a, MPSF97, NP96a, NMvB+98, Nic96, NG96, PM97, PS93, PSD97, Pen93, Pen96, PAT93, Rat92]. **Electronic** [RHC96, RW98, RKPE95, RAA94, RS97b, Sah95b, SD96a, SPFL93, SBL+94, SAFK97, SG92, SG93, SST93, SST94, SR96, SRM98, SBIP97a, SBIP97b, SMO+96, SAL+94, SG96b, SG97, SGB97, SGB98, Sta93, SL98, Tac96, TKO+92, TTOY93, TH97, TCA+91, TPR96, TZCT97, TIPM96, TCM98, VR95, Wil90, Wil96, WDCA97, WTS93, XYC98, YK97, AEHM91, AKS+90, BDZ94, Ano92o, Ano93g, BGS99, BOL+90, BBZ91, Ber96b, BAL95, BS92, Bro95a, Cal90e, CLC90, CPA98, CP99a, CJX+92, Cio90b, CC91b, Cio91, Cio93, CCS99, CML92, Coo92, DFGB99, DD89, Dia99, FLWZ90, FLLZ91, FMD+94, FMD+96, FKR92, FJR96, GVV+90, GS91, GRBA92, Gur99, I'H90, JMS95, KTK+90, Kha92, KH90, KJL96, KPTVT+97, Kov90a, Kov90b, KG98, LMC97b, Lan95, LU92a, Lás93, Li97, LVCP91, xLTY92, LG96]. **electronic** [Mar94c, MCOS94, MW92, MBG90, MECE97, MLL99, MS93a, Mez90, METHH94, Muk92, Nob99, Nor91, NMCK92, PK90, Pet92, PCF94, RRC94, RD90, Res99, REKP92, RK91, SP92a, SX96, SGGC99, SK91, SP91, SWD+99, SSM90, SLDB91, Spr93, Suh91, Suh92, TJ97, TMA97, TFSZ95, Tit96, TŚPKM94, VX99, WL92, XKB+99, XSG97, YG90, YBZ92, BSS+97b, FS99, LFD99]. **Electronic-phase** [TKO+92, TTOY93]. **electronically** [PY92]. **electronics** [Avi92, Bir94, Sla92, Mic97]. **Electrons** [BRZY97, BW97, BL92b, BO93, GFRR94, Hag98, OKI98, TAY+97, Bar90, Hag99b, Har90, LB93, LG92, SMH92, TP92]. **Electrons-in-a-Box** [OKI98]. **Electrophilic** [MKM97, PHM+91, AFM99, DGMW90, TFR99, Yu95]. **electropolymerization** [HDY+91]. **Electrostatic** [BMP93, BMVV93, DDG93, DD93, FT95, FP96, GJOV97, HS92a, JSG97, KM90c, KMM95, MK99, MKM96, MKM97, MM98, MM95, MSCP92,

MAAP+98, NK96a, PRC98, SKTN97, SM94, SGK+95, SG94, BMP92, CMSF93, CA90b, FT96, FT97a, KY92, KKM99, LLL92, MEP90, MSRP90, MBP91, MPIP99, RAM91, SCMF93, SHF94, SLL+91, WGP99].
Electrostatics [Bec97b]. **Element**
[Eid99, LVL+93, SGB97, SGB98, MSC92, NPL90]. **Elemental**
[KL94, Mur90]. **Elementary** [Str92, TMDB98]. **Elements**
[ČHM95b, DKM97, DV98, FBKD97c, GMI95, GKS99, Iga95, Jur97d, KJ93, LBMR95, Mar97b, Mik94, Pal93b, Sam97, Sch95b, ZWZ96b, ZARB96, BCLS94, Brä98b, BG98b, BG98c, BG98d, CC92c, DW90, For92b, FJR96, GVV+90, HW04, JRS+99, JF92, Kov90b, KA95b, Lin92, Lon99, MD99, PZ91, SP90, Sch95a, Tit92, WDS97, ZFZ92]. **ELF** [Fue98]. **Elimination**
[CC96, FLF96, Kat97, MR94, Cun92]. **Ellinger** [Enk97]. **Ellipsoidal**
[KZ99, LB97, LB98, MBA97]. **Ellipsoidal-Coordinate** [KZ99]. **Ellis**
[Cal90d]. **Elongation** [ASI94b, IAN+94, MAI95, MAI97, RAI99]. **Elsevier**
[Ågr90, Tay91, Tri96]. **Embedded**
[EDF+98, PB95b, RS94, TJ95, VR95, SRP+98]. **Embedded-cluster**
[PB95b]. **Embedding** [Zou92, Bre99, TS92]. **embodiment** [TD03].
Emission [Hag97, FSW+91, TR91]. **emitted** [DMR96]. **Empirical**
[Löw99, MS98, RWT91, RWT92, Roś96, GBVM93, LK90, LZ91, TD03].
Employing [JKK+92, KCI98, PPP97]. **Enantioselective** [SWMB94].
Encapsulated [LEG+94]. **Enclosed** [Aqu95, A.95]. **end** [Dia99, PTC94].
end-group [Dia99]. **Endo** [MV98a, SLG+96]. **Endo-Lone-Pair** [MV98a].
endohedral [HRRBL97]. **Ene** [Pra97]. **enediyne** [BS95]. **Energetic**
[VDD96, KSN93]. **Energetics**
[AL95, BFP93, WR96, Fra99, SPM+96, SZCO99, WTD+94]. **Energies**
[AR93, ADPS98, BT95, BF95, BKL97, BLK97, BMP93, BZQ95, BDH+97, CV99, CM94, CS98, De 97, DMFR93, DZO97, EPB97, FR93b, GSD97, GSJS97, JKRW98, JGR98, JMR98, Jos97, JM96c, KSH94, KGv93, KKE+96, LP97c, LS92a, LP94, LTP96, Loh96, Mar95b, MHÅ98, Maz98, MV99, NBS95, Pai97, PL98, Pec93, PAAM98, RS98, Roś96, ST93, SDG97, TVP93, Wen98, Ada91b, Ada96a, AMH+92, BHGC99, BCY95, BKL98, CA91, CB91, DKTZ94, EKI94, HC96c, HZF+91, Ish91, Ish92, Jur99d, Jur99c, KSSG95, LU92a, MK90, MSPS90, MBP91, NL96b, Ort92, Pai99, PG96, RR95, SF94, SCP91, SS98, SJR91, VES+99, VA90, VZ92, YAD92, WB93]. **Energy**
[AR92, ART94a, ASP97, AP93, AM98a, AMKS93, Aqu95, BBOR96, BE98, BP93c, BG95, BRA+99, Bra97a, BJLK98, BP95, BCL98, CCM+96, CM96b, CH91, CC97b, Csa96, DP93, DM96, DTM96, DDG93, DPP+94, FP94, Fer95, FT97b, FDF97, FS93a, FS94, FS95b, Fue94, GS94, GR96a, GG97a, GBS+93a, GBS93b, Gin95, Gin97, GBRA94, GLMP98, GP97, HMGP93, HLS94, HA93, HM95, IK94, IY99, JKK+92, Jas94, Jur97b, Jur97e, Jur98a, KPR97, KNA94, KS95b, KSY97, KT96, KPTŚ94, KH96b, KCI98, KL90, Lad97b, LRM96, LKLBD98, LBKLC98, MMP+94, MK97a, MSM96, MD93a, Mez94a, Min94b, MPJ97, MPJ98, MJS93, MV99, NM95, NS97b, Pal92b, PM97, PLA98, PV98, PPSK96, PPK97, PR97, Rot96, RK95, RRS97, SMPJ94, Sch97, SZL95,

SIM93a]. **Energy**
[SZC97, STMR97, SATP94, Suz99, SV95, Sza95, Tac96, TBČP95, Taş93, Taş96a, TDO97, Val94, VV95, WS94b, WTSN94, XR94, Žit94, A.95, AS99, ACHT95, AGNS92, And93a, AKCS91, AH92a, Bec94, BDK90, BP93b, BML98, BRV99, BV93, BFW92, ČDM91, CCS98, Cim96, CJM+91, CA90b, CEM+96, CTC95, Csa90a, Csa91, Csa92, DS99, DI95, DLF99, DS93, EC96, EMP92, Fer91, FGM90, FF90, FS92, GRBA92, GRB+93, GL92, GVB96, GZSvD99, GSKC99, GH92, Gut99b, HFM91, HC96a, HC96d, Hir92, Jac92, JK90, JM94, KBKT93, KR93, KMP+90, KCLI95, KK92b, LCB98, Lás93, Lei99, LH94, LP99, LV97, LFD99, Löw90d, LLB99, LM92, MD92a, MS91, MNT96, MKRW99, MCOS94, MG93a, Mez90, MT91, MYPL90, MSF91, MD92c, Mur90, NNH98, NST94, NÅJ91, NÅJ92, NOS94]. **energy**
[OSS95, OYNY98, Ort92, OYL91, PGM95, PK90, PMDM97, PMDM98, PP90, PČP92, PFK99, RG99, RSCP91, RK92, Rot97, RBB+94, RNS93, SK99a, ST97, SKE92, SEKEB98, STS95, SN90a, Sin92, SS91, SLS91, SES93, TCS+90, TMA97, VÅJ+92, WP91, WDS97, WW97, WI98, Yu95, ZP90, ZBL99, ZGPS97, Zho93, AST95, Loh91, NOY98, Ano92l]. **energy-based**
[FF90]. **Energy-Evaluating** [Fer95]. **Energy-Partitioning** [JKK+92]. **Engineering** [Enk97, Lun92]. **Englewood** [Str92, Wha96]. **enhanced**
[MVL98]. **Enkephalin** [PLV92, LS99, LVCP91, PVU+93]. **Enolate** [PBB92]. **enolates** [SCA93]. **Enrico** [And93b, Ano92m, Ano92-46, KK92b]. **Ensemble**
[CC95, CCWCF96, HLJ96, OGK90, WT98, Nag95b]. **Ensemble-density**
[OGK90]. **Ensemble-representable** [CCWCF96]. **Ensembles**
[BRA+99, Nag95a, Nag98b]. **entanglements** [Art94b]. **Enthalpic** [BPVP92]. **Entities** [BPL94]. **entropic** [BPVP92]. **Entropies** [YAD95, HSWS95]. **Entropy**
[AZAC97, GH96a, GLMP98, NP96a, Wal94, Zie95, AYAZ95, GJPZ97, MP91]. **envelope** [Hos97]. **Environment**
[DB99, FVN98, JCÁ96, Löw97b, Sch99b, CRK+91, NGM+95, RK91]. **environmental** [LF90, SLDB91]. **Environments** [ZLWES99, Mar92b]. **Enzymatic** [GLBM96, SHB+96, BBSS96]. **enzymatically** [HDB+95]. **Enzyme** [ECBH96, HM99, KK92a, Kov98b, RMH+99]. **enzyme-inhibitor**
[RMH+99]. **epitaxial** [Mil97]. **epoxides** [KM90c, WP92]. **EPR**
[Krü97, MA99a, PLBB99, VABM94]. **Epstein** [Cim96]. **EPV** [SB92b]. **Equalization** [GJ95, Nal91, Nal92c, Yor95]. **equally** [AEJ91]. **Equation**
[Aon98, BD94a, BD94b, Boe95, CV94, DZF93, Eid99, Hag98, IK94, LVL+93, Maz98, MS97a, MS97b, NOYY94, PTH+97, RW98, Sch93, ST96a, Sim97, Taş96b, TE96, TZ97b, Zha96, AGH91, AA92, BS91a, BD95a, CC91a, CP92, FKK99, Fer90, Geg91a, Geg91b, Hag95, KH96c, PZDM97, PZDM98, Rod91, SN99, Sim95, Sim99c]. **Equations**
[Áng93, Bec97b, BG95, Chr94, FK94, GRT96, Gin96a, HM97c, JM93a, JKJ94, JKJ95, Mar93a, Mar98b, NS93a, SE97, Ste96, Ter97, BBS91, CTF92, ČPV90, CGMG92, Har99, JKGM99, Kry96, Nal91, Nal92c, New97, PP91, Roc99, Sch92c, SE95b, Vin92, WW97, ZZW94]. **equilibria** [Nal98].

Equilibrium [Gui98, KH90, MTD93, METHH94, Cab96, EMS92, NWT92, PSAUS90, Sla92, Zha92b, Boe95]. **Equivalence** [HM97a, NYY96]. **equivalent** [PC91]. **Erdahl** [Cal90a]. **ergodography** [OYNY98]. **Ergotamine** [MM95]. **Ermer** [Tri98c]. **Erratum** [AR99a, CB94a, DJ12, FS95b, FS09, Her93a, Iva97, Jac98, KN99a, MD95, MT90a, MC91b, PMDM98, PZDM98, RDK02, Rot97, SKN95a, Sim99b, Vol90, Wen96a]. **Error** [CSS93, Ney95b]. **errors** [SEKEB98]. **ESR** [HZ99]. **essay** [HZ92]. **essential** [DBM99]. **Ester** [HBH98]. **Esters** [FLRV97, KE91, MKBP97, PHBB92, PBHB95, PRB96, TSS95]. **estimate** [JS91]. **Estimates** [GP97]. **estimating** [SN90b]. **estimation** [BPHB96]. **Estimations** [Roś96]. **Etching** [Jen94]. **Ethane** [MSM96, TI94]. **ethene** [TSRP99]. **Ether** [FDD+93, Jur99c]. **Ethyl** [NSS+95, RT98, BH92, HJ94]. **Ethylene** [Bra97b, DC97, FK98, MÅ99b, Sak97, YNNY99, YTYS97, AFM99, Cab96, CDP+99, TFR99, Men99]. **Ethylenes** [KM92, AEHM91]. **Ethylenic** [Shu96]. **ethylester** [BS91c]. **ethylguanidino** [TBP99]. **Etiocholanes** [KGVM97]. **Eu** [DDN95]. **EUCHEM** [Fuk90]. **Euler** [FCMB99, PZDM97, PZDM98]. **Eulerian** [BRV90]. **Evaluate** [SPH98, HK97]. **evaluated** [MK90, SC96, ZZ93]. **Evaluating** [Fer95, Mar95c]. **Evaluation** [Bud92, BFW92, CDDV93, DPP+94, DV98, FS93a, FS93b, GWCT97, GİA96, Gus98, HNB92, HS92f, Ish96, JJ96, Jur97a, KZ99, LKBJ97, LDP93, LS96, Mik94, PCO+94, PD93, SPH98, Sch95b, TP94, US97, WS94b, YD97, BBB+95, Cim96, FJR96, GB90, JRS+99, Jur99c, Kin99, LP97d, Sch95a, Whi99, ZFZ92]. **Even** [RR94]. **evenly** [JL91]. **Event** [Voj96]. **events** [Lev99]. **Evidence** [GHB+99, KCP90, RW92, YJL92]. **Evolution** [AD92, BSB94, BM96, CG95, Fan97, KEP93, Mic96b, PGS97, RJ97, SB98, YBM97, Kha91]. **evolutionary** [GHB+99]. **Ewald** [Har98a, LS93a, TW90, TW92]. **Exact** [AM97, BBC+96b, CD92, CR96a, CFB97, FS97, Gör98, HM95, HM97b, Hol98, JGP91, KCI98, LP94, LG95a, MAD98, Nag95b, SMH92, Taş96b, vDvLR99, DB94b, Iva96, Iva97, NM91, OM91, PČP92, TD99, FS09]. **Exact-Exchange-Mixing** [KCI98]. **Examination** [CSZ97, DE92, MDM94, Ney95a, PKM93, Cul91, Jac92, JGCJ96]. **Example** [BRV90, KBBK90]. **Examples** [UWB94, BFW92, ZWD98b, And90]. **excess** [SLS91]. **excess-energy** [SLS91]. **Exchange** [AC95, ABR95, BZQ95, BP95, BCL98, CGLP96, CGR+94, CA97, FDF97, GR96a, GBRA94, GNF90, GGSA98, Gör98, GvLB96, GVB97, GY95, HH97, HM97b, KLLB98, KCI98, KO95, Lah92, LP94, LG95a, LBKLC98, LR94, MS93b, PP98b, PS94b, QS98, SKN95a, SKN95b, San97, SS95, SS97b, SV95, AM93, Bec94, BCY95, CFMA95, CLGW95, Csa90a, Csa91, Csa92, EMS92, FWS97, FDAC90, FADC91, GRBA92, GRB+93, GL95, GVB96, KLI92, KCLI95, LCB98, MS91, MS92, Nag95b, PRVS95, SS99a, SS91, SS92e, TUK90, VBN95a, VBN95b, YOTY93, KL92a]. **exchange-** [Csa91]. **Exchange-Correlation** [BP95, CGLP96, GGSA98, GVB97, HM97b, PP98b, Bec94, GVB96, KCLI95, LCB98, SS91]. **exchange-coupled** [YOTY93].

Exchange-Energy [LBKLC98, Csa90a, Csa92]. **exchange-like** [CFMA95]. **exchange-only** [SS99a, KL92a]. **exciplex** [MTTS93]. **excitable** [KO91]. **Excitation** [CS98, DlD99, DP93, DM96, DTM96, DMFR93, LD94, LD95, Oht98, ST93, SDG97, Wen98, YLD97, DS99, IHG95, JY94, KSIH92, LHNK99, LP99, PK90, SF94]. **Excitations** [GS97a, MVL96, Ada91a, BAL95, Cio91, GZDZ97, Sas90, STM96b, WB93, ZM95]. **Excited** [BLB95, BČ96b, CLSI94, CCS98, CGLP96, DD97a, Dau94, FSBS+95, Kan93, MB98, Nag95a, Nag98a, Nag98b, NS91, Nic96, PCC93, PTP95, RSD97, SE95a, SC98a, SE95b, SGB98, Sza95, TG95, The97, TC98b, TCM98, VZ93, WS95, WD97, BGS99, BJ92, BRL92, CC91b, Cio91, DDC97, IHG95, KP92, MLB92, MHG95, MLL99, MAAP90, MPP92, MDM94, MSS99b, NNH98, OGK90, SE93a, SKC99, SKRK90, TGS99, VX99]. **Excited-State** [CGLP96, CCS98, SE95b, DDC97, MLB92, SKC99]. **Exciton** [ÅGL97, DP93, DM96, RM99, SCC91, DS99, VCMLL90, VZ92]. **Exciton-Depleting** [DP93]. **Exclude** [GRT96]. **excluded** [Art94b]. **excluded-volume** [Art94b]. **exclusion** [SB92b]. **exemplified** [BP92a]. **EXGEM** [Røe90]. **Existence** [AFTM95a, AFTM95b, AFO+97, AFTM98, AFZ+99]. **exo** [SLG+96]. **exo/endo}** [SLG+96]. **Expanded** [GM94, PP98b, CÅ92a]. **expanding** [PCO+94]. **Expansion** [BF94, DLV95, GLMP98, JM93b, Kut94, MJS93, NS95b, Pan95, PB95c, SP94, SV95, TBČP95, TZ97b, TM93, WBD97, Hol98, Ish92, Le 97, LP97d, LK92, Mar92a, MFH91, Mur90, Pri98, RLR90, SPS96a, SKE92, SS91, SS92e, TH90, VFBP96]. **Expansions** [BK94b, CB93a, GM93, HM95, Jon94, KZ99, KMP94, KMP97, KF98, MZM94, McD97, MS93b, MTL97, PR97, Sch95b, BBMM99, Ell91, JE90, MS92, Sch95a]. **Expectation** [KS98, NS93b, Núñ95a, EMP92]. **Experiment** [BMG+98, Kar93, SSK+92, SB97b, Ågr91, GS97b, HW84, HW87b, MA99a, RTKP95, Sem94, TGDS97]. **Experimental** [BKWL97, HH92, Jur96b, SBM97, SS97a, BBB+95, HW87a, LHL91]. **experimentellen** [HW87a]. **Experiments** [HZ93, HWB05, Mar98a, Brä95, Brä98b, HW92, HW94, HW96, HW00, HW04, LM93, Mon94, OS92, TD99]. **explain** [Bha99]. **Explanation** [VS95]. **Explicit** [ČPV90, LBPL97, LBLKC98, Kin99, Sim99c, KK92b]. **Explicitly** [GKKA97, JM93b, JBS97, KM99b, Ryc94, KA95b, ZA95]. **Exploiting** [RH96b, LP92]. **Exploration** [Jur98a, MB97a]. **Explorations** [Sjö96, Sil95]. **exploratory** [FMD+94]. **Exploring** [Sch97, TCS+90, MD92a]. **explosion** [BCC99]. **Exponent** [GM94]. **Exponential** [Gho95, Gra97a, HS91, HS92f, HS92e]. **Exponential-Type** [HS91, HS92e, HS92f]. **exponents** [ISOA99, TTM99]. **Expressions** [GRK96, IP93, LBPL97, Pal93b, Pan95, WWM+98, CXFP99, CTC95, DW90]. **EXRHF** [Røe90]. **Extended** [Cal96a, Day96, DP97, DMB97, HBJ+92, Kov98a, KL97b, LLL97, MAI95, Mor97b, Mor94, PV94, SGGMGFS96, YO92, AMC97, AM92, AM93, BA90, BHH92, BC93, CD92, DGMW90, HK95a, HS92c, Loh91, MHN98, MD92b,

MW90a, MDM94, Oza92, Røe90, Røe91, YNO94, DMFR93]. **extending** [PRVS95]. **Extension**
[DHPC95, DKM97, Jug96, Pop98, PSS97, TV92, XSA+92, Zho94]. **extensive** [HC96c, LS99]. **External** [JOC97, Mar98b, NONY97, OK96, CA90b, KS95a, KA96, Mar92b, MCA92, NMN+99]. **extracule** [KM99b]. **Extrapolation** [NV94a, NV94b, NV97a, WL90]. **Extremal** [KV96, TSPK97]. **Extreme** [Can94, Eng92, Mar92b].

F [Brä98c, Eri92, GSSD+96, GARC97, Lin96a, MTNF99, Moc99, Mon94, NL96a, SKE92, STMR97, FAV92, MHM95a, Ort98a, Ort98b, Pal94, RK92, TGS99, TPR96, WY99]. **F.** [Ano92n]. **Face** [CF96]. **Face-Sharing** [CF96]. **Factor** [DBF+96, Fue94, GP95, MC94, MPJ97, MPJ98, LBBK91, MSF91]. **Factored** [BGS98]. **Factorization** [MD93c, SM96b, MAPLB92]. **factorized** [MW92, WL92]. **Factors**
[AD97, ALRP96, BDNT97, LKMCVT95, LKMCVT96, Pal97a, PM95, Bud92, BFW92, Kin99, PRSDS92, PSM94, RSCP92]. **failure** [SWD+99]. **famous** [Klo90]. **Faraday** [Aon99]. **Fast** [HO94, DD97b, Cim96, RW98]. **fate** [MG91]. **fatty** [SJB90]. **Favorable** [Gut99b]. **FCP** [DKWM97, DKM97]. **Fe** [BUZ94, MECE97, MNC95, SG96b, SGB97, SGB98, CdBKZ99, Cas97, Cze99, DFL98, DLF99, GSSD+96, ZC96]. **Fe-Al** [DFL98]. **Fe-His** [GSSD+96]. **feasibility** [DO90]. **features** [CWZ98b]. **FeCO** [XLW+99]. **feedback** [MVL98]. **Feenberg** [HC96d]. **Fellows** [Ano99n]. **Femtosecond** [DD98a, KDHW90]. **FeN** [ZTC97]. **Ferguson** [Lun91]. **Fermi** [Csa92, GC91, MHN98, ZP92b, BSS96, Csa96, HS99, MK97a, WS95, WG95, Xu96]. **Fermi-Edge** [BSS96]. **fermion** [Jør92, CBG94, Col97]. **Ferredoxin** [CSZ97]. **ferrocene** [Coo92]. **ferromagnets** [CEZ+99]. **Feshbach** [MTTS93, ZZW94]. **Few** [FS97, AGAP98, FS09, OCK99, PA99]. **Few-Body** [FS97, FS09]. **few-electron** [PA99]. **Feynman** [CBG94, Kry95, Pop98, VCCM92]. **FF** [Boe93, Boe95]. **FFT** [RW98]. **FH** [TGS99]. **fibered** [MV92]. **Fibonacci** [SBM97]. **Field** [ABB93, ADB96, AM98a, AGNS92, Bau97, CPA95, DD98a, Dun99, Eng95, Hag97, HC96e, Huz96, JDJP99, Jos97, Kar98, KBA96, KPTŚ94, Kol97, Lef97, MB97a, MB98, MKM93b, MLT+96, NONY97, NG95, Ols96, OK96, Pan93, PVLG93, RB95, SKTN97, Sch97, SB96, SG98, SKZ96, STM96a, Ste96, TMP97, TKMA92, TSS97, VdV96, WHF92, AS93, ACC92, ASM91, BBS91, BZMR92, Cha92, DD95, DB94b, FNSV99, GRTR96, Hag99b, Ish90, KTK+90, KA96, Kie97, KKNY99, Kla93, KKL90, KY91a, KY91b, KL92a, KBM92, Kum93a, LK90, LKM99, LM91, LF90, MCA92, MRT95, MC91a, MC91b, Moh92, NSTFC94, NMN+99, ROL+90, SM94, SBAD90, SES93, SJ97, VR90, VES+99, ZWD98b, ZJ89, ZJ93, ZJ96, ZJ02]. **Field-Theoretic** [Dun99]. **Fields** [BRZY97, BG95, CFB97, DlD99, HHHP99, JOC97, Ken97, Ken98, KL97a, KMM95, Mar98b, MS98, Moi97, NY98, RS94, RS97b, RS97a, SC97, Sch98, SS97a, Sul97, TC98a, YXX99, Adl95, Fer92, Hua92, LTSL96, Mar91, Mar92b, RR95, SC91, Sem96b, TC98c, Deu96]. **figures** [Brä95, Brä96c, Dun96b]. **File** [She91]. **Film** [MPV94, Boe91]. **Films**

[MPV94, Bat92, Boe92, BBRT94, MV90, WTSN94]. **find** [AI99, Smi90]. **Finding** [KM92, Sim93b, CLZ99, Hag96]. **Fine** [MLB92]. **Fine-structure** [MLB92]. **Finite** [Art97, BČ96b, Cal96a, CW97, Eid99, FS97, GP97, KPR97, KKNN97, LVL$^+$93, Lin92, Mey94, Mey97, Mon94, NV94a, NV94b, RPKM95, Tac92, Ale95, Cal90c, CMA93, CDG04, FS09, Hag94, JPP87, Kir92, KS92, LTY90, MC91a, MC91b, MSC92, NPL90, NV97a, Rep96, WDS97, WL90]. **Finite-Dimensional** [KPR97, RPKM95]. **Finite-Element** [LVL$^+$93]. **Finite-Size** [Art97, NV94a, NV94b, Tac92, NV97a]. **First** [BBS91, BA97a, BLB95, Cal90d, Can97, Cha97, Dat95, DLG95, FT95, Fri93a, Fri93b, GKKA97, Gin97, Hil98, HU94, KI94, KJ93, PCC93, Rep96, Roś96, SE95a, SCS98, SC98a, SPG97, Sie93, SGB98, TN96, YDFS98, DS90, EDH$^+$92, EMP92, Lad94, STS95, TMR99, TSS95, VX99, Lon99]. **First-** [DLG95, Gin97, KJ93, DS90]. **first-excited** [VX99]. **First-Order** [BBS91, Sie93, EMP92]. **First-Principles** [Fri93a, Fri93b, KI94, EDH$^+$92, TMR99]. **First-Row** [BA97a, Can97, Dat95, Roś96, YDFS98]. **Fisher** [Kum93b]. **Fission** [KF96]. **Fitted** [ÁC94, GGSA98, Sim95]. **Fitting** [BBC$^+$96b, Boe96, Ran94]. **five** [GX98]. **Fix** [JK92b]. **fixed** [CE90]. **flames** [GX95]. **flat** [MVS97, MD91]. **FLATER** [WP91]. **Flatland** [NK96b, PZ91]. **Flavins** [WDCA97]. **Flavone** [FT95, FT96, FT97a]. **Flavoproteins** [WDCA97]. **Flexibility** [RWT92]. **flexible** [CLR$^+$93, Cor92, Duc90, WP91]. **Flipping** [Tew94, SSM$^+$99]. **Floppy** [ZZCSE94, Brä96b]. **Floquet** [LP97c, Lef99, PLA98, TC98a]. **Flow** [Suk95, AB99, Lei99]. **Fluctuating** [SB97b, MCB99]. **Fluctuation** [O'C96, Pon98, BKY99, PCD99]. **Fluctuations** [Tob99, YDFS98, Art93, NOY98, TD99]. **Fluid** [CSP98, DD98a, DD98b, Cha92, DD95]. **fluids** [GG84, Cal90f]. **Fluorescence** [GSM$^+$92]. **fluorescences** [GS90b]. **Fluoride** [BPL94, FLF96, GBS93b, Pan93, VZ92]. **Fluorides** [BPL97b, KJ93]. **fluorinated** [DO90]. **Fluorination** [KEMM93, CL90]. **Fluorochloroethanes** [CV99]. **Fluoroethylidenes** [KW92]. **fluoroketene** [FF96]. **fluoroketene-imine** [FF96]. **Fluoronium** [GBS$^+$93a]. **Fluorophores** [CDD$^+$99]. **fluoropropane** [RK92]. **fluorotoluene** [JDJP99]. **Fluorouracil** [MRT97]. **Flux** [LMR94]. **Flux-Flux** [LMR94]. **fluxes** [LA97]. **FNO** [CWX93]. **Fock** [CC97a, Ish90, AOH96, AA92, BBTU97, BDNT97, BP93d, BGS97, BJLK98, CD92, CZ94a, CMA93, Cha97, CH94, CMA$^+$99, Cul91, CGMG92, Dat95, Day96, DN96, DDD93, DHPC95, DPP$^+$94, DRBE96, FSBS$^+$95, FGS92, GR96a, GJPF92, GL98, Gre94, HGC93, Hol98, HS92d, HGL99, HK95b, IK94, IY99, KLO$^+$98, KWT95, KKWT99, KS90, KC97, Kry95, Kun90, KL92b, LV98, LBL98, LLB99, MYN$^+$96, MS91, MKRW99, MSRSP93, MR99, MW90a, MC91a, MC91b, Moh92, MSS99b, NNMH96, NM96, NU95, NL96b, OS90, PA92, PDT97, PDO92, PAAM98, Pra97, PZ91, RHC96, Scu95, SB92a, SGGMGFS96, SAL$^+$94, Sta97, Sta98b, Sta98a, Sta98e, SZ97b, SO97, SPL97, TTM99, TKO$^+$92, TTOY93, VA90, VIK98, VZ93, WB94, YITY93, ZC95].

Fock-CI [DN96]. **Fockian** [Gin98]. **Fold** [HL93b, PM95, SM96b, She90d]. **folded** [GSM+92]. **Folding** [Luo95, Art94b, KM99a, RK99, Urr94]. **Forbidden** [Pon97, OS90]. **Force** [FGRS98, HM97c, JDJP99, Kry95, MS98, Mez94a, MLT+96, SB97b, SS92c, VdV96, WHF92, YXX99, ACC92, Hua92, KS95a, KKL90, Sem96b, Sta91, Tac94]. **Forced** [RJ97]. **Forces** [LAS+95, Mar97a, Mez97b, Pie93, JMP99, LM93, Mon94, Sco90, VCCM92]. **Forecast** [NTL96]. **Foreword** [Ave96, CP96]. **Form** [BDNT97, FDD+93, GP95, Gin99, PIG94, PLV92, ČPV90, FL95, GC91, MZ91, McW99, NM91, Sch94]. **formacetal** [BV93]. **Formal** [GJOV97, LZ96]. **Formaldehyde** [MB98, CCS98, GH96b, KL92b, STKK92, TFYY91]. **Formalism** [BD94a, BD94b, FBKD97a, MR99, NOYY94, Sah95a, Sah95b, Sur95, BD95a, FL91, KS90, LP93, Sch90, Pet92]. **Formalisms** [PTP95]. **Formamide** [AL95, BTTS97, OMTS97, SS92c, TT98, WFS93, WFS93]. **formamidine** [AKCS91, NOY98]. **format** [She91]. **Formation** [HPSC97, NK98, RC97, SBZ92a, YAD92, ZGPS97, CPN91, NMSJ99]. **formed** [Bar90]. **Formhydroxamic** [YW92]. **Formhydroximic** [YW92]. **Forming** [NFVM94, CR96b]. **Formosinho** [Ano93h]. **Forms** [AC97, MD92c, PA99, SE92]. **Formula** [DW97, MMP+94, Nag95a, PZW93, BP92a, FGM90, HC96a, HK97]. **formulae** [For92b]. **Formulas** [AM98b, KP97, Lai94, Mor96a, Pal97a, Roś96, Sza95, BG98d, GL95, Hos97, MGLBP95, Sin92]. **Formulation** [BD94b, CPA95, För92a, GR94, GR95b, GR96b, GSM98, JKRW98, KNN96a, KLM91, KL92a, Pri95, Tac96, TC98a, The98, CT95, Cam92, Geg91a, GLM91, MP91, Sut99a, Yor95, ZC99, OS90]. **formulations** [DBLV94, TCM99]. **Formyloxyl** [KVS98]. **Förner** [Brä96c]. **Forward** [LDP93]. **Foundation** [LZ94, HW87a]. **Foundations** [Emc97, CC92a, GZ97, GZ06]. **Four** [CN99, Cai93, GBL97, PPP97, VDD96, Jon92b, LU92a, MS92]. **Four-Body** [CN99, PPP97]. **four-center** [Jon92b, MS92]. **Four-Membered** [GBL97]. **Fourier** [RW98, ABLA97, CM99, CJH98, DB94b, FD93, FFD96, FFD98, HS92e, Pah98, Rod91, SB98, TZ97b]. **Fourth** [Ano91g, Bir94, DM96]. **Fourth-Order** [DM96]. **FPLMTO** [MGNK95]. **Fr** [ERC91]. **Fractal** [LL97, PV94, SLtM+94]. **Fractals** [AR96]. **fraction** [MM91]. **Fractional** [BK94a, BKM93, GW91, HLJ96]. **Fractionally** [Nag95a, PCC93]. **Fragment** [RWT92, FNSV99, MZ91, NSTFC94, NSS92, PA92, RWT91, RK92]. **Fragment-Based** [RWT92, RWT91]. **Fragmentation** [PPSK96, PPK97, Man95a, Man95b, MG93a]. **Fragments** [BC96a, BLBP97, JTZ+96, SC98b]. **Frames** [Nal97]. **Framework** [DDG93, KEG+97, Lad97a, MPJ97, SB98, MRT95, MSF91]. **Frameworks** [LV98]. **France** [CD81]. **Franck** [AD97, LKMCVT95, LKMCVT96, PRSDS92, PSM94, Pal97a, PLS99, RSCP92]. **Frank** [Jør92, Str92]. **Free** [BO93, CM96b, Gre94, HRRBL97, KVS98, Mar94b, MNT96, MHÅ98, MPOG99, OMTS97, Ter97, WWM+98, BW90, CTC95, FJR96, HVS98, Mar90, Mat96, MV91, MVHV96, OYNY98, TNS92, VM92, YNO92, FGRS98]. **free-base** [YNO92]. **Free-Energy** [CM96b]. **Free-Radical** [Gre94].

Freedom [NP96b]. **Freeman** [Jør92]. **Freeon** [Cam92, MC97a, MC97b, Mat99]. **Frequencies** [AML+95, BP93c, GL97, Hea97, HZ94, JAG95, Jur97c, KLC98a, STMR97, BP93b, FB90, FR93a, Kal90, MHL94, MSS99b, NL96b, PSAUS90, TBP99, Zha92b, Pro95]. **Frequency** [ASI94a, Bau97, BP96b, Far97, JR96, KSY97, Lef99, LG95b, Mor96b, PLA98, SB95a, SB97a, CT95, CPA98, Fan90, RH92]. **Frequency-Dependent** [ASI94a, JR96, KSY97, LG95b, Mor96b, CT95, RH92]. **Frictional** [NYY96]. **Friedel** [DMB97]. **Friedrichs** [RG96]. **Friend** [Par94a]. **Frohlich** [TMM97, MVL98]. **frontier** [MCA92, RD90, SCA93]. **Frontiers** [Yur95, Yur95, Kar96]. **Frost** [Zho94]. **Frozen** [Fer96, LY98, SZ96, RK92]. **Frozen-Core** [Fer96, SZ96]. **FSGO** [KR91]. **Fukui** [KN92, NM95, Nal97]. **Fukutome** [WT98]. **Full** [BEG94, DREW98, DQB97, SR96, TMSI98, WKP+95, ANB94, BE93, GR95a, Nag96, Nes94, SS92d, PR97]. **Full-CI** [PR97]. **Full-Electron** [SR96]. **Full-Potential** [DREW98, Nes94]. **Fullerene** [Kup98, LSC98, LEA+94, Sur97, AS99, HRRBL97, LSS96, LCS98, SZCO99]. **fullerene-related** [LSS96]. **Fullerenes** [BT95, HT97, LT99, TH97, TL98, TLC98]. **fullerides** [BSS+97b, MCCF95]. **Fullerites** [Sta98c]. **Fully** [CTG97, FSVZ97, FADC91, PP91, TTM99]. **Function** [AC97, AB97, AYDR96, BSB94, BBC+96b, BK94b, BGS98, CZ94b, DLV95, Fer96, Fue98, GVC96, GBS+93a, Har97b, Har98b, KZ99, KN92, Kry95, LMR94, LDP93, LTP96, NP96a, NM95, Nal97, NS93a, PO97, PMN+92, SD96a, SB96, SN98, BE93, Boe96, BC93, CT95, CC91a, CB96a, DDA92, DHDP92, DWM90, FG99, FKK99, GC91, HS92d, Jak93, JDB99, Jon92a, JJ96, Lip91a, Lip91b, MM91, Mez90, MD93b, MIW91, Mur90, NOYF92, NS92, PSO90, PTM92, Pri98, RLR90, SNNY99, Sir99, Sme92, TWK98, Urr94, WN90]. **Functional** [AMRT94, ART94a, AL95, ASP97, ABR95, ASI94b, BDG96, BIM97, Bér97, BCRL94, BG98a, Bra97b, BS94, CM96b, CdBKZ99, CG97a, CJA94, Cha98, CB94a, CGLP96, CSP98, Cio94, Coh97, CPA95, CGR+94, CA97, Dau94, DPP+94, DZ94, DD98b, DZ96a, Dob98, Dun96a, Dun97, Eng95, EMMS94, EMMS97, FP94, FT97b, FWC+93, Fue94, GMS97, GR94, GG97a, Gho94, GD94, GSD97, GD96, Gör98, GPD94, GG97b, Gre94, GWCT97, GLBM96, HMGP93, Hag97, HHKM95, HM95, HBH98, JBT+95, Jou97, JZ95a, JZ95b, JM96c, Jur96a, Jur96b, Jur97a, Jur97b, Jur97c, Jur97e, Jur97d, Jur97f, Jur97g, Jur98a, KD98, KS94b, KVS98, Koh95, KH96b, KL97c, LLC+94, Lev97, LLZ98, LKLBD98, LBLKC98, Lu99, LLBM+95, LAS+95, Mar95b, MK97a, Mar98a, MRT97, MO98, MFP96, MFAT98, MDJ98, MSCP92, Nag94]. **Functional** [Nag98a, NV97b, OHSF97, PCE95, PP98a, Per98, PB96, PEBS97, PGS97, PSCZ97, PAAM98, PS94b, PSS97, RL95, RB95, RHC96, RPB+97, RP98a, RSD97, RRS97, SPH98, SPOAS97, San97, SSO+97, SD97, Sch95a, SZL95, SZ96, SZ97a, Scu95, SCP93, STY+98, STMR97, SFM94, SAL+94, SG97, ŠH96, SDG97, SATP94, Suk94, Suk95, TKNI96, Tac96,

TC98a, TG95, The97, TŚPKM94, TB95, Wło95, WR96, YNY99, ZC95, Ali99, AC95, ABSW95, Ano92l, AH92a, BAR94, BOA95, BMDM90, BDK90, BAL95, BDPS97, BS92, BYE+97, BPVP92, CCS98, CZ94a, CB93b, Cha92, CLGW95, CP99b, CH94, CMA+99, CA91, CEM+96, Csa90a, Csa90b, CK91, Cze99, DI95, DA91, DDC97, DM92, EDH+92, FEE+98, GWB97, GJPF92, GNF90, GK91, GW91, HCRR94, HMG+92, Har94]. **functional** [HK95a, HLJ96, Iva96, Iva97, JWG95, JH90, Jur99d, Jur99c, KK99a, KSSG95, KMP+90, KWZ98, KC97, KL90, KLM91, KL92a, KK92b, KPB99, LBL98, MG97, MM99a, Mar95a, Mar99a, MVS97, MECE97, MSMR99, MLL99, MRT95, MRST95, MR97, Min90b, MSF91, MCA95b, MNC95, Nal95b, OGK90, PWL95, PY89, PMDM97, PZDM97, PMDM98, PZDM98, PP90, PG96, PA99, RVP92, Rey95, RDY95, SH90a, SCP91, SP92b, SP95, Sem96a, SPM+96, SNNY99, SSC92, SCS94, SS91, SG96b, Spr93, SC99, SNH99, TNSM99, Tet93, TP90, The94, TC98c, TGDS97, Tri96, Van96, VVO98, WW97, WI98, WGP99, WMZ98, Yor95, YNNR97, ZC96, ZTC97, ZY94, Zie96, ZPBC97, Cal93]. **Functional-Based** [JBT+95]. **functional-group** [MM99a]. **Functionals** [ABR95, ADM98, FS93a, FS94, FS95b, GR96a, GBRA94, LP94, LBKLC98, MPJ97, MPJ98, PV98, RRS97, SMPJ94, SDW+98, SKN95a, SKN95b, SF95a, Val94, VB94, Cal90a, CLGW95, CES87, Csa90a, Csa91, Csa92, Fer91, GRBA92, GRB+93, GSKC99, KCLI95, MSMR99, OYL91, Per93, PG95, PRVS95, Sem94]. **Functions** [AL98, And94, AM98b, BDT96, BR94, CM96a, CWZ98a, CC98, CJH98, CPTR96, CTG97, DTS97, DKWM97, DKM97, FK94, Fer95, FFD98, Flo97a, FS93b, FS97, GM94, GT93, Gra97a, Gui98, GOAY98, HS91, HS92f, HS92e, Hoo94, IP93, KSG93, Kin96, KKJ94, Kut94, LB98, LDP93, Maz98, Mic96b, MCM98, Moi97, MV99, Núñ95a, Núñ95b, Núñ97, Oht98, OK96, PVLG93, Pen93, Pen96, RH95a, RH96a, RP96, Ryc94, SPH98, TKMA92, TM93, US97, US96, Wil96, AS93, AH92b, AA92, BBS91, BS91a, BCC99, BBMM99, BRV90, BGS97, Ced90, CÅ92a, CM99, DBLV94, DKM96, DBF+92, DW90, DS92, Flo97b, FS09, FM92b, Geg91b, GL99, GJP91, Har90, Hos97, HYS91, ITK91, JL91, JEB92, KE90, KFK91, KKWT99, KT95, KRZ91, KA95b]. **functions** [LP97d, LV97, LDJH92, LDHJ92, MT90b, MVHV96, MD99, MR92a, MPSLB91, MYPL90, MP91, NE95, Par92b, PDO92, PK92b, RC92a, Res99, SG90, SKRK90, SH90b, VA90, Wil99b, YKN+99, YG90, ZP92a, ZA95]. **fundamental** [AH92a, Cha96, Del90, Gre98, MM93]. **Fundamentals** [BCD95, Löw95e, HW84, HW87b, Cal90f]. **funnel** [MTTS93]. **Furan** [LX95, MKK98]. **Furfuryl** [MH98, Tew92]. **Furfuryl-** [MH98]. **Further** [CK91]. **Fused** [EMMK94]. **fusion** [SJ91]. **fuzzy** [MM99a]. **fuzzy-set** [MM99a].

G

[Ano90z, Ano92j, Ano93h, Ano94-37, Ano99d, Brä96b, Cal90f, Cal93, Deu98b, Lun91, Wha96, DDC97, Ano94i, CD93, CPGC99, FMS+99, FL95, HBJ+92]. **G*** [Les92]. **G1** [Jur97a]. **G2** [Jur97a]. **GA**

[SST94, BC97b, Bau98, DKM97, HBJ+92, MMRSN92, PCF94, SPFL93].
GaAs
[BP96c, CFDS90, FS95a, LMAK93, Por98, SMM+90, SPFL93, SBL+94].
GABA [MG90]. **GABAB** [LBBE98]. **Gadolinium** [SD97]. **galactose** [RC99]. **Gamma** [LDP93]. **Gap**
[Ott94, TDK+94, GSKC99, KPM+90, NNH98, SBZ92a]. **gaps** [BRS96].
Garrod [Mic96a]. **Gas** [BMP93, BZQ95, ET99, FY95, GD96, HPSC97, KO95, MLR+98, Oku98, PP98a, SM98, VBUS99, WG95, ZL98, Csa94, DDN99, Eng92, FSW+91, GL96, GSKC99, Lei99, TCS+90]. **Gas-Phase** [BMP93, BZQ95, ET99, Oku98, VBUS99, DDN99]. **Gas-Surface** [KO95].
Gases [NTL96, KSK+99, MAK+91, MK90]. **Gauche**
[DZ96b, FF96, WBH90]. **Gauge** [FCVL98, Lef97, KKNY99, SS92g, Woo99].
gauge-invariant [KKNY99]. **Gauges** [LA97]. **Gauss** [JS91, Mor96a].
Gaussian [AM98b, BNLF96, BC97b, Boe96, BJA99, BB97b, BS92, ČHM95a, ČHM95b, ČHMA95, CM99, DTS97, FFD98, FR98, FS93b, FM92b, GM93, GJP91, GKKA97, HBJ+92, HH97, Hil98, Ish96, JL91, JBS97, JM99, JZ95a, JZ95b, Jur96a, Jur97c, Jur98b, Kin96, KH95, KA95b, KL97a, Kut94, Le 97, MSD95, MRT95, MR97, MS92, MS93b, MTL97, PG94, PDT97, REU+91, SP92b, SSC92, TH90, TKSH93, US97, WBP91, Wil96, Wil99a, ZA95].
Gaussian-2 [Jur98b, SP92b]. **Gaussian-based** [SSC92].
Gaussian-Orbital-Type [Jur96a]. **Gaussian-Type**
[AM98b, Ish96, JZ95a, Jur97c, KL97a, BJA99, FM92b, HBJ+92].
Gaussian-Type-Orbital [JZ95b]. **Gaussians** [ITK91, KP97, PK96, SF95b].
GC [RP98a]. **GCA** [BKLV94]. **GCOSMO** [TNS96]. **Gd** [Li93, KLT97].
GdNbO [DDN95]. **Ge** [BL99, MECE97, STMR97, BML98]. **GeCH**
[BML98]. **GeH** [MRST95]. **Gelfand** [BG98b]. **Gell** [MHN98]. **Gell-Mann** [MHN98]. **Geminal** [Hil98, JBS97, PB95c, SP94, Røe90, Røe91]. **Geminals** [GKKA97, Sur94, LDJH92, LDHJ92]. **geminate** [LM91]. **General**
[AM97, BA97b, CC95, Cha98, FBKD97a, IP93, Lad97a, LF99, Löw93c, McD97, Muk96, Núñ95b, SC97, Sza95, OS95, PS92c, ST91, BG98d, FKK99, Geg91a].
Generalization
[MPP+97, Pen96, Val94, Csa90b, CK91, She90b, TR91, HVS98, MVHV96].
Generalized [ANB96, AH97, AT93, BPE97, CLZ99, Cul95, Day95, Day96, FR98, Gra97a, KMP94, KMP97, LDGA96, MS97a, MS97b, MPOG99, MMD96, MTL97, MT96, NOYY94, PP98a, RG94, RG96, She90a, TC98a, TM99, TNS96, ZC95, Ave00, GLM91, JK92b, KC93, KT95, KS90, KLI92, LH90, Mar99a, PK92b, VV91, Yor95]. **Generalized-Gradient** [PP98a].
Generalized-Overlap [Day95]. **generalized-valence-bond** [KT95].
Generalizing [Kat93]. **Generated** [RP96]. **Generation**
[BNLF96, CV98, LBLKC98, Mik94, SLtM+94, Har99, TC98c]. **Generator** [PDT97, BG98c]. **generators** [BG98b, BG98c, BG98d, Tit92]. **genesis** [Par90b]. **genotoxicity** [BTKVG99]. **Geometric**
[SL98, EZ93, KSN93, Nal92d, MM93, VX99]. **Geometric-phase** [VX99].
Geometrical

[AKS+90, BPL94, GMR+93, RHC96, Zap95, Art96, BBS91, BR92]. **Geometrically** [KN99b, NK98, KN99a]. **Geometries** [AR93, AMKS93, Jur97c, RGHH94, STMR97, LS93b, MHL94, PSAUS90, SCP91, Zha92b]. **Geometry** [GL97, Min90b, MAI97, MT96, TJ95, VFHL93, ZM97, Bro96, CTC95, FMD+94, HSWS95, Kal90, KMR92, METHH94, SE92, Sch92b, SG90, WD91, XKB+99]. **George** [Ano99d, Deu98b]. **German** [Brä95, HW87a]. **Germanium** [NN94, VBD+98]. **Germany** [Brä95]. **germination** [HB94]. **Gerratt** [Ano99f, Ano99p, WRC99]. **GeSiH** [BML98]. **Get** [PZW93]. **GGAs** [KPB99]. **Giant** [KLT97, Nes94, RG99]. **Ginzburg** [Aon98]. **glass** [Tet93]. **GLF** [BD94a, BD94b, BD95a]. **Global** [Löw97b, BA90, LM92]. **globular** [Kid99]. **Glutathione** [VC92, BMVV93]. **Gly** [GJLA99, LU92b]. **Gly/NMDA** [GJLA99]. **Glycine** [MTD93, Ram90, RC92a]. **glycol** [Cab96]. **glycolic** [FR92]. **glycylcarbonyl** [Tew94, Tew97]. **Glyoxalase** [VC92]. **glyoxylic** [BS91c]. **Go** [BPE97]. **gold** [Boč96, HCRR94]. **Golden** [Lef99]. **Goldstone** [PR97]. **Goldstone-Type** [PR97]. **Good** [Roś96, KTCN93]. **Goodman** [Ano99c, Ano99g, Ano99h, Ano99o, Ano99n, Kas99]. **Gordon** [Mon93]. **Gradient** [BPE97, EMMS94, EMMS97, FGRS98, GR96a, GvLB96, HC96e, HM95, KS94a, KP97, Min94b, PP98a, PB96, RRS97, SV95, Tri97, ZC95, ASM91, BDPS97, CLGW95, IHG95, JH92, Per93, SS91, SS92e, ZPBC97]. **Gradient-Corrected** [EMMS97, PB96, RRS97, BDPS97, CLGW95, Per93]. **Gradient-Dependent** [Tri97]. **Gradient-Optimization** [FGRS98]. **Gradients** [NG95, SZL95, SE97, MHN98, Ort92, SBAD90, SE95b]. **Gradus** [And93b]. **grafted** [Art96]. **Graph** [JM96b, KP90, LL94b, MD93c, PM95, PMM97, PV99, SYZ96, ZLHZ94, Ano92k, DM97a, Hal93, LTY90, Mon93, Rom92, She90b, She90c]. **Graph-Theoretic** [PMM97]. **graph-theoretical** [Rom92]. **Graphical** [KSS92, KŽ90, RP96, SAR96, SGK99, RTS91, She90a]. **graphite** [BLC95, LaF90]. **Graphs** [Gin96b, GLLY94, LNT99, SM96b, SBM97, BKM90, BBLK94, LLSY92, She90a, She90c, She90d]. **Gray** [Cal90f]. **Great** [Kra96]. **Green** [Ced90, DDA92, DHDP92, EP98, FL91, HS92d, MM91, MD93b, NS92, NS93a, SNNY99]. **Green-matrix** [FL91]. **Greenstein** [Deu98b]. **Grid** [ADB96, ČHM95a, ČHM95b, ČHMA95, SB98, DB94b, New97]. **Grids** [GPD94]. **Griffin** [CGMG92]. **GROMOS** [FVN98]. **GROMOS-MD** [FVN98]. **groove** [HGP91]. **groove-binding** [HGP91]. **Ground** [BEG94, BLB95, BK94b, Bra97a, CLSI94, CAJ95, DTA+96, DD97a, DLV95, DMB97, FSBS+95, Fri93b, GFRR94, KA95a, Mar98b, MW90a, NS93b, NOS94, PCC93, RR95, RS94, SE95a, Sch98, SIM93a, SGGMGFS96, SGB98, STM96b, SNH99, TBČP95, Ced94, CEZ+99, DDC97, EJ93, KSW98, LS93b, MUL99, MG97, MHM95a, MLL99, MB93, NM91, New97, Ort91, Ort93, PFK99, PZ91, RVP92, RK92, SE93a, SM92a, SW95, SSM90, Tri98c, UJS90, WI96, WW97, ZA95]. **Ground-State** [Bra97a, DLV95, FSBS+95, GFRR94, Mar98b, NS93b, SIM93a, TBČP95, MW90a, NOS94, RR95, STM96b, SNH99,

CEZ+99, DDC97, MUL99, MG97, Ort93, PFK99, RK92, SM92a, WW97]. **grounds** [SC96, TM99]. **Group** [BMP93, CL95, Fer95, Fer96, FBKD97a, FBKD97b, FBKD97c, Flo97a, GPč94, GKS99, JPJ95, KSG93, KP93, Kat93, Kat97, Kat98b, KN92, LV93, MFAT98, PZW93, RP96, SAR96, SB96, SSMK93, WFK97, YPC97, Zer99b, BCLS94, BRV90, Cam92, Dia99, FC99, Flo97b, HGL99, KSSG95, Kat91, Kat98a, KSS92, KP92, KS92, KM90b, KH97, LP98, MM99a, PK92a, Pau95, RAM91, Sta91, TP94, ZP92a, ZYZ90, FC99, Kum93b]. **Group-Adapted** [Flo97a, Flo97b]. **Group-Function** [SB96]. **Groups** [Gin97, LJ95, Mey94, Mey97, ŠH96, WZ94, ZYY95, DM92, Ell92, FCMB99, LBBK91, Les92, PC99, RWT91]. **Grown** [SLtM+94]. **Growth** [GŁ94, Mil97]. **Grundlagen** [HW87a]. **GT** [SST94]. **GTF** [TTM99]. **GTO** [BGS97, Dat95, VCCM92]. **GTOs** [SAW97]. **guanidinium** [MG97]. **Guanine** [FW92b, FW92c, GL97, MKM93b, BHV96, FL95, SM92a, TG96]. **guanine-cytosine** [BHV96, TG96]. **Gubbins** [Cal90f]. **guide** [Qui02]. **Guidelines** [Ano92o, Ano93i, Ano93j, Ano97d, Ano97e, Ano97f, Ano97g, Ano97h, Ano97i, Ano97j, Ano97k, Ano97l]. **gulf** [VRR92]. **GVB** [FG99, PČe90]. **GVB-RP** [FG99].

H [Ano92k, BML98, Brä95, Brä98b, Brä98c, BDH+97, Cal90a, CMF+98, CR96b, CB93b, CB94a, CF93, CXFP99, CEM+96, DZ97, Gao93, GPS90, IBS95, JKK+92, Jur97e, KP96, KJ95, KGv93, LCS98, MLL99, MW90b, MLK94, Mon93, Nag96, PZTPMC99, RG99, RA91, RCWN94, RNS93, RKG96, SDP+95, Ska92, SL97, SC98b, SC99, TJ97, WFS93, WI96, WMD95, ZBL99, GV93, ACHT95, Ata97a, ADM98, BA91, BZMR92, BDNT97, BBC+94, BP93c, BP93b, BP96b, BK94b, Brä93b, BYGA99, CAK+96, CLOFR98, CPBC95, CR96b, CDB90, CD93, CPD+98, Csa96, Cun92, DE92, DSS90, FCVL98, GJPZ97, HMG+92, Hag99a, HB95, HZ94, JMP99, JKJ94, JG95, JEB92, JM99, Jur97e, KS95a, KKWT99, Kor90, LJ95, LA97, LGT94, MCL95, MALT96, MTP+98, MHM95b, MK90, MTD93, MTTS93, MD91, NYKY98]. **H** [OSS95, Ort98b, PBS99, PPSK96, PPK97, RCWN94, RS97b, RNS93, Sch97, SP92b, Sem94, STC96, TMA97, TUK90, Úle92, UJS90, WYZ+92, WY99, WDS97, YD96, YSHD97, HP98]. **H-Bond** [Brä93b, CD93]. **H-Bonding** [CAK+96, DE92]. **H.-J** [Brä98c]. **Haken** [Brä95, Brä98b]. **Half** [BP93d, FSBS+95, MSS99b, OS90]. **Half-Projected** [FSBS+95, BP93d, MSS99b, OS90]. **halide** [NMCK92]. **halides** [BRS95]. **Hall** [Str92, Wha96, Ano99d, Gut99a, HLJ96, Sch99a, Sri97]. **Halogen** [Lu99, RL95]. **Halogen-** [RL95]. **Halogenated** [ET99, BMP92]. **Halogenobenzoic** [BKWL97]. **halogenofurans** [NVR+91]. **Halogens** [TV92]. **Hamilton** [Sch90]. **Hamiltonian** [AS96, Aon98, Bro95b, DB94b, EKI94, Ell91, Ell92, Gin96a, Jug90b, KBWJ96, KH95, KS90, Kru92, Löw90d, May98, Oku98, RPKM95, RABZ94, SB98, SZ97a, Sen96, SS99b, STM96a, STM96b, SJ97, SKS98, Tom91, VDBPR97a, VDBPR97b, ZM95].

Hamiltonian-crystal [SJ97]. **Hamiltonians** [BSS97a, CT96, CB99, CYY95, CL94, DP96, KDB90, MPKR94, PZWJC96, SB98, TS92, vvBS96]. **Hammond** [MBM92]. **Handbook** [Coo05, Atk91, Str93]. **Handed** [PFMC97]. **Hans** [Car96]. **Harbola** [SS92b]. **hard** [KSH92]. **hardbound** [Ano92l]. **Hardcover** [Brä95, Brä96c, Car96, Dun96b, Kar96, Mic96a]. **Hardness** [AK97, BKR97, DLG95, FSVZ97, GR94, GG97a, Gho94, GWCT97, KZ94, RR94, WG94, Pea95]. **hardnesses** [GW91]. **Harmonic** [MS98, MPOG99, Pal91, PV91, Pal93b, Pal97b, Pal98, SB95a, SB97a, SB97b, SF95b, STMR97, WBD97, DW90, JE90, Lev94, NL96b, PSAUS90, TC98c]. **harmonically** [OM91]. **Harmonics** [ABLA97, CV98, Jon94, Ave89, Ave00, Cal90b]. **Harris** [Jør92, LLC+94]. **Hartree** [CGMG92, Dat95, DN96, KC97, SB92a, YITY93, AOH96, AA92, BBTU97, BDNT97, BP93d, BGS97, BJLK98, CD92, CZ94a, CMA93, Cha97, CC97a, CH94, CMA+99, Cul91, DDD93, DHPC95, DPP+94, DRBE96, FSBS+95, FGS92, GR96a, GJPF92, GL98, Gre94, HGC93, Hol98, HS92d, HGL99, IK94, IY99, KLO+98, KWT95, KKWT99, KS90, Kry95, Kun90, KL92b, LV98, LBL98, LLB99, MYN+96, MS91, MKRW99, MR99, MW90a, MSS99b, NNMH96, NM96, NU95, NL96b, OS90, PA92, PBB94, PDT97, PDO92, PAAM98, Pra97, PZ91, RHC96, Scu95, SGGMGFS96, SAL+94, Sta97, Sta98b, Sta98a, Sta98e, SZ97b, SO97, SPL97, TTM99, TKO+92, TTOY93, VA90, VZ93, WB94, ZC95]. **Having** [Löw96c, Ols96]. **HBr** [TUK90]. **HCCCC** [CMF+98]. **HCCH** [MZ91]. **HCl** [BYGA99, CEM+96, BCS96, Del92, Jen94, JC90, WY99]. **HCN** [AOH96, Del92, Sch99a]. **HCO** [BLB95, DQB97]. **HCOOH** [PZTPMC99]. **hcp** [Boe95]. **HCSe** [LHL91]. **HCuCH** [CPN91]. **HD** [KA95a, Voj96]. **He-like** [BD95a]. **head** [GJDD97]. **head-to-tail** [GJDD97]. **heat** [NOY98, Pal93a, ZGPS97]. **heats** [BP90, YAD92]. **heavier** [BCLS94]. **Heavy** [GLMP98, KUN+98, RDK97, EMS92, JC90, KSSG95, RDK02, Tit96]. **heavy-light-heavy** [JC90]. **HeH** [BCMÖ97, EJ93, KA96, SEKEB98, TNSM99]. **HeI** [GZDZ97]. **Heiberger** [JK92b]. **Heidelberg** [Brä95, Brä96b, Brä96c, Dun96b]. **Heidrich** [Mat97]. **Heights** [ADPS98]. **Heisenberg** [BHX96, Bra97a, KBWJ96, KS92, MC97a, VBN95a, VBN95b]. **held** [Cal90d, CD81, JPP87]. **Helical** [AP93, Pal92b, VZ92]. **Helices** [PFMC97, ITT+94, TWK+92, Woo98]. **Helium** [CBT93a, DLV95, DD98a, DD98b, GD96, GS97a, LKFF98, LB95, PM93, PK96, RS94, WBD97, BGS99, BP92a, BP93b, Cha92, FDAC90, LKVS97, New97, PFK99, Whi99, ZW96a, vMVvLvD97]. **Helium-like** [CBT93a]. **Heliumlike** [KKT93, TN96, WD95, WD97, CBT93b]. **helix** [PBR96]. **Hellmann** [Kry95, Pop98, VCCM92]. **Help** [NV97b, SF94, Tos95, YNNR97]. **heme** [CL92, PLBB99]. **heme-protein-derived** [PLBB99]. **Hemeproteins** [ATP+96]. **Hemimercaptal** [VC92]. **Hemocyanin** [BBC+96a]. **Hemoglobin** [GSSD+96, BPVP92]. **Hendrik** [Jør92]. **heptane** [CAM+97, MMCC99]. **heptane-2.1** [CAM+97]. **Heritage** [Emc97]. **Hessian**

[AB97, KPA95]. **heteroanalogs** [EMMHP92]. **heteroaromatic** [DT96]. **heteroatom** [ŠG96a]. **Heterocumulenes** [MV98a]. **Heterocycle** [JSKC95]. **Heterocycles** [Roz97]. **heterocyclic** [METHH94]. **heterofullerene** [Eva97]. **Heterogeneous** [LL97, BH99, EZ92, Mar92b]. **Heteronuclear** [FWT+96, CKM91]. **Heterosiliranes** [LS96]. **Heterosubstituted** [HZ94]. **heuristic** [NOYF92]. **Hexagonal** [RAA94, BBRT94, VCMLL90]. **Hexamers** [Kry98]. **hexanuclear** [BUZ94]. **Hexatriene** [DC97, HRH99]. **hexyl** [XSA+92]. **HF** [Kar90, RCWN94, BFV94, CWJ+99, DSS90, Del92, FCVL98, FL95, Jen94, Les92, LCLO95, MR94, NG97, TB95, WY99, Bec97a, RCWN94]. **Hg** [MTL97]. **HgC** [BBTU97]. **HgO** [SBD+92]. **HH** [BD94a]. **HH-GLF** [BD94a]. **HI** [CM96a, KLO+98]. **Hierarchical** [KRB+97, Wil99b]. **Hierarchies** [Jak93]. **Hierarchy** [Sah95a]. **High** [ACHT95, BP96b, Che93, CSZ97, CC96, DMB97, ELMY96, Fri93a, Gin95, GBL97, HK95b, Jur97a, Jur99b, Jur99a, Jur99c, Ken93, Kup98, Lef99, LJN+98, MB97a, PLA98, RL98, RS97b, Sim99c, Sul97, TD96a, TWWC91, WS94b, WL99, AI99, Bar90, BSS97a, BB91, DBM99, KCP90, Mar94c, MS94, SGK99, SB92a, TC98c, WO92, Fri93b, Li93, JMS95]. **High-** [CSZ97]. **High-Energy** [Gin95, WS94b, ACHT95]. **High-Frequency** [Lef99, PLA98]. **High-Level** [GBL97, Jur97a, Jur99b, Jur99a, ELMY96]. **High-Order** [BP96b, LJN+98, SB92a, TC98c]. **High-resolution** [TWWC91, WO92]. **High-Spin** [Che93, TD96a, AI99, SGK99]. **High-Symmetry** [Kup98]. **High-T** [Fri93a, MS94, Fri93b, Li93, JMS95]. **High-Temperature** [WL99]. **High-Valent** [CC96]. **Higher** [CJM+91, Eid99, PNB94]. **Highly** [AEAO99, Brä98c, GH96a, PV98, BKS97, EZ93, SB90, Sla92]. **Hill** [CGMG92, Str92]. **Hinchliffe** [Cal90g]. **Hindered** [Fir94, HRRBL97, PHBB92]. **Hindrance** [TI94]. **Histamine** [MTP+98, TCS+90]. **histogram** [BRV99]. **Historical** [Löw95a]. **HIV** [BRA+99, Mav98, DZB92b]. **HIV-1** [BRA+99, Mav98, DZB92b]. **HLA** [NWG+99]. **HMO** [RPT90]. **HNBH** [MZ91]. **HNNH** [DZ97]. **HOCO** [DQB97]. **Hoffmann** [SS92g]. **Hole** [CH94, DHPC95, DP97, FT97b, KSKJ94, KM92, Xu96, FAV92, Xu99, YJL92]. **hole-mixing** [YJL92]. **Holes** [BKS96, WS95]. **Holland** [Cal90c]. **Homeomorphism** [KBA96]. **homogeneous** [Mar92b]. **Homologs** [KUN+98]. **Homology** [Bla99]. **Homonuclear** [Mar94d, MP93, Suz99, YDFS98]. **honor** [Mic92]. **Honvood** [Cal90d]. **HOOH** [SLL+91]. **Hooke** [BCL98, LCB98]. **Hopping** [DP93, jYL94, TIA+92]. **hormone** [Bla99]. **HSAB** [BTKVG99]. **HT** [PW97]. **Hubbard** [Ara94, BXZ95, BČ96b, Che93, ČB96b, DMB97, GPč94, Mat90, Oza92, TBČP95, Vin92, Yam90, YO92]. **Hückel** [DGMW90, Gra97b, Jur98b, Loh91, OKY+99, TBČP95]. **Hückel-based** [DGMW90]. **Human** [Fuk95, BPVP92, YSJ94]. **Hund** [Nor91, PKM93]. **Husimi** [HC93, MP91]. **HXC** [NL96a]. **HY** [NL96a]. **Hybrid** [BC96a, CCM+96, Cha98, ECBH96, GL96, GY95, Her97, Jur98a, Jur99d, MLT+96, FG96, GJPF92, Min90a, RK91, ZFZ92]. **Hybridization**

[KN99b, KMM95, MK99, MKM96, MKM97, MM98, KN99a, KKM99]. **Hybrids** [HR97, Lin97, RH95b]. **Hydrated** [BSHP97, MFP96, KRZ91, OSS95, PS92c]. **Hydration** [SD97, SSMK93, DKTZ94, MG90, PTM92, PHBB94, RWT91, TFT+91, TFYY91, TNS92, WBH90, WO92]. **hydrazine** [MSRP90]. **Hydride** [CAK+96, SFG+98, BK97, BFV+93, CPN91, FNSV99]. **Hydride-Transfer** [CAK+96]. **Hydrides** [BA97a, BMP93, DHL+94, DLG95, DZ96b, KJ93, PZ95]. **hydrido** [Gal98]. **Hydrocarbon** [Che93, EMMS94, KGv93, Sak98, KM90c, LE92, RG99, RA91]. **Hydrocarbons** [GRK96, HA93, HZ94, LFD94, ML97, Mon98, Mor97b, RL94, Ran97, SF96, AH92a, BTKVG99, DHDP92, Dia99, GX98, GH92, Gut99a, HGP+92, Luk92, MAC96, MBP91, PVN90, SPM+96, VRR92]. **hydrochloric** [TFR99]. **Hydrodynamics** [MKM93a]. **Hydrogen** [Aqu95, AK97, BA97b, BP96c, BCS96, CCB+97, CBSR+98, CDD+99, CMFA93, CAÖ96, CR93, CLKMTA95, DTS97, Del92, DC95, FF94a, FT95, FT96, FT97a, FWBT94, FLF96, GBS93b, Jur97a, Jur98b, KS94a, KS94b, KY93, KH97, Kry98, LKMC93, LJS94, MtPC+96, Mor96a, MTD96, MPJ98, Pan93, PLA98, PTC94, PB97b, RL95, RGT95, SM98, SSP98, SC94, SG98, SS92c, Suh94, SFGW96, TNM98, Taş97, TT98, VBV92, VBUS99, YNMT98, A.95, AGNS92, AZ99, BJMK92, CCC+95b, CMG92, CSH99, Cul91, DS93, DSW93, Fer92, Flo95, FDAC90, GT97, Jur99d, Kar90, KSH92, Mar97c, MKDL93, MMRSN92, MSS99b, NF92, NWT92, PZTPMC99, RFG99, Ram90, RC92a, Ram94, SY91, SLG+96, TKSH93, The94, TG96, VM92, VZ92, WG99, WBS99, WSTB90, ZW96a, LaF90]. **hydrogen-bond** [SY91]. **Hydrogen-Bonded** [AK97, BA97b, KS94a, KS94b, Kry98, VBV92, Cul91, Kar90, RFG99, VM92, WG99, WBS99]. **Hydrogen-Bonding** [FT95, FT96, FT97a, KH97]. **Hydrogen-like** [Taş97]. **Hydrogen-Substituted** [RL95]. **Hydrogen-Transfer** [BCS96]. **Hydrogen-Type** [DTS97]. **hydrogenase** [PBS99]. **hydrogenases** [DFGB99]. **Hydrogenated** [AST93, HU94, KI94]. **Hydrogenation** [SWMB94, SZ98]. **Hydrogenlike** [HFM91, MFH91]. **hydrogens** [SN90b]. **Hydrolases** [HBH98]. **Hydrolysis** [HBH98, PHBB92, STS95, TSS95, WJC+98, WP92]. **Hydrolytic** [PBHB95]. **Hydrophobic** [AV92, NK96a, PB97b, Urr94]. **Hydroxides** [BK94c]. **Hydroxo** [CdBKZ99]. **Hydroxo-** [CdBKZ99]. **Hydroxy** [MRT97]. **hydroxyketones** [FWZ97]. **Hydroxyl** [BHPB93]. **hydroxylamine** [MR92a]. **hydroxylation** [SRP+98]. **hydroxylations** [CD90]. **hydroxypentanoic** [Flo95]. **Hydroxypropanal** [OSA+97]. **Hydroxypropionic** [CFR96]. **Hydroxypyridine** [MTD93]. **Hydroxytetronic** [BKEMM94]. **Hydroxyurea** [LB96a]. **Hylleraas** [BKL98, FR98, HMLK98, KL93b, KBL95, LH90, PCO+94, US96]. **Hylleraas-CI** [BKL98, HMLK98, KBL95]. **Hyper** [JCA97]. **Hyperboloidal** [LKMC93]. **Hypercoordinate** [CCG+96]. **Hyperfine**

[Bec97a, EMMS94, Kar98, NG95, For94]. **Hypermodified** [Tew94, SSM+99, Tew97]. **Hyperpolarizabilities** [ASI94a, BP96b, Cha97, LL92, Mor93a, NYKY98, SAS99, Shu96, YNY99, AD92, BP93b, KMR92, Kur90, LKM99, LYSL95, MD92b, MPP92, Mun92, RH92]. **Hyperpolarizability** [JR96, KUN+98, Kan93, Mor96b, NONY97, SC98a, TSRP99, YNNY99, BP92a, CPA98, CP99a, DBF+92, LL99, NYKY98, NYNY99]. **hyperradius** [AGH91]. **Hyperspherical** [Ave89, AH92b, Ave00, BD94a, BD94b, CN99, DZF93, WBD97, Zha96, BZMR92, BD95a, NZ92, Cal90b]. **Hypersurface** [RRS97, AKCS91, TCS+90]. **hypersurfaces** [BML98]. **hypervalence** [JF92]. **Hypervalent** [Har96, DA91]. **hypervelocity** [WSM+94]. **Hypervirial** [LBMR95]. **hypothesis** [Jac92]. **HZSM** [MMCC99].

Iachello [Lin96a]. **IBM** [Mic96a]. **Ice** [TNM98, KY91b]. **Icons** [Alt92, Lin93]. **Icosahedral** [TH97, TLC98]. **Idazoxan** [HS92b]. **Idea** [Sut96]. **Ideal** [NV94a, NV94b, NV97a]. **idempotency** [MYPL90]. **Identical** [TDO97]. **identify** [Bla99, DRGC90]. **Identifying** [MPR97]. **Ih** [KY91b]. **II** [BB94, ELMY96, FWS97, MDS98, ROL+90, SBIP97b, SJ97, YDDP92, Str93, AFTM95b, Bec97a, BB95, BFW92, BG98c, CC92b, ČHM95b, CCWCF96, CPN91, CV99, ČB96b, CF99, DKWM97, FT96, FLLZ91, FBKD97b, FW92c, Fri93b, GK90b, GR95b, GR96b, Geg91b, GS90a, HBJ+92, HC96b, JKJ95, JM96a, JGR98, JDB99, KP93, KLC98a, KC97, KY91b, LCV92, LDGA96, LRM96, MC97b, MFH91, MKBP97, NS95b, NWG+99, NV94b, Pal93b, PZDM97, PZDM98, PACO90, PPK97, Pos91, RWT92, SOK+98, SNNY99, SR96, SGW+92, Sta95, TYTY91, VDBPR97b, VM92, YOTY93, ZWD98b]. **II-VI** [CF99]. **III** [BHL+99, BPL94, CdBKZ99, HBGR99, SBIP97b, AFO+97, BKM90, Bou96, BG98d, ČHMA95, CRK+91, CDB90, DP93, DKM97, FT97a, FBKD97c, GSSD+96, GC91, HC96c, JMR98, KC98b, LV93, LX95, Mat99, MVHV96, NE95, NV97a, SD97, SD98, Sta98d, Sur94]. **III-V** [SD98]. **Ill** [JK92b]. **Ill-conditioned** [JK92b]. **Illustration** [DC95]. **Image** [MV90]. **images** [DVL+91]. **Imaginary** [BP93c, BP96b, BP93b]. **Imaging** [SLD95, BCC99, HBGR99]. **imidazole** [SE92]. **Imidazolidines** [BP92b]. **imine** [FF96]. **Iminium** [LX95]. **Imino** [MH98]. **immobilized** [Kov98b]. **IMOMM** [MSM96]. **Impact** [JKRW98, JGR98, JMR98]. **impacts** [WSM+94]. **Impenetrable** [Aqu95, A.95]. **implantation** [NST94]. **Implementation** [FGRS98, KP97, PTP95, SWF93, SZL95, Ter97, CJM+91, EDH+92, FKHD97, ZYZ90, HC96b, ZWD98b]. **Implications** [DZB92a, HM95, JH92, Nal94, WDCA97, BDP+92, XSA+92]. **Implicit** [GSM98, KK92b]. **Imply** [MSP94, Ber96c]. **Importance** [HH92, Löw97b, TN96, Löw92g]. **Important** [MPR97, MKM96]. **Improved** [AR99b, GD94, HS91, HS92e, KH96b, MGLBP95, TR94, TKMA92, ZDO99, Zha96, CF93, Hua92, AR99a, YNNR97]. **Improvement** [JO94, HC96d]. **Improving** [LG95a, RSCP92, LH94]. **impulses** [TBW90]. **Impurities** [TIPM96, RD90]. **Impurity** [AMC97, DDN95, Wil90]. **in-plane** [LTSL96].

Incidence [RRC94]. **Include** [PSS97, DD90b]. **Including** [AL95, LAS+95, Mey94, Mey97, TAY+97, FKR92, GJPMML91, KKL90, KRZ91, Mar94c, Moh92, RH92, SCA93, Suh91]. **Inclusion** [Boč90, RL92, ČPV90, HWB97b, HWB97a, RWT92]. **Incomplete** [LDP93, KB92]. **Incorporating** [RPB+97]. **Increase** [KKT97]. **Increased** [Har96]. **Increased-Valence** [Har96]. **Indacene** [HHKM95]. **Indefinite** [Löw96c]. **independence** [Lev99]. **Independent** [KFS92, MS97a, MS97b, Mey94, Mey97, SB98]. **Index** [AV92, KPA95, GSPSM93, Kin93, Kin94, Luk92]. **Indexes** [TSS97]. **Indexing** [FJRS97]. **indicators** [BMP92]. **Indices** [MK98a, MK98b, Nal97, NMM97, SP94, TKNI96, GB90, HGP+92, NM94, NM96]. **Indigoid** [Che96]. **Indirect** [AO93, SD98, TMDB98]. **INDO** [DM95, FKR92, HZ99, JKK+92, KRZ91, KSIH92, PSBL98, RL92, SJ97]. **INDO/S** [HZ99, KRZ91]. **indol** [RTKP95]. **indol-3-ylacetic** [RTKP95]. **Indole** [FSHC99, RTKP96, RT99, RT98]. **indole-3-acetic** [RTKP96]. **Indoles** [WGP99]. **Induced** [BS93, Gui98, MB98, MLK94, MSS99a, RM99, Tew94, Ata94, Ata97a, CA90b, FSW+91, NMN+97, NMN+99, Pal93a, SPFL93, SSM+99, TBW90]. **Induction** [Pie93]. **industrial** [RVL97]. **Inelastic** [GYDY97, CF93]. **inequalities** [Csa93, Csa95]. **inequality** [TNSM99]. **Infinite** [CW97, Del96, FUI97, LKMC93, NV94a, NV94b, Suh94, Ale95, CA90a, CMA93, FS92, LKVS97, MFCA94, NV97a, Suh92, Suh93, TKO+92, TTOY93, YITY93]. **infinitely** [Dia99]. **inflammatory** [BD95b]. **Influence** [BKY99, BFV94, DWR99, GS94, JCÁ96, Lei99, MDD93, MKM97, PB97a, Tew97, BBS90, MT91, NGM+95, PACO90]. **Information** [NP96a, YAD95, Zie95, Ano90h, Ano94i, HSWS95, Rig92]. **Infrared** [GSSD+96, HJ94, MDD93, ZJS99, HS95, Lin91, TWWC91]. **Inhibition** [Mav98, RAM91]. **Inhibitor** [BBD97, RMH+99, SHB+96]. **Inhibitors** [KKS99, MBV+98, ARBB95]. **inhibitory** [HB94]. **Inhomogeneous** [HM97c, Fer92, HLJ96]. **initial** [GZDZ97, Hag96]. **Initiation** [Lad97a]. **Initio** [AKD96, AST93, BTTS97, BBC+96a, BLB95, BAK96a, BL92b, BCS96, BDH+97, Bue96, BDD93, CWX93, Cai94, CMF+98, CLSI94, CMFA93, CAÖ96, Cha97, CFR96, CPTR96, DS96, DRBE96, DZ97, EMMK94, FF94a, FF94b, FT95, FLRV97, FWC+93, GDID98, GBS+93a, GL97, GL98, GW98b, GP97, HP97, HHKM95, HBH98, Huz96, Jen94, JZ95a, JZ95b, JM96c, Jur96b, Jur97a, Jur97b, Jur97e, Jur97d, Jur97g, Jur98a, Jur98b, Jur99b, Jur99a, KUN+98, KKNN97, KL97a, Kry98, KG97, KG99, LV93, LJ95, LRM96, Löw99, LBG95, MSD95, MCE+93, MF96, MDD93, MS98, MRL99, MTD93, MSCS95, MR94, NNMH96, NBS95, OSA+97, OHSF97, Par97, PVLG93, Pen93, Pen96, PFMC97, RKN97, RM96, RML97, RKPE95, Ryd94, SE95a, Sak97, SKTN97, SNMB97, SPS96b, SG93, SLA97, SMO+96, SHC+98, ŠH96, Sta96a]. **Initio** [Sta97, Sta98a, TB95, VH96, YY96, Yam97, YD97, YK97, YW92, ZL98, Ågr90, ADB95, ACC92, ACB+99, AGAP98, AGM99, ANB94, AKCS91,

ABCM93, BL99, BMA90, BHL+99, BILA95, Bha99, Bla99, BB93, Bre99, BHV96, BMG95, BCY95, CLOFR98, CA92b, CMA93, CPA98, CRK+91, CKB91, CP99b, CEM+96, DFGB99, DV91, DLF99, DBF+92, DO90, ERC91, ELMY96, Eva97, FAV92, FF92, FT96, FF96, FT97a, FWS97, FFD96, FMD+96, FL91, FR92, FR93a, For94, Fra99, FADC91, GE92, GX98, HSES94, HGL99, ISOA99, IBS95, JMP99, Jur99c, KK99a, KPW+95, Kar90, KNN96b, KR93, KJL96, KH96a, Kir92, KKL90, KK93, Kor90, KYW95, KG98, KL92b, LCV92, Les91, Les92, LW92, LXWZ99, LBG97, MD92a, Man95a, Man95b, Man99, MKK96, MCOS94, MW92, McW99]. **initio** [MLL99, MR92a, Mil97, MFCA93, MFCA94, MRBM91, Nov92, NL96a, OTG91, OS92, PVČ+90, Pal94, PAF91, PTKS+92, Ram94, RTKP95, RTKP96, RD97, REU+91, REL+90, REKP92, RK91, RK92, RC99, SE92, SE93a, STKN90, SDP+95, SAB+97, SRP+98, SS90, SX96, SP91, SCP93, Sem94, SPM+96, SKE92, SG92, Ska92, SKRK90, SLL+91, SLG+96, Suh91, SPR94, TCB99, VR92, WFS93, WLB+94, WSB94, WL92, WKP+95, XSG97, XFF98, YNO92, YNO94, YD96, YSHD97, YAD92, ZGPS97, LHL91]. **innate** [Chu99]. **Inner** [BZQ95, BDH+97, JM96b, BCY95, ČVW91, ZBL99]. **Inner-Sphere** [BZQ95, BDH+97, BCY95, ZBL99]. **Inorganic** [KN92, Lun91, OCK99]. **Insecticide** [NAK95, KKS99]. **insertion** [RD97, SM96a, WY99]. **insight** [BADM97, VABM94]. **insights** [FMS+99, VR92, Woo98]. **inspired** [Rau02]. **Instability** [ATI97, CC97a, LN96, Sim93b, YOTY93, YO92, RNS93, TKO+92]. **Institute** [CD81, Yur95]. **Instructions** [Ano95f, Ano95g, Ano95h, Ano95i, Ano95j, Ano95k, Ano95l, Ano95m, Ano95n, Ano95o, Ano95p, Ano95q, Ano96h, Ano96i, Ano96j, Ano96k, Ano96l, Ano96m, Ano96n, Ano96o, Ano96p, Ano96q, Ano96r, Ano96s, Ano96t, Ano96u, Ano96v, Ano96w, Ano96x, Ano96y, Ano96z, Ano96-27, Ano96-28, Ano97a, Ano97b, Ano97c]. **insulating** [MS93a]. **Insulator** [Dun99, Kov98a, NMN+98, MCCF95, NMN+97]. **Integer** [Sri97]. **Integral** [AH92a, CBG94, Ish96, KNA94, KNN96a, KKNN97, Mar94a, NONY97, PTH+97, She91, Whi99, Zap95, BA91, JS91, Jon92a, KNN96b, Nag96, PLS99, Roc99]. **Integral-Geometrical** [Zap95]. **Integrals** [AM98b, BR94, BB97b, DW97, FS93b, GY95, GİA96, Gus98, GOAY98, HO94, HS91, HS92f, Jon94, Jon97, KZ99, Kin96, KBL95, LKBJ97, LDP93, LR94, MBA97, MS93b, PMN+92, SPH98, SBD+92, US97, US96, Bud92, BFW92, CM99, DD97b, FM92b, GP91a, GJP91, JE90, JEB92, Jon92b, Jon93, Kin99, LH90, LK93, MRC99, MT90b, MHS95, MS92, MGLBP95, MFCA93, Ort95, PCO+94, PW91, RLR90, REU+91, Smi99, SH90b, TNI96, ZZ93, ZFZ92, ZB92]. **Integrand** [FS94, FS95b]. **Integrated** [CDDV93, KM97, MSM96, MK97b, KKK90, KK91, MK95, MK96]. **Integration** [FS93a, IYFI99, Csa92, JO94, Roc99]. **integrations** [JE90]. **Intelligent** [JCM+92, PS92a]. **Intense** [BRZY97, CFB97, DlD99, DD98a, NY98, Cha92, DD95, Mar91, Mar92b]. **intensities** [KSF91, Lin91, MSS99b, OTG91]. **Intensity** [DMR96, GDID98, BBS90, MLK94, PC91, McH91]. **Inter** [Par92a]. **Inter-**

[Par92a]. **Interacting** [CBG94, GJOV97, MR99, GT97, Mar93b, Nak92, OM91, SMH92]. **Interaction** [Ågr91, BHL+99, BEG94, BP96c, BL98, CCB+97, CF96, DS96, DDG93, DFL98, DM94b, ESP98, EBG95, GRT96, HP98, Huz96, JKK+92, JTZ+96, KSR95, KKE+96, MALT96, MC97a, MR92b, NTL96, PS96, Pec93, PRC98, PFMC97, SWF93, SM96b, SF95a, Sch99b, Sur94, Sur95, TMDB98, VA90, Ada96a, Art94b, Bat92, BE93, BHV96, BLG95, CC91a, CPBC95, CCC+95b, CGG96, CLR+93, CDP+99, DI95, DS93, Duc90, EVSN92, FM92b, GVB96, HC91, ISOA99, Ish91, IHG95, KBKT93, KSS92, KRZ91, KK90, LB94, LLB99, MMRSN92, MMCC99, MLT98, MHG95, Men99, Moh92, NL96b, NI94, Pai91, Pet92, Pro94, Pro95, RTS91, SWD+99, SBPPH92, SEKEB98, SG90, SCS94, SBZ92d, SJR91, Tac92, TSY99, TYY91, TC98c, VÅJ+92, WP90, WMW92, YZX96, YDDP92, YJL92, Yu95, PTL90]. **Interactions** [BP93c, DE92, GBVM93, Gin97, KSN95, Kar98, LV93, LS93a, May98, NNMH96, OLC+96, SE93b, SD98, SGB97, ŠH96, SPL97, TWK+92, ZRNZ97, Ada90, Ada91b, AGM99, And90, BP93b, BH92, BMP92, CG97b, CMSF93, CPGC99, GPS90, GP91b, HVS98, HZ92, JMP99, KPTS+93, KPTVT+97, KY92, KH97, LaF90, Man95a, Man95b, Man99, MV91, May92, MVHV96, MK90, OB95, PWL95, PA92, RMH+99, SCC91, VR90, VM92]. **interactive** [Qui02]. **Interatomic** [RA96]. **Interband** [SMM+90]. **Interbasis** [KMP94, KMP97]. **Interbond** [Sur95]. **Intercalated** [Sta98c, MCA95a, VS95]. **intercalates** [BLC95]. **intercalators** [HGP91]. **interchain** [TIA+92]. **interchange** [She91]. **Interconversion** [TCB99]. **Interconversions** [BHPB95, HRH99, Sla92]. **intercorrelation** [HGP+92]. **interdisciplinary** [LF94]. **Interelectronic** [GR95b, GR96b, Lah92]. **Interface** [CCT98, Kov98a, Sjö96]. **interfaces** [WGP99]. **interference** [May92, Sil95]. **Interim** [Har97a]. **Interionic** [Mez94a]. **interlayer** [LaF90]. **Intermediate** [NMN+97, NMN+98, Pai97, PL98, SS99b, ACZ91, BZ92, BHGC99, CPN91, EZ92, FF96, Pai99, ZM95]. **Intermediates** [BP92b, EMMK94, HS95, HDB+95]. **intermetallic** [MECE97]. **Intermolecular** [Ada96a, Ada99, BH92, EE91, GBVM93, May98, McH91, Pie93, SPL97, TT98, VH96, VR90, Ada90, Ada91b, BMP92, HVS98, HZ92, JMP99, KBKT93, KY92, Löw90d, MV91, MVHV96, MR92a, MRBM91, Sco90, SJR91, VM92]. **Internal** [BW99, Che97, GWCT97, KC98a, KLC98a, KC98b, Nal92b, Pal97b, ZZCSE94, CLZ99, CTF92, GX98, GS90a, MJLL99, Sch92b, WFS93]. **internally** [SS92d]. **International** [Deu96, Kra96, Löw91c, Löw91d, Löw92a, Löw95f, MDS98, Str92, Ano91g, Lad94, Löw90c, Löw91a, Löw91b, Löw91e, Löw92b, Löw92c, Löw92d, Löw93a, Löw93b, Löw94b, Löw95c, Löw95d, Löw95b, Löw96a, Löw96b]. **Interpair** [JJ97]. **Interpolant** [BČ96b, ČB96b]. **Interpolation** [DQB97, CLZ99]. **Interpretation** [BDG96, Gin95, Gin97, Pec93, PEBS97, Cio93, Kat98a, SH90a, SBZ92b, Tom91]. **Interpretations** [ÅGL97]. **Interreactant** [Nal97]. **Intersecting** [BW97, Nal94]. **intershell** [DI95]. **Interstellar**

[AST93, PMM97]. **Interstitial** [EDF+98, LFD99]. **Intersystem** [KMVÅ95]. **Intra** [JJ97]. **Intra-** [JJ97]. **Intracules** [KKT93]. **Intramolecular** [ADPS98, CDD+99, Flo95, GSPSM93, GL98, HP97, Ram90, SSP98, CSH99, DS93, MKK96, NOYF92, Par92a, RC92a, Ram94, Sem96b]. **intrasupermolecular** [NOYF92]. **Intrinsic** [DZ94, MD93a, NSS+95, SX96]. **intrinsically** [AMH93]. **Introduction** [ASH91, AVV93, Ano91h, Ano91i, Ano91j, Ano92p, Ano97m, Ano98n, Ano98o, Ano99e, Brä93a, Brä95, Brä98b, Cal92, FR94, HWB05, Kas99, KWZ98, Loe92, Löw90a, LZ92, Löw92e, Löw92f, LZ94, Löw97a, MCA92, Mor98b, NOYY94, ÖSZ90a, ÖSZ90b, ÖSZ92, ÖSZ93, ÖSSZ93, ÖSZ94a, ÖSZ94b, ÖSZ95a, ÖSZ95b, ÖSZ96a, ÖSZ96b, ÖSZ97a, ÖSZ97b, ÖSZ99a, ÖSZ99b, ÖSZ99c, OAG99, RS97a, Smi96, Tri98a, UH95, HW84, HW87a, HW87b, HW92, HW94, HW96, HW00, HW04, Kum93b, Rat92, RS00, Kla93]. **Introductory** [Kys90, Ber96a]. **Invariance** [CAK+96, Jou97, JH92, Woo99]. **invariant** [KKNY99, OS95]. **Invariants** [BDT96]. **Inverse** [RL98, Aon99, Kin93]. **Inversion** [Sen96, ITK91, SP92b, WSB94]. **Inversion-Bending** [Sen96]. **inverted** [TMA97]. **Investigated** [KUN+98, ST93, Mar97c]. **Investigating** [KM92]. **Investigation** [BBS90, BČ95, Bra96a, Cha95, Cha97, CFR96, CS98, Csa90b, Csa96, DP93, EK94, EMMS97, JTZ+96, Jay92, JZ95a, JZ95b, KBKT93, KY92, Lah92, LLZ98, MCE+93, MV98a, MFP96, PKM93, PSCZ97, SWMB94, STS95, STMR97, YZX96, YK97, And93a, BBCL92, BB93, BS91c, BV93, CEM+96, CK91, DM97b, DFGB99, FLWZ90, FR92, GWB97, GJPF92, HSWS95, HB95, JMP99, KR93, KS94c, KE91, MG91, MFCA94, NGM+95, PTM92, Ram94, RBB+94, ŠG96a, TFR99, WBH90, WMZ98]. **Investigations** [BTN98, Bou94, KS94a, KVS98]. **Involved** [DTM96]. **Involving** [BF96, GH96a, LX95, Nic96, PVLG93, WR96, Bud92, BFW92, HBJ+92, MBG90, MK90]. **Iodides** [Sta97]. **Iodine** [DYD96, EMMS97, GZSvD99]. **Iodine-doped** [DYD96]. **Ion** [BCMÖ97, BD94a, CA91, DD98b, GBS+93a, HNB92, PBB92, Ryd94, SD97, Sch97, TKNI96, ABCM93, BLC95, BILA95, BJMK92, DMR96, DKTZ94, EC96, FMR91, Khu92, KRZ91, MG97, NST94, RMF90, TMR99]. **ion-atom** [DMR96]. **Ion-Helium** [DD98b]. **Ion-Molecule** [TKNI96]. **Ionic** [AMD+97, CBAM97, CLSI94, GD96, KSKJ94, KM92, BRS96, CLOFR98, CDB90, GPS90, KTK+90, Lun92, MAAP90, PBPN90, SP91, YNNR97]. **Ionization** [AR99b, BMP93, CDDM96, CGR+94, FLRV97, GW91, Jur97d, KCI98, LD95, MG93b, Moi97, Mor94, NKUS97, Par97, PAAM98, STMR97, Voj96, AR99a, CB96a, CFB97, DDA92, GL95, KSSG95, KTCN93, KCLI95, MHY98, MDM94, MSPS90, MBP91, SP92a, SPB90, SZ95]. **Ionization/Dissociation** [Moi97]. **Ionized** [IK97, NS97a, NS97b, ZRNZ97, NS91, SB90]. **ionizing** [CH91, WK90]. **ionone** [TCB99]. **Ions** [BF96, BPL94, CBT93a, GS94, GH96a, IK97, KKT93, KGv93, PAT93, RDK97, VIK98, AMH+92, BUZ94, BKS97, BMG95, CBT93b, CFB97, Dav90,

FAV92, Har94, II94, LRM93, LHL91, LBG97, Mar91, MLB92, MDM94, NM91, NMCK92, Par99, PZA92, RDK02, SC91, SBPPH92, YDDP92, Brä98c]. **IPGG** [LCP+91]. **Ir** [NG95, NG96, SC99, GL97, KL92b, KL97c, MS98, YXX99]. **Ira** [Str92]. **IRC** [FF94a]. **Iridium** [CBSR+98]. **Iron** [RP98a, UWB94, HE90, PBS99, RKH+98, SJ97]. **Iron-Porphyrin** [RP98a, RKH+98]. **Irreducible** [ZWZ96a, CXFP99, Ell91, Ell92, PC99]. **Irreversibility** [BA93, Brä93a, KEP93, Pri95, BR92]. **Irreversible** [Mav98]. **ISBN** [Ber96b, Brä95, Brä96b, Brä96c, Car96, Deu96, Dun96b, Kar96, Lin96a, Mic96a, Sjö96, Str93, Tri96]. **Ising** [CM96b, Mat96]. **Iso** [Mez94a]. **Iso-Energy** [Mez94a]. **isobutylbenzene** [LCV92]. **isochromenes** [RC92b]. **isocitrate** [GVK99]. **isocyanates** [TF92]. **Isocytosine** [KL97c, YXX99, ZL98]. **Isocytosine-Cytosine** [ZL98]. **Isoelectronic** [BKL97, BLK97, Bec97a, LBM94, RSD97, STC96, KD92, LMMK93, SC98b, TFSZ95, Yam90, YAD92, SS92b]. **Isomer** [DZ97, Har97a, HP98, Su93, MZ91]. **isomerase** [FNSV99]. **Isomeric** [BHPB95]. **isomerism** [KL94]. **Isomerization** [ART94a, Jur97f, Lei99, LAM92, MRB+96, NOY98, SP92b]. **Isomers** [AK97, MF96, Oli99, WG94, AS99, CSH99, JH90, KP96]. **Isopropylamine** [ZJS99]. **Isopycnic** [Cio90a]. **Isospectral** [TDO97]. **Isotherms** [NTL96]. **Isothiazolones** [MC95]. **Isotope** [Ata94, HMLK98, LE92]. **isotopic** [AS95, FV96, PVČ+90, TUK90]. **Isotopomers** [BCMÖ97, ZJS99, RN96]. **Isotropic** [TZ97a, DOPS91, For94, MK90]. **ISQBP** [Ano92q]. **Israel** [JPP87]. **Issue** [MDS98]. **Issues** [PK94]. **Iteration** [AA92, DDD93, DC95, KG92]. **Iteration-Variation** [DC95]. **Iterative** [MS97a, MS97b]. **IUPAC** [Kra96]. **IV** [AFTM98, Boč90, BB97a, Cio93, DM96, FDC92, Flo97a, Flo97b, HVS98, HC96d, KLC98b, KLM91, LLSY92, Ney95a, Pal97b, Pau92, RML97, Sur95, SB92b, TGS99]. **IVA** [CL95]. **IVA-Group** [CL95]. **IVB** [CL95]. **ix** [Cal93, Mun92].

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[NS95a, Ney95a, Ney95b]. **Justin** [Kum93a].

K-region [KL93a]. **Kajzar** [Eri92]. **Kaku** [Kla93]. **KALA** [NAK95]. **kapton** [Por97, Por99]. **Kármán** [CW97]. **Karo** [Mic92]. **Kasha** [Ano91f, Ano91y]. **Kato** [Csa90b, CK91]. **kbar** [SCP95]. **KCl** [CBAM97]. **Keeping** [Hed95]. **Keggin** [CJX+92]. **Kekulé** [GH92, Hal91]. **Kemer** [Yur95]. **Kepler** [DJ12, DJ95, KC93, KMP94]. **Kernel** [Gör98, HMK96, MHK95]. **Ketene** [FF94b, Fir94, FF92, STKK92]. **ketoenolyl** [For94]. **Ketoesters** [SWMB94]. **Ketone** [SC94]. **ketones** [TKK+90]. **Key** [GDID98, Löw91e]. **kinds** [LDJH92, LDHJ92]. **Kinematic** [MIW91]. **Kinetic** [AS99, AM98a, Csa96, GR96a, GBRA94, GX95, HM95, KT96, LKLBD98, LBKLC98, MK97a, QS98, SS97b, VAVN91, Zho93, Bec94, Csa90a, Csa91, Csa92, GRBA92, GRB+93, MS91, Moc99, MC91a, MC91b, MYPL90, OYL91, WW97, BFW92]. **Kinetic-** [LBKLC98, Csa91]. **kinetic-energy** [Bec94, Csa90a, Csa92, GRBA92]. **Kinetics** [Gre94, OB95, FWZ97, Mon93]. **KKR** [WTS97]. **KLI** [KLLI97]. **Kluge** [Brä98c]. **Kluwer** [Ano92l, Ano93h, Ber96b, Cal90e, Cal90b, Eri92, Kar93, Kar96, Lun91, Lun92]. **knots** [DM98]. **Kohn** [Fau92, Bec97b, BKL91, CZ94a, Egu96, GR94, GvLB96, GVB97, Hag97, HS93, KLI92, KCLI95, KLLI97, NMM97, Nal98, PGH95, PS94b, QS98, Roc99, Sah95a, SS99a, SS97b, Ter97, The98, TŚPKM94, WT98, WW97]. **Koopmans** [Day96, Mor94, MDM94]. **Korringa** [Fau92]. **Kotani** [Ohn95]. **Kr** [BC97b, HBJ+92]. **Kramers** [Chr94, KLO+98, Sch93, VDL95]. **Kramers-restricted** [VDL95]. **Kratzer** [Coo94, RABZ94]. **KRb** [YLLJ96]. **Kroll** [Boe97]. **Kryachko** [Ano92l]. **krypton** [KSK91, Pai99]. **Kynurenic** [GJLA99].

L [Ano93h, Ano96-58, Deu96, Jør92, Str92, SC99, GK90a, GK90b, NAK95, RKN97, Sme92]. **L-KALA** [NAK95]. **L-Proline** [RKN97]. **Labarthe** [RL97]. **Labeled** [JM96b]. **Lability** [TSS97]. **LaC** [WMZ98]. **Lack** [TBBE98]. **LACO** [Nes94]. **Ladder** [MV98b, MPSLB91, NYLBNSB97, KTCN93]. **LADH** [TCA+91]. **Ladik** [Brä96c]. **lag** [Sim99c]. **Lagrange** [PZDM97, PZDM98, Sch90]. **Lagrangian** [Kry96]. **Lagrangians** [RVP92]. **Laguerre** [AM98b, CM99, FM92b, Taş97]. **Lamb** [BJMK92]. **lamella** [AS93]. **Lanczos** [GW98a, KBGE97]. **Landau** [Aon98]. **Landscapes** [BRA+99, BRV99]. **Langevin** [NOYY94]. **Langhoff** [Ber96b]. **Language** [GMI95, TP94]. **Lanthanide** [JKK+92, BB94, BB95, Bou96, BB97a, HBGR99]. **LaO** [MCOS94]. **LAP** [PSS97]. **Laplace** [CP92]. **Laplacian** [SR96]. **LAPW** [KYW95]. **Large** [BBS+97, BLBP97, CL94, DKWM97, DKM97, Dun96a, Dun97, HL93a, JCM+92, KSH94, MALT96, MAI95, MLT+96, PDC96, RM99, SMPJ94, SPOAS97, Sta96a, TJ95, VHFL93, BK95, BMFPV92, CRK+91, CDG04, CE90, DKM96, Dia99, DBF+92, FG99, I'H90, JMP99, JJ96, KS94c,

MKRW99, NSTFC94, PAF91, PA92, RRC94, RD90, Rey90, REU+91, Sæb90, Sae92, JPP87, Cal90c]. **Large-** [KSH94, BK95, Rey90]. **Large-Dimension** [KSH94]. **Large-Scale** [BBS+97, HL93a, BMFPV92]. **larger** [OSS95, RAI99]. **Laser** [Ata97a, BRZY97, CFB97, DlD99, DDH+96, DD98a, GW98a, Hag97, Hag98, MY99, TC98a, Ata94, BCC99, Cha92, DD95, Hag94, TC98c]. **Laser-Assisted** [Hag97, Hag94]. **Laser-Driven** [GW98a]. **Laser-induced** [Ata97a, Ata94]. **Late** [BC97a]. **Lattice** [Bra96a, LS93a, PP98b, SIM93a, TD96a, Bar90, BX94, FDAC90, FADC91, KPW+95, KYW95, RVP92, WP91]. **Lattices** [BKS96, CBAM97, MCM98]. **Law** [Mor96a]. **layer** [Boe91, MW92]. **layered** [AST95]. **Layers** [CV98, SMM+90, SBL+94]. **LCAO** [BKR97, CZ94a, EJ93, LMC97b, MW92, OK96, SPOAS97, SPF96, SLD95, WL92, ZWD98a, ZWD98b, ZC95]. **LCAO-DFT-LDA** [SPF96]. **LCAO-LSD** [LMC97b]. **LCGTO** [Boe93, Boe95, Boe97, GGSA98, Min90b, PSAUS90, WS92]. **LCGTO-DF** [GGSA98]. **LDA** [AMC97, LMC97a, MB97b, MVV+97, SPF96]. **LDF** [BPL94]. **LDF-Based** [BPL94]. **Lead** [DREW98, MLR+98, YK97]. **Lead-Alkali** [MLR+98]. **Leaky** [Har97b, Har98b]. **learning** [PS92a]. **Least** [BBC+96b, Fir94, DBLV94]. **Least-Motion** [Fir94]. **least-squares** [DBLV94]. **Lee** [Iva96, Iva97]. **Left** [PFMC97]. **Left-Handed** [PFMC97]. **Legendre** [Ced94, NS95b]. **Length** [BSB94, DWR99, DB94a, LP96, ST93, CP99a, GFS92]. **Lengths** [HH92, EMS92, Zha91]. **less** [LSS96]. **Leu** [NSS92, HMK96]. **leucine** [SKM99]. **leucinostatin** [NSS92]. **Leupeptin** [BBD97]. **Level** [ABB93, ADB96, ANB96, BDH+97, CMCR96, CSS93, GBL97, Jur97a, Jur99b, Jur99a, KSY97, Lad97b, PP95, RS98, See97, SPL97, CT95, DCK92, ELMY96, GSPSM93, GX98, Jur99c, Kun90, LO93, LG96, NM91, NL96b, Sin92, SJ97, VG90]. **Levels** [HLS94, KVB97, LKMCVT95, LKMCVT96, Suz99, AR92, AMC97, ČDM91, GZSvD99, HFM91, Lás93, PVČ+90, TYY91, TYTY91]. **Levin** [Mon94]. **Levine** [Lin96a, Str92]. **Li** [Ali99, BSHP97, HZ91b, SP91, SL97, TST+99, WMD95, BRL92, BKL97, BLK97, BDNT97, Csa96, DS90, DSS90, EBG95, FSBS+95, HBJ+92, KKWT99, KBBK90, LBG97, MCA95a, MW90b, MDM94, Pro94, Pro95, SKE92, STC96, VX99, WBP91]. **LiAr** [SE95a]. **LiB** [CWZ98b]. **LiBeH** [Boe91, Min98]. **Library** [ZCT98]. **librational** [KY91b]. **lidocaine** [DB97]. **Lie** [DlD99, GYDY97, GDYY97, KS90]. **Lieb** [Csa96]. **LiF** [JJ97, WTS93]. **Life** [Kor95, Roo93a]. **lifetime** [BRL92, GSM+92]. **Lifetimes** [NBS95, SPS96b, KSF91]. **LiFH** [SATP94]. **Ligand** [BRA+99, DDH+96, DL92, MHÅ98, MBA94, PW97, STM96a, Bla99, BRV99, BDPS97, TWK+92]. **ligand-activation** [TWK+92]. **Ligand-Protein** [BRA+99, BRV99]. **Ligand-Triggered** [PW97]. **Ligands** [GJLA99, TSS97, CLR+93, GVV+90, VL91, WD91]. **ligated** [HCRR94]. **Light** [KH95, Mar93b, Mar97b, YBM97, DMR96, JC90, SBZ92d, VPŠ+90]. **LiH** [HZ91b, HZ91b, MDM94, PVČ+90, RS97b]. **like** [BJM+94, BD95a, CBT93a, CFMA95, LMV92, LADV92, MLB92, MVL98,

PVU+93, Taş97, TNS96, WI98]. **Limit** [GLMP98, KSH94, KTT97, Sie93, TBČP95, BK95, GR95a, PP91, PČP92]. **Limited** [LL94a, LKMC93, WZW96, LKVS97, Was91]. **Limits** [Ada96b, MDM94, Rom92, PL93]. **LiN** [SK91, YK97]. **Lincoln** [Str93]. **Line** [Min94b, Eng92, SE93a, CLZ95]. **line-shapes** [Eng92]. **Line-Then-Plane** [CLZ95]. **Linear** [AM92, Áng93, AFTM95a, AFTM95b, AFO+97, AFTM98, BBMM99, CDDM96, Egu96, GR95b, GGSA98, GH92, Hil98, IK94, Jas94, Löw93c, Löw96c, LG95b, Mat99, NY98, OKI98, PP95, Pie93, RR94, SB95a, SB97a, Shu96, Su93, SV95, Wil96, Yam97, AFZ+99, BJA99, CT95, DS93, For92b, GL96, hJH97, KYW95, LP99, NYKY98, NNH98, Par92b, TWK98, TNI96, TBW90]. **linearization** [DM97a]. **Linearly** [Mey94, Mey97]. **Liner** [GR96b]. **Lines** [HA93]. **Lineshape** [PLBB99]. **Link** [PS94a]. **Linkage** [GSSD+96]. **Linked** [KBL95, BKL98, KL93b]. **Linking** [CCE+93]. **links** [DM99]. **Lionel** [Ano99c, Ano99g, Ano99h, Ano99o, Ano99n, Kas99]. **Liouville** [NY98, NYNY99]. **Liouvillean** [RB95]. **Lipid** [JI95, WP91, Woo98]. **Lipids** [CDDV93]. **lipoxygenase** [ARBB95]. **Lippert** [Dun96b]. **Lippmann** [DJ12, CG95, DJ95]. **Lipscomb** [Ano91-27, Ano91z]. **Liquid** [CT96, GS97a, JCÁ96, Kry98, MLR+98, OMTS97, TT98, Wal94, Cor92, FDD95, KY91b, Mar97c, MR92a, SB95b, SCP95]. **Liquids** [HL93a, HM97c, Mar94c]. **List** [Ano92q, Ano93k, Ano95r, Ano96-31, Ano96-29, Ano96-30, Ano97n, Ano99i, Ano99j, Ano99k, Ano99l, Ano99m, Par94c, Tri98b, Zer98b, Ano90a, Ano90b, Ano91a, Ano91b, Ano92a, Ano92b, Ano93a, Ano93b, Ano94a, Ano94b, Ano92-46, Ano95a, Ano95b, Ano96a, Ano96b]. **Lithiated** [RM96, TSRP99]. **Lithium** [FDF97, GKKM96, JR96, KTT97, KJ93, MSCS95, MMD96, RSD97, YK97, BLC95, BK97, KI94, LK94, MESH93, SK91, SP91, LBL98]. **Lithium-Cation** [GKKM96]. **Liver** [CAK+96]. **LiX** [SL93]. **LM** [GRK96]. **LM-Conjugated** [GRK96]. **LMO** [Sur94]. **LMSS** [Ran93]. **LMTO** [MGNK95, Spr93, WTS97]. **LMTO-ASA** [MGNK95]. **Ln** [Bou96, Bou96]. **Ln=Pr** [Li93]. **LnBa** [Li93]. **Local** [ADB96, BP93e, BMP93, CGR+94, CA97, Cze99, Day95, GR94, GD94, HMGP93, Hag97, KLLB98, KS94a, Kir95, LP97a, LBPL97, LBKLC98, LBLKC98, LLBM+95, MI93, MBM92, MECE97, MSCP92, Per93, PAAM98, SGK+95, Sha95, SLD95, TP90, Tri97, ZC95, BA90, BDPS97, DB97, DA91, GRTR96, GT97, KR91, Kov90a, KLI92, LF99, LBL98, MS91, Min90b, MSPS90, MBP91, PSAUS90, PMDM97, PZDM97, PMDM98, PZDM98, PP90, SH90a, SCP91, SN90a, Tos95, WS92, YB99, HMG+92, Kov90a]. **local-density** [DA91, Min90b, YB99]. **Local-Exchange** [KLLB98]. **Local-Scaling** [LBPL97, LBKLC98, LLBM+95, LBL98, PMDM97, PZDM97, PMDM98, PZDM98]. **local-spin-density** [WS92]. **Locality** [HH97, MA99a]. **Localization** [BBK90, Fue98, HR95, HS92c, Moi97, PM97, PVN90, SGGMGFS96, ZP92a, ALS+91, Cio90a, Lei99]. **Localization-Consistent** [PM97]. **Localized** [KBT94, KK90, KKE+96, MYN+96, MCM98, PBB94, PV94, RH95a, RH95b, RH96a, RMPR98, SBIP97a, Spr96, Ste96, Sur94,

Ter97, CKB91, DRGC90, För92a, KBB+90, KH96a, MAC96]. **locally** [CÅ92a, KH96a, NE95]. **Locate** [BLRD92]. **Located** [Kov98a]. **locations** [BA92]. **logarithm** [BJMK92]. **logarithmic** [KE90]. **Logic** [Löw95e]. **Logical** [BCD95]. **London** [Ano93g, Cal90e, Cal90b, Mon94]. **Lone** [BL92b, MV98a]. **Long** [AL98, BL92b, DMB97, GVB97, KPTS+93, KPTVT+97, LM93, Mik94, NB97, Pie93, TKMA92, Löw90d, PA92, PBR96, ZP92b, PAC90, Mon94]. **Long-** [GVB97]. **Long-Range** [BL92b, DMB97, Mik94, NB97, Pie93, TKMA92, KPTS+93, KPTVT+97, LM93, PA92, PBR96, ZP92b, PAC90, Mon94]. **Longitudinal** [FCVL98, MCA95b]. **Look** [HR95, LADV92]. **Looking** [FD93]. **loop** [ML99]. **loop-to-edge** [ML99]. **LORG** [KH96a]. **Louis** [Löw96d, Pau97]. **Low** [BS94, CWX93, Cai93, Cai94, CL97, CR96a, CR93, CSZ97, HM97b, Lad97b, MR92b, Ott94, RB93, SK99a, Sch95c, SC98a, ST93, TD96a, TT98, Ukr94, WDS97, BFRN90, CWZ98b, DDC95, GSKC99, KÅ99, KSK+99, LL99, Mar99a, MCOS94, NST94, PVČ+90, PGM95]. **Low-Dimensional** [Lad97b, Ukr94]. **Low-energy** [SK99a, WDS97, PGM95]. **Low-Gap** [Ott94]. **Low-Lying** [BS94, CWX93, Cai93, Cai94, CR96a, MR92b, SC98a, ST93, RB93, Sch95c, BFRN90, CWZ98b, DDC95, GSKC99, MCOS94, PVČ+90]. **low-molecular-weight** [KÅ99]. **Low-Order** [HM97b, Mar99a]. **low-Rydberg** [KSK+99]. **Low-Spin** [CSZ97, TD96a]. **Low-Temperature** [CL97]. **Low-Wave-Number** [TT98]. **Löwdin** [Jon92a, Mez97b]. **Lower** [Csa96, DTA+96, HMLK98, TVP93, Taş96a, Žit94, Csa94, Csa95, Fer90, GZDZ97, KE90, KD92, LK94, PFK99]. **Lower-Bound** [HMLK98, KD92]. **Lower-Lying** [DTA+96]. **Lowest** [HHKM95, SZC97, TPR96, Gut99b, KD92, LHNK99, MSS99b, ST97, TGS99]. **Lr** [KWT95]. **LSD** [GJDD97, Bou94, KPB99, LMC97b, RRC94, RP98a]. **LSD-CGA** [GJDD97]. **Ltd** [Cal90d, Kra96]. **LTP** [CLZ95]. **Lu** [JKK+92]. **Lucas** [SBM97]. **Ludeña** [Ano92l]. **Lund** [Lun92]. **Lyapunov** [KB93]. **Lying** [BS94, CWX93, Cai93, Cai94, CR96a, DTA+96, MR92b, SC98a, ST93, BFRN90, CWZ98b, DDC95, GSKC99, MCOS94, MSS99b, PVČ+90, RB93, Sch95c].

M [ANB94, Ali99, BDH+97, Cal90e, DKWM97, DKM97, JKK+92, Kra96, Kum93b, Lun92, NG95, SM96a, Sjö96, SG96b, SGB97, SGB98, SL97, SC98b, SC99, SNH99, TST+99, Tri96, Wha96, ANB94, Ali99, BDH+97, DKM96, DKM97, GK90a, GK90b, SG96b, SL97, SNH99, ZBL99]. **M.** [Enk97]. **machine** [Sin92]. **machinery** [DD99]. **Macintosh** [Mic96a]. **Macomber** [Dun96b]. **macrocyclic** [Bha99]. **Macromolecular** [Mez97b, SCL96]. **macromolecules** [MM91]. **Macroscopic** [MB98, Res99, Sim99a, Sim99b]. **made** [AZ99, BAF+95]. **MAF** [SR99]. **Magnesium** [ALRP96]. **Magnet** [BMG+98]. **Magnetic** [BK96, BRZY97, CdBKZ99, FCVL98, GMR+93, Gus98, JOC97, Jos97, KL97a, LZ96, MB97a, NONY97, NG95, Ols96, PO97, RS94, RS97b, RS97a,

SSK+92, Sch97, SC97, Sch98, SG98, SS97a, Sul97, TMDB98, ARDP92, Cas97, Fer92, FWS97, GR95a, HBGR99, Jur99d, KKNY99, LM91, LTSL96, LBG97, MTNF99, Mar91, MCT99, RR95, SC91, WO92, Yam90, YKN+99, BUZ94]. **Magnetism** [MC97a, MC97b, PEBS97, Mar94c]. **magnetoresistance** [Nes94]. **Magnets** [MC97b, Mat99, MNT96]. **Main** [DKM97, BCLS94]. **Main-Row** [DKM97]. **major** [XSA+92]. **Making** [ÖOD96]. **Maksić** [Cal90d]. **malarial** [TCZ91]. **maleic** [HMK99]. **malonaldehyde** [LS93b]. **Malononitrile** [ET97]. **malononitriles** [METHH94]. **Manifestations** [ZH99b]. **manifold** [Ada91a, CCS98, DDN95, Man99]. **Manipulation** [BB97b, TP94]. **Mann** [MHN98]. **Mannich** [LX95, MKK98]. **Manuscript** [Ano93i, Ano93j, Ano92o]. **Many** [Ber96c, BD94a, BD94b, CBG94, Cim96, IK97, JOC97, KBT94, KNN96a, KZVGB97, Koh95, Lin96b, LFD94, Mar96, Mar99a, MHM95b, MS93b, Muk96, NNY+96, NMKP94, NB97, Oht98, Pie93, SAR96, SD96a, SN98, Sta93, SPL97, SKS98, TC98a, TM93, VVS94, YAD95, Ano92l, Ano93g, AGH91, BD95a, Cam92, DWM90, HC96a, HC96b, HC96c, HC96d, Ish92, Jør92, KSF91, KL90, Kry96, MHM95a, MUMH97, Muk92, Mur90, Pos91, PK92b, SH90a, SKE92, SD91, VCMLL90, ZC99, ZP90]. **Many-Body** [BD94a, BD94b, IK97, JOC97, KBT94, KZVGB97, Lin96b, LFD94, MHM95b, NB97, Pie93, Sta93, SPL97, SKS98, VVS94, Cim96, Ano93g, BD95a, HC96a, HC96b, HC96c, HC96d, Ish92, KSF91, MHM95a, MUMH97, Muk92, Mur90, SH90a, SKE92, VCMLL90, ZC99, ZP90]. **Many-Center** [MS93b, SN98]. **Many-dimensional** [Ber96c]. **Many-Electron** [KNN96a, Mar96, Muk96, NMKP94, Oht98, SAR96, SD96a, SN98, TC98a, TM93, YAD95, Mar99a, Ano92l, Cam92, DWM90, KL90, Kry96, PK92b, SD91]. **Many-electron-wavepackets** [NNY+96]. **Many-Fermion** [CBG94, Jør92]. **many-particle** [AGH91]. **Many-Photon** [NMKP94]. **MAPLE** [McD97, Pie93, TP94, Lai94]. **Mapping** [MKM93b, MM98, KM90c, KBM92, SM94]. **Maps** [AP96, MK99]. **Masao** [Ohn95]. **Mass** [Ara94, MMP+94, MG93a]. **massively** [Ken93]. **Masten** [Ano92n]. **Master** [BG95]. **Masthead** [Ano90k, Ano90l, Ano90m, Ano90n, Ano90o, Ano90p, Ano90q, Ano90r, Ano90s, Ano90t, Ano90u, Ano90v, Ano90w, Ano90x, Ano91k, Ano91l, Ano91m, Ano91n, Ano91o, Ano91p, Ano91q, Ano91r, Ano91s, Ano91t, Ano91u, Ano91v, Ano91w, Ano91x, Ano92r, Ano92s, Ano92t, Ano92u, Ano92v, Ano92w, Ano92x, Ano92y, Ano92z, Ano92-27, Ano92-28, Ano92-29, Ano92-30, Ano92-31, Ano92-32, Ano92-33, Ano92-34, Ano92-35, Ano92-36, Ano92-37, Ano92-38, Ano92-39, Ano92-40, Ano92-41, Ano92-42, Ano92-43, Ano93l, Ano93m, Ano93n, Ano93o, Ano93p, Ano93q, Ano93r, Ano93s, Ano93t, Ano93u, Ano93v, Ano93w, Ano93x, Ano93y, Ano93z, Ano93-27, Ano93-28, Ano93-29, Ano93-30, Ano93-31, Ano93-32, Ano93-33, Ano93-34, Ano93-35, Ano93-36, Ano93-37, Ano94j, Ano94k, Ano94l, Ano94m, Ano94n, Ano94o, Ano94p, Ano94q, Ano94r, Ano94s, Ano94t, Ano94u]. **Masthead** [Ano94v, Ano94w, Ano94x, Ano94y, Ano94z, Ano94-27, Ano94-34, Ano94-35,

Ano94-28, Ano94-29, Ano94-30, Ano94-31, Ano94-32, Ano94-33, Ano95s, Ano95-45, Ano95-46, Ano95t, Ano95u, Ano95v, Ano95w, Ano95x, Ano95y, Ano95z, Ano95-27, Ano95-28, Ano95-29, Ano95-30, Ano95-31, Ano95-32, Ano95-33, Ano95-34, Ano95-35, Ano95-36, Ano95-37, Ano95-38, Ano95-39, Ano95-40, Ano95-41, Ano95-42, Ano95-43, Ano95-44, Ano96-32, Ano96-33, Ano96-34, Ano96-35, Ano96-36, Ano96-37, Ano96-38, Ano96-39, Ano96-40, Ano96-41, Ano96-42, Ano96-43, Ano96-44, Ano96-45, Ano96-46, Ano96-47, Ano96-48, Ano96-49, Ano96-50, Ano96-51, Ano96-52, Ano96-53, Ano96-54, Ano96-55, Ano96-56, Ano96-57]. **Materials** [Coh97, DJF98, SB96, Mar94c, Tos95, YNNR97]. **Mathematical** [DB99, PV94, Ano91g, CDB99]. **Matrices** [CB94b, FBKD97b, Gin96a, HH97, HM97b, KSG93, KBWJ96, Maz98, Mez97b, PRTV97, PK96, Sam97, SFM94, Spr96, Zap95, Cal90a, CES87, Ell92, GL96, Hol98, HMK96, Mar95a, Mar99a, MHK95, MYPL90, MP91, NZ92, PC99]. **Matrix** [Bad95, BM96, BG98b, BG98c, BG98d, ČHM95b, DV98, DKBB97, FBKD97c, Gin98, Gin99, GMI95, Iga95, JBT$^+$95, Kin96, KA95b, KMM96, LY98, LBMR95, Mik94, Mor93b, Pal93b, Sch95b, Tit92, Tit93, TCM98, TNM97, WT98, ZWZ96b, ZARB96, BCD91, DW90, Ell91, FL91, For92b, FJR96, ITK91, JRS$^+$99, Kov90b, MD99, NM94, NE95, PAC90, PACO90, PNB94, PK92b, SN99, SP90, ŠG96a, Sch95a]. **Matter** [Ino96, Löw90c, Mar94b, BCD91, CDB90, Löw91a, Löw91b, Löw91c, Löw91d, Löw92b, Löw92c, Löw92d, Löw92a, Löw93a, Löw93b, Löw94b, Löw95c, Löw95f, Löw95d, Löw95b, Löw96a, Löw96b]. **Maxima** [Che96]. **Maximum** [AYAZ95, AZAC97, CC91b, GH96a, TŚP97, WG94, ZZ91, Zha92a, MP91, Pea95, Zha92b]. **Maximum-Entropy** [AZAC97, AYAZ95]. **May** [Cal90d, FG96, JPP87, Kar93, Bha99]. **MBOHO** [HZ94]. **MBPT** [GR95a, GS97b, KBB$^+$90]. **MC** [FZZ92]. **McClelland** [She90c]. **McGraw** [Str92]. **McGraw-Hill** [Str92]. **MCH** [SGB98]. **MCl** [SNH99]. **MCLR** [NÅJ91, NÅJ92]. **MCM** [AT99]. **McMurchie** [JGP91]. **MCO** [SG96b, SGB98]. **MCP** [PSAUS90]. **MCSCF** [BBS91, FG99, JR96, KSIH92, NÅJ91, NÅJ92]. **MCSCF/MCLR** [NÅJ92]. **McWeeny** [CS96b]. **MD** [FVN98, LSGS91]. **MDGI** [SJB90]. **Me** [Sta98b, CRK$^+$91, GARC97]. **Mean** [ADB96, Gui98, Mez94a]. **Mean-Field** [ADB96]. **meaningful** [Ada91b]. **Means** [Gin98, LBPL97, LBKLC98, LBLKC98, MBA97, MS93b, BMA90, MS92, SO97]. **Measure** [Mez97a, NP96a, BR92, MM99a]. **measured** [Hal91]. **measurement** [Kar93, CPW92]. **Measures** [HM97a, HSS$^+$95, Mez97a, Mez97b, MFAT98, SMO$^+$96, BBSS96, CC92a, CC92b, HSWS95, Mez94b]. **Measuring** [BCC99]. **Mechanical** [AV92, AM97, ALRP96, BLBP97, CDC98, ECBH96, FLRV97, GDID98, JDJP99, KL97b, NFVM94, RL94, TNM98, TTK99, Tch96b, Tch96a, VBV92, Wal94, Wen96a, ZWPJ94, Ano96-31, Ber96b, BV93, CBL95, DV96, FNSV99, Fer91, FG96, KJL96, KS94c, Lan95, NOY98, NPL90, NGM$^+$95, OM91, SH90a, SR99, Wen96b, YUSM99]. **mechanically** [GSM90]. **Mechanics** [BLBP97, Emc97, O'C96, Pri95, RKN97, Wło94, Wło95, Wul94,

Adl95, BD95c, Chr89, Deu96, Gar95, Gin91, GZ97, GZ06, LCP+91, LU92b, MA99a, Mic96a, Pos91, PK92b, RTKP95, RS00, SR93, SR02, Sch94, SN97, Wha96, WP90, Car96, Str91]. **Mechanism** [DDP96, FF94b, HBH98, LX95, OSA+97, AKCS91, BBTU97, BP90, CLOFR98, DV91, DD99, FMS+99, FF92, FF96, FWZ97, GWB97, Jug90a, KO91, NOY98, DZB92b, SBZ92d, TF92, TCA+91, ZH99a]. **Mechanisms** [BAK96a, BAK96b, Cha95, ECBH96, Sak97, Sak98, BH99, BDP+92, CH91, DRGC90, KWZ98, MV92, Nes94]. **mechanistic** [Ano96-58]. **mechlorethamine** [BVV91]. **Media** [Chr94, Dun99, JSKC95, SM98, Chr92]. **Mediated** [DDH+96, NMN+97, NMN+98, BBB+95, HDB+95, PBR96]. **mediators** [MG90]. **Medium** [GJOV97, MCT99, NOYY94, TCM99, BKY99]. **Meeting** [Bir94, FR94, FG96]. **MEH** [BB91, BBC92, BB94, BB95]. **Melbourne** [Mon93]. **melittin** [LS99]. **Melts** [WGR+94]. **Membered** [BT95, GBL97, Ran95]. **Membrane** [PW97, DS99, LS99]. **membrane-bound** [LS99]. **membranes** [Kov98b]. **Memorial** [Mic92]. **memoriam** [FMT93, Tri95]. **Memories** [Roo93a]. **Memory** [Löw96d, Ohn95, Ano99e]. **Menton** [CD81]. **merocyanine** [MUL99]. **MEs** [BG98b, BG98c]. **Meso** [MZ93]. **Meso-** [MZ93]. **Messier** [Eri92]. **Met-Enkephalin** [PLV92, LVCP91, LS99]. **met-enkephalin-like** [PVU+93]. **meta** [KPB99]. **meta-GGAs** [KPB99]. **metabolique** [GK90b]. **metabolism** [KKS99]. **metabolites** [KL93a, VS95]. **Metal** [BKWL97, BA97a, BC97a, BCRL94, BK94c, CF96, DHL+94, DDH+96, Dun99, LRM97, LLZ98, MMP+94, MPV94, MBA94, MCCF95, NMN+97, NMN+98, NN94, PAT93, SZL95, SZ97a, SS97b, STM96a, ACZ91, BUZ94, BCLS94, BDK90, Boe93, BDPS97, Bro95a, Bro96, CKM91, EDH+92, FMR91, FZZ92, HS93, JWG95, hJH97, Kap99, KF96, KBBK90, Li92, MSMR99, MAC96, MS93a, MV90, Nor91, PBPN90, PTL90, PZA92, ROL+90, REL+90, SM99, SCA93, SBPPH92, SS95, STM96b, SC99, Van96, YDDP92, ZBL99, KK99a]. **metal-CO** [hJH97]. **Metal-Insulator** [Dun99, NMN+98, NMN+97]. **Metal-Ligand** [DDH+96, MBA94, BDPS97]. **Metal-Metal** [CF96]. **Metal-Nitrosyl** [BCRL94]. **Metallacyclobutadienes** [Rin94]. **Metallic** [AMD+97, FDF97, Mar97a, TSPK97, ARDP92, CD92, GRB+93, REKP92, The94]. **Metallocenes** [Coo95]. **metalloenzyme** [KK99a]. **metalloproteins** [BBCL92]. **Metals** [BTN98, Jur97g, KPTŚ94, MBP97, PP98b, SDE94, Egu96, LB94, Lun91, PO91, WY95, WS92]. **Metastable** [ABB93, ANB96, Bar90, KA96]. **Metathesis** [RC97]. **Methacrylic** [FY95]. **Methane** [CC96, Jur99b, YNMT98, BYE+97, CRsP93, CMG92, YNST99]. **Methanediol** [BAK96a]. **methanes** [BMP92]. **Methanetetraol** [BAK97]. **Methanetriol** [BAK96b]. **Method** [ADB96, AB97, ASI94b, BCMÖ97, BLBP97, BD94a, BD94b, BR94, CMCR96, CZ94b, DE92, DM95, DM97a, DDD93, DKWM97, DKM97, Dun99, FSBS+95, GGSA98, GH96a, GMI95, GG97b, GLBM96, Hag98, HK95b, Huz96, IK94, Iga95, IAN+94, JM95, JGR98, JMR98, KUN+98, KBGE97, KKNN97, KPA95,

KSY97, KY93, KLLI97, Kry95, LVL+93, MV98b, MSM96, MB98, MS97b, MBA97, Mik94, MAD98, MAI95, MAI97, NONY97, Nag98b, NS93a, PIG94, Pec93, Pen93, Pen96, PDT97, RDF98, RL95, RL92, SWF93, SPOAS97, SZL95, SS99b, Sim98, SBD+92, STM96a, SDG97, TMSI98, TR94, US96, VJ95, VJ97, WTS97, YD97, ZLHZ94, ZWJP95, Zou92, Ada91a, AS99, Bal90, Bat92, BD95a, BA90, Boe95, BRV99, BS95, CC91a, CS96a, ČVW91, Cul91, DKM96, DWM90].
method [Duc90, Fau92, FNSV99, Fer92, FZZ92, FW92a, FHHE90, GHB+99, GRTR96, GB90, Hag96, Har94, HZ91a, HZ99, HK97, Ish92, JM96a, hJH97, Jon92b, Kal90, KG92, KNN96b, KF96, KY92, KB92, LO93, LK90, LKM99, LH94, LP97d, LP98, LJS94, LH90, MRC99, MHS95, MFH91, MHY98, MB93, MW90a, MRT95, MR97, MC91a, MC91b, Moh92, MAPLB92, MPP92, NSTFC94, NNY+96, NKS+96, Nag96, Nes94, New97, NZ92, Pal92a, PSAUS90, Par90a, Pau92, PCO+94, PL91, PTL90, PZA92, RAI99, RRC94, Réa90, Rin96, Roc99, Rom92, RL97, RK92, ŠG96a, SWD+99, SPB90, She90c, SS92d, Sin92, Sme92, STM96b, TSY99, TR91, Tho96, Tit96, VR90, WS92, YITY93, ZM95, Zha92b, Zho93].
methodological [GDB98].
Methodology [BPL97b, Del92].
Methods [ASP97, BIM97, BLE96, BBS+97, BLRD92, BF94, BL92b, CCM+96, DRBE96, DZO97, DKBB97, GD96, HS92b, Her98, HS91, HS92e, Jug96, JM96c, Jur97a, Jur97b, Jur97e, Jur97d, Jur97g, LZ92, Löw99, Mar95c, Nic99, PMN+92, PTH+97, RL94, RHC96, RWT92, Roz97, Sæb90, SAW97, Sch95c, SRM98, Sim97, SAL+94, SG97, SGB97, SGB98, Sta93, SATP94, Sza95, UWB94, VFHL93, WR96, ZON+96, ZZZY96, ANB94, ACAT92, Ano90g, Ano90i, Ano93g, BMA90, BBTU97, Boč90, CZ93, CMA+99, DS90, DSS90, FG96, FGS92, GL92, Gut99b, Hag92, Hag95, HK95a, HC96c, HSES94, Iac92, Jak93, JO94, Jør92, JK92a, KK99a, KLO+98, KLI92, LZ91, LS92b, MG97, Muk92, PAF91, RPT90, RWT91, RC92b, SGGC99, SSC92, Sim95, Sim99c, SES93, SG96b, WGP99, YBZ92, ZFZ92, BBSS96].
Methoxy [HS99].
Methoxyidazoxan [HS92b].
Methyl [MZ93, NSS+95, PSCZ97, BH92, CMG92, HDY+91, MJLL99, PVF+92, RT99, STS95, SCJK90, VS95, SSM+99].
Methyl-Ethyl- [NSS+95].
Methylacetamide [TT98].
Methylamine [AMKS93].
Methylated [VDD96, HWB97b].
Methylation [FW92c].
methylcopper [CPN91].
Methylene [Oli99].
Methyleneimminium [MKK98].
methylenimine [FF92].
Methylformamide [TT98].
Methylglyoxal [VC92].
Methylpyridones [RM96].
methylthio [SSM+99].
Metiamide [MTP+98].
Metric [Löw96c, Mez97a].
meV [Eng92].
MFI [MBML91].
Mg [BZQ95, NBS95, Csa96, FR93b, Pro94, Pro95, YDDP92].
MgAl [BILA95].
MgC [DDC95, DTA+96].
MgF [LG96].
MgI [MBG90].
MgO [LXWZ99, AMT+99, FP96, PCB92, YNNR97].
MH [SNH99, SM96a].
micelle [SWK90].
Micelles [ZLWES99].
Micha [Mon94].
Michael [Ano91f, Ano91y, Ano92-45, Ano92-44, FMT93].
Michio [Kla93].
microclusters [SPR94].
microdynamics [BC93].
microflows [SBZ92c].
microscope [DVL+91].
Microscopic [BXZ95, BHX96, Brä93a, MO98, MBA94, NOYY94, NYY96, BADM97, BA90, SBZ92b, Sim99a, Sim99b].

microscopy [Hag94, Ike99, VBD+98]. **Midgap** [TYY91, TYTY91]. **Midpoint** [Mar94d]. **midrange** [Tos95]. **Mills** [EMMHP92]. **Mimics** [LJ95]. **mind** [Cha96, Gre98]. **minima** [Sch92a]. **minimal** [PCD99]. **Minimization** [FP94, Pai97, PL98, KM99a, Pai91, Pai99, WP91]. **Minimum** [Gui98, NM95, Pon98, Gut99b]. **Minimum-Energy** [NM95, Gut99b]. **Miniplasmids** [Tob99]. **Mirror** [PM95]. **Mismatched** [PS99]. **Mivazerol** [VDD96]. **Mixed** [JCÁ96, MLR+98, STM96a, Sch92b, TC98c]. **Mixed-Ligand** [STM96a]. **Mixing** [AT93, FD96a, HOF+97, KCI98, GVB96, YJL92]. **Mixtures** [SSK+92]. **ML** [SC99, Zha91]. **MM** [BLBP97, MSM96, Tho96]. **MMVB** [BBOR96]. **Mn** [LW92, SZ97b, VR92]. **Mn-related** [LW92]. **MnC** [SGB97]. **MNDO** [BP90, Ert90, GL92, MAL93, MALT96, MZ91, TV92, HNB92]. **MO** [Csi77, AKD96, Boč96, BB91, BB94, BB95, Bou96, BB97a, CWZ98b, CS96a, Csi76, Del96, FAV92, FZZ92, HHKM95, JK92a, MF96, MSM96, MZ95, MAAP90, STKN90, SKTN97, Sin92, SHC+98, WMW92, And94, SR96]. **mobile** [LB93, Sla92]. **Möbius** [Jur98b, LR94, SH90b, Zho94]. **Möbius-type** [SH90b]. **Mode** [AMD+97, DJ95, KLC98a, Lef97, MD93c, DJ12, LF99, MSS99b]. **Model** [AT99, Amo96, ATI97, Ara94, BE95, BE98, BČ96b, Bra97a, CLSI94, CA90a, CMFA93, ČB96b, Col97, CPA95, CSZ97, DDH+96, DL92, DMB97, EMMK94, FT97b, Fue94, GPč94, GSM98, Huz96, JKJ94, JM95, JKRW98, JGR98, JMR98, JSG97, KBWJ96, KPR97, KPTS97, Kon94, Lah92, LCLO95, LB95, LEA+94, MI93, MHM95b, Mat99, MAD98, MAI95, MPV94, Nal94, NM95, OKI98, PW97, PPP97, PTC94, PS94b, RPKM95, RABZ94, RML97, RG96, Sak98, SB98, Sch99a, Sch99b, SBIP97a, SLS91, ST96b, SFGW96, TSPK96, WPB98, Wil96, YO92, Zha92a, AEJ91, ACZ91, AD92, BZ92, BOA95, BPHB96, BL91, CT95, ČPV90, Con92, CF99, DVJ93, Del90, DDA92, DCK92, EZ92, FKR92, FM92a, GSPSM93, GWB97, GJDD97, GL96, HFM91, JM96a, Jug90b, KR91, KF96, KSH92]. **model** [KB92, MUL99, MBM92, MMCC99, MFH91, MRB+96, MCA95a, MCT99, MCA95b, MRD92, Nak92, Nal92a, OS90, Oza92, PBPN90, PCB92, PČe90, PZTPMC99, PP91, PČP92, RWT91, RC99, Sas90, SS92g, SZ95, SN90b, TFT+91, TFYY91, TIA+92, TLTL92, TD99, TWK+92, TCM99, TNS96, Vin92, WLB+94, WDS97, YNST99, YNNR97, ZP90, KY91b, MLK94]. **Model-Systems** [Sch99b]. **modeled** [Csa92, CPGC99]. **Modeling** [ADB96, BOL+90, CAK+96, CL95, DBF+96, DS92, DSW93, GJ95, Jen94, LV93, MLT+96, MCB99, NTL96, NG97, RMH+99, SD97, SKZ96, SM92b, TBP99, VS95, AFM99, Bla99, BHV96, BS95, DGMW90, GJPMML91, GRTR96, GX95, KÅ99, KE91, Kun90, Smi96, TSS95, YDDP92]. **Modelization** [LADV92]. **Modelling** [SKJ98, Mak87, Cal90d]. **Models** [ÁC94, BXZ95, BHX96, BMK96, Bra96a, CAÖ96, FP96, JG95, KD98, LV93, MALT96, PFMC97, PTH+97, SG94, Tch96b, Tch96a, Yam97, Ano93h, BRS96, CL92, DFGB99, Fer91, FCA91, HS92a, HDB+95, KS92, LCV92, MAL93, MCB99, OCK99, PP92, PMO90, Røe90, Røe91, REL+90, SAB+97,

SRP+98, Sim99a, Sim99b, SMH92, STZ96, Yam90, ZP92b]. **moderately** [DBF+92]. **Modern** [Amo96, CTG97, KGC+96, Löw97b, Oli99, SP95, TC98b, GZ97, GZ06, Kla93, Kry96, Sem96a, Tri96]. **Modes** [KC98a, KC98b, PP98b, BZMR92, HZF+91, HW91, JDB99, KLC98b, WD91]. **Modification** [DD90b, FW92a, GRT96, GRTR96, Gin91, Iva96, Iva97]. **Modifications** [Sta98a, WZW96]. **Modified** [BE95, Fue98, MMP95, MK99, NM94, Pec93, Por99, RL92, SWMB94, Taş97, Was91, ZARB96, BGS97, FHHE90, Hol98]. **modified-Hartree** [Hol98]. **Modifying** [ZZZY96, ISOA99]. **modulated** [Lin91]. **MoF** [FAV92]. **Molecular** [AEAO99, AP96, ÁC94, Ano92j, ATI97, AM98b, Art96, Art98, BKR97, BC96a, BSB94, BM96, BCMÖ97, BLBP97, BSHP97, BG98a, BBLK94, BR94, BFH96, BMP93, Cal90d, CCM+96, CC92a, CC92b, CMCR96, CFB97, CC97a, Cio94, CG96, Coo94, Cor92, Csi82, DR92, DE92, DP93, DM96, DTM96, DN96, DBF+96, DZF93, Dun98, ESHP99, Enk97, ECBH96, Fan97, FM92b, FWT+96, GBVM93, GVK99, GJ95, Gho95, GRT96, Gin99, GT93, GPD94, GG97b, GGHP94, GLBM96, GW98a, Gus98, GLLY94, HW04, HAEMA92, HS92b, HGC93, HL93a, Her97, IYFI99, JM96b, Jon94, Jos97, KUN+98, KFS92, KPD93, Ken97, Ken98, KK92a, KM97, KN99b, KE91, Krü97, KPB99, KL97c, LB96a, LJ95, LZ96, LP97b, LLC+94, LDP93, Lip91a, Lip91b, Löw99, LH90, LTY92, LL92, LU92b]. **Molecular** [Lun92, LBG95, Mar90, Mar94d, Mar95b, MHÅ98, MKM93a, Mar95c, MC97b, Mat99, MR99, Mez90, MK99, MAI95, MH98, MSCS95, MK97b, MK98a, MK98b, Mor97a, MV99, MSCP92, MAAP+98, NK96a, NY98, NP96b, OMTS97, ÖOD96, OSA+97, PCB92, Pen93, Pen96, PVU+93, PC95, PAAM98, PJ96, RKN97, RK97, RD98, RWT92, RW98, Roś96, SM98, SM96b, Sch95b, Sch95c, SNMB97, SCP95, SS99b, SRS92, SG94, STMR97, SGGMGFS96, SMO+96, SM92b, ŠH96, Ste96, SP94, Sul97, Suz99, SBZ92a, TMSI98, Tal93, TMP97, TD96a, Tho96, TC98b, TNM97, TD96b, US97, US96, UWB94, VBV92, VFHL93, WS94b, Wan94, WP90, Wil96, WGR+94, WP92, Wul94, YTYS97, Zha92b, Zha92a, ZLHZ94, ZM96, ZM97, Ågr91, ARDP92, ACAT92, Ano90i, Ano96-31, AM90a, AM90b, Art93, Ata94, AD92]. **molecular** [Avi92, BBSS96, BJ92, BKL92, BKM90, BVV91, BVV92, BMVV93, BMFPV92, BJMK92, Cal90f, CM99, Chr89, Cio91, Con92, CA90b, CB91, CE90, DS99, DCK92, DRGC90, DÖ94, DO90, FMR91, FMD+96, Geg91a, Geg91b, GJDD97, GP91b, GG84, HSWS95, HDB+95, HOF+97, Iac92, JO94, JE90, Jon92b, KDB90, KKK90, KK91, Kin93, Kin94, KH96a, KKNY99, KWZ98, KÅ99, Kov90a, Kov90b, KK90, Kry96, KSW98, KSK+99, KKM99, KL92b, LK99, LYSL95, LADV92, Lei99, LF99, LHL91, Les92, LV97, LTY90, LUU90, LCP+91, MD92a, Mar92a, MT90b, MLL99, MM94, MCA92, Mez94b, MLK94, MK95, MK96, Mun92, MSC92, MPIP99, NKS+96, NMN+99, NYNY99, Nal92d, DZB92b, NL96a, NL96b, OKY+99, PBPN90, Pic92, RTKP95, Rau02, RFM90, RWT91, REU+91, RK91, RK92, RC99, RCWN94, RAM91, RMF90]. **molecular** [Sae92, SCA93, SX96, Sch95a, SC96, SGGC99, SCP91, SOK+98, SCJK90, Sla92, Smi96, SKRK90, Str91, TTM99,

TH90, TYY91, TW90, TW92, TCB99, The94, Tom91, Tul91, UBA92, VES+99, WM92, WLB+94, WW97, WGP99, Woo99, AEHM91, AHM97, Bir94, Brä98b, KMR92, KN99a, SK99a, SHF94, Mic97].
molecular-electronics [Sla92]. **molecular-orbital** [Mar92a].
molecular-state [KSW98, KSK+99]. **Molecule**
[AS96, BBC+94, BvL96, CWX93, CCB+97, DB99, Del96, Gin98, GV93, GYDY97, HBL99, JCÁ96, KM92, Kon94, KA95a, LD95, MB98, Mon99c, MTD96, MPJ98, PVLG93, PLA98, Pie93, PTC94, RGT95, SG93, SZ98, TKNI96, TMSI98, VDBPR97a, YTYS97, BSS+97b, CRsP93, CCC+95b, CRK+91, CWJ+99, Coo92, DDC95, GSM90, GJPZ97, HGL99, Ike99, LLL92, MMRSN92, MHM95a, MUMH97, Nak92, Nal91, Nal92c, NWG+99, OTS+95, PGM95, Ran93, Røe91, SOK+98, SG92, TGS99, TG96, XSA+92, Zha91].
Molecule-Surface [GYDY97]. **Molecules**
[AHI96, AZAC97, BBOR96, BKM93, BEJ98, BZQ95, BK98, CT96, CAK+96, CC95, Che97, CL94, DTA+96, DlD99, DDH+96, DHPC95, DKWM97, DKM97, FCVL98, FSF96, GG97a, Gra97a, Har96, HP97, Hil98, HHHP99, IP93, JOC97, JCM+92, JAG95, JM96c, Kan93, KVB97, KD95, Kru92, KMM95, Kup98, LDGA96, LKMCVT95, LKMCVT96, LTP96, LN96, LSC98, Mar94b, Mar98b, MRL99, MR92b, MKM96, MKM97, MLT+96, Mor93a, MP93, NK98, Pal97b, PP98a, PBB94, PDC96, PPK97, RPJZW96, RD98, RL98, RABZ94, Roś96, RS97a, Ryc94, SC97, Sch98, SD96a, SPF96, Shu96, Sta96a, Su93, Suk95, Suz99, TNS+94, TDO97, VdV96, VHFL93, WP93, WS95, Was96, WZW96, YDFS98, ZWJP95, ZZCSE94, AI99, BJ92, BZMR92, BKY99, BJM+94, BK95, BL91, Bro95b, BPVP92, BLG95, Cal90d].
molecules [Cal90e, CCWCF96, CTF92, CXFP99, CS99, CBL95, CLGW95, CTC95, Csi76, DKM96, Deu98a, DA91, DT96, DBF+92, EMS92, Eri92, FLHT90, GFS92, GS92a, GSPSM93, GL99, GS91, GDYY97, GDF92, GS90a, GS90b, HS95, HZF+91, IL95, hJH97, JY94, KM90a, KPTS+93, KY92, KT95, Kov98b, LU92a, LCS98, Mar93b, MKDL93, MSMR99, MHG95, MKP91, MB92, MW90b, Min90b, MC91a, MC91b, Moh92, MKBP97, MAAP90, MPP92, MJLL99, MIW91, MSPS90, NE95, OS91, OS92, PY89, Par99, PK94, Rat92, RF94, RD90, RTS91, RSCP92, Sæb90, SM99, SC91, Sco90, SPB90, Sin92, SSM90, SKRK90, SLDB91, SN90b, ST91, TFSZ95, Tit96, TKK+90, VA90, VPŠ+90, Wil99a, WMW92, WZ96, YB99, YKN+99, ZB92, ZM90, DD89, Mak87, Ågr90, Cal93, Lin96a]. **Molin** [Kra96]. **Møller**
[Cim96, HC96d, Hir92, KLO+98, Kir95, KSY97, MJS93, Pra97, SAS99, Suh93, VCMLL90, vDvLR99]. **Molten** [BPL97b]. **Molybdenum**
[Boe98, CF96, TGDS97]. **Moment**
[Fer92, Gus98, KJ93, MS98, McD97, MK98b, RDF98, Sut99b, ZZ93].
Moment-method [Fer92]. **Momenta** [Kru92, YPC97]. **Moments**
[BOX94, CJA94, KBWJ96, KY93, MZM94, Mon98, SPS96b, DOPS91, GB90, KSF91, LBG97, PSO90, PTL90, PNB94, SSC92, SKRK90, TP90, TK92].
Momentum [AZAC97, AH96, AHWA96, BDT96, BDNT97, Can97, DDD93, HSS+95, Mar96, MAC96, Ols96, Pal93b, Sch94, TP90, TK92].

Momentum-Space [AH96, MAC96, Sch94]. **monitoring** [MBM92]. **Monkhorst** [Jør92]. **Mono** [Bér97, Cha97, GL97, WSTB90]. **Mono-** [Bér97, Cha97, GL97, WSTB90]. **monobridged** [OTS+95]. **Monocarbides** [DTA+96]. **monocation** [TCS+90]. **Monoconfigurational** [MR99]. **Monographs** [Deu96]. **Monohydrated** [GL98]. **Monohydration** [KO91]. **monolayer** [WTS93]. **monolayers** [Boe93, MVB92, WM92]. **Monomers** [Mor97a, HDY+91]. **mononucleotide** [Sta95, Sta96b, Sta98d]. **mononucleotides** [Sta95]. **monoprotonated** [DB97]. **Monosubstituted** [MG93b]. **Monotonicity** [AYDR96]. **Monoxide** [MR92b]. **Monte** [BBMM99, ACB+99, ACAT92, ACHT95, BRL92, BBC+94, BBC+96b, BRA+99, BRV99, CDC98, KNN96b, KKNN97, KI94, Kid99, Mar97c, MB97b, MR92a, Rey90, Rot96, Rot97, UBA92, VBD+98]. **MoO** [BS92, BS94, Bro95a]. **Morse** [AD97, BR97, Coo94, LKMCVT95, LKMCVT96, MPOG99, NYLBNSB97, PRSDS92, SP90]. **Mössbauer** [EMMS97]. **Motion** [AS96, BCMÖ97, Fir94, GSM90, JDB99, KY91b, RGO94, TW90, TW92, VBD+98]. **Motions** [Mic96b, Par92a]. **Mott** [MS93a]. **Mott-insulating** [MS93a]. **Moving** [TSPK97, DM94a]. **MP** [Les92]. **MP2** [AOH96, GX98, KC97, YTYS97]. **MP6** [HC96c]. **MRCI** [hJH97]. **MRD** [BMG95, CRK+91, CKB91, LG96, PPSK96, SKRK90]. **MRD-CI** [CRK+91]. **MRSDCI** [Cai93]. **MS** [NMCK92, RRC94, VABM94]. **MS-X** [NMCK92]. **MSH** [JI95]. **MT** [Geg91b]. **Mu** [CML92]. **muffin** [RRC94]. **muffin-tin** [RRC94]. **Mukherjee** [Ano93g, Sta93]. **Mulliken** [LV98]. **Multi** [Pen96, ZP90]. **Multi-Configuration** [Pen96]. **multi-reference** [ZP90]. **Multicavity** [DKTZ94]. **Multicenter** [GKKA97, IYFI99, JE90, Jon94, PMN+92, Smi99, TH90, DD97b, MHS95, DBLV94]. **Multicolor** [TC98a]. **Multiconfiguration** [Huz96, MB98, Mic96b, Pen93, FGS92, SO97]. **Multiconfigurational** [AR93, Kup98, LP93, MR99, SAFK97, VIK98, ZON+96, BBS91, MHY98]. **Multidimensional** [EP98, PL91]. **multielectron** [DBLV94]. **Multifractal** [LL97]. **Multigrid** [BIM97, Bec97b, BBS+97]. **multilevel** [AEJ91, Nal92a, LLSY92]. **multilocal** [BA90]. **Multiminima** [Taş93, Žit94]. **Multiparticle** [Mon94]. **multipartitioning** [ZC99]. **Multiphoton** [Ata97b, BFV92, DlD99, Moi97, Ata94, Ata97a, BFV94, Hag99b, JY94, KSK91, LA97]. **Multiple** [AT99, BC97a, GR95b, GH96a, HGC93, JM93a, JKJ94, JKJ95, JSG97, MKM97, YPC97, And93a, HHPT91, MBML91, Sch92a, SBL+94, TC98c, GR96b]. **multiple-minima** [Sch92a]. **Multiple-Reference** [GR95b, GR96b]. **multiple-transition-point** [And93a]. **multiplet** [PG96]. **Multiplets** [KT96, Nag95b]. **Multiplication** [KL93c, FCMB99]. **multiplicities** [STM96b]. **multiplicity** [MW90a]. **multiply** [BCLS94]. **Multipolar** [BP96b, LS93a]. **Multipole** [Gus98, KY93, KJ93, Le 97, McD97, Pan95, KY92, PA92, PNB94, SPS96a, SKRK90, SLL+91, ZZ93]. **Multipoles** [ÁC94]. **Multiquantum** [Kov98b]. **Multireference** [DM94b, Hir92, JG95, KD95, WSW96, Wen98, vDvLR99, Cim96, LC90, MUMH97, SS92d, TGS99]. **multishell** [BG98b, BG98c, BG98d]. **muon** [SJ91]. **Mushrooms** [Art97].

mustard [BVV92, BHV96]. **Musulin** [Zho94]. **mutagenic** [PWL95]. **mutation** [LF90]. **mutations** [NWG+99]. **Mutual** [GJ95]. **Mutually** [Bro93, CDG04, DMFR93]. **MVO** [Was91]. **My** [Roo93a, Cle92a]. **Myb** [JTZ+96]. **mylar** [Por97]. **Myoglobin** [SPC96, PS92c]. **mystery** [Sil95, Sjö96].

N [CEM+96, Eri92, Kor90, Kum93b, MM94, SP91, SSM+99, Str92, WYW96, YK97, ZC96, IP93, KSN93, Tit92, AEAO99, ABDM94, ASM91, BMA90, CLGW95, DSS90, DOPS91, DZ97, Eva97, FDC92, GV93, Hir92, HB95, Kal90, KBGE97, LC93, MK90, MZ95, PGM95, PGS97, RK95, SE93b, SK99a, SP92a, SW95, SSM+99, SES93, STC96, Tew94, Tew97, Yam90]. **N-** [LC93]. **N-Acetyl-2** [RK95]. **N-band** [Yam90]. **N-Sulfinylanilines** [AEAO99]. **N-threonylcarbonyl** [SSM+99]. **Na/W** [KO95]. **NaBr** [MTNF99]. **NaCl** [JMD95, JSG97]. **NADP** [GVK99]. **NaK** [Man99]. **naked** [HCRR94]. **NaN** [YK97]. **nanometer** [KDHW90]. **Nanoparticles** [ZLWES99]. **Nanotubes** [TAY+97]. **naphthalene** [VDBPR97b]. **naphthalenophane** [RGHH94]. **naphthalenophane-1** [RGHH94]. **Narrow** [Ara94]. **Narrow-Band** [Ara94]. **National** [Bir94]. **native** [TD99]. **NATO** [Ano92j, Ano93h, CD81, Eri92, Kar93, Yur95]. **Natta** [Nov92, Sak97]. **Natural** [BW99, BCD95, Löw95e, Löw97b, PKM94, WZ94, BP93d, BC93, Cio90a, LO90]. **Nature** [Bad95, DP94, Fuk95, Kap99, SG93, CP99b, MZ91, SG92, SLL+91]. **NB** [JMP99, SAB+97]. **NbIr** [CKM91]. **NBMO** [AI99]. **Nd** [Bou96, Li93, AS93]. **NDDO** [Ney95a, Ney95b, Cul95, FZZ92, NSTFC94, SGGC99, ZFZ92]. **NDDO-based** [SGGC99]. **NDDO-type** [ZFZ92]. **Ne-Isoelectronic** [SS92b]. **Near** [Bad95, Dat95, GSSD+96, Kov98a, MVL96, NWT92, PDO92, KSH92]. **Near-equilibrium** [NWT92]. **Near-Hartree** [PDO92]. **Near-Infrared** [GSSD+96]. **Near-Sighted** [Bad95]. **nearly** [vMVvLvD97]. **need** [RWT91]. **Negative** [BJLK98, Sie93, ZW96a, Har94]. **Negative-Energy** [BJLK98]. **Negatively** [HL93b, NS97a, TIA+92]. **Neglect** [NS95a, NS95b, NE95, Ney95a, Ney95b, ACZ91, BZ92, EZ92, NSTFC94]. **NEH** [UJS90, PHH94]. **Neighboring** [Gin97, SY91]. **Neocarzinostatin** [MC94]. **Neon** [PL98, YM99, TKSH93]. **Nesbet** [Cim96]. **Nesting** [Mez97a, Mez94b]. **Net** [GLLY94, MSP94, LLL91]. **netropsin** [BS91b]. **Network** [AFTM95a, AFTM95b, AFO+97, AFTM98, AFZ+99, BHH92, Hop90, Rig92]. **Networks** [VHFL93]. **Neumann** [Emc97]. **Neural** [BHH92, Hop90, Rig92]. **Neuroleptic** [CMA+99]. **Neuromolecular** [WPB98]. **Neutral** [CBAM97, CDDV93, KSN95, RKN97, CKB91, DB97, DS90, Ram90, SB90, TK92]. **Neutron** [Mar98a]. **Newman** [Kum93b]. **Newton** [ZA95]. **NEXAFS** [PÅS+97]. **NF** [WSB94]. **NH** [BBC92, PPSK96, TFSZ95, XFF98, JMP99, DR92, DWB98, FCVL98, GWB97, LDGA96, MLT98, MHY98, PS93, PPSK96, PPK97, SL93, SPS96b, WY99, YD96]. **NHDP** [GVK99]. **NHNH**

[Gao93]. **NHO** [Mar97c]. **Ni** [BDD93, ROL+90, SG96b, SGB97, SGB98, BDD93, BL98, Cas92, CCS99, FWS97, GMR+93, KJ97, MtPC+96, SW92]. **Ni-Al** [KJ97]. **Nickel** [BDD93, ETV94, LEG+94, MDJ98, BT96, PBS99, BB93]. **nickel-iron** [PBS99]. **NiCO** [XLW+99]. **nicotinamides** [AHM97]. **nicotinic** [AHM97]. **NiFe** [DFGB99]. **NiFeSe** [DFGB99]. **NiMo** [XYC98]. **nine** [Ran95]. **nine-membered** [Ran95]. **Ninth** [MDS98]. **NITM** [Ell92]. **Nitrate** [CXL97, ESP98, PSCZ97, ESHP99, Pro95]. **Nitric** [JZ95a]. **Nitride** [BKS96, DJF98, SP91, VCMLL90, ZSK97]. **Nitro** [DB94a, PGS97, SSMK93, Shu96]. **Nitro-Substituted** [SSMK93, Shu96]. **nitroaniline** [LKM99]. **nitrocubanes** [CKB91]. **Nitrogen** [CCG+96, GBL97, HDB+95, Jur96b, Jur98a, Jur99b, RD98, SZ98, WYW96, CS96a, CS99, OS92]. **Nitrogen-Containing** [RD98]. **Nitrogenase** [SZ98]. **Nitroimidazoles** [WR96]. **Nitromethane** [Jur97c, SCP95]. **Nitronyl** [YNY99]. **Nitrophenylcyanate** [Mor96c]. **Nitrophenylthiocyanate** [Mor96c]. **Nitrosyl** [BCRL94]. **Nitroxide** [TD96b, YNY99]. **Nixon** [EMMHP92]. **NJ** [Str92]. **NMDA** [GJLA99]. **NMR** [LSGS91, BZ92, DM98, EB97, FWT+96, Gal98, GARC97, LT99, LUU90, LCP+91, Mon98, NN94, SCL96, SZ96, SZ97a, SD96b, TL98, Tos95]. **NN** [CP99b]. **NNO** [CRK+91, SP92b]. **NO** [Cai94, SZCO99, EKI94, BK94b, GWB97, HMGP93, HHPT91, RKH+98, VJ95, VJ97]. **no-pair** [EKI94]. **Noble** [NTL96, Csa94]. **Nodal** [SD96a]. **NOESY** [LSGS91]. **Non** [CFB97, GS90a, MS91, Mor93b, HS92d, II94, KR91, Per93, KLM91, OK96]. **Non-** [Mor93b, Per93]. **non-adiabatic** [II94]. **Non-Bloch** [OK96]. **Non-Born** [CFB97, KLM91]. **non-Hartree** [HS92d]. **Non-local** [MS91, KR91]. **Non-radiative** [GS90a]. **Nonadditive** [KSN95]. **Nonadiabatic** [Ata97b, BS93, BM96, BK94b, BKLv95, KA95a, KO95, MPR97, NKS+96, Pet92, SOK+98, SBZ92b, SJ91, Tul91, CSG99, GPS90, xLTY92, PY92, SBZ92c, TFT+91]. **Nonadiabaticity** [BSS96]. **nonapeptide** [NSS92]. **Noncanonical** [Gin99, NU95]. **Noncommutative** [Gin98]. **Nonconventional** [SKS98]. **noncorrosive** [KPM+90]. **noncovalent** [WP90]. **nondegenerate** [Pal91]. **nondisjoint** [AI99]. **Nonempirical** [BDH+97, DKM96, DKWM97, DKM97, FDD95, NS95a, NS95b, Ney95a, Ney95b, HBJ+92, NE95, ROL+90]. **Nonequilibrium** [CT95, GG97a, RB95, KH90]. **Noninteger** [KKT97]. **Nonintegrable** [Pri95]. **Noninteracting** [HM95, OYL91]. **Noniterative** [NU95]. **Nonlinear** [Áng93, BZ90, CV98, CT96, DB94a, Hom93, Kie97, Kir92, LFS94, Mar93a, Mor93a, Ott94, PB95c, PB99, PK94, SPH98, SM99, SB97a, Sas90, Sch93, Wen96b, AMC97, ADB95, DCK92, Eri92, GFS92, KMR92, MKP91, MB92, PFK99, Rat92, Sch94, SB92a, SMH92, Wen96a]. **nonlinearities** [Hei90]. **nonliner** [LO93]. **Nonlocal** [ABR95, AS95, CGR+94, CA97, EMMS94, FT97b, FSVZ97, GRBA92, GRB+93, GBRA94, JWG95, RRS97, VB94, Sem94]. **nonlocality** [MA99a]. **Nonmetallic** [RMPR98]. **Nonorthogonal**

[DV98, Fer96, Iga95, CB99, RTS91]. **Nonorthogonality** [Sin92]. **nonparabolicity** [EC96]. **Nonperfect** [CR96b]. **Nonperiodic** [MAI95]. **nonplanarity** [HGL99]. **nonproduct** [DD97b]. **nonradiative** [BKY99, Chr92]. **Nonrelativistic** [AH97, BKL97, BLK97, BKL98, GLMP98, HMLK98, RW99]. **Nonresonant** [CPA98]. **Nonrigid** [BK98, Kel97, SSM90]. **nonrigidity** [HGL99]. **Nonseparable** [TE96]. **Nonsingular** [BSS97a]. **nonspherical** [LB96b]. **Nonstandard** [SJB90, JM96a]. **Nonstationary** [NMKP94]. **nonsteroidal** [BD95b]. **nonuniform** [Iva96, Iva97, OYL91]. **Nonunitary** [BA93]. **nonvariational** [Geg91a, Geg91b]. **nonzero** [BG98c]. **norbornenone** [KH96a]. **Normal** [DJ95, KC98b, Nal91, Nal92c, NK98, PP98b, DJ12, HW91, KLC98b, TFYY91]. **Normal-Mode** [DJ95, DJ12]. **Normalized** [Ell91, Ell92]. **Norman** [Ano96-58]. **North** [Bir94]. **Note** [BDT96, BNLF96, CC97b, DC95, AB99, TMH94, Wen93]. **notes** [Ano92i]. **Nova** [Ano92k]. **Novel** [DBG92, DQB97, EK94, SP94]. **novo** [SKM99]. **NR** [PZTPMC99]. **NSF** [Ano96-31, FG96]. **Nuclear** [AS96, AO93, BCMÖ97, HS91, JBT$^+$95, Mic96b, PTC94, RGO94, SPH98, US97, BCC99, Bla99, DRGC90, DÖ94, DM92, FV96, GSM90, GR95a, Hag99a, KH96a, MTNF99, MM93, MC91a, MC91b, PVČ$^+$90, SK99b, SBZ92c, VPŠ$^+$90, WO92, ZP92b]. **nuclei** [ASM91, VCCM92]. **nuclei-centered** [VCCM92]. **Nucleic** [AP96, RFG99, Tew94, ACC92, FHHE90, Les92, PTM92, SSM$^+$99, Tew97]. **Nucleophiles** [PBB92]. **Nucleophilic** [DD93, DGMW90]. **nucleotide** [LJS94, YJL92]. **nucleotides** [KJL96]. **nucleus** [BBCL92, HFM91, MFH91]. **Number** [JM96b, TT98, TMH94]. **Numbers** [KKT97, KS96, HS92c, KTCN93, LG92]. **Numerical** [AHI96, AH97, Bra97a, CGS$^+$94, CFB97, Csa96, DP93, FDF97, FS93a, GPD94, GWCT97, Hag98, IYFI99, KWT95, Loh96, NY98, NYNY99, Núñ94b, Roc99, SB95a, SB97b, BFW92, Csa92, Hag95, Hag96, JE90, KT95, SN99, Tal93, DD89, Cal90e]. **Numerov** [Sim97]. **Numerov-Type** [Sim97]. **Nunn** [Ano91z, Ano91-27]. **NWChem** [BAF$^+$95]. **NY** [Ano92k].

O [BA91, BILA95, BB91, BFRN90, BDH$^+$97, CLOFR98, CJX$^+$92, GPS90, IBS95, JH90, Jur97e, Li93, LF95, MGNK95, Min94a, MZ95, NM95, Ort98b, REU$^+$91, RCWN94, SRP$^+$98, SBAD90, TJ97, WI96, WL99, WMD95, XYC98, ZBL99, ABDM94, BMA90, BA91, BZMR92, BRV90, BB91, BYE$^+$97, BYGA99, CGG96, CLGW95, Csa96, DSS90, FCVL98, FSW$^+$91, HJ94, HP98, KS95a, KH96a, MCL95, MALT96, MTD93, MLK94, NL96a, OSS95, RKH$^+$98, SCA93, Sem94, SGB97, TFSZ95, WFS93, WY99]. **O-Acylation** [SCA93]. **O-ethyl** [HJ94]. **O/** [MTD93]. **object** [WP95]. **objects** [CC92a, CC92b]. **Observable** [JM93b]. **Obstacle** [Art97]. **Obtain** [PM95]. **Obtained** [HLS94, KY93, MSCP92, Par92b]. **Obtaining** [Val96]. **OC** [Bou96]. **occasion** [Ano94-36]. **Occupancies** [PS96]. **occupation** [HS92c]. **Occupied** [Nag95a]. **occur** [FL95]. **occurrence** [BCD91]. **Occurring** [FS94, FS95b].

Occurs [Sim93b]. **OCl** [Fra99]. **Octabisvalene** [Gal96]. **Octahedral** [LT99, BUZ94, Bro96, Ell92, FC99]. **Octakis** [Boč96]. **Octamers** [Kry98]. **octatetraene** [YAD92]. **Octupole** [BOX94, BP93c, BP93b]. **odorant** [WMW92]. **Off** [DMB97, Lás93, MTNF99, Whi99]. **off-center** [MTNF99, Whi99]. **Off-Diagonal** [DMB97, Lás93]. **Ögretir** [Ano92j]. **OH** [Jen94, Ort98a, SZCO99, BA91, CLOFR98, CDB90, FV96, Her93a, Her93b, Jur97e, SL93, VES$^+$99]. **Öhrn** [Ano94-36]. **Olefins** [BTN98, NHN97]. **oligomer** [Kir92]. **oligomeric** [CPA98, DDA92]. **Oligomers** [ÅGL97, BSB94, DWR99, JSKC95, CA90a]. **oligopeptidase** [JGCJ96]. **Oligopyrroles** [TTK99]. **OM** [RKG96]. **OMe** [NSS92]. **On-Top** [PEBS97]. **oncogene** [YSJ94]. **Oncoprotein** [JTZ$^+$96]. **One** [Bad95, BP96a, BF94, CL94, Day95, Day96, DDP96, Eid99, Flo97a, Fri93a, Gin96a, HWS92, IY99, KD95, Kup94, MBA97, MAD98, NV94b, NB97, NYLBNSB97, NB93, Núñ95a, Núñ96, Núñ97, OKY$^+$99, SP90, SB97b, SSD96, Spr96, TBČP95, WT98, Wil96, ZYY95, BL92a, BS91a, CAM$^+$97, Cio90b, DD99, Flo97b, For92b, JGP91, KG92, LC90, LLL91, MZ91, Mic96a, MD93b, NYKY98, PP92, PVN90, PKJ99, RLR90, RSCP91, Sil95, Sjö96, Spr93, SBZ92a, TKO$^+$92, TTOY93, ZFZ92, DB94b]. **One-** [IY99, SB97b, SSD96, LLL91]. **One-Band** [MAD98, For92b]. **One-Center** [BF94, SP90, JGP91, ZFZ92]. **one-component** [BSS97a]. **One-Dimensional** [Eid99, Kup94, NV94b, NB97, Núñ95a, Núñ97, TBČP95, BS91a, KG92, MD93b, NYKY98, RSCP91, TKO$^+$92, TTOY93, DB94b]. **One-Electron** [Bad95, CL94, Day95, Day96, Flo97a, Fri93a, KD95, MBA97, Núñ96, Wil96, Cio90b, Flo97b, PVN90, PKJ99]. **One-Matrix** [WT98]. **one-particle** [LC90, SBZ92a]. **One-Range** [HWS92, RLR90]. **One-Step** [DDP96, DD99]. **Ones** [CCE$^+$93]. **onions** [DI95]. **only** [KL92a, SS99a]. **ONOO** [KK93]. **ONOOH** [KK93]. **Onset** [GBJMA94]. **Open** [BMA93, BG95, DZ96b, GV93, HT97, JPJ95, KSY97, Kol97, NU95, PAT93, PGH95, Was96, HVS98, KMP$^+$90, KM90b, KS90, LP98, MHG95, Pal92a, PMDM97, PZDM97, PMDM98, PZDM98, YOTY93]. **Open-Chain** [DZ96b, GV93]. **Open-Shell** [BMA93, JPJ95, KSY97, Kol97, PGH95, Was96, HVS98, KS90, LP98, MHG95, Pal92a, PMDM97, PZDM97, PMDM98, PZDM98, YOTY93]. **Opened** [KMVÅ95]. **Opening** [JZ95b, CAM$^+$97, LAM91]. **Operator** [CG95, DJ95, Day95, Day96, EP98, Her97, RJ97, ZWZ96b, BG98b, DJ12, KRRB99, KS90, PZA92, VÅJ$^+$92]. **Operators** [AFTM95a, AFTM95b, AFO$^+$97, AFTM98, FBKD97c, Flo97a, KFS92, Löw93c, MV98b, NYLBNSB97, NB93, Núñ94b, Oht98, Pal93b, RH96b, Sie93, AFZ$^+$99, ERC91, Flo97b, FJR96, Hud99, KLO$^+$98, KA95b, MPSLB91, NI94, Ort98a, Smi99, Tom91]. **Opiatelike** [ZCT98]. **opioid** [PVU$^+$93, CML92]. **OPP** [LAM92]. **Oppenheimer** [AZ99, CFB97, KLM91, RL98, STY$^+$98, SNNY99, Sut99a]. **Opportunities** [SS97a, PK94]. **Optical** [AL98, BMG$^+$98, DWR99, DB94a, DREW98, HU94, LFS94, LEG$^+$94, Mor93a, Ott94, PO97, STM96a, SDG97, ZLWES99,

AMC97, ADB95, Aon99, DCK92, GFS92, KMR92, Kir92, LO93, Lev94, MB92, PK94, Rat92, SM99, SB92a, SMH92, VABM94]. **optics** [Eri92, MKP91]. **Optimal** [BJLK98, RD98, GVB96]. **Optimally** [TM93]. **Optimization** [BBC+96b, CTG97, FGRS98, GVC96, Hoo94, Kol97, Kov90a, Kov90b, MAI97, MT96, VHFL93, CTC95, CGMG92, KP92, Min90b, OYNY98, Sch92b, TTM99, ZA95]. **Optimizations** [TJ95, VFHL93]. **optimize** [Sir99]. **Optimized** [Ada91a, BC97b, EBG95, GG97b, GvLB96, Huz96, MKM96, MS93b, Nag98b, PG94, Pen93, Pen96, RSGC96, Sch95b, WBP91, GV92, HZF+91, MM99b, MS92, TC98c]. **Optimized-Basis-Set** [Pen93, Pen96]. **Optimum** [FB90]. **Options** [MPR97]. **optoelectronics** [Mun92]. **Optogalvanism** [YM99]. **Orbit** [HBL99, KMVÅ95, RL92, SFG+98, BG98b, BG98c, BG98d, ERC91, JRS+99, KLO+98, KRZ91, Man95a, Man95b, Man99, PW91, TSY99, Tit92, VÅJ+92]. **Orbital** [AEAO99, And90, ATI97, BR94, BFH96, BEJ98, Bro93, Cio94, DE92, GBVM93, HAEMA92, HS92b, Hed95, Hil98, IYFI99, JKRW98, JGR98, JMR98, JZ95a, JZ95b, Jur96a, KUN+98, LP97b, MH98, MSCS95, Mor97a, NS95a, NS95b, Ney95a, Ney95b, OSA+97, PS96, SRS92, SGGMGFS96, Sta96a, Sta97, Sta98a, TMSI98, TMP97, TD96b, Wan94, Zha92a, ZLHZ94, AEHM91, AHM97, Ada91a, Cio90a, CA90b, DO90, FMR91, GV92, HS92c, KDB90, KH96a, KCLI95, LMMK93, LO90, LTY90, Mar92a, MKDL93, MLL99, MCA92, NE95, OKY+99, PCB92, Pau92, PP90, RK91, RMF90, SCA93, SX96, SCJK90, SKRK90, Sta95, Sta96b, Sta98b, Sta98d, Sta98e, SS98, TTM99, TH90, TYY91, WB94, WL90, WP92, Zha92b]. **orbital/molecular** [RK91]. **Orbitally** [GWCT97, NM92, Nal92b]. **Orbitals** [BW97, Bro93, BJLK98, Coo96, DTS97, DDD93, EBG95, FD93, GM94, GVC96, Gin95, Gin99, GY95, GİA96, Gus98, GOAY98, Her97, HO94, Huz96, Ish96, Jon97, Jur97c, LLL97, MYN+96, MBA97, Mey94, Mey97, MR92b, MS93b, NMM97, NU95, PBB94, PGH95, RSGC96, RMPR98, Spr96, Ste96, TV92, WZW96, BBK90, BJA99, BP93d, Bud92, BFW92, CKB91, Cio90a, CC91b, Cio91, DM94a, DRGC90, EJ93, För92a, HS92d, HOF+97, JE90, JEB92, Jon92b, Jon93, KKNY99, Kov90a, KK90, Le 97, LLB99, MAC96, Min90a, Nob99, Ort98a, Ort99, RD90, RTS91, Sir99, Tal93, TMD96, Was91, ZZ91, ZZ93, ZWD98a, ZWD98b]. **Orbits** [Ols96]. **Order** [ASP97, AR93, BBS91, BSB94, BP96b, CV94, CB94b, DM96, DB94a, DM94b, DMB97, Eid99, FR93b, HM97b, KSY97, KD95, LS93a, LFS94, LJN+98, Mor93b, Ort98b, Sam97, Sie93, Sim93b, Sim98, SP94, SATP94, SPL97, TD96a, VVS94, VIK98, VFHL93, ZO95, Ada91a, Ada91b, BSS97a, BKL91, BCD91, Cim96, DHDP92, DCK92, EMP92, GFS92, HC91, HC96a, HC96b, HC96c, HC96d, KMR92, KLO+98, LYSL95, MNT96, Mar99a, Ort97, RNS93, SDO91, SB92a, Sim99c, Suh93, TFYY91, TC98c, Tos95, VÅJ+92, VCMLL90, WKP+95, ZM95, ZC99]. **Ordered** [LRM96]. **Ordering** [DTA+96, FD96a, LFD99, MGNK95, MVB92, NWT92, SB95b]. **Orders** [RG94, RPT90]. **Ore** [US96]. **Organic** [Jen99, KM97, Mor93a, Sta97, TMDB98, Ano92j, Ano93h, Ano96-58, AI99,

BLC95, BHH92, Csi76, Csi77, CD81, FCA91, FKR92, FS99, GFS92, HS95, KMR92, MKK96, Mar93b, MAAP90, MPP92, OCK99, Pár98, PSBL98, SPB90, Smi96, Sta98b, Yam90, MKP91, Eri92]. **Organization** [Lun92, TD03]. **Organized** [AR96]. **Organomagnesium** [OSA+97]. **Organometallic** [DDH+96, DRBE96, Tch96a, ARDP92, BDPS97, CEZ+99, KR91, Yam90]. **Organonickel** [TB95]. **organophosphorus** [Kin94]. **orientation** [CL90, Tew97]. **Orientational** [Kry98, MVB92]. **Oriented** [SWF93, WP95]. **Origin** [BDT96, MBA94, Sak98, TBBE98, TI94, ZH99b, KMP+90, Le 97, Pop90]. **Origin-Shift** [BDT96]. **origins** [Par90a, Cio93]. **Orthogonal** [Bro93, GPč94, KL93c, WZ94, Ban91, KM90b, MM94, MPSLB91, Pau92]. **orthogonality** [Wil99b]. **Orthogonalization** [KRB+97]. **Orthogonalized** [GVC96, LLB99, NE95]. **Orthogonally** [PTP95]. **Orthonormalization** [Löw93d]. **Oscillations** [ANB96, DMB97]. **Oscillator** [CB93a, Coo94, DBB94, KMP97, LDGA96, Lef97, MS97b, Pal93b, Pal97b, Pal98, RJ97, SB95a, SB97a, AR92, BRL92, BADM97, DOPS91, DW90, KSF91, LC90, MLB92, MK90, PRSDS92, Pal91, PV91, Réa90, SP90, YBZ92]. **Oscillators** [NYLBNSB97, RDF98, SB97b, TZ97a, DB94b, Fan90, WN90]. **OsO** [NS91]. **Other** [CCE+93, CRK+91, FLWZ90, Hag92, HC96d, SPM+96, SKM99]. **Our** [Löw97b]. **Outlines** [Lad97a]. **outlook** [KK92b]. **Outperform** [JCM+92]. **Overcoming** [Rey90]. **Overcomplete** [Per98]. **Overlap** [Day95, Day96, GİA96, GOAY98, HO94, HS92f, Jon97, MMD96, NS95a, NS95b, NE95, Ney95a, Ney95b, VR95, Zha92a, ACZ91, BZ92, EZ92, Jon92a, JEB92, MRC99, NSTFC94, ZZ91, Zha92b]. **Overlapping** [Fer95, KPTS97]. **overlaps** [GV92]. **overtone** [KSF91]. **Overture** [Bal96]. **overview** [TCM99]. **Ovomucoid** [NK96a]. **oxepins** [Tri98c]. **Oxford** [Cal90f, Cal93, Deu96, Jør92, Kla93, Kum93b, Kum93a, Lin93, Lin96a, Mic96a, Str93]. **oxidase** [RC99]. **Oxidation** [NHN97, BBB+95, LC93, PHBB94, YNST99]. **oxidative** [HDB+95]. **Oxide** [HLS94, JZ95a, Jur98a, Bro95a, GWB97, KCP90]. **Oxides** [BK94c, ETV94, Jur96b, SDE94, MS93a, Nor91, Yam90]. **Oxidized** [TTK99]. **Oxirane** [KMVÅ95]. **Oxo** [GL97, MRT97]. **Oxo-amino-Tautomers** [GL97]. **Oxo-Hydroxy** [MRT97]. **Oxohalides** [CCG+96]. **Oxohydride** [RKG96]. **Oxygen** [BLE96, BvL96, GMR+93, JM96c, KFS92, LV98, MGNK95, Min96, RP98a, SFGW96, UWB94, YNMT98, YTYS97, CSH99, FEE+98, Kha91, Li97, MLK94, OS92, SAB+97, SM92a, SKC99, SW92, BB93]. **Ozone** [RRS97, BH99, NÅJ91, NÅJ92].

P [BKL97, Brä98a, Brä98c, BCY95, BZQ95, CRsP93, Eri92, Kar93, Kor90, SPFL93, SP91, Sjö96, Str93, TIPM96, Tri96, BLK97, DWR99, LB94, MEP90, BRL92, Man99, Mar97b, PWL98, RSCP91, SC95, STC96, WG94, PAT93]. **p-phenylenevinylene** [DWR99, LB94]. **P450** [CL90, KKS99, LC93]. **P450cam** [CLR+93]. **Package** [BFH96]. **packet** [BYGA99, PY92, PL91].

packets [Bar90]. **Packing** [RK95]. **Padé** [CG95, CB93a, HC96d, LKLBD98, LBPL97]. **Padé-Type** [CB93a]. **PAF** [DBF+96, DBF+96]. **page** [Ano90-29]. **pages** [Car96, Lin96a, Sjö96, Kla93]. **PAH** [VS95]. **Pair** [CJA94, CPTR96, FW92b, KM92, MV98a, PEBS97, PS94a, PB95c, PJ96, Pon97, Pon98, ROSM96, SP94, WS94a, ZH99b, AS95, BHV96, EKI94, FL95, GDF92, Ish92, KSIH92, LK90, MRD92, PCD99, PB99, Røe91, TGS99, TG96, Zie96, FW92c]. **Pair-Density** [PEBS97]. **pair-excitation** [KSIH92]. **Paired** [KSG93, GT97, Pau92]. **Pairing** [DMB97, May97, Pon98, She90b, Ukr94, KŽ90, LRM93, PS99, Tac94]. **Pairon** [CYY95]. **Pairs** [BL92b, Brä93b, CD93, HNB92, KV96, SM98, ZL98, AGNS92, LM91, LJS94, RFG99]. **Paldus** [BG98b]. **Palladium** [MÅ99b, AGNS92, FS99, SCP93]. **Panacea** [Coh97]. **Papain** [DV91]. **Paper** [LZ92, LZ94, Ano90g, Ano90i, LZ91]. **paperback** [Str93]. **para}** [LKM99, TKK+90]. **para}-nitroaniline** [LKM99]. **Para-quinones** [TKK+90]. **Parabolic** [LP97c]. **Paraboloidal** [CLKMTA95, LKFF98, LKVS97]. **paradigms** [TD03]. **paradox** [Ran94]. **Parallel** [BAF+95, EP98, GSSD+96, HL93a, PSS97, Xu96, ACB+99, Fer92, FKHD97, Har91, KJD+93, Ken93, LGBL94, LS99, Suh91]. **Paramagnetic** [LZ96, BBCL92, BUZ94]. **Parameter** [DFL98, GSM98, KCI98, JJ96, KKK90, MNT96]. **parameterized** [Loh91]. **Parameters** [BDD93, EMMS97, GİA96, MM98, NG95, Por98, TV92, DLF99, MSS99b, NL96b, PACO90, Por97, Por99, SC96, WA94, WZ99]. **Parametric** [MK98b, RJ97, SRM98, HDB+95, YG90]. **Parametrization** [AV92, GLBM96, JK92a]. **parametrizations** [WW97]. **parametrized** [SGGC99]. **Parentage** [BK94a]. **Pariser** [Ano90-27]. **Párkányi** [Jen99]. **parnassum** [And93b]. **Parr** [Cal93, Ano90z, Ano94i, Ano94-37, Iva96, Iva97, Par94a]. **Parrinello** [Kry93]. **Part** [DPP+94, MDS98, GVB96]. **Partial** [Kat97, LB96b, MTTS93, Ort97, RH96b, GZDZ97, Kat91, Lin92, SN99, VA90]. **Partially** [GVC96, GV92, PK90]. **participants** [Ano90a, Ano90b, Ano91a, Ano91b, Ano92q, Ano92a, Ano92b, Ano93k, Ano93a, Ano93b, Ano94a, Ano94b, Ano95r, Ano95a, Ano95b, Ano96-31, Ano96-29, Ano96a, Ano96b, Ano97n, Ano99i, Ano99k, Ano99l, Ano99m, Zer98b, Ano96-30, Ano99j, Tri98b]. **Particle** [Bla96, DP97, Ino96, Lev97, MPOG99, ZWZ96b, AGH91, BMDM90, CC91a, LC90, LLL91, NM94, NS92, Sch92c, SD91, SBZ92a, WA94]. **particles** [BMFPV92, GSM90, KSH92, KSW98, Mar93b, OM91, Woo99]. **Partition** [RWT92, Kin94, Luk92, RWT91]. **Partitioning** [Cio90b, IY99, JKK+92, KS90, MR99, Muk96, SKS98, MG93a]. **Partitions** [FJRS97, PM97]. **Partner** [MPOG99]. **parts** [Ska92]. **Path** [BA91, CBG94, KNA94, KNN96a, KNN96b, KKNN97, Mar94a, Min94b, NONY97, Oku98, Pon97, BA92, Hei95, Mat97, Nag96, RD97, ZB92]. **path-integral** [Nag96]. **paths** [AM90a, AM90b, CE90, LAM91, LAM92, MBM92]. **pathway**

[SHF94, WJC+98, WJC+99]. **Pathways** [Fir94, FK98, LB93, CF99, TCB99]. **Pattern** [Kry98, LBBE98, Mar95c, TBBE97, LaF90]. **Patterns** [WBD97, Sin92]. **Pauli** [NM91, Pec93, QS98, SZ97a]. **Pauli-Type** [SZ97a]. **Pauling** [Zha91]. **Pauncz** [Zer99b]. **PaX** [NMCK92]. **Pb** [GARC97, YK97]. **PBE** [MSMR99]. **PC** [NSÁS+90]. **PCM** [AGAP98, TCM99]. **PCO** [HZ91a]. **Pd** [BYE+97, CCB+97, SZC97, SCS94, XKB+99]. **PdO** [BYE+97]. **peculiarities** [BSS+97b]. **Peel** [FHHE90, HE90]. **Peierls** [ATI97, Kup94, LN96]. **Pentacoordinated** [DBG92]. **Pentalene** [BBOR96]. **pentamethyl** [BB94]. **pentamethyl-cyclopentaldienyl** [BB94]. **peptidase** [DD99]. **Peptide** [NAK95, PFMC97, SKJ98, WHF92, Jac92, JGCJ96, KM99a]. **Peptides** [PFMC97, NMSJ99, PVU+93]. **Percival** [Kar93]. **Perfluorodimethyl** [FDD+93]. **Performance** [AHI96, JG95, Mar95c, RAI99, BDPS97, CLGW95, GJPF92, Gut99b, Ken93]. **Pericyclic** [Pon97, JK90, OS90, PS92b]. **Perimetric** [LKBJ97]. **period** [Cle92a]. **Periodic** [ANB96, GKS99, LV98, MCM98, NNMH96, NK96b, NB97, PSBL98, ZYY95, For92b, LO93, VZ92, ZWD98a, ZWD98b]. **periodically** [FS95a]. **Periodicity** [Har98a]. **periods** [Kor90]. **Peripheral** [MZ93, GVV+90]. **permanent** [KY91a, KY91b]. **Permanganate** [DZ96a]. **Permethylated** [RM99]. **Permutation** [KSG93, SAR96]. **permutations** [Che92]. **peroxidase** [CL92]. **peroxide** [MSS99b]. **peroxy** [BHGC99]. **Personal** [Par94a]. **Perspective** [Rin94, SS92e, TD99]. **Perspectives** [CCM+96, Mos98, SC97, Hei95, Roo93a, Mat97]. **Perturbation** [Ada90, Ada91b, Ada96b, Ada99, AR93, Áng93, CJA94, CZ93, CB93a, CJH98, Gin98, IK97, KBT94, Kir95, KSY97, KD95, LD94, MHM95b, MV98b, RDF98, SG98, SAFK97, SAS99, Su93, SPL97, SJR91, TBČP95, Wen98, vDvLR99, Ada94, Ada96a, Cim96, Fer92, GL95, HC91, HC96a, HC96b, HC96c, HC96d, Hir92, Hol98, Ish92, KSF91, KLO+98, LC90, MHM95a, MUMH97, MRD92, MD92c, Suh93, SO97, VCMLL90, ZC99, ZP90, Suh92]. **perturbational** [TFYY91]. **Perturbations** [ANB96]. **Perturbative** [Gho95, LLB99, SB95a, ZON+96, IHG95, MD99, SS98]. **Perturbed** [AEAO99, DP97, LB98, MD93a, Nic99, Sur94, ABCM93, BILA95, Pic92]. **PES** [Ell91]. **PEt** [BUZ94]. **PF** [FAV92]. **PH** [SC99, PS93, WY99]. **Pharmacophores** [MBV+98]. **Pharmacophoric** [LBBE98, TBBE97, GVV+90]. **Phase** [BDT96, Boe98, BMP93, BZQ95, CM96a, CT96, CCZ97, DBB94, ET99, FY95, FD96b, HPSC97, Her98, JI95, JCÁ96, Mar97b, MSS99a, MLR+98, Oku98, SM98, Sim97, Sim98, SD91, VBUS99, VZ93, Wło94, Wło95, ZL98, BKL92, Cab96, CFMA95, DDN99, DLF99, FSW+91, Har90, KFK91, Mez90, Sas90, Sim95, Sim99c, TKO+92, TTOY93, TCS+90, VX99, WSM+94, ZDO96]. **phase-fitted** [Sim95]. **phase-lag** [Sim99c]. **Phase-Shift** [Sim98, KFK91]. **Phase-Space** [DBB94, Wło94, Wło95]. **Phases** [Mar94b, Mar97a, Lei99, NMN+99, NWT92, Lun92]. **PhD** [Ano99n]. **Phe** [LU92b]. **Phenanthrene** [CR96a]. **Phenol** [SC98a, HWB97a, WI96].

phenolic [PHBB92, PBHB95]. **phenols** [BP90, BHPB93, HB94, VES+99]. **Phenomena** [IK94, MÅ96, O'C96, Kum93b, Tom91, ZJ89, ZJ93, ZJ96, ZJ02, Kum93a]. **phenomenological** [DBM99]. **Phenomenon** [GMMH97, TMM97, ÅC92, BR92, SBZ92c]. **phenoxypropanolamine** [WTD+94]. **Phenyl** [MH98]. **Phenyl-** [MH98]. **Phenylene** [JKK+92, Lah92]. **phenylenevinylene** [DWR99, LB94]. **phenylethynyl** [TSRP99]. **PHGLF** [WD95]. **Philadelphia** [Mon93]. **Phloroglucinol** [MCE+93]. **Phonon** [BS93, KCP90]. **Phonons** [LMAK93]. **Phospha** [Jay92]. **phosphatase** [KÅ99]. **Phosphate** [FLRV97, KJL96]. **phosphide** [GL92, SP91]. **Phosphinidenes** [BC97a]. **phosphodiester** [BV93]. **phospholipid** [CPGC99]. **Phosphorescence** [FSHC99]. **Phosphorus** [CCG+96, GBL97, PD93]. **phosphotriesterase** [KK99a]. **Photo** [Ano99o, NMN+97, NMN+99]. **Photo-induced** [NMN+97, NMN+99]. **photobiology** [ESTM95, Kra96]. **photocaged** [RC92b]. **Photochemical** [DHL+94, FK98, Kha91]. **photochemistry** [CPN91, SCMF93]. **Photochromic** [MRRA92]. **Photodecarboxylation** [FY95]. **Photodesorption** [DDH+96, YBM97]. **photodetachment** [MCB99]. **Photodissociation** [DDH+96, Man99, MY99, GL96, II94, MIW91]. **photoelectrochemical** [KPM+90]. **Photoelectron** [DZOR98, Gin95, KM90a, LFD94, MKBP97, NVR+91, NV97b, TKK+90, KJL96, Ort97, PVF+92, YJL92]. **Photoemission** [BSS96]. **Photoenolization** [SC94]. **photoexcited** [TYY91, TYTY91]. **photofragments** [MIW91]. **Photoionization** [CM96a, DC97, LD94, LEA+94, SLD95, DD96, DD95]. **photoisomerization** [Ert90]. **Photon** [NMKP94, Hag99b, OB95, PSO90]. **photonics** [MKP91, Eri92]. **photosynthesis** [DM97b]. **Photosynthetic** [DTM96, SKTN97, CMSF93, STKN90]. **phototransfer** [LM91]. **Phthalocyanine** [GBVM93, HE90]. **phycoerythrocyanin** [SCMF93]. **Phyllosilicates** [NTL96]. **Physical** [BDD93, HSS+95, WK90, Del90, HYS91, JKGM99, Pea95, SS92e, DS99]. **physicist** [Roo93a]. **Physicists** [Mon99c]. **Physicochemical** [RVL97]. **Physics** [Deu96, HWB05, Löw90c, Löw94c, BKL92, Brä95, Brä98b, ČVW91, HW84, HW87a, HW87b, HW92, HW94, HW96, HW00, HW04, Hei90, Kry96, Lad94, Löw91a, Löw91b, Löw91c, Löw91d, Löw92b, Löw92c, Löw92d, Löw92a, Löw93a, Löw93b, Löw94b, Löw95c, Löw95f, Löw95d, Löw95b, Löw96a, Löw96b, Rau02]. **Phytochrome** [GDB98]. **phytohormone** [RTKP95, RT99]. **Phytohormones** [RT98, RTKP96]. **PI** [DD90b, AH92a]. **Pi-electron** [AH92a]. **Picture** [AH96, KS98, PS94a, BD95c, Car96]. **Pike** [Deu97]. **Pilar** [Str92]. **pilocarpic** [KE91]. **Pilocarpine** [EK94, KE91]. **Pilot** [ZM95]. **Pines** [Dun99]. **Pinnacle** [WP95]. **pinocarveol** [PRB96]. **piroxicam** [BD95b]. **pitfalls** [DVJ93]. **pK** [MK95]. **place** [WI96]. **plan** [Avi92]. **Planar** [JM96b, Jur98b, RH95b, KH96c, MFCA94]. **Planarization** [Tri98c]. **Plane** [PM95, BK97, HK95a, LTSL96, WM92, CLZ95]. **plane-wave**

[HK95a]. **Planes** [Mar97a]. **planning** [FG96]. **Plants** [ML97]. **Plasma** [YM99]. **plasmas** [Mar90, WYZ+92, ZW96a]. **plastoquinone** [MD94, MD95]. **Platelet** [DBF+96]. **Platelet-Activating** [DBF+96]. **Platinum** [BC97a, Boč96, MÅ99b, SFG+98, TSS97, SBPPH92, SC96]. **Platinum-Centered** [Boč96]. **Playground** [BA97a]. **pleated** [Suh91]. **Plenum** [Ano93g, Mon94]. **Plesset** [Cim96, HC96d, Hir92, KLO+98, Kir95, KSY97, MJS93, Pra97, SAS99, Suh93, VCMLL90, vDvLR99]. **plicies** [Löw95c]. **PM** [BHKK93]. **PM3** [DZ96b, GKKM96, LJS94, MALT96, MC94, NSS+95, HS92b]. **PMO** [SBM97]. **PNA** [ITT+94]. **Point** [AL95, LMR94, Mey94, Mey97, Sta91, And93a, AH92a, BA92, FCMB99, GKM90, KDB90, LF90, Mar92a, Mez90, PC99, Smi90]. **Points** [AB97, BLB95, BLRD92, KPA95, CE90, HR99, Mez90]. **Poisson** [PWL98, LP97a, PTH+97]. **Polar** [HP97, Mor97b, PRC98, BKY99, Ert90, KY92, RWT91]. **polarity** [DR92]. **Polarizabilities** [BSB94, BP93c, Can97, CMCR96, CZ94b, CMFA93, CAÖ96, DT96, KSY97, LL92, SS92b, SO94, AD92, BP93b, CA90a, CA92b, CMA93, Har94, JCA97, SDO91, SSC92]. **Polarizability** [GG97a, MRL99, TSRP99, CP99a, DBF+92, MFCA94, MCA95b, Par92b, PNB94, SGGC99]. **Polarizable** [FM92a, JCÁ96, PRC98, CT95, Cor92, MCT99, TCM99]. **Polarization** [AP96, AO93, CMFA93, DD93, GJ95, KL93a, MB98, OS91, SO94, DMR96, DD90a, DRGC90, JMP99, RC92a, Res99, SDO91, Smi99, WWFR99]. **Polarization-Induced** [MB98]. **Polarized** [Boe93, BS94, GR94, KLI92, McH91]. **Policies** [Löw90c, Löw91c, Löw91a, Löw91d, Löw92c, Löw92d, Löw93a, Löw93b, Löw94b, Löw95f, Löw95d, Löw96b, Löw91b, Löw92b]. **Politzer** [Tri96]. **Poly** [DWR99, Lah92, BL92a, GT97, LB94, GT97, LU92b]. **polyacènes** [GK90a, GK90b]. **Polyacetylene** [DD97a, GP97, LRM96, LRM97, MI93, RML97, VZ93, AKS+90, CMA93, CP99a, DY96, LTY92, xLTY92, Sas90, Sta98e, TIA+92, TYTY91, TTOY93, WL90, YYLB90, YITY93]. **Polyallyl** [Che93]. **polyamides** [ITT+94]. **Polyatomic** [BLBP97, DQB97, KPD93, LDGA96, WP93, Cal90e, CTF92, DD89, FLHT90, ZM90]. **Polyatomics** [MSD95]. **polyazamacrocyclic** [HBGR99]. **Polycation** [Lah92]. **Polycentric** [Wil96]. **Polycyclic** [LL92, RL94, BBLK94, KM90c, LYSL95, VRR92]. **polycycloalkanes** [DD96]. **Polyelectron** [PKM94]. **Polyene** [Mat99, CA90a, PP92, PP91, PČP92]. **Polyenes** [ATI97, BEG94, BE95, BE98, BČ95, BČ96b, GP97, IK94, JCA97, KBT94, KBGE97, LP96, RR94, ST93, KKL90, Kur90, LRM98, LP99, NNH98, Suh92, TWK98, MD92b]. **Polyethylene** [Gin97, And90, CA92b]. **polyethylenes** [DO90]. **Polyhedral** [MFAT98]. **polyhexapeptide** [LUU90]. **Polyiodide** [Sta97]. **polyisocyanates** [RBT99]. **Polymer** [Art97, LRM97, MAI95, PV99, PÅS+97, Sur97, PK90]. **Polymeric** [CMFA93, And90, BL92a, Dia99, FADC91, MFCA93, MCA95b].

Polymerization [Sak97, BT96, Jug90a]. **Polymers** [ÅGL97, ASI94b, CAÖ96, IAN+94, JSKC95, MAI97, NV94b, Ott94, PB97a, Sta96a, SL98, TMDB98, AMH93, Art94b, Art96, CA90a, CA92b, CFMA95, För92a, GJDD97, HZ91a, Kir92, LO93, LB94, Nob99, PK94, Sta98e, Suh93, TYY91, TYTY91]. **polymethine** [BBS90, Rep96]. **polymorphism** [CDM+94]. **Polynomial** [BČ96b, ČB96b, LKLBD98, NS95b, PM95, SYZ96, TZ97a, ZW96b]. **Polynomials** [Gin96b, KL93c, NS95b, DM97a, KRBT94, MPSLB91, SS92a]. **Polynuclear** [ML97]. **polynucleotides** [ITT+94]. **polyolefins** [BP90]. **Polyoxometallates** [DRBE96]. **Polyoxymethylene** [FFD98]. **Polypeptide** [Jac97, BOL+90, Jac98, Sch92a]. **Polypeptides** [DRBE96]. **polyphenyls** [MD92b]. **Polyphosphorus** [DZ96b]. **polypropylene** [FMD+94]. **Polysila** [KGv93]. **Polysilane** [RM99, And90, CA92b, CPA98]. **Polysilanes** [Yam97]. **Polystyrene** [LCV92, LV93, Por97]. **Polytetrafluoroethylene** [MVV+97]. **polytetrapeptides** [LCP+91]. **Polythionylphosphazene** [LJ95]. **Polythionylphosphazenes** [RL95]. **polythiophene** [MFCA94, Sta98e]. **Polyynes** [JCA97, Mor93a, MD92b]. **Pople** [Ano90j]. **Population** [PKM94, PS94a, PB95c, PJ96, Pon97, Min90a, OKY+99, PB99]. **Populational** [Nal97]. **Populations** [CPTR96, YBM97, MIW91]. **porphin** [YNO92]. **Porphine** [GBVM93]. **Porphyrazine** [LEG+94]. **Porphyrin** [RP98a, RKH+98]. **Porphyrins** [MZ93, HE90]. **Portable** [Har91]. **portion** [LS99]. **Poschl** [RABZ94, ZARB96]. **Position** [Mar96, Sch94]. **position-** [Sch94]. **positioned** [Whi99]. **Positive** [BJLK98, MVL98, SIM93a]. **Positive-** [BJLK98]. **Positive-feedback-enhanced** [MVL98]. **Positively** [NS97b]. **Positivity** [BA93]. **Positron** [TMSI98]. **Positron-Molecule** [TMSI98]. **Positronium** [BD94a, Ike99]. **Possibilities** [NMN+97, Rom92]. **Possibility** [KM92, NMN+98, NMN+99]. **Possible** [CAK+96, DS96, DZ97, SM98, KBM92, DZB92b, WJC+98, WJC+99]. **Post** [Ano99n, GL98, NL96b, BBTU97, HGL99, KL92b, MYN+96]. **Post-Doctoral** [Ano99n]. **Post-Hartree** [GL98, NL96b, BBTU97, HGL99, KL92b, MYN+96]. **postulate** [MBM92]. **Postulates** [Urr94]. **Potassium** [MBV+98, Bre99, ESHP99, KO91]. **Potential** [ASP97, AL98, AP93, AP96, AR99b, AK97, ABLA97, AD97, BBOR96, BR97, Bla96, CGLP96, Coo94, CL95, DFDK99, DREW98, DD93, FT95, FP96, FCVL98, GPS90, GBS+93a, GG97b, Gra97a, GvLB96, GVB97, GSM98, GW98b, HM97b, HWS92, Huz96, IP93, Jas94, Jur97e, Jur98a, KLLB98, KY93, KLLI97, LB97, LX95, Lio92, LCLO95, LBMR95, MD93a, Mez94a, MTD93, Min94b, MPR97, MK99, MM98, MPV94, Mor96a, MTL97, Nag98b, NK96a, OSS95, Pai97, PL98, PLA98, PPSK96, PPK97, QS98, RRS97, SS92b, Sch97, SGK+95, SR96, ST93, SS97b, SATP94, VH96, XR94, ZARB96, ACB+99, ARBB95, AGNS92, AKCS91, AR99a, ALS+91, BCLS94, BJM+94, Ber96c, BKL91, BML98, BFW92, ČDM91, CCS98, Cor92, CEM+96, Dav90, DBR+96, FT96, FT97a, FDD95, Gao93, Geg91a, Geg91b]. **potential** [Hag95, Hag96, Hag99b, HS93, Hir92, KR93, KY92, KLI92, KM90c, LLL92,

LV97, LM92, MD92a, MCOS94, MVS97, Mez90, MR92a, MPSLB91, MGLBP95, Mur90, NOYF92, NM91, Nal92a, Nes94, NÅJ91, NÅJ92, Pai91, Pai99, PW91, RSCP91, RA96, RK92, RAM91, SH90a, SP92a, SM92a, SM94, SPS96a, STS95, SN90a, Ska92, Sla92, Smi99, TNSM99, TCS+90, TM99, TŚPKM94, TC98c, VÅJ+92, VVO98, WDS97, ZP90, GZSvD99, SES93]. **Potential-Barrier** [MPV94]. **Potential-Derived** [KY93, KY92]. **potential-energy** [AGNS92]. **Potentials** [BP96a, BMP93, CDDM96, Coo95, Coo94, CGR+94, ECBH96, FLRV97, FD96a, Jur97d, KMM95, LG95a, LKMCVT95, LKMCVT96, MG93b, MKM96, MKM97, MPOG99, Mor94, MPJ98, MTL97, MM95, MSCP92, MAAP+98, NKUS97, NC95, Núñ94a, PG94, Pie93, RABZ94, ROSM96, STMR97, Sie93, Taş93, Taş96a, TE96, TSPK96, WR96, YY96, Žit94, Ano96-31, BC97b, BMP92, CÅ92a, CB99, DGMW90, DDA92, DSW93, ERC91, GW91, KLW92, KLO+98, KCLI95, KKM99, LRR92, MD94, MD95, MHY98, MDM94, MEP90, MSRP90, MBP91, MPIP99, Nag95b, PO91, Rey95, SPB90, SLL+91, SS95, Van96, WBP91, YNNR97]. **Power** [De 97, Ino96, Por98, Sie93, Por97, Por99, WTS93]. **Powerful** [Val96]. **Powers** [PZW93]. **pp** [Ano92l, Ber96b, Brä95, Brä96b, Brä96c, Cal93, Dun96b, Kar96, Mic96a, Str91, Str92, Str93, Kum93b, Kum93a, Str92]. **PPAR** [Bla99]. **PPO** [LAM92]. **PPP** [Bal90, BEG94, BE95, BE98, BČ96b, CR96a, ČPV90, ČB96b, Del90, FHHE90, HE90, I'H90, Jug90b, MAAP90, Par90a, PČe90, PVN90, Pop90, RPT90, SM96b, Sas90, SPB90]. **Practical** [Pan95, CC92b]. **practice** [Csi76]. **Prasad** [Eri92]. **PRDDO** [DKM96, DKWM97, DKM97]. **PRDDO/M** [DKM96, DKM97]. **PRDDO/M/FCP** [DKWM97, DKM97]. **Precision** [Csa92, KL97b]. **precrystalline** [EZ93]. **precursors** [CF99]. **Predict** [Far97, Fir94, DO90]. **Predicting** [TSS97, CMA+99, Gut99b, MG93a, VVO98]. **Prediction** [AST95, GL97, HJ94, BDP+92, Mez90, SP92a, Sco90, TGDS97, Woo98]. **predictions** [GS97b, PWL95, SKM99, TFSZ95]. **Predictive** [Gre94, SRM98]. **Predictor** [Sim95]. **predissociation** [GZDZ97]. **Preface** [JZ96, Lad94, Ska90]. **preferences** [Tew92]. **preferential** [AGM99]. **preferred** [LE92]. **prefixed** [GV92]. **Pregnanolones** [KG99]. **Preliminary** [FDD+93, HDY+91, JTZ+96, PPP97, ŠH96, MG91, MG93a, KY91b, PWL98]. **Prentice** [Str92, Wha96]. **Prentice-Hall** [Str92]. **preparatory** [Cle92a]. **Preparing** [Ano93i, Ano93j, Ano92o]. **Presence** [OK96, Sch97, Lás93]. **Present** [Dav98]. **Present-Day** [Dav98]. **Press** [Cal90f, Cal93, Deu96, Jør92, Kla93, Kum93b, Kum93a, Lin93, Lin96a, Mic96a, Mon93, Mon94, Str93]. **Press/Gordon** [Mon93]. **Pressure** [MSS99a, Bar90]. **Pressure-Induced** [MSS99a]. **Price** [Cal93]. **Primary** [WWM+98, MG93a]. **Principal** [KKT97]. **Principle** [CG95, CT96, Pal95, Tit93, Wło94, BTKVG99, Dia99, SB92b, ZB92, Pea95]. **Principles** [Fri93a, Fri93b, HU94, LZ94, SPG97, TŚP97, Chr89, EDH+92, KI94, SCS98, SHB+96, Str91, TMR99]. **prism** [GP91a]. **Pro** [LU92b]. **Probabilities** [SPS96b, GZSvD99, Mar99b, Sme92]. **Probability** [Far97].

Probed [GSSD+96]. **Probes** [CDD+99, MRL99, Egu96, KK92a]. **Problem** [AM97, CN99, CB93a, CM94, DJ95, Fri93a, Gin98, LVL+93, Löw95a, May98, Muk96, NS97a, PTC94, Sad97, Sim98, TŚP97, Ada90, Cam92, DJ12, Fan90, JGP91, JK92b, KP92, KE90, KFK91, OM91, Rey90, Sch92a, Sme92, SB92b, Úle92]. **Problems** [Bec97b, BBS+97, BKLv95, CCE+93, LS96, Löw94c, Nic96, NYLBNSB97, SN98, Brä95, BMA99, Löw91e, LTY90, PAC90]. **Procaine** [DB97]. **Procedure** [DMFR93, XY98, CLZ99, JK92b, Sir99, SZ97b, TSS95]. **Procedures** [CGS+94, Löw93d]. **Proceedings** [Cal90d, Cal90c, Cal90a, Kar93, Nal95b, CES87, Csi77, CD81, JPP87, Lad94, Yur95]. **Process** [DDP96, Jur99a, Mor97a, NSS+95, NFVM94, ST96b, TNM98, CAM+97, II94, KSK91, Nov92, RVL97, SAB+97, ZBL99]. **Processes** [BMA93, BF96, CSP98, DP93, DTM96, EEL97, NP96b, RC97, XY95, BFV94, BCY95, CR96b, Chr92, DM97b, DS99, ESTM95, Hag96, Hag99b, Kov98b, Kra96, OS90, Rid82, Rid88, Rid93, Rid99, Sta90, TMA97]. **Processing** [BMG+98, REU+91]. **processus** [GK90b]. **Prodrugs** [EK94, KE91]. **Produce** [Reg92]. **Produced** [CAK+96]. **Product** [HS92e, PBB94, Cam92]. **Products** [Flo97a, Kat93, Kat97, Kat98b, Flo97b, Kat98a, LM91]. **Professor** [Ano91y, Ano96-58, Ohn95]. **Profile** [VDD96, TMA97]. **Profiles** [AK97, MRL99, MD93a, AYAZ95, NST94, RK96, SAW97]. **progestins** [KG98]. **Program** [Löw90c, Löw91c, SSO+97, Löw91d, SGW+92, WP91, Löw91b, Löw92b, Löw93b, Löw95f, Löw91a, Löw92c, Löw92d, Löw93a, Löw94b, Löw95c, Löw95d, Löw96b]. **programming** [PFK99]. **Progress** [McW90]. **project** [PS92a, Ran93]. **Projected** [FSBS+95, Iga95, RP96, BP93d, MSS99b, OS90]. **Projection** [Her97, ČVW91]. **projector** [HMK96, MHK95]. **Proline** [RKN97, SKJ98]. **prolonged** [AKS+90]. **Proof** [May97, Mez97a, PZW93, She90b]. **Propagation** [DM96, GW98a, Lin94]. **Propagator** [AO93, BG95, CMFA93, DP97, DZO97, DZOR98, Ort98b, Par97, SO94, SM96c, ZO95, ZON+96, DRGC90, LO90, MHY98, MM94, MB93, OS91, Ort91, Ort92, Ort93, Ort95, Ort98a, Ort99, Pic92, SDO91, ZO94, ZDO99, ZZW94]. **Propanal** [VBUS99]. **Properties** [Amo96, ABDM94, AYDR96, BK96, BA97b, BS94, CdBKZ99, CR96a, Coh97, CB94b, DWR99, DJF98, DB94a, DP94, FCVL98, Gal96, GP95, Gho95, Gin96b, GMR+93, GPD94, GFRR94, HU94, HSS+95, JCÁ96, KF98, KEMM93, KTCN93, KD95, LZ96, LEG+94, Löw93c, Löw96c, Lun92, MZM94, Mar97b, MPKR94, Mez97a, MTD93, Mor93a, MC95, Mor96c, Mor97b, Mor98a, MPSF97, NTL96, NG97, Núñ96, OK96, Ott94, PP95, Reg92, RAA94, RS97b, RS97a, Sen96, SG97, SL98, TSS97, UWB94, VL91, WDCA97, ZLWES99, ZC95, Ågr90, ARDP92, AMC97, ADB95, ACAT92, AST95, BL99, BUZ94, BJM+94, Bha99, BA90, Boe91, Boe92, Boe95, BJA99, BKM90, BCD91, BMVV93, Cal90d, Can94, Cas97, CZ94a, CJX+92, Cio90b, CCS99, DB93, DWB98, DDC97, DBM99, DB94b, EMP92, FDC92, FDAC90, Gal98]. **properties** [HHPT91, Hud99, Jur99d, KSN93, KPW+95, KI94, KKNY99,

Kir92, KSH92, LO93, LG92, Les91, LDHJ92, LVCP91, Mak87, Mar94c, MCOS94, MCT99, MB92, NGM+95, NÅJ91, NÅJ92, OS91, Pal92a, Pic92, RP98b, SBL+94, SK91, SP91, SB92a, She97, SG96b, Spr93, Suh92, SNH99, TCM99, TGDS97, VABM94, WBH90, WW97, XYC98, Brä98a]. **Property** [BO93, Mar95c, PL91]. **propiolactone** [BH92]. **Proposed** [DBF+96, Csa90a, Csa91, She91]. **Proposition** [DDP96]. **Propylene** [Sak97]. **Propyne** [Par97]. **Prospects** [Dob98, McW90]. **protactinium** [NMCK92]. **Protease** [BRA+99, Mav98]. **Proteases** [BBD97, DDP96, RMH+99, TNS92]. **Protein** [BMK96, BRA+99, Luo95, SD96b, BOL+90, BCX92, BRV99, Chu99, FMS+99, Kid99, KÅ99, NH90, Pal93a, PLBB99, SCMF93, Sch92a, SJB90, Urr94, WP91, WO92, CPGC99]. **Protein-coupled** [CPGC99]. **Protein-Water** [BMK96]. **Proteins** [För97, FWT+96, Mik94, PFMC97, SKTN97, SSO+97, SM92b, jYL94, ACC92, BDP+92, CLR+93, CL92, GSM+92, Pal92b, Par92a, RK99, Sim99a, Sim99b, Suh91, TD99, TBP99, YSJ94]. **Protocol** [BA97b]. **Proton** [BDG96, BOA95, CMSF93, GKKM96, GBS93b, GL98, KS95a, OS92, PD93, SHF94, BZ90, BHKK93, CDB90, DS92, DSW93, EMS90, EBMS92, Gao93, KK99b, LF90, LS92b, MKK96, MA99a, OSS95, PMO90, SY91, WG99, WI96]. **proton-transfer** [KK99b, WI96]. **Protonated** [FDD+93, RRS97, BGS99, TCB99]. **Protonation** [EMMK94, FW92b, Tew94, DBL+90, SSM+99, Tew97, TNS92]. **Protonation-Induced** [Tew94]. **Protonic** [CD93]. **protons** [NST94, WTS93, WTSN94]. **Prototropic** [FW92b, FW92c]. **Prototypical** [ABB93]. **prüfer** [Úle92]. **PS** [HBJ+92, Ike99, KP97]. **PS-21** [HBJ+92]. **Pseudo** [GPč94, LX95, Shu96]. **Pseudo-Linear** [Shu96]. **Pseudo-Orthogonal** [GPč94]. **Pseudoaromatic** [BBOR96]. **Pseudoclosed** [HT97]. **pseudohalides** [PVF+92]. **Pseudomagnetic** [Ken97, Ken98]. **Pseudopotential** [BNLF96, BFRN90, KR91, RP98b]. **pseudopotential-based** [BFRN90]. **Pseudopotentials** [Coh97, FSVZ97, ANB94, HBJ+92, MB97b]. **Pseudospectral** [DDN99]. **Pseudospinors** [MTL97]. **pseudosydnone** [SCJK90]. **Pseudotetrahedral** [BCRL94]. **Psychoactivity** [Reg92]. **Pt** [CDP+99, MtPC+96, SWMB94, XSG97]. **Pt/Alumina** [SWMB94]. **Pt/Ni** [MtPC+96]. **PtAu** [CDP+99]. **PtCl** [RD97]. **PtH** [SFG+98]. **PtSn** [CPBC95]. **Pu** [ERC91]. **Publication** [Par94c]. **Publications** [Ano90y, Ano92-46, Ano99h, Ano99p, Kum93a]. **Published** [Ano97o, Ano98p, Kra96]. **publisher** [Ano92h]. **Publishers** [Ågr90, Ano92k, Ber96b, Cal90e, Cal90b, Kar93, Kar96]. **Publishing** [Ano93g]. **Pull** [JCA97, KM92, MB92]. **Pullman** [Cal90c, Ano99a, Ano99e]. **Pulse** [Hag98]. **Pulsed** [BMG+98]. **Pulses** [MY99, YBM97]. **pumping** [TR91]. **Pure** [Kra96, SF95b]. **purine** [Tew92]. **pursuant** [HZ93]. **Push** [JCA97, KM92, MB92]. **Push-Pull** [JCA97, KM92]. **PW** [CJX+92]. **Pyramidal** [NG95]. **pyrazole** [DBR+96, RAM91]. **pyrene** [KL93a, WP92]. **pyridine** [TWWC91]. **pyridinecarboxylic** [KBM92]. **pyridinium**

[PBBH93]. **Pyridone** [AL95, MTD93]. **Pyridyl** [MH98, MZ93]. **Pyridyl-Substituted** [MZ93]. **Pyridylacetic** [NSS+95]. **pyroelectrics** [MNT96]. **Pyrolysis** [GZ98, SL93, BS91c, FWZ97]. **Pyrrole** [BSB94, BL92a].

Q [DM97b, CMSF93, DM97b, RSCP91]. **QCISD** [Bau98]. **QCISDT** [HKC96]. **QCT** [TUK90]. **QDPT** [LD95]. **QED** [Lin96b]. **QM** [BLBP97, Tho96]. **QM/MM** [Tho96]. **QR** [BB97a]. **QR-SCMEH-MO** [BB97a]. **QSAR** [BBE95, Rom92]. **Quadratic** [HKC96, Shu96, CGG96, Fau92, HC91, KMR92, PSO90, Par92b, SN90a]. **Quadrature** [DW97, HS91, HS92e, DD97b, SH90b]. **Quadratures** [Sch95b, SS92a]. **quadruple** [Li92, TKSH93]. **Quadruply** [PTP95]. **quadrupolar** [SCL96]. **Quadrupole** [BOX94, BP93c, BP93b, FV96, PVČ+90, VPŠ+90]. **Quality** [NP96a, Roś96, SS92f]. **Quanta** [Atk91, HWB05, Brä95, Brä98b, HW92, HW94, HW96, HW00, Str93]. **Quantal** [CSG99, HM97c, LLL91]. **Quantenphysik** [HW87a]. **Quantification** [Mar94a, WK90]. **quantiques** [GK90a, GK90b]. **Quantitative** [BBSS96, HB94, AM90b, BTKVG99, HZ91a]. **Quantities** [Nal94, Chu99, Nal92a]. **Quantization** [BK94a, GMI95, KK92a, SR99]. **Quantum** [AV92, AM97, AR96, ALS+91, AAS93, ALRP96, BW97, BLBP97, BBC+94, BBC+96b, BSHP97, BHX96, BG95, BBRT94, BG98a, BR94, BVV91, BVV92, BFV+93, BBE95, BYGA99, Cal90b, Cal96b, CCM+96, CCC93, CC98, CMG92, CB93b, CB94a, Cha92, CSP98, CD93, CBL95, Con92, CDC98, DHL+94, DBB94, Deu98b, DD98a, DD98b, Dun98, ESP98, EP98, Emc97, Enk97, ECBH96, ETV94, Far97, FLWZ90, FLLZ91, FNSV99, FLRV97, FS99, GKM90, GDID98, GJPMML91, GJOV97, GJLA99, GZ98, GLBM96, GW98a, Gur99, Hag92, HMK99, JCÁ96, JDJP99, JPP87, KSKJ94, KPD93, KS94c, Kir95, KKT97, KL97b, KY91a, KY91b, Lan95, LBM94, LB98, LGT94, Löw90c, Löw91a, Löw91b, Löw92b, Löw92c, Löw92d, LZ92, Löw93a, Löw93b, Löw94b, LZ94, Löw95c, Löw95d, Löw95b, Löw96a, Löw96b]. **Quantum** [Löw99, MUL99, MKDL93, Mar99b, MHK95, Maz98, Mez97b, MY99, MLT+96, MDS98, Mos98, NY98, NFVM94, NS95a, NS95b, Ney95a, Ney95b, Nic99, NV94a, NV94b, O'C96, Deu97, PZ95, PS94a, Pop98, Pri95, RL94, RB95, RT99, RM99, Rid82, Rid88, Rid93, Rid99, RW99, Ryd94, Ryl99, SH90a, SKJ98, SB95a, SB97a, SB98, SR93, SR02, SDE94, SN97, SMO+96, SS97a, SES93, Sri97, SFGW96, TNM98, TTK99, Tch96b, Tch96a, Tob99, TSS97, VR95, VdV96, VBV92, Wen96a, Wło94, Wło95, Wul94, Zer99b, ZZZY96, ZWPJ94, ZJ89, ZJ93, ZJ96, ZJ02, Ada94, Adl95, Ano90g, Ano90i, Ano96-31, Ave89, BZ90, Bha99, BX94, BS91c, BSP98, Brä96b, Brä98b, BD95c, BMVV93, BV93, Cal90g, Cal90c, CDB99, CC92a, CC92b, Car96, Chr89, Coo05, CPW92]. **quantum** [DVJ93, DV96, Deu96, DD95, EC96, EVSN92, Fer91, FG96, FL95, GSM90, Gin91, GB90, GZ97, GZ06, GL96, HZ93, Hag94, Hag96, HW84, HW87a, HW87b, HW04, HLJ96, HZ91b, Hin88, JY94, Kar93, KC93, KJL96,

KTCN93, KH95, KH96c, KSH92, LMMK93, Lei99, LTSL96, LZ91, Löw91c, Löw91d, Löw91e, Löw92a, Löw95f, MD94, MD95, Mat96, MA99a, MB97b, MCB99, NPL90, NE95, NV97a, OS95, OM91, Pau95, PS95, Pos91, PK92b, Qui02, RS00, Rey90, RSCP91, SPS96a, SHB+96, Sil95, SR99, Sjö96, SMH92, Str91, Str92, TIA+92, TMA97, UBA92, WJC+98, Wen96b, WP95, YUSM99, CPW92, Löw91e, Löw95f, Löw95b, Ber96b, Kar93, Kla93, Kum93a, Sta90, Str92, Tay91, Wha96]. **Quantum-Chemical** [GJPMML91, GJLA99, VdV96, FLWZ90, HZ91b]. **Quantum-Classical** [GLBM96, JCÁ96, Ryl99]. **Quantum-Mechanical** [ALRP96, TTK99, KS94c, SH90a, Fer91, OM91]. **quantum/classical** [GL96]. **Quartet** [Jur99b]. **Quartic** [DBB94, MS97b, SB95a, Taş96b, AR92]. **Quasi** [CC91a, CJA94, Gin96a, GPč94, JG95, KSY97, LP97c, LD94, MHM95b, NMCK92, SZL95, Spr96, ZYY95, BL92a, BMDM90, KSF91, LO93, MHM95a, MM93, MRD92, Spr93]. **Quasi-Degenerate** [CJA94, JG95, LD94, MHM95b, KSF91, MHM95a, MRD92]. **Quasi-Energies** [LP97c]. **Quasi-Energy** [KSY97]. **Quasi-One-Dimensional** [Gin96a, Spr96, ZYY95, BL92a, Spr93]. **Quasi-particle** [CC91a, BMDM90]. **Quasi-Relativistic** [NMCK92, SZL95]. **Quasi-Spin** [GPč94]. **quasi-symmetric** [MM93]. **quasidiabatic** [Nob99]. **Quasienergy** [CJH98]. **Quasiparticle** [VCMLL90, Egu96, GNF90, Ort97]. **Quasiperiodic** [ANB96]. **Quasispin** [Vin92]. **quaternary** [SKM99]. **Quaternionic** [Adl95, Deu96]. **quinoid** [GJDD97]. **quinone** [MD94, MD95, Rey95]. **quinonenediimine** [SWD+99]. **quinones** [TKK+90]. **Quintet** [BS92, BS94].

R [Ber96b, Cal90a, Cal93, Lin96a, Mic97, PZTPMC99, Deu97, BHGC99, BPVP92]. **R2R3** [JTZ+96]. **rôle** [GK90b]. **Rabi** [ANB96]. **Radial** [KTT97, ST96a, Sim97, TZ97b, TN96]. **Radiation** [Brä98c, TNS+94, BKS97, CH91, Hag99b, PS95, WA94, Deu97]. **radiationless** [SLS91]. **radiations** [WK90]. **Radiative** [SPS96b, GS90a, KSF91]. **Radical** [AKD96, Cai93, Cai94, EMMS94, Gre94, Jur98a, Jur99a, PZ95, TPR96, UWB94, WR96, YNY99, HDB+95, KTK+90, Kha92, LE92, MCL95, SP92a, SW95, Lun92]. **radically** [BBB+95]. **Radicals** [ET99, KVS98, PBB92, Yam97, BAR94, BHGC99, For94, HZ99, PLBB99]. **Radius** [RM99, YD97]. **radon** [RP98b]. **rainbow** [MEB91]. **Ralph** [Str91]. **Raman** [GSSD+96, HJ94, McH91, OTG91, WKP+95]. **Ramon** [Tay91]. **Random** [CM96a, JCM+92, VZ93, CFMA95, CDG04, ZDO96]. **Random-Phase** [CM96a, VZ93, ZDO96]. **Randomly** [SB97a, SB97b]. **Range** [BL92b, DMB97, GVB97, HWS92, Mik94, NB97, Pie93, TKMA92, KPTS+93, KPTVT+97, LM93, PA92, Per93, PAC90, PBR96, RLR90, RBB+94, ZP92b, Mon94]. **Raphson** [ZA95]. **Rapid** [Cul95, DV98, Ish96, MBV+98, JS91]. **Rare** [GD96, PP98a, GL96, KSK+99, MK90]. **Rare-Gas** [GD96, PP98a]. **ras** [YSJ94]. **Rate** [Chr94, Chr97, FF94a, Luo95, Núñ97, RZ96, Sch93, Chr92, TFT+91]. **Rates**

[LMR94, Oku98, DM97b, EBMS92, GS90a]. **Rational** [De 97, ZCT98, KKS99, RSCP91]. **ratios** [BPHB96]. **Ratner** [Wha96]. **Ray** [ÅGL97, DC97, Mar98a, TNS+94, ACHT95, BKS97, DD96, GGHP94, WS94b, Brä98c]. **Rayleigh** [Ada91b, Ada96b, Áng93, Gin98]. **Rb** [KSW98]. **Reactant** [NOYY94]. **Reaction** [AT99, ADPS98, BCS96, CN94, CPA95, CF99, DZ94, FF94a, FF94b, FY95, FK98, FB96, Gre94, Jur98a, Jur99b, KTK+90, KO95, LMR94, LX95, MKK98, MB98, MD93a, Min94b, Oku98, PBB92, Pon97, Pra97, RZ96, RD97, RW92, Sak98, SKTN97, Sch99a, SPM+96, TKNI96, TMP97, VdV96, VC92, XY95, YNST99, YTYS97, AM90a, AM90b, BA91, BH99, BHGC99, BP90, BS95, BYGA99, CLOFR98, CRsP93, CR96b, CB93b, Chr92, CMSF93, CE90, DGMW90, FF92, FF96, FEE+98, FNSV99, Hei95, HZ91b, JC90, LK90, LKM99, LAM91, LAM92, MBM92, Mat97, MRT95, MV92, Nag96, NOY98, NH90, OYNY98, STKN90, TFT+91, TFYY91, TP92, TF92, TMA97, UJS90, VR90, WJC+98, WJC+99, WI96, XFF98, YD96, YSHD97]. **Reaction-Field** [MB98, LKM99]. **Reactions** [ART94a, BPL97b, Bra97b, BZQ95, BK98, CR93, Chr94, CCT98, DHL+94, GLBM96, Jen94, Jur97a, LL94a, LL97, MV98a, NOYY94, PMM97, Pon97, RC97, Sch93, WR96, ABSW95, BBSS96, BS91c, BCY95, CDB90, CWJ+99, ELMY96, EZ92, JK90, KK99b, LM91, LAM91, ML99, NOYF92, OS90, PB95b, PHBB94, RK91, SLG+96, TLTL92, TUK90, WY99, WY95, WP92, WZ96, ZM90, Deu98a]. **Reactive** [KEG+97, HS95, LGBL94, Nal98]. **Reactivities** [RL94]. **Reactivity** [ET99, FSF96, MV98a, Mon93, MM95, Nal95a, Nal97, TKNI96, Tch96a, WDCA97, BBB+95, Cas91, FS99, GRTR96, MCA92, PS92b, RFM90, Yu95, Ano92j]. **Reagent** [LX95]. **Reagents** [OSA+97]. **rèagion** [GK90b]. **Real** [Bad94, Bec97b, BBS+97, BP93c, BP95, NV94a, NV94b, ZWZ96a, BOL+90, BP93b, BRV90, BW90, NV97a, NZ92, YB99]. **Real-Space** [Bec97b, BBS+97, BP95, NV94a, NV94b, NV97a]. **realistic** [BL91]. **Reality** [CG97b]. **realization** [LP92, SN99]. **Rearrangement** [KW92, Mic94, PRB96]. **received** [Ano98a, Zer98a]. **recently** [Csa90a, Csa91]. **Receptor** [GJLA99, MTD93, PW97, ARBB95, Bla99, CML92, CPGC99, FMS+99, GHB+99, PVU+93, VL91, WD91]. **receptor-bioligand** [CPGC99]. **receptor-G** [FMS+99]. **Receptors** [GJOV97, PW97, GVV+90]. **Reciprocal** [TŚP97, BBLK94]. **Recognition** [Mar95c, BDP+92, FMS+99, DZB92b, PVU+93, Rig92]. **Recollections** [Hal99]. **recombination** [GL96, LM91]. **Reconciliation** [KLI92]. **Rectifier** [MBV+98]. **Recurrence** [AM98b, FS93b, Kat93, Pal97a, Kat91]. **Recursion** [LDP93, DW90, MGLBP95]. **Recursive** [Mik94]. **redistribution** [TP92]. **Redox** [BDH+97, CdBKZ99, WWFR99]. **redox-active** [WWFR99]. **Redshifts** [Her93a, Her93b]. **Reduced** [CYY95, DQB97, Fer96, MPKR94, Maz98, Mor93b, PRTV97, Sam97, VDBPR97a, YNMT98, BCD91, Hud99, Kat91, Kat98a, Kov90b, KPM+90, KG98, MHN98, Sim99c, VDBPR97b, YNST99]. **Reduction** [BP92b, FBKD97b, ZWZ96b, GWB97, MD94, MD95, PBBH93, WSW96].

redundancy [Sta91]. **Reference** [GR95b, JKJ94, JKJ95, JKRW98, MCM98, Nal97, NU95, PPP97, LP93, WB94, ZP90, GR96b, HFM91]. **Reflecting** [Nal97]. **reflections** [Hal99]. **refractive** [GSPSM93]. **Regime** [TMM97]. **regimes** [CSG99]. **Region** [AP93, NMN+97, NMN+98, KL93a, VRR92, VS95]. **Regional** [GSM90, Tac96, Zou92, GS92a, TNSM99]. **Regions** [CW97, MPR97, WP93, GK90b, GK90a]. **Regular** [Gin96a, LNT99, vvBS96, NYKY98]. **Reichardt** [BDZ94]. **Reidel** [Cal90c, Cal90a]. **Reinterpretation** [Sah95a]. **Related** [BHPB95, DZB92a, FT95, KM92, LEA+94, Mez97a, MFAT98, MGK99, PBB92, RGHH94, TVP93, FT96, FT97a, FEE+98, FLWZ90, FLLZ91, Gal98, JY94, KTCN93, LSS96, LW92, MEP90, Nal92a, PAC90, RC92a, Tom91]. **Relating** [JDB99]. **Relation** [AMKS93, Aon98, Coo94, JBT+95, Mar98a, See97, WTS97, AMH+92, Kat91, MS91, Mar94c, MNT96, Mar99a, MBP91, PMS94]. **Relations** [DM92, FS93b, HM97a, Kat93, Kün99, LG95a, Pal97a, BS91a, CSH99, DW90, GSM90, GS92a, GS92b, NM92, Sch92c]. **Relationship** [GG97a, HSS+95, Mon98, RF94, SM94]. **Relationships** [BMP93, GJOV97, BTKVG99, HB94, Khu92, KBM92]. **Relative** [BBB+95, HPSC97, KSN95, WR96, AGAP98, BKEMM94, BDPS97, Jur99d, MSRP90, Zha91]. **Relativistic** [AO93, AAS93, Boč96, Boe98, BJLK98, Del98, EKI94, FBKD97a, FBKD97b, FBKD97c, Flo97a, HCRR94, Ish92, IK97, KS98, KLT97, LMMK93, LBM94, LKBJ97, LLZ98, Lin96b, MSD95, Mey94, Mey97, MTL97, NKUS97, NG96, NMCK92, PG94, RP98b, SZL95, SZ97a, SRW96, SB90, SM95, SO97, WS92, XKB+99, vvBS96, BSS97a, BC97b, Boč90, Boe97, Bro95b, BLG95, ERC91, Flo97b, Ish91, KLO+98, SNH99, TM99, VAVN91, WBP91, Boč90, EKI94]. **Relativistically** [Loh91]. **Relativity** [DN96]. **Relaxation** [GH96a, Her98, TD96a, SCL96, Sim99a, Sim99b]. **Relaxed** [CB94b]. **relay** [LF90]. **release** [SHF94]. **Relevant** [RL94, VDBPR97a, VDBPR97b, BH99, SJ91]. **reliability** [MVS97]. **Reliable** [MK90, VCCM92, FG99, RCB+99]. **remark** [Ber96a]. **Remarks** [GŁ94, Ino96, Löw93d, Kys90, Löw90d]. **Reminiscences** [McW96, Pau97, Mat92]. **Removal** [vMVvLvD97, AM93]. **Renner** [Pet92]. **Renormalization** [Her96, KSH94, BK95, CDG04, Kum93b, Sme92]. **Renormalized** [Ort91, RDF98, ZDO99, Ada96a]. **Reorganization** [BZQ95, BDH+97, LRM96, MB98, Pon97, BCY95]. **Reorientation** [HHHP99]. **Replacements** [NK96a]. **Report** [FG96, Har97a]. **reports** [Lun91]. **Representability** [Mor93b, Sam97, Har90]. **Representable** [CC95, SFM94, CCWCF96, KLM91, KL92a]. **Representation** [CBG94, KSG93, KBT94, KKE+96, KO95, KMM96, OLC+96, Ryl99, VJ95, VJ97, WM92, Wło94, WZ94, AS95, AH92a, BRV90, CC92a, CC92b, Ced94, HC93, KBB+90, KH95, MM91, MPSLB91, Nal91, Nal92c, RCB+99, She90c]. **Representations** [DJ95, Flo97a, LKLBD98, PZW93, RP96, SAR96, Wło95,

WFK97, Flo97b, DJ12]. **Representative** [ART94a, BF95]. **Representing** [AFTM95a, AFTM95b, AFO+97, AFTM98, AFZ+99]. **repressor** [KRRB99]. **reproduce** [GVK99, GV92]. **Repulsion** [Che93, FS93b, Ish96, US97, GJP91, MT90b, MHS95, MFCA93, SH90b, TNI96]. **requirement** [OYL91]. **requirements** [CML92, Iva96, Iva97, WI98]. **Requisites** [Jou97]. **Research** [Kar93, Kas99, BTKVG99, Cle92a, GZ97, GZ06]. **Resemblance** [Löw93d, SC96]. **Reservoir** [Del96]. **Residue** [Mik94, NK96a, LS99]. **Residues** [SKJ98, BOL+90]. **Resistance** [LNT99, BBLK94, MD93b]. **Resolution** [AFTM95a, AFTM95b, AFO+97, AFTM98, LVL+93, AFZ+99, TWWC91, WO92]. **Resolutions** [BG95]. **Resolved** [GWCT97, LM91, Nal92b, NM92, PL91, YCML91]. **Resonance** [BT95, IK94, KLT97, Moi97, Ran97, RG99, SSP98, AS99, BW90, Eng92, Hag99b, HBGR99, MTNF99, McH91, MM94, WO92]. **Resonance-Stabilized** [SSP98]. **Resonances** [BR97, Brä93a, KEP93, Sim97, And93a, HS99, MM94, MTTS93, ZZW94]. **Resonant** [RG96]. **respect** [YG90]. **Response** [CDDM96, CJH98, CB94b, Gho95, Hag98, JBT+95, Jas94, KKJ94, LG95b, LJN+98, Nal97, NS93b, PP95, PO97, SV95, TCM98, BBS91, CT95, DB94b, Egu96, Hag96, KMR92, Kie97, KK91, KYW95, LKM99, MCT99, Pal92a, PSO90, Par92b, Pic92, Rat92, SM99]. **restraining** [KS95a]. **Restricted** [AB97, GT93, JEB92, Kol97, NU95, SE97, SBIP97b, VDL95]. **Restrictions** [PS96, Wil99b]. **Results** [AOH96, CR96a, Dat95, KP97, KWT95, Pra97, SBM97, TV92, BFW92, KY91b, LG96, OS90, OS92, PČP92, RDY95, UBA92]. **retards** [TW90, TW92]. **Retrospective** [KK92b]. **Returning** [BKM93]. **revealed** [AS99, ITT+94]. **Reversal** [Mey94, Mey97]. **Reverse** [ZLWES99, DZB92b]. **reversed** [BS91b]. **Reversible** [SCMF93, BMFPV92, KL93a]. **Review** [Ågr90, Ano92l, Ano92k, Ano92j, Ano93g, Ano93h, Ber96b, Brä95, Brä96b, Brä96c, Brä98b, Brä98a, Brä98c, Cal90g, Cal90d, Cal90f, Cal90c, Cal90e, Cal90b, Cal90a, Cal93, Car96, Deu96, Deu98a, Dun96b, Eri92, Gre98, Jen99, Jør92, Kar93, Kar96, Kla93, Kra96, Kum93b, Kum93a, Lin93, Lin96a, Lun91, Lun92, Mat97, Mic96a, Mic97, Mon93, Mon94, Deu97, Sjö96, Sta90, Sta93, Str91, Str92, Str93, Tay91, Tri96, Wha96, Zer99b, Deu98b, Mic99, Mon99a, Mon99b, RKS99, Tri99, Zer99a, Deu99, Pau99, Jør92]. **revised** [MSMR99]. **Revision** [TGS99]. **Revisited** [GR94, JKJ94, KTT97, MHM95b, CZ93, DT96, PL93]. **Revisiting** [CEM+96]. **Rh** [NG95, SM96a, SC99, EZ92, EZ93]. **RHF** [BE98, FFD96, FMD+96, FFD98, FDAC90, GJDD97, RT98]. **rhodium** [CCC+95b]. **RI** [FKHD97]. **ribbon** [NMSJ99]. **Rich** [WZW96]. **Ridley** [Sta90]. **Right** [PFMC97]. **Right-** [PFMC97]. **rigid** [FKR92, KY91a, KY91b, WLB+94]. **rigidified** [Tho96]. **Rigorous** [Cio93, The98, Geg91a, Geg91b, RDY95, KY91a]. **Rigouous** [Kry93]. **Ring** [ACPR98, Bla96, JZ95b, KMVÅ95, LN96, MZ93, MGK99, MJS93, RMPR98, SF96, BJM+94, CAM+97, DD90b, KLW92, LAM91, MMCC99, Yu95].

Ring-Opened [KMVÅ95]. **ring-opening** [CAM+97]. **Ring-Shaped** [Bla96, LN96, KLW92]. **Rings** [BT95, GBL97, Tri98c, DV99, Les92, Ran95]. **Rn** [HBL99, MTL97, RP98b]. **RNA** [PS99]. **RNase** [KW98]. **RnXe** [RP98b]. **RO** [BHGC99]. **Robert** [Deu98a, Mic97, Ano90z, Ano94i, Ano94-37]. **Robust** [Dav98]. **ROHF** [LG96, LBG97]. **Role** [BP96a, DL92, GDID98, GFRR94, LRM98, Li97, LZ94, Mar94d, Min96, PFMC97, Sak97, SM98, SC94, ŠH96, Cas97, CMSF93, DV91, MS94, PTM92, RC92a, SBZ92a, SB92b, LBBK91, LSGS91]. **Roothaan** [CC97a, GRT96, KMP+90, KM90b, Mar93a]. **Rostoker** [Fau92]. **rotamers** [WBH90]. **Rotating** [Loh96]. **Rotation** [BW99, Bue96, Che97, PO97, VJ97, Aon99, BFV94, CTF92, GX98, MJLL99, ST91, TS92, WFS93, YZX96]. **Rotation-Vibration** [VJ97]. **Rotational** [AST93, GH99, HMGP93, Jou97, LKMCVT96, RBT99, YLD97, MIW91]. **Rotationally** [GYDY97, CF93, She90d]. **Rotations** [Pal97b, BRV90, CLZ99, HRRBL97, Löw92h]. **route** [CB99]. **Routes** [PSCZ97]. **Rouvary** [Mon93]. **Rouvray** [Ano92k]. **Rovibrational** [XY98, FV96, PVČ+90]. **Rovibronic** [YLLJ96]. **Row** [BA97a, Can97, Dat95, DLG95, DKM97, Jur97d, KJ93, PDT97, Roś96, WFK97, YDFS98, ACZ91, Bro96, DS90, JF92, Lon99]. **Roy** [CS96b]. **RP** [FG99]. **RPA** [GARC97, PP95, Per93]. **RPA-AM1** [GARC97]. **Rps** [CMSF93]. **Ru** [SBIP97b]. **Ruben** [Zer99b]. **rubredoxins** [SZ95]. **Rudolf** [Ano90y]. **Rudolph** [Ano90-27, Ano90-28]. **Rule** [PKM93, AI99, Gut99a, MPP+97, Nor91, Par99, Lef99]. **Rules** [AMH93, Kat97, DD97b, She90a, SR99, SS92g, VV91]. **Rumer** [KRZ91, LP92, SA96]. **RuO** [NS91]. **rupturing** [CR96b]. **Ruthenium** [BC97a, SBIP97a]. **Rutile** [RHC96, Bre99, HSLL92]. **Rydberg** [CBT93a, KSK+99, MBG90, MKDL93, MCL95, RL98, TGS99]. **Rydberg-like** [CBT93a]. **Rydberg-valence** [TGS99]. **Rys** [SS92a].

S [Ano92l, Ano92-45, Ano92-44, Ano93h, BUZ94, Ber96b, BP93b, BCY95, BZQ95, CRsP93, Cze99, JH90, Mon94, MNC95, Deu97, RNS93, SES93, TIPM96, BRL92, BP93b, BGS98, CG97b, GS90b, HJ94, HS92b, HZ99, JL91, JH90, KRZ91, LC93, LK94, Man99, SP92a, VG90, WBD97, WY99, ZGPS97]. **S-2-diisopropylaminoethylmethylphosphonothiolate** [HJ94]. **S-containing** [LC93]. **S-Type** [BGS98, JL91]. **SA** [BBS91]. **SAC** [NS91]. **Sachs** [HK97]. **Saddle** [Mar92a, Smi90]. **Saddle-point** [Mar92a]. **Sahni** [SS92b]. **salicylaldehyde** [CSH99]. **Salt** [LX95, MKK98]. **salts** [PBBH93, Sta98d]. **Salvetti** [FGM90, Mor93b]. **Same** [GİA96, Sta98a]. **Sample** [VM92]. **Sampled** [BBC+96b]. **Sampling** [CDC98]. **Sanibel** [Ano90a, Ano90b, Ano91a, Ano91b, Ano92a, Ano92b, Ano94a, Ano94b, Ano95a, Ano96a, Ano96b, Ano93a, Ano93b, Ano95b, Pul90]. **Sarkar** [Deu97]. **satellite** [Nal95b]. **Satellites** [BL98, LEA+94]. **satisfy** [Iva96, Iva97]. **Saturated** [GBL97, Mon98, GS91, KH96a]. **Sayed** [Kra96]. **Sb** [CFDS90]. **Scalar** [Boe97, Del98, Hei90, SZ97a, SNH99]. **Scalar-relativistic** [Boe97].

Scale [BBS+97, HGC93, HL93a, BMFPV92]. **Scaled** [JDJP99, Val94, KKL90]. **Scales** [CCE+93]. **Scaling** [Art98, CB93a, GGSA98, Her96, KB93, KE93, LL97, LBPL97, LBKLC98, LBLKC98, LLBM+95, Mez97a, Nag95a, PV98, WSW98, GS92b, Iva96, Iva97, LL99, LBL98, OYL91, PMDM97, PZDM97, PMDM98, PZDM98, SN90b, WI98, Mez94b]. **Scaling-Nesting** [Mez97a]. **scanning** [DVL+91, Hag94, Ike99, VBD+98]. **scattered** [BUZ94]. **Scattering** [ČHM95a, ČHM95b, ČHMA95, Del98, EP98, GYDY97, GBJMA94, Ken97, Ken98, LVL+93, LB97, LB98, Mar98a, Pai97, PL98, PM93, RGT95, Sim98, TNS+94, WS94b, YLD97, ACHT95, CF93, HHPT91, KFK91, LGBL94, Lin92, MM94, MEB91, Nes94, Pai99, PGM95, STKK92, WDS97]. **SCCEH** [VABM94]. **ScCO** [hJH97, SBOB97]. **SCF** [AS93, BP93d, CT95, CFR96, CJM+91, CPTR96, CSZ97, DV91, FGRS98, FZZ92, FL91, FR92, FKHD97, GS97b, GP91b, Gra97b, HLS94, HVS98, HZF+91, KLLB98, KR93, KMP+90, Kup98, Les91, LW92, MD92a, MV91, MVHV96, MSC92, NC95, Pec93, PPP97, PZA92, RC92a, Ram94, RTKP95, RTKP96, REU+91, SLA97, SHC+98, TSY99, Tal93, VM92, VHFL93, WMW92, YNY99, ZWD98a, ZWD98b]. **SCF-LCAO** [ZWD98a, ZWD98b]. **SCF-MO** [SHC+98]. **Schatz** [Wha96]. **Scheme** [Del96, FS93a, FJRS97, IY99, KSG93, Kry93, LV98, MR99, MK99, MD93c, SPF96, Zha96, DBLV94, Del90, FF92, FADC91, Hol98, PMDM97, PZDM97, PMDM98, PZDM98, Rom92, ZWD98b]. **Schemes** [Fer95, RP98a, NPL90]. **Schiff** [DBL+90, TCB99]. **Schlüter** [FMT93]. **Schrödinger** [Ada91b, Ada96b, Áng93, AGH91, AA92, BS91a, BD94a, BD94b, BD95a, CP92, CV94, DZF93, Eid99, FK94, FKK99, Fer90, Geg91a, Geg91b, Gin98, Hag95, Hag98, HYS91, KH96c, KEP93, LVL+93, Maz98, MS97a, MS97b, New97, NB93, NI94, Núñ94b, RH96b, RW98, Rod91, Ryl99, Sah95a, Sch93, Sie93, Sim95, ST96a, Sim97, Sim99c, Taş96b, TE96, TZ97b, Zha96]. **Schwartz** [RDK97, RDK02]. **Schwinger** [CG95]. **Science** [Ågr90, Ano92k, Kra96, Kum93a, SB96, Klo90]. **Sciences** [BCD95, Cal90d, Löw95e, Löw97b, Löw92g]. **Scientific** [Ano99p, Mat92, McW96]. **SCMEH** [BB97a, Bou96]. **SCO** [SE93b]. **SCO/He** [SE93b]. **SCO/N** [SE93b]. **Screened** [GSM98, Núñ94a, PS94b, ST93, US97, WTS97, CB99]. **Screened-Coulomb** [PS94b]. **Screening** [GİA96, VVS94, EC96, TNS96]. **SCRF** [DKTZ94, FL95]. **Se** [JH90, ANB94, CG97b]. **Search** [AB97, JCM+92, KPA95, Par94b, PP98b, Reg92, Val94, Cha96, Gre98, JGP91, LS99, SM94]. **Searches** [BML98]. **Searching** [CLZ95, PK99]. **Second** [ASP97, AR93, BK94a, BKL91, CV94, CB94b, DLG95, DB94a, DHDP92, FR93b, Gin97, GMI95, Hil98, Jur97d, KUN+98, KSY97, KJ93, KD95, Mor93b, NONY97, Ort98b, PDT97, RNS93, Sam97, SDO91, Sim93b, SP94, SATP94, TFYY91, TSRP99, VVS94, VIK98, YNY99, YNNY99, ZM95, Ada91a, Ada91b, ACZ91, BP92a, BP93b, BCD91, Bro96, CPA98, CP99a, Cim96, DS90, DBF+92, FT96, GFS92, JF92, KMR92, KLO+98, Kor90, LYSL95, Lev94, NYNY99,

Nor91, Sem96b, Str93, VÅJ+92, VCMLL90, WKP+95, ZC99, NYKY98].
second-derivative [Sem96b]. **second-harmonic** [Lev94].
Second-Neighboring [Gin97]. **Second-Order**
[ASP97, AR93, CV94, CB94b, DB94a, FR93b, KSY97, KD95, Mor93b, Ort98b, Sam97, Sim93b, SP94, SATP94, VVS94, VIK98, BKL91, DHDP92, RNS93, SDO91, TFYY91, ZM95, Ada91a, Ada91b, BCD91, Cim96, GFS92, KMR92, KLO+98, LYSL95, VÅJ+92, VCMLL90, WKP+95, ZC99].
Second-Row [DLG95, Jur97d, KJ93, PDT97, ACZ91, Bro96, DS90, JF92].
Section [CM96a, ČHMA95, CCS98]. **Sections**
[RH96b, SLD95, WS94b, KSW98, SK99a, WM92]. **Sectors** [HK95b]. **Secular** [Gin96a, Gin96b]. **Sediments** [ML97]. **see** [TD99]. **Selected**
[MC94, WN90, UBA92]. **Selection** [RPJZW96, Par99]. **Selective**
[BF96, GBS93b, GWB97, MM99b, VL91]. **selectivity** [Bla99, KO91]. **Self**
[AGNS92, AR96, BG95, BKM93, BZQ95, CV94, CM94, CE90, DM94a, DTM96, Fer96, Huz96, KSKJ94, KKNY99, Kol97, KE93, MHN98, MB98, MRT95, Pan93, RM99, Sch95c, SG98, SMO+96, Ste96, TKMA92, VVS94, VFBP96, Wło94, Wło95, BBS91, BZMR92, BHGC99, BCY95, Con92, FCMB99, FEE+98, FNSV99, GRTR96, Ish90, KL92a, MC91a, MC91b, Moh92, NSTFC94, TC98c, TD03, ZWD98b]. **Self-Adjoint** [KE93].
self-assembly [Con92]. **Self-avoiding** [CE90]. **Self-Consistency** [DTM96].
Self-Consistent [CV94, CM94, Fer96, Kol97, MB98, Pan93, Sch95c, SG98, Ste96, VVS94, DM94a, MHN98, BBS91, FCMB99, FNSV99, GRTR96, Ish90, KL92a, MC91a, MC91b, Moh92, NSTFC94]. **Self-Consistent-Field**
[AGNS92, Huz96, TKMA92, KKNY99, BZMR92, ZWD98b]. **Self-Dual**
[Wło95, Wło94]. **Self-Energy** [BG95]. **Self-Exchange** [BZQ95, BCY95].
Self-expansion [VFBP96]. **self-interaction** [TC98c]. **self-organization** [TD03]. **Self-Organized** [AR96]. **self-reaction** [BHGC99, FEE+98].
Self-Returning [BKM93]. **Self-Similarity** [SMO+96]. **Self-Trapped**
[RM99]. **Self-Trapping** [KSKJ94]. **Semi**
[GBVM93, KSKJ94, LKMC93, Löw99, LK90, LKVS97, LZ91, Sta98b].
Semi-Empirical [Löw99, GBVM93, LK90, LZ91]. **Semi-Infinite**
[LKMC93, LKVS97]. **Semi-Ionic** [KSKJ94]. **Semianalytical** [Jon92b].
Semiclassical [DPP+94, Her98, Mar94a, SG98, Sie93, YLD97].
Semiconducting [Mar97a]. **Semiconductor**
[DKBB97, Kov98a, LRM97, SD98, Bat92, GDF92].
Semiconductor-Insulator [Kov98a]. **Semiconductor-Metal** [LRM97].
semiconductors
[DD90a, FDC92, Gur99, GC91, Rid82, Rid88, Rid93, Rid99, WKP+95, Sta90].
Semidirect [ZO94, ZO95]. **Semiempirical** [BBD97, BLRD92, BL92b, BS95, BL98, Cha95, Cul95, Dew92, GKKM96, Gho94, HSLL92, HS92b, JBT+95, Jug96, JSKC95, KG97, Kur90, Lah92, Lio92, LB94, LZ92, LL92, MD94, MD92b, MGK99, MBP97, MR94, PIG94, PD93, PZWJC96, SRS92, SBIP97b, SLA97, SBD+92, SL97, Ste96, TMP97, VC92, WYW96, ZZZY96, BH92, CAM+97, CS96a, CMA+99, DBR+96, FZZ92, HSES94, HZ99, IGK+92,

JK92a, KDB90, OS92, WG99, WMW92, ZFZ92, MD95, WJC+98, YAD92]. **Semimetals** [Sta98c]. **Seminario** [Tri96]. **semiquinones** [TKK+90]. **Semisimilarity** [Mez94b]. **Sensitivities** [MM95, SN90b]. **Sensitivity** [BFL91, CB94a, JBT+95, Nal94, Nal95a, NM95, CB93b, Eng92, KMR92, Nal92d, Nal92b, NM92]. **Separable** [LB97]. **separated** [OCK99]. **separated-bond** [OCK99]. **Separation** [RL98, SGK+95, AGH91, JM94, LK90, MHS95]. **Separations** [STMR97]. **September** [Yur95]. **Septet** [BS94]. **Sequence** [GBS99, LBM94, RSD97, Wen96a, BS91b, BDP+92, Csa94, LSGS91, MBG90, Wen96b]. **Sequence-dependent** [GBS99, BDP+92]. **Sequences** [Bec97a, Bor94, SBM97, LMMK93, WP90]. **Sequential** [BPL97a]. **Ser** [CAK+96]. **Ser-48** [CAK+96]. **Series** [Ano92j, Ano93h, BKL97, BLK97, BKLV94, De 97, Deu96, Eri92, FS97, MI93, MAI95, Mon94, SS92b, SBM97, ČVW91, FS09, HC96d, Kin94, KD92, Kra96, LMV92, MBG90, MBP91, PHM+91, SM94, Sch95a, Tri96]. **Serine** [DDP96, DD99, HBH98, RMH+99]. **session** [Mic92]. **Set** [ČHMA95, CSS93, Coo94, EMMS97, FFD98, Jur98a, Jur98b, MSD95, PHH94, Pen93, Pen96, SMPJ94, AM92, BD95a, Bro96, Cul91, CB91, FR93a, ISOA99, Ish91, JGCJ96, JL91, Les91, MM99a, MFH91, PCO+94, PB99, Qui02, UBA92, WSW96, YNO94]. **Sets** [AHI96, AMKS93, AHWA96, BEJ98, Bro93, ČHM95a, ČHM95b, ČHMA95, Dat95, HH97, Hil98, JM99, KKT97, KL97a, LJ95, LTP96, NNMH96, PG94, PMN+92, RPJZW96, Sad97, SPOAS97, Ter97, TJ95, Wil96, ZWZ96a, BC97b, Boe96, DBF+92, FR98, HBJ+92, KH96a, LO90, Lon99, MHS95, PKJ99, RAI99, REU+91, SS92f, Sta98d, TKSH93, VAVN91, WBP91, Wil99a, vMVvLvD97]. **settings** [Woo98]. **seven** [BOL+90]. **seven-component** [BOL+90]. **Several** [CSZ97, GW98b, TSRP99, GZSvD99]. **Sextet** [KEG+97]. **SGA** [MD99]. **SH** [SC99, Man95a, Man95b, Moc99]. **Shake** [BL98, EEL97, Mor94, ÅC92]. **Shake-Up** [BL98, EEL97, Mor94]. **Shakeup** [Ort98b, Ort98a]. **Shallow** [BP96c, Kov98a]. **Sham** [Bec97b, BKL91, CZ94a, Egu96, GR94, GvLB96, GVB97, Hag97, HS93, KLI92, KCLI95, KLLI97, NMM97, Nal98, PGH95, PS94b, QS98, Roc99, Sah95a, SS99a, SS97b, Ter97, The98, TŚPKM94, WT98, WW97]. **Shannon** [GLMP98, HSWS95]. **Shape** [Art97, Art98, FP96, KN99b, LAM91, LAM92, PV94, ZM96, AM90a, Art93, Art96, Geg91a, Geg91b, KN99a, MM94, PVN90, RAM91]. **Shaped** [Bla96, LN96, KLW92]. **Shapes** [MFAT98, NK98, Eng92]. **Sharing** [CF96]. **Shedding** [HM97a]. **sheets** [Suh91]. **Shell** [AM98a, BMA93, BEG94, GP95, GM94, HT97, JPJ95, KFS92, KSY97, KS96, Kol97, NU95, PKM93, PGH95, SPC96, SR96, Was96, BFP93, BG98b, BG98c, HVS98, KMP+90, KM90b, KF96, KS90, LP98, MHG95, MC91a, MC91b, Moh92, MCB99, Pal92a, PMDM97, PZDM97, PMDM98, PZDM98, VDL95, YOTY93, ZYZ90]. **shell-structure** [BFP93]. **Shells** [KPTS97, PAT93]. **Shepard** [DQB97]. **Shepard-Type** [DQB97]. **Shevelko** [Brä98a, Brä98c]. **Shielding**

[SZ96, SZ97a, GR95a, GS97b, KH96a, RN96, Tos95]. **Shift** [BDT96, Sim98, BZ92, BJMK92, BG98c, FNSV99, KFK91, XSA+92]. **Shifting** [RS98, CA90b]. **Shifts** [Mon98, NN94, PRC98, See97, Sim97, TMP97, BRS95, DO90, VG90]. **Shiotani** [Lun92]. **Shock** [KDHW90, TBW90]. **shocked** [SCP95]. **Shopping** [PB96]. **Short** [GVB97, CLC90, Per93]. **Short-Range** [GVB97, Per93]. **SI** [Kor90, BL99, BCY95, BZQ95, GARC97, STMR97, FS95a, Jen94, KGv93, MKRW99, Mil97, SMM+90]. **Si-** [FS95a]. **SIC** [FB90, RAA94]. **Side** [LJ95, PFMC97, AGM99, HGP91, LBBK91, TBP99]. **Side-Chain** [PFMC97]. **Side-Group** [LV93]. **Siegert** [BW90]. **Siegmund** [Car96]. **SiGeH** [OTS+95]. **Sighted** [Bad95]. **Sign** [DFL98, LLL91]. **signal** [TWK+92]. **Signed** [LL94b]. **significance** [Sla92]. **Significant** [PSD97]. **Signs** [GLLY94]. **SIH** [Pal94, MRST95, WY99]. **silacarbonyl** [TFOY92]. **silagermylyne** [OTS+95]. **Silatranes** [DS96]. **Silica** [NNMH96]. **Silicon** [DBG92, DJF98, HU94, LV98, Mar97a, PB97a, TIPM96, Tri97, Boe96, GKM90, KPW+95, MD92a, PDO92, SBL+94, Suh93]. **silicon-based** [Suh93]. **Silole** [YY96]. **Silver** [KSN95]. **Silverman** [Sjö96]. **Similar** [MRL99]. **Similarity** [HM97a, Mez97b, MFAT98, SMO+96, SP94, AM90b, BBSS96, CC92a, CC92b, CC91b, Kin93, LM92, LAM92, MM99a, Mez94b, PS92b]. **Simon** [Lin93]. **Simple** [CCE+93, Hoo94, Iva96, May97, PPP97, PZW93, PP98b, RC97, ROL+90, Roś96, Sch99b, TSY99, US96, ZWPJ94, ZZCSE94, Ada94, AI99, BE93, Brä96b, GSPSM93, Ken93, LLL91, PTL90, PA99, TYY91, Iva97]. **Simplified** [HWS92, KLLI97, SPF96, Cio91, DCK92]. **Simulate** [GBVM93]. **Simulated** [BLRD92, MT96, IBS95, JH90, KI94]. **simulating** [CL92]. **Simulation** [BBC+94, BPL97a, CGS+94, DHL+94, Jug96, LMC97b, LL94a, MKM93a, OMTS97, PW97, SWK90, Ano96-31, BCX92, Cor92, FG96, GGHP94, Jak93, Kid99, Mar97c, MR92a, NH90, OTG91, PLBB99, SCP95, TW90, TW92]. **Simulations** [BM96, BRA+99, CCE+93, CDC98, DDH+96, FVN98, FWT+96, GLBM96, Hag97, KSKJ94, LLC+94, Loh96, MHÅ98, SSD96, SM92b, WGR+94, ACC92, ACB+99, CBL95, DHDP92, GVK99, KJD+93, LADV92, LSGS91, SKC99, The94, VBD+98]. **Simultaneous** [TTM99]. **Simultaneously** [KM92]. **Sinanoglu** [She90a]. **Sinc** [KH96c]. **SINDO1** [JAG95]. **Single** [BR94, Cio91, GM94, Hag99b, JKJ94, JKJ95, JKRW98, KP93, KSK91, KSW98, Lef97, Lev97, PPP97, Ada91a, BMA90, CS99, IHG95, LP93, MHG95, NS92, PK92a, SK99a, SD91, PMDM97, PMDM98]. **Single-active** [KSK91]. **single-bonded** [CS99]. **Single-Center** [BR94]. **Single-Cycle** [KP93, PK92a]. **Single-density** [PMDM97, PMDM98]. **single-electron** [BMA90, SK99a]. **Single-electron-capture** [KSW98]. **single-excitation** [IHG95]. **Single-excitations-adapted** [Cio91]. **Single-Exponent** [GM94]. **Single-Mode** [Lef97]. **single-particle** [NS92, SD91]. **Single-photon** [Hag99b]. **Single-Reference** [JKJ94, JKJ95, PPP97, LP93]. **Single-Reference-State** [JKRW98]. **Singles** [HKC96, WB94, SWD+99]. **Singlet** [HHKM95, Jur97c, MR92b, Sak98,

STMR97, SC98b, YTYS97, Kha91, KBBK90, LMMK93, MSS99b, OS90]. **Singlet-Triplet** [STMR97, SC98b]. **Singly** [IK97]. **Singular** [BP96a]. **singularities** [TS92]. **Singularity** [Sie93, AM93]. **sinusoidally** [Hag95]. **SiO** [WL92, ABCM93, Jen94, Ali99]. **SiOSi** [Jen94]. **Site** [BBC+96a, KW98, RML97, SZ98, Boe96, DFGB99, GK92, HM99, KK99a, SJB90, TNS92, WD91]. **site-centered** [Boe96]. **Sites** [CDD+99, MKM97, SHC+98, Pro95]. **Situ** [Nal94]. **Situations** [GG97a]. **Sixfold** [Che97]. **Sixth** [HC96a, HC96b, HC96c, HC96d, HC91]. **Sixth-order** [HC96a, HC96b, HC96c, HC96d, HC91]. **Size** [Art97, BDD93, ČHMA95, FP96, LP99, NV94a, NV94b, SM96c, vDvLR99, BBRT94, Bre99, Gur99, HC96c, MC91a, MC91b, NV97a, Tac92, VCCM92]. **size-effects** [Gur99]. **size-extensive** [HC96c]. **Sketch** [Ano99c, Ano91f]. **Slater** [BR94, BFH96, BEJ98, Bud92, BFW92, EJ93, GM94, GY95, GİA96, Gus98, GOAY98, HO94, Iga95, JE90, JEB92, Jon92b, Jon93, Jon97, KKT97, KLI92, Mar98b, MT90b, MHS95, MBA97, MS92, MS93b, RLR90, VV91, ZZ93]. **Slater-Type** [BR94, BFH96, BEJ98, GY95, GİA96, Gus98, GOAY98, HO94, MBA97, Bud92, BFW92, EJ93, JE90, JEB92, Jon92b, Jon93, Jon97, KKT97, MHS95, ZZ93]. **Slow** [Mic94, DMR96, JDB99, TMR99]. **Sm** [BB94, BB95, Bou96, BB94, BB95]. **Small** [ABR95, BLE96, HLS94, MDJ98, NS97a, PZ95, RM99, Ryc94, STKK92, AGNS92, BGS99, BOA95, BMDM90, BFP93, Cas97, CCS99, Dia99, DBF+92, FLHT90, Kap99, KM99a, LHL91, MD92a, Mat96, MSMR99, RF94, Sem94, XKB+99, Gur99]. **Small-angle** [STKK92]. **small-bipolaron** [Mat96]. **Smart** [Kid99]. **SmCp*** [BB97a]. **Smith** [Cal90a]. **Smoothly** [DPP+94]. **Sn** [GARC97, GFRR94, STMR97, Oku98, MECE97]. **SnCl** [RD97]. **SnH** [MRST95]. **SnO** [YNMT98, YNST99]. **Sobolev** [Hil98]. **Society** [Bir94, Löw97b, Lad94]. **Sodalite** [NNMH96]. **Sodium** [AML+95, BPL97b, PCC93, YK97, MESH93, SWK90, LB94, Sta96b]. **Soft** [Kon94, PP98b]. **Softcover** [Brä96b]. **software** [Mic96a]. **solar** [KPM+90]. **Solid** [EDF+98, FD96b, GS97a, LCLO95, LZ92, Pan93, WGR+94, Ano90g, Ano90i, BJ92, BK97, BSS+97b, CRK+91, FDD95, HR99, Kun90, KPB99, LZ91, LXWZ99, RK91]. **Solid-State** [LCLO95, LZ92, Ano90g, Ano90i, HR99, KPB99, LZ91]. **Solids** [CLSI94, CM94, NC95, SPF96, ZC95, CZ94a, CMB95, GRTR96, MESH93, NGM+95, PDO92]. **solitary** [TBW90]. **Soliton** [LRM96]. **solitonlike** [NYKY98]. **Solitons** [För97, DY96, TIA+92]. **solubility** [BHH92]. **Soluble** [Bra96a]. **Solute** [OLC+96, WWFR99, KH90]. **Solute-Solvent** [OLC+96]. **Solutes** [CCM+96]. **Solution** [AM97, Bec97b, BD94a, BD94b, Bra97a, CCT98, CV94, DZF93, Eid99, FD96b, Gin98, GH99, JI95, NOYY94, Nic96, Rod91, Ste96, Taş96b, WR96, AGAP98, AFM99, AMH+92, BD95a, BPVP92, CAM+97, CP92, CTC95, DV91, ESHP99, FG96, Geg91a, Geg91b, Hag92, HB95, NOY98, New97, OYNY98,

OM91, PP91, RBB+94, SWK90, Sim99c, TKO+92, TTOY93, Tom91, WO92].
Solutions
[BDNT97, EDF+98, JM93a, JKJ94, JKJ95, Sad97, YO92, Ada90, Brä95, BMA99, CDB90, FC99, Hal93, JM96a, JKGM99, JGP91, KS92, Oza92].
Solvation [Cas91, EBMS92, OLC+96, PTH+97, RPB+97, AMH+92, CT95, CA91, FM92a, KH90, STZ96, TFT+91, TLTL92, TNS96]. **Solvatochromism** [CDD+99, DV96]. **Solve** [Zha96]. **Solved** [Löw94c]. **Solvent** [AL95, BDZ94, CPA95, CCZ97, CDC98, Gao93, GSM98, Jug90a, MAK+91, MB98, MR97, NP96b, OLC+96, PCE95, SAFK97, SM92b, FKR92, GJPMML91, MRB+96, MRT95, MT91, PZTPMC99, RCB+99, SCA93, Tom91]. **Solver** [RW98].
Solving [CM94, Gin96a, Hag98, IK94, MS97b, TZ97b, Fan90, Hag95, JK92b, Sme92, KH96c]. **Some**
[AEAO99, BP92b, BF94, BPL94, Bra96a, Brä93b, BDD93, BK94c, BMG+98, CL97, CDB99, Che97, CSS93, EMMK94, EK94, FSBS+95, GŁ94, Hal93, HAEMA92, Hom93, Hud99, Jur97d, LLL92, Löw91e, Löw93c, Löw93d, Löw94c, Löw96c, Löw97b, LJN+98, Mar97b, McW96, MKM93b, MKM96, PBB92, PSCZ97, RC97, SSK+92, SM96b, Sch92a, SC97, Sha95, SS97a, Spr93, TKNI96, TBBE98, TSS97, UWB94, ZJS99, ZZZY96, AHM97, BS91a, BBS90, BE93, Bha99, DBM99, FLLZ91, FHHE90, GFS92, HBGR99, Kan93, KR91, Kha92, Kin99, KY92, KBM92, LLSY92, Li92, Löw92h, LE92, MCOS94, MSPS90, MEP90, MSRP90, OS90, Par99, PHBB92, PBHB95, PG95, RAM91, SM94, SJ97, TCZ91, TG96, Wen93, WD91, Kha91, RDY95]. **Something** [Cal96b]. **Sons** [Cal90g]. **SOSCF** [TSY99]. **Space**
[AH96, AHWA96, Bad94, Bec97b, BBS+97, BDT96, BDNT97, BP95, DBB94, DDD93, EBG95, FFD98, FBKD97b, GT93, HK95b, KPR97, Kir95, LKMC93, Mar96, MSRSP93, NV94a, NV94b, RPKM95, RS98, SBIP97b, Val96, VDBPR97a, Wło94, Wło95, Wul94, DM92, FT97a, FFD96, Har90, ISOA99, KB92, LS99, LKVS97, Mar90, MHY98, MAC96, MM93, MV92, NV97a, NZ92, Pau92, Sch94, VDBPR97b]. **Space-Restricted** [GT93]. **space/bond** [ISOA99]. **spaced** [AEJ91, JL91]. **Spaces** [CLKMTA95, Hil98, JM95, Löw96c, Mar95c, PS96, BP93d, BC93, Duc90, JGCJ96, JM96a]. **Spanning** [JM96b, TMH94]. **Spatial** [BGS99, ZWJP95, Csa90b, CK91, PKJ99].
Spatially [PZWJC96, ZWPJ94, SR99]. **Special**
[MDS98, The97, The98, Geg91b, HR99, LK90, LLSY92, Löw92h]. **Species** [AST93, STC96, TD96b, WR96, ACZ91, CLOFR98, LSS96, LHL91, Moc99, OS90, PVČ+90, XKB+99]. **Specific** [Nic96, RWT91]. **specificity** [HGP91].
Spectra [ÅGL97, AEAO99, BSS96, CYY95, DC97, DZOR98, FSHC99, Gin95, HAEMA92, HJ94, Kar94, KVB97, Ken97, Ken98, KC98a, KLC98a, KC98b, KL97c, LFS94, LT99, LD94, LFD94, LD95, Löw99, MS98, MH98, MK97b, NV97b, Par97, PÅS+97, SAFK97, SBIP97a, SBIP97b, STM96a, TL98, TZCT97, TT98, TDO97, YXX99, YLLJ96, ZJS99, AEHM91, AHM97, CB96a, DHDP92, DD96, DM98, FLHT90, FLWZ90, FLLZ91, FHHE90, FL95, GX95, HS99, HS95, Kar90, Kha92, KLC98b, MKBP97, NÅJ91, NÅJ92, NVR+91, OSS95, PVF+92, PLBB99, RCWN94, SE92, SJ97, SZ95, TLC98,

TST+99, TFSZ95, TBP99, WKP+95, WBS99, YJL92, ZFZ92]. **Spectral** [AT93, AFTM95a, AFTM95b, AFO+97, AFTM98, BG95, FUI97, Gin96b, KBWJ96, RPKM95, TMP97, AFZ+99, CÅ92a, DB93, DOPS91, GS90b, LMV92, Lin91]. **spectrometric** [MG93a]. **Spectroscopic** [BS94, CWZ98b, DBL+90, Gal96, GMR+93, MCOS94, MRST95, WBS99, ZH99b, Brä98a, Dun96b, LG92, LM95, MSS99b, OS91, She97, SSM90, SZ97b, Sut99b, RC92b]. **Spectroscopical** [BPL94]. **Spectroscopies** [TN96, Ågr91]. **Spectroscopy** [CSZ97, EB97, FWT+96, GDID98, KPD93, KW98, Sta93, Sul97, Ano93g, BBZ91, GK92, KM90a, McH91, Muk92, TKK+90, WO92, YCML91]. **Spectrum** [BJ98, CCZ97, DZ96a, KLT97, MDD93, Nic99, Taş93, Taş96a, Žit94, BDZ94, Geg91b, KL92b, NE95, Ort97, RSCP91, SP92a, Sme92, SZ97b, SCC91, VX99, VCMLL90]. **speculation** [Tri98c]. **speech** [Rig92]. **Sphere** [BZQ95, BDH+97, RH96a, SD97, BCY95, HFM91, MFH91, ZBL99]. **Spherical** [Aqu95, FS93b, HR97, Jon94, SF95b, A.95, BRV90, CM99, EMS92, EC96, TH90, Whi99]. **spherically** [SAW97]. **Spheroidal** [CLKMTA95]. **Spherulitic** [GŁ94]. **Spin** [AO93, BHX96, Boe93, Bra96a, BS94, CCC93, CDDM96, Che93, CPTR96, CSZ97, EEL97, FBKD97b, FBKD97c, Flo97a, FWC+93, FJR96, GR94, GL99, GVC96, GPč94, HBL99, Iga95, JPJ95, KSG93, KFS92, KBWJ96, KPR97, KS95b, KMVÅ95, Löw96c, MPKR94, Mat96, MCM98, MÅ96, MÅ99b, NMN+97, Nag94, NU95, Oli99, PKM93, Pen93, Pen96, PEBS97, PRTV97, PG96, PTP95, PW91, PGH95, PSS97, RSGC96, RFG99, RPKM95, RP96, RL92, SFG+98, SZ97b, Sur97, TD96a, TD96b, VDBPR97a, WWM+98, AI99, BG98b, BG98c, BG98d, Che92, CEZ+99, Cze99, DWM90, DRGC90, ERC91, Flo97b, JRS+99, KSS92, KLO+98, KRZ91, KLI92, LP93, Löw92h, LBG97, Man95a, Man95b, Man99, Mar99a, MHY98, MM99b, MD99, MW90a, MNC95, OCK99, PSAUS90, Per93, Pet92, RBT99, RGO94, SGK99]. **spin** [Sir99, TSY99, TFR99, Tit92, VÅJ+92, VDBPR97b, WS92, Wil99b, LP97d]. **Spin-** [BHX96]. **Spin-Adapted** [CDDM96, JPJ95, KPR97, MPKR94, NU95, PRTV97, PTP95, RPKM95, VDBPR97a, JRS+99, LP93, MD99, VDBPR97b]. **Spin-averaged** [SZ97b]. **Spin-Catalysis** [MÅ96]. **Spin-Coupled** [CPTR96, GVC96, Oli99, Pen93, Pen96, RSGC96, GL99, RFG99, MM99b, OCK99, RBT99, Sir99, TFR99, Wil99b]. **Spin-Dependent** [FBKD97c]. **spin-extended** [MW90a]. **Spin-Free** [WWM+98, FJR96, Mat96]. **Spin-Independent** [KFS92]. **Spin-Mediated** [NMN+97]. **Spin-multiplet** [PG96]. **Spin-Orbit** [HBL99, KMVÅ95, RL92, SFG+98, PW91, BG98b, BG98c, BG98d, ERC91, JRS+99, KLO+98, KRZ91, Man95a, Man95b, Man99, TSY99, Tit92]. **Spin-Paired** [KSG93]. **Spin-Polarized** [Boe93, BS94, GR94, KLI92]. **Spin-Projected** [Iga95]. **Spin-Spin** [AO93, DRGC90]. **Spin-Unrestricted** [CCC93, PGH95]. **spinel** [BILA95]. **spinless** [Mar99a]. **Spiral** [LCP+91, LU92b]. **spiro** [CAM+97]. **spirochromics** [YUSM99]. **spironaphthoxazines** [MRRA92]. **Spline** [DLV95, FGS92, DBLV94]. **split** [Sta98d]. **Splitting**

[PM95, She90d, CB96a, KBBK90, ROL+90, She90c, SC98b, PL91]. **Splittings** [STM96a]. **sponsored** [Bir94]. **Spontaneous** [SW97]. **spontaneously** [RVP92]. **spore** [HB94]. **Springer** [Brä95, Brä96b, Brä96c, Car96, Dun96b, Sjö96, Str91]. **Springer-Verlag** [Brä95, Brä96b, Car96, Dun96b, Sjö96, Str91]. **Square** [HM97a, NG95, WM92]. **Square-Cell** [HM97a, WM92]. **Square-Pyramidal** [NG95]. **Squared** [MSRSP93]. **Squares** [BBC+96b, DBLV94]. **Squeezed** [MSRSP93, Pal97a, PSM94]. **Squeezing** [Fan90]. **SSCH** [SLL+91]. **SSH** [SLL+91]. **ST** [PTP95]. **Stabilities** [RGHH94, KP96]. **Stability** [Boe98, BMG95, CAJ95, GD96, HU94, KSN95, LN96, PHBB94, RKG96, SL93, SM98, YNMT98, AS99, AGAP98, BKEMM94, CPN91, Cio93, FAV92, LaF90, LAM92, MW90b, Moc99, PBHB95, SPR94, TFOY92, WYZ+92]. **Stabilization** [HP98, BB93, BHGC99, LRM98, YAD92]. **Stabilized** [SSP98, VBF95, BFP93, VFBP96]. **Stabilizing** [PFMC97]. **Stable** [Can97, FT95, Hag98, HO94, IBS95, Lás93, Su93, FT96]. **stack** [Sta98b, She90c]. **stacked** [CEZ+99]. **Stacking** [MAI95]. **Stages** [Hoo94, SL93]. **staggered** [Pal94]. **Standard** [DRBE96, She91, ZL98, DBF+92, MD94, MD95, VCCM92]. **Stands** [SL93]. **Stark** [ABDM94, HHHP99]. **starting** [AA92]. **State** [ABB93, Ale95, BF96, BEG94, BLB95, BK94b, Bra97a, CLSI94, CGLP96, CAJ95, DTA+96, DLV95, DMB97, FSBS+95, Fri93b, GFRR94, JKRW98, JMR98, KA95a, KMM96, LCLO95, LZ92, Mar98b, MM99b, MTD93, NYY96, Nal94, Nic96, NS93b, Pan93, RS94, RW92, SE95a, SIM93a, SGGMGFS96, SDG97, TBČP95, TT98, WT98, ARDP92, Ano90g, Ano90i, BBSS96, BBS91, BRL92, BP93b, Boe95, BSS+97b, BMA99, CCS98, CEZ+99, DDC97, EJ93, FV96, GH96b, GK91, Gut99b, HR99, KA96, KSW98, KSK+99, Kun90, KPB99, LKM99, LZ91, LS93b, MUL99, MG97, MLB92, MHM95a, MB93, MW90a, NM91, New97, NOS94, OYNY98, Ort93, PY92, PFK99, RR95, RA96, RK92, SK99a, SM92a, SKC99, SE95b, SW95, SSM90, STM96b, SNH99, TWK98, TG96, Tri98c, TNS92, UJS90]. **state** [VX99, WI96, WW97, YITY93, ZA95]. **state-averaged** [BBS91]. **State-Selective** [BF96, MM99b]. **State-Specific** [Nic96]. **State-Universal** [JMR98]. **States** [ART94a, BKL97, BLK97, Bec97a, BR97, BČ95, BČ96b, BS94, BGS98, CWX93, Cai93, Cai94, CBT93a, CLZ95, CLSI94, CR96a, DTA+96, DD97a, Dau94, FSBS+95, FS95c, Gre94, GSJS97, HHKM95, HMLK98, Jac97, JM95, JKJ95, JG95, Kan93, KBGE97, KS95b, KN99b, Kov98a, MSRSP93, MHM95b, MB98, MR92b, MR94, Nag95a, Nag98a, Nag98b, NMKP94, Nic96, NK98, Nic99, Núñ94b, Pal97a, PS93, PCC93, RDF98, RL98, RSD97, Sch98, SZC97, SC98a, SG93, Sim93b, SGB98, Sza95, TPR96, TG95, The97, The98, TC98b, TCM98, TD96b, VJ95, VJ97, VZ93, WS95, WD97, WBD97, Was96, BGS99, BOL+90, Bar90, BFRN90, BS92, BFV+93, Cam92, CBT93b, CWZ98b, CLZ99, Ced94, CB99, CC91b, Cio91, DDC95, DWM90, FKK99, GDF92, GSKC99, HC93]. **states** [IHG95, Jac98, JKGM99, KP92, KD92, KN99a, xLTY92, LK94, MCOS94,

MHG95, MLL99, MV90, MAAP90, MPP92, MDM94, MSS99b, NS91, NNH98, Nob99, NÅJ91, NÅJ92, NI94, OGK90, Ort91, PVČ+90, PSM94, PZ91, RVP92, RB93, Roc99, REKP92, SE93a, SHB+96, SPFL93, SWD+99, ST97, SG92, SKRK90, TGS99, Wil90]. **Static** [ABDM94, BA97b, CZ94b, Gho95, JCA97, MFP96, Ols96, SS92b, SB95a, SO94, Voj96, CP99a, DBF+92, DB94b, MFCA94, MCA95b, Pal92a, MCB99]. **Stationary** [AL95, AMKS93, AB97, BLB95, BLRD92, Gho95, KPA95, BA92, HC93]. **Statistical** [BC93, CBT93b, Gar95, Gui98, Kar94, MPKR94, NOY98, PV97, Pop98, Wal94, BZ90, BSP98, VX99, Mic96a]. **Statistical-mechanical** [NOY98]. **Status** [AMKS93]. **steepest** [BA92]. **Step** [AB97, CAK+96, DC95, DDP96, ST96a, DD99, FNSV99, STS95, Tit96, TSS95]. **Stephen** [Deu96]. **stepped** [Mil97]. **Steps** [SZ98, MG93a]. **Stepwise** [Fir94]. **stereoelectronic** [Bha99, ISOA99]. **Stereoisomers** [BjH97]. **stereoregular** [CFMA95, FMD+94]. **Stereoregulation** [Sak97]. **stereoselectivity** [SLG+96]. **Steric** [BW99, CLC90, TI94]. **sterically** [PHBB92]. **steroidal** [KPTS+93]. **Stieltjes** [SLD95]. **Stilbene** [MGK99, MRB+96]. **stimulated** [TR91]. **STM** [MD93b]. **STO** [LDP93, PMN+92]. **Stochastic** [BCX92, Chr97, Nag96, Chr92, SN99, Wil99a, SKC99]. **stoichiometry** [DM92]. **Stokes** [BRS95]. **STOP** [BFH96]. **Stopping** [Ino96, Por98, Por97, Por99, WTS93]. **Stopping-Power** [Por98]. **storage** [GJPMML91]. **Story** [McW96]. **STOs** [GM93, Jon94, KZ99, LR94, MRC99]. **Strain** [LS96, LMAK93, DD90b]. **strained** [MW92, MSPS90, Tri98c]. **strained-layer** [MW92]. **strand** [CH91, PWL98]. **stranded** [ITT+94]. **strategic** [Avi92]. **Strategies** [Enk97, Sae92, SN90a]. **Strategy** [CTG97, Jon97, WWM+98]. **Stratified** [CV98]. **stratospheric** [BH99]. **Strength** [YDFS98, Zie95, BRL92, BBTU97, DOPS91, Eng92, MK90, SY91, YBZ92, Zha91]. **Strengths** [LDGA96, BADM97, KSF91, MLB92, MSRP90]. **stretch** [DS93]. **Stretching** [GSSD+96, HP97, HZ94, SS92c, BHPB93]. **Strictly** [Sur94]. **String** [TFT+91, TFYY91]. **Stripped** [DD98b]. **strips** [Dia99]. **Strong** [Che93, FUI97, KL97a, Pal95, RS94, RS97a, Sch97, SC97, Sch98, KCP90, SC91, BMDM90]. **Strongly** [MCM98, BOL+90, Che92, Mar94c, PČP92]. **Structural** [Ali99, Ano96-58, AFTM95a, AFTM95b, AFO+97, AFTM98, AFZ+99, Boe98, BJA99, CML92, DS96, DJF98, GVV+90, JI95, KBA96, KEMM93, LL99, MPSF97, PCF94, Suh92, ZYY95, ZC95, AM90b, Cas97, CZ94a, CCS99, DFGB99, FDC92, HGL99, JMP99, KPW+95, MEP90, PACO90, RA91, RBB+94, Sin92, TTOY93]. **Structure** [AL95, ATP+96, AH97, ALRP96, BKWL97, BS91b, Bec97a, BBS+97, BTN98, BFH96, BCD95, BS94, BJLK98, BK94c, CCC+95a, CAK+96, CXL97, CFR96, Che93, CCT98, Cio94, CG96, CM94, CSZ97, CF96, DZB92a, DWB98, DL92, EDF+98, FFD98, GP95, GD96, Gin95, GV93, GJOV97, GJLA99, GvLB96, GP97, GLLY94, HNB92, HL93b, IAN+94, Ino96, Kan93, KGC+96, KEG+97, Khu92, KM97, KS96, KGVM97, KG97, KG99, KL97c,

LB96a, LMC97a, LRM96, LY98, Les91, LEG+94, MRL99, MVV+97, MW90b, MK97b, MK98a, MC95, Mor96c, Mor97b, Mor98a, NMvB+98, NAK95, Nic96, NG96, NC95, NS97b, PW97, PVLG93, PS94a, PJ96, QS98, RHC96, RW98, RKPE95, RAA94, RKG96, Sah95b, SD96a, SC98a, SST93, SBIP97a, SS97b, SAL+94, SG97, SGB97, SC95, SPR94, Suz99, TWK98]. **Structure** [TH97, TIPM96, VR95, VR92, VHFL93, Wil96, Xu96, YNNY99, YK97, ZL98, ZY94, ZM96, ZRNZ97, Ågr90, ANB94, Ano92j, BTKVG99, BL92a, BILA95, BUZ94, BBZ91, Ber96b, BJM+94, Boe93, BFP93, Bro95a, VD90, Cal90d, Cal90e, Cas91, CJX+92, Coo92, Csi82, DR92, DD89, FS95a, FLWZ90, FLLZ91, FMD+94, FFD96, FKR92, FS99, Gal98, GK92, GS91, GL92, GDB98, Gur99, GH92, Gut99b, HS93, HB94, Iac92, JDB99, JMS95, KK99a, KTK+90, KH90, KJL96, KWZ98, KT95, Kov90a, Kov90b, KG98, KBM92, KL92b, LMC97b, Lan95, Lip91a, Lip91b, LFD99, LTY92, Mak87, MW92, MLB92, MMCC99, MS93a, MB92, Min98, MK96, METHH94, Muk92, NSS92, NMSJ99, Nor91, OTS+95, PTM92, Rat92, RRC94, REKP92, RK91, RCWN94, SM94, SX96, SBAD90, SK91]. **structure** [SST94, SKM99, SLDB91, SG96b, Suh91, TJ97, Tit96, VRR92, VCMLL90, WA94, Wil90, WL92, Woo98, XYC98, XKB+99, XSA+92, Xu99, YYLB90, YSJ94, ZGPS97, ITT+94, Kar90, MK95, Pul90, She91, Sta93, Ano93g, Lun91]. **Structure-Activity** [GJOV97, BTKVG99]. **Structure-Affinity** [GJLA99]. **Structures** [AMKS93, ADPS98, BK98, CL97, Coo95, EMMS94, Har96, Jur96a, KGv93, Lad97b, LJ95, LRM96, LS92a, Li93, LF95, Loh96, MI93, MAI95, NOYY94, PV99, RW92, Spr96, TZCT97, AKS+90, And90, ABCM93, BL99, BGS99, BBZ91, BJM+94, BT96, BCD91, Dia99, EZ93, FLLZ91, FB90, FMD+96, Fra99, GJDD97, Hal91, IBS95, JK90, KP96, KSN93, KSSG95, KI94, LO93, Li97, MECE97, Min94a, NMCK92, PS99, PMS94, Sch92a, SZCO99, SLDB91, TST+99, TFSZ95, WG99, XSG97, BHGC99, KJ97]. **Strumian** [AH92b]. **Students** [Ano99n]. **Studied** [FWT+96, PIG94, RHC96, Ryd94, SAFK97, TNS+94, GZSvD99, hJH97, LSGS91, NS91, ZY94]. **Studies** [ART94a, AK97, BKWL97, BZQ95, BCS96, BDH+97, Cai93, CL97, CCC+95a, CBSR+98, CXL97, CDC98, EZ92, FF94a, FF94b, FT95, FB96, FLF96, GBVM93, GJLA99, Har97a, HS92b, HHKM95, HBH98, I'H90, Jur98b, KSR95, KS94b, KN92, LKM99, LX95, MZ95, MR92b, MZ93, MGK99, MC95, Mor98a, NNMH96, NONY97, NHN97, Pau92, PVLG93, PBB94, PS94b, RKPE95, RKG96, Sak97, SA96, Sta98a, SZ98, TZCT97, TSPK96, TB95, TD96b, WO92, YXX99, YTYS97, ZYY95, BJM+94, BH99, BD95b, BHH92, CPBC95, CLGW95, CP99b, DB97, DBL+90, DP96, FT96, FF96, FT97a, GFY+99, GL96, HCRR94, Hag99a, HWB97b, HWB97a, JY94, Kar90, KL92b, LYSL95, LSS96, Les92, LC93, LB94, LUU90, LCP+91, MFCA93, NMN+99, Nak92, NÅJ91, Nov92, NL96b, PVN90, PCF94, Rat92, RTS91, REKP92, RC99]. **studies** [SS90, SP92b, SCP93, Ska92, SSM90, Spr93, TCZ91, Tri98c, TNS92, VRR92, WJC+99, WY95, WP92, YOTY93, NÅJ92]. **Study** [AL95, AKD96, AP93, AMT+99, AHI96, AMKS93, AR96, ADPS98, BA97b,

BBD97, BBOR96, BTTS97, BJ98, BEG94, BLE96, BBC+96a, BSP97, BSHP97, BHX96, Boč96, BP92b, BjH97, BAK96a, BAK96b, BAK97, BCRL94, BPL97b, BRA+99, Bra97b, BHPB95, Bue96, BDD93, BK94c, BvL96, CBAM97, CWX93, Cai94, CdBKZ99, CCB+97, Che96, Che97, CA97, CCZ97, CD81, DS96, DD97a, DN96, DB94a, DZ96a, DZ97, DD93, Dun99, ESP98, EMMK94, ET97, ET99, EDF+98, FY95, FLRV97, FDF97, FDD+93, FWBT94, Gal96, GG97a, GD96, GBL97, GL98, HZ91a, HP97, JKK+92, JKRW98, JGR98, JMR98, JDJP99, Jur96b, Jur97f, Jur99b, Jur99a, JSKC95, KW92, KH96a, Kry98, KGVM97, KG99, KL97c, LV93, LJ95, LMV92, Li92, LH94, Lio92, LFD94, LSC98, Lu99, LBG95, MKK98, MRT97, MALT96].
Study
[MTP+98, MDD93, Mav98, MB98, MG93b, MRL99, MTD93, MDJ98, MY99, MK99, MC94, MKM96, Mor97a, MBP97, NSS+95, NN94, NFVM94, NM95, Oli99, Pan93, PMM97, PP98a, PHH94, PFMC97, PLV92, PPP97, PM93, PBB92, PZ95, RL95, RM96, RC97, RGHH94, RP98a, RK95, Roz97, ROSM96, SE93b, SE95a, SKTN97, SL93, SNMB97, SZC97, SPS96b, SDE94, SR96, SGGMGFS96, SGB97, SGB98, SHC+98, Sta97, SC95, STC96, SFGW96, TTK99, TB95, VDBPR97a, VDD96, VBV92, VC92, VZ93, WYW96, XLW+99, Yam97, YW92, Yur95, ZJS99, ZL98, ZWJP95, AEHM91, ADB95, AGM99, ANB94, AKCS91, ABCM93, ABSW95, AH92a, AD92, BL99, BMA90, BLC95, BHL+99, BJ92, BAR94, BOA95, BBTU97, Bat92, BILA95, BCLS94, BBMM99, BH92, BHH92, BHGC99, BRV99, Bre99, BHPB93, BVV91]. **study** [BVV92, BMVV93, BYE+97, BMFPV92, BS95, BMG95, BYGA99, BLG95, CWZ98b, CLOFR98, Cas92, CPN91, CRsP93, CCC+95b, CAM+97, CWJ+99, CS99, CSH99, CCS99, CMA+99, CL92, CDP+99, CF99, DD90a, DBR+96, DSS90, DD96, DI95, DV91, DV99, DDC97, DLF99, ESHP99, EVSN92, Ert90, Eva97, FMS+99, FF92, FEE+98, FWZ97, FNSV99, FV96, FMD+94, FGM90, FL95, FKR92, Fra99, Gal98, GE92, GPS90, GX98, GJDD97, GBS99, GS90a, HK95a, HDY+91, HBGR99, HRH99, HZ91b, HGL99, HHPT91, II94, JMS95, Jur99d, KP96, KK99b, KSN93, KI94, KA96, Kha92, KC93, Kor90, KC97, LCV92, LHNK99, Les91, LHL91, LGT94, LCS98, LU92b, LBG97, MUL99, MG97, MG90, MRRA92, MKK96, MCOS94, MBG90, MKDL93, MMRSN92, MMCC99, MAL93, MLT98, MSMR99, MLL99, Men99, Mil97]. **study** [Min98, ML99, MBML91, MCA95b, MRBM91, NF92, NNH98, NL96a, OTS+95, PCB92, Pal94, PČe90, PB95b, PB99, PHM+91, PHBB92, PBBH93, PBHB95, RFG99, RTKP96, RBT99, Réa90, RCB+99, RD97, RK91, RCWN94, RKH+98, SCL96, SE93a, SM96a, SDP+95, SAB+97, SCS98, SM92a, SRP+98, SCA93, SX96, SP91, Sem94, ST97, SEKEB98, SCJK90, SW92, SCS94, SW95, SLS91, SBOB97, SLL+91, Sta98b, SC98b, SC99, SLG+96, SBZ92d, TIA+92, TLTL92, TF92, TST+99, TCB99, Tho96, TUK90, TC98c, UJS90, WP91, WFS93, WLB+94, WJC+98, WG99, WY99, WB94, WSB94, WMD95, WBS99, WMW92, XSG97, XFF98, YD96, YSHD97, YDDP92, ZC96, ZTC97, ZP90, ZBL99, ZGPS97, ZSK97, JGCJ96, KR91, VDBPR97b]. **Studying** [CL94, KKE+96, SKS98]. **Sturmian** [AHWA96]. **Sturmians** [Ave00].

Stuttgart [Brä95]. **Styrene** [RW92]. **sub** [KDHW90]. **sub-nanometer** [KDHW90]. **Subgraphs** [ZW96b]. **Subgroup** [PC99]. **Subgroup-chain** [PC99]. **subject** [KKWT99]. **Subjected** [Bla96]. **Submission** [Ano95f, Ano95g, Ano95h, Ano95i, Ano95j, Ano95k, Ano95l, Ano95m, Ano95n, Ano95o, Ano95p, Ano95q, Ano96h, Ano96i, Ano96j, Ano96k, Ano96l, Ano96m, Ano96n, Ano96o, Ano96p, Ano96q, Ano96r, Ano96s, Ano96t, Ano96u, Ano96v, Ano96w, Ano96x, Ano96y, Ano96z, Ano96-27, Ano96-28, Ano97a, Ano97b, Ano97c, Ano97d, Ano97e, Ano97f, Ano97g, Ano97h, Ano97i, Ano97j, Ano97k, Ano97l]. **Subsets** [WBD97, GS92b]. **Subshell** [GM94]. **Subspace** [GW98a]. **Subspaces** [GM93, Ban91]. **Substates** [GSSD+96]. **Substituent** [CV99, CC96, FLF96, KZ94, KN92, HZ91a, Tew97, PHBB94]. **Substituents** [DWR99, Jay92, JM94, KPTS+93, XSA+92]. **Substituted** [Bra97b, MZ93, RL95, SSMK93, Shu96, BHPB93, HB94, KBM92, PHBB94, RC92b, SLG+96]. **substitutes** [BBS90]. **Substitution** [Gra97b, KK99a, LE92, MZ91, PHM+91]. **substitutional** [RD90]. **substitutions** [DGMW90, MHG95, MBML91]. **substrate** [TNS92, WMW92]. **substrate-free** [TNS92]. **Substrates** [SD98]. **subsystems** [GSM90]. **subtilis** [HB94]. **Subtle** [Mar95b, GVK99]. **Subunit** [CMFA93, SCMF93]. **Success** [DVJ93]. **successive** [LP97d]. **succinonitrile** [WBH90]. **Suited** [Ada99]. **Sulfides** [Jur97b, Mor98a, CMB95]. **Sulfinylanilines** [AEAO99]. **Sulfones** [Mor98a]. **Sulfur** [AHI96, LS92a, MV98a, BVV92, FWS97, Les91, SLG+96]. **sulfur-bridged** [FWS97]. **Sulfur-Centered** [MV98a]. **Sulfur-Containing** [AHI96]. **Sum** [Mar98b, Kat98a, MPP92]. **Summation** [LS93a, ČVW91, TW90, TW92]. **Summations** [Har98a, FDAC90]. **Sums** [KP93, Kat93, Kat97, Kat98b, Sie93, CFMA95, FADC91, PK92a]. **suosan** [SM94]. **Super** [NV94a, NV94b, AMH93, CDG04]. **Supercell** [EDF+98]. **supercells** [NV97a]. **supercluster** [Cze99]. **Superconducting** [Fri93b, LK99, LG95b, Bar90, GK91, Tac92]. **Superconductivity** [BS93, Fri93a, Fri93b, SBZ92d, SBZ92c, WL99, AS95, Mat96, NMN+99, SBZ92a, SBZ92b, LRM93]. **Superconductors** [BSS96, CL97, CG97a, DMB97, Li93, Min96, NMN+97, NMN+98, Suk95, BB91, DBM99, JMS95, KCP90, MS94, Min94a, Yam90]. **Superdirect** [DM94b]. **superlattice** [MW92]. **superlattices** [BL92a]. **Superposition** [CSS93, Ell92, FW92a]. **superstrong** [RR95]. **superstructures** [BDP+92]. **Supersymmetric** [Bla96]. **Supersymmetry** [DJ95, DJ12]. **suppressants** [GX95]. **Surface** [ASP97, AT99, AP93, Art98, BMP92, BMP93, DP94, FP96, GMR+93, GYDY97, GBJMA94, Jur97e, Jur98a, KM99a, KO95, LCLO95, Min94b, MPR97, MAI95, MBP91, MAAP+98, NTL96, NMvB+98, NHN97, OMTS97, PLA98, PM93, Sch99a, See97, SATP94, SFGW96, TNM98, WG95, YNMT98, ČDM91, CEM+96, EDH+92, Eng92, FMR91, Gao93, GE92, GL92, GRTR96, GZSvD99, JWG95, KR93, Kie97, KK92a, LMC97b, MD92a, MLT98, Mil97, MD91, MPIP99, Nak92, NF92, OYNY98, PCB92, PSBL98, RK92, SAB+97, SCS98, SM92a, SRP+98, SBPPH92, STS95, Ska92, SS95,

WY95, YNST99, MKRW99]. **surface-molecule** [Nak92]. **Surfaces** [AMT+99, BBOR96, DDH+96, GW98b, Hea97, Jug96, JSG97, LL94a, LL97, Lio92, MALT96, MD93a, MPV94, NTL96, PPSK96, PPK97, PAAM98, RK97, Sch97, SS97b, WGR+94, XR94, AGNS92, Ber96c, BDK90, GPS90, HS93, LV97, Löw90d, LM92, MVS97, Mez90, MD93b, MSPS90, NÅJ91, NÅJ92, OSS95, PBPN90, PTL90, RAM91, SM99, SX96, SW92, SN90a, Sut99b, VBD+98, WM92, ZP90]. **Surprises** [LS96]. **Surrounding** [SKTN97]. **survey** [OCK99]. **susceptibilities** [GFS92, Lev94]. **Susceptibility** [KM97, LFS94, SSK+92, DCK92]. **Suspending** [ZYY95]. **Sutcliffe** [Sut99a]. **sweeteners** [SM94]. **Switching** [SB98]. **sydnone** [SCJK90]. **Symanzik** [CB93a]. **Symbolic** [BB97b, ČVW91, Pie93, CP92, TP94]. **Symbols** [Lai94, Roo93b, RL97]. **Symmetric** [FBKD97a, FBKD97b, FBKD97c, Flo97a, Flo97b, HHHP99, IP93, KP93, Kat93, Kat97, Kat98b, KS92, Mez97a, PM95, RP96, WZ94, WFK97, YLD97, Zer99b, AFM99, JK92b, Kat91, Kat98a, MM93, NZ92, PK92a, Pau95, She90d, SS92g]. **Symmetric-group** [KS92]. **Symmetric-Top** [HHHP99]. **Symmetrical** [DD97b, HW91]. **symmetrically** [PC91]. **symmetricized** [Kov90a]. **Symmetries** [Alt96, The97, The98, Alt92, KŽ90, Lin93]. **Symmetrized** [Ada96b, CWZ98a, PZW93, DWM90, ZWD98a]. **Symmetrizing** [CC98]. **Symmetry** [BK98, CC98, CGG96, GS94, GLM91, GKS99, Her97, HC96e, JBS97, Kup94, Kup98, Mey94, Mey97, Mez97a, SM96b, Sen96, SW97, TMDB98, WT98, YO92, Zha92a, ZWZ96b, ZM97, And90, CLZ99, Coo92, Kov90a, Kov90b, LV97, Mez90, MJLL99, Nob99, Oza92, PC99, Sta91, Vin92, VZ92, ZZ91, Zha92b, ZWD98a, ZWD98b]. **symmetry-adapted** [CLZ99, LV97, PC99, ZWD98a, ZWD98b]. **symmetry-reduced** [Kov90b]. **Symposia** [Ano97o, Ano98p, Ano93a, Ano93b, Ano90a, Ano90b, Ano91a, Ano91b, Ano92a, Ano92b, Ano94a, Ano94b, Ano95a, Ano95b, Ano96a, Ano96b, Pul90]. **Symposium** [Cal90d, JPP87, LZ92, LZ94, Ano90g, Ano90i, Ano92q, Bir94, Cal90c, LZ91, Nal95b, CES87, Cal90a]. **synchronization** [CR96b]. **Synchrotron** [TNS+94]. **synthase** [ARBB95]. **Synthesis** [ASI94b, Cio94]. **synthetic** [PBHB95, RC99]. **synthons** [KP90]. **syntopy** [MM93]. **System** [ABB93, ANB96, BW97, BMK96, FK94, Fer95, GW98a, GKS99, KPR97, KNN96a, KMP94, KMP97, Muk96, NV94a, NV94b, See97, SSD96, SC95, TBČP95, Voj96, ZYY95, AZ99, BPHB96, Cas92, Eng92, KC93, Nag96, Nal92a, NV97a, OM91, PS92a, Ska92, SGW+92, Sut99a, TKO+92, TTOY93, TŚPKM94, TNSM99]. **System-Partitioning** [Muk96]. **Systematic** [Bou94, CV99, RTKP95, SZC97, ST97, Les91]. **Systematics** [LS96]. **Systems** [AT99, ADPS98, AT93, ACPR98, Ara94, AFTM95a, AFTM95b, AFO+97, AFTM98, AK97, BMA93, BA97b, BLBP97, BG95, BGS98, BAD99, Cal96a, CBG94, CV98, CMFA93, CCE+93, Col97, Dun96a, Dun97, DQB97, EMMK94, Eng95, FS95c, FUI97, GD94, Gin96a, GBRA94, GG97b, Har98a, Her98, KS94a, KSY97, Koh95, KN92, Kup94, Lad97b, Lah92, LLL97, Lin96b, LG95b, LEA+94, Mar96, MB97a, MS97b, MR99, MCM98, MK99, MAI95,

Mon94, MV99, NFVM94, Nal94, NM95, NU95, NB97, NP96b, OLC+96, PKM93, PV94, PAT93, PZWJC96, PGH95, Pri95, RMPR98, SE93b, SLtM+94, SPOAS97, SDW+98, SAR96, SSP98, Sch99b, SS99b, STMR97, Spr96, Suh94, Suk94, TKNI96, Taş97, TC98a, TDK+94, Ukr94, VBV92, WS94b, WD95, WD97, Wil96, YAD95, ZWPJ94, ZRNZ97]. **systems** [Ada94, AM92, AM93, Ale95, AEJ91, AB99, AI99, AST95, AFZ+99, BOA95, BE93, BD95a, BA90, BX94, BSP98, BB94, BB95, Bou96, BB97a, BFV92, BC93, Cal90c, CD92, CSG99, CPBC95, CAM+97, CB99, Che92, Cio90b, CDG04, CE90, DDA92, DWM90, DÖ94, DB94b, FG99, FFD96, For92b, FKR92, FS92, Gal98, GPS90, GRBA92, GJDD97, GBS99, GDF92, HVS98, HK95a, HS92c, HLJ96, I'H90, JPP87, KG92, KR91, Kel97, KL90, LO93, LC90, LBBK91, LMV92, LLL91, LM93, LL99, LTY90, Lun92, MBG90, MECE97, MD92b, MVHV96, MCT99, MM93, MtPC+96, MFCA93, MEP90, MRD92, NSTFC94, NKS+96, NMN+99, NYKY98, Nak92, Nal98, NV97a, OCK99, PAF91, PA92, PMO90, PMDM97, PZDM97, PMDM98, PZDM98, PZTPMC99, PAC90, PACO90, RFG99, RC92a, RCB+99, ROL+90, RSCP91]. **systems** [SCL96, Sae92, SGK99, ŠG96a, Sch90, SC96, Sem94, SR99, SES93, Spr93, Suh93, SD91, SBZ92c, TP92, TCM99, TD03, VZ92, Yam90, YOTY93, YITY93, ZM95, Ano92l, Brä96b, Mon94].

T [Bau98, AS93, BB91, BPVP92, DMB97, Fri93a, Fri93b, JMS95, KCP90, Li93, LBPL97, LSGS91, Mar94c, MS94, MCA95a, PTP95]. **Table** [Ano95-47, Ano96-59, Ano96-60, Ano96-61, Ano96-62, Ano97p, Ano97q, Ano97r, Ano97s, Ano98q, Ano98r, Ano98s, Ano98t, Ano98u, Ano99q, Ano99r, NK96b]. **tables** [Brä96b, Dun96b, FCMB99]. **tail** [GJDD97]. **Tails** [ADM98]. **take** [WI96]. **Taken** [SRM98]. **Talc** [NTL96]. **Tamm** [DP97, VZ93]. **Tamoxifen** [BHPB95]. **Tanaka** [Kra96]. **target** [PGM95]. **Targeted** [ZCT98]. **Targets** [TN96]. **Tautomeric** [MTD93, MKK96]. **Tautomerism** [Enc96, MRT97, PCE95, YW92, HB95, TCS+90]. **Tautomerization** [AL95, ADPS98, BTTS97]. **Tautomers** [BP93e, GL97, GL98, BKEMM94]. **Taylor** [Sch95a]. **TB** [WTS97]. **TB-LMTO** [WTS97]. **TCNQ** [Sta98b]. **td** [SJ91]. **TDHF** [CPA98]. **Te** [GFRR94]. **Teacher** [Par94a]. **Technique** [BČ96b, ČB96b, PM95, Boe93, CB96a, ČVW91, CGMG92, ML99]. **Techniques** [CSZ97, JCM+92, PHH94, AR92, ACHT95, Chr89, MM91, MK90, RF94, SNNY99, Str91]. **Technology** [Bir94]. **TeCl** [KC97]. **Teller** [Cas97, GMS97, Pet92, RABZ94, RNS93, Sim93b, Suk94, Suk95, ZARB96]. **Temperature** [CL97, CR93, KKNN97, Pal93a, WL99, KS92]. **Temperature-induced** [Pal93a]. **Temperatures** [CR93]. **template** [RFM90]. **Temporal** [DTM96, Mic94]. **tendencies** [LFD99]. **Tennyson** [Sut99a]. **Tensor** [GWCT97, BRV90, Cam92, LG96, MHY98]. **Tensorial** [Pal97b, ZWZ96a, Ell91, Ell92]. **Tensors** [GARC97, LBG95, Pal93b, Pal97b, Pal98, SZ96, SZ97a, GS97b, HZ99, Pal91, PV91, PNB94, Sem96b]. **tentative** [GK90a, GK90b]. **teratogenicity** [CLC90]. **term** [SBZ92a, TGS99]. **Terminal** [ZYY95]. **Terms** [AM98a, DTS97, GR95b, GR96b, Gin95, Gin96b,

Gin97, GGSA98, KBL95, KC98b, NS95b, Ort98b, HC91, KE90, KL93b, MHN98, PCO+94, SLDB91, Sut99a, SB92b]. **tert}** [CAM+97]. **tert}-butylcyclopropanone** [CAM+97]. **Tesla** [BMG+98]. **Test** [AR93, KP97, Lef99, LD95, MSM96, SKN95a, SKN95b, BA91, BHKK93, LO90, KLO+98, Van96]. **Testimony** [I'H90]. **Testing** [ČB96b, KLC98b]. **Testosterone** [KG97]. **tests** [Bec94, KPB99]. **tetracaine** [DB97]. **tetrachlorodibenzo** [MEP90]. **Tetrachloromethane** [GMS97]. **Tetracyanoethylene** [Cio94]. **Tetrafluoride** [SM95]. **Tetrafluorobenzene** [MSS99a]. **tetrahedral** [EMS92]. **tetrahedrane** [SPM+96]. **Tetrahydrocannabinols** [BjH97]. **Tetrahydrofuran** [KUN+98]. **Tetrakis** [TSRP99]. **tetrameter** [BB95]. **tetramethylene** [Jug90a]. **tetranitroimidazole** [CP99b]. **tetrapeptide** [NSS92]. **Tetrasilane** [Yam97]. **Tetratomic** [AS96]. **tetrazine** [Ort97]. **tetrazole** [IGK+92]. **TG** [SST94]. **théaories** [GK90a, GK90b]. **Theinyl** [MH98]. **Theinyl-Imino** [MH98]. **Their** [ADM98, BDG96, BMP93, CDD+99, Flo97a, GBVM93, Gin96b, HH92, Her98, HSS+95, HM95, IK97, Jur96b, Löw97b, Lu99, NK98, Núñ95b, Ott94, PZ95, SSK+92, Sch99b, See97, SGB97, ŠH96, STC96, YO92, AMH+92, BDP+92, BSS+97b, Brä98a, Ced90, CSH99, CBL95, CMA+99, Flo97b, GVV+90, Jur99d, Löw91e, MRST95, MKBP97, MBP91, NNH98, RF94, SC96, She97, TTM99]. **Them** [BP93c, Ber96c]. **Theorem** [Day96, HWS92, KCI98, LBMR95, May97, Mor94, Nag94, Csa90b, CK91, Ell92, Gin91, GLM91, KS90, LV97, MDM94, PLS99, She90b, SN90b, DMFR93]. **Theorems** [AFTM95a, AFTM95b, AFO+97, AFTM98, HM95, KL93c, Löw93d, Pop98, AFZ+99, BP93a]. **Theoretic** [Del98, Dun99, PMM97]. **Theoretical** [AP93, AMT+99, AFM99, AMKS93, ADPS98, ASI94b, BMA90, BMA93, BKWL97, BF95, BA97a, BSB94, BSP97, BH99, BD95b, BjH97, Boe91, BDP+92, BHGC99, BZQ95, BK94c, Cas92, CRsP93, CPBC95, CCC+95b, CCB+97, CBSR+98, CWJ+99, CS99, CSH99, CPD+98, CDP+99, CDDV93, DB97, DDC95, DTA+96, DM97b, DB94a, DD96, EK94, ET97, ET99, Eng95, ECBH96, FMS+99, FY95, FWZ97, FL91, FDD+93, FB96, FLF96, Gal96, Gal98, HJ94, HWB97b, HWB97a, II94, Jug90b, JZ95a, JZ95b, KW92, KSN93, KA96, KCI98, KMM96, LYSL95, LHL91, LFD94, LRR92, LC93, LBBE98, Löw94c, LSC98, LCS98, MV98a, MKK98, Mar95c, MBG90, MMRSN92, MMCC99, MALT96, MTP+98, Mav98, MG93b, Men99, MY99, MBML91, MPOG99, MC95, Mor96c, Mor98a, NONY97, NMN+99, NTL96, Nak92, NF92, NN94]. **Theoretical** [NHN97, NNH98, NST94, OLC+96, Ott94, PWL95, Pár98, PP98a, RGHH94, RCWN94, RKG96, RW92, Sak98, SKTN97, SL93, SP92a, SRP+98, SCA93, SWMB94, SBOB97, SGB97, SGB98, TLTL92, TF92, TST+99, TC98a, TFSZ95, TZCT97, TCZ91, TB95, Tri96, UJS90, VDCK97, VPŠ+90, WBH90, WY99, WJC+99, WY95, WMD95, WMZ98, XY98, XY95, YXX99, ZJS99, ZBL99, ZM90, BLC95, BAR94, BBB+95, CPN91, CS96a, CD81, DD90a, DS90, DSS90, FMD+94, GBS99, HW87a, HDY+91, HRH99, HB95, JMP99, Kha92,

KE91, KPM+90, Lad94, MRRA92, MRB+96, Mun92, PHM+91, PHBB92, PBBH93, PBHB95, Rom92, SM96a, SM92a, SW92, Smi96, SES93, STZ96, SC98b, TP94, WBS99, YDDP92, ZSK97, CC92a, CMA+99, DM98, FCA91, GS90a, GS90b, KP96, KWZ98, Tit96, TM99, YOTY93, Ano93h, Jen99]. **Theoretically** [FF90, YLLJ96]. **Theoretically-derived** [FF90]. **theoretischen** [HW87a]. **Théorie** [GK90b, GK90a]. **Theories** [BG95, KS98, Lev97, NS95a, NS95b, Ney95a, Ney95b, KDB90, NS91, NE95]. **Theory** [ÅGL97, Ada96b, Ada99, ASI94a, ABR95, And94, AR93, Áng93, Aon99, AO93, BDG96, BIM97, BG98a, BA93, BAD99, CG97a, CC95, CJA94, Cha98, CGLP96, CSP98, CDDM96, CJH98, Chr97, Coh97, CA90b, CPA95, Csi76, CB94b, Dau94, DHPC95, DZ94, DD98b, DZOR98, Eng95, EMMS97, FP94, Fri93a, GDID98, GR94, Gho94, Gin98, Gin99, Gör98, GG97b, GG84, Gra97b, GWCT97, Hag97, HWB05, HHKM95, HBH98, IY99, IYFI99, JG95, JM93b, JPJ95, JM96c, Jur96b, Jur97a, Jur97b, Jur97c, Jur97e, Jur97d, Jur97f, Jur97g, Jur98a, KBT94, Kar93, Kar98, Kar94, Kir95, KZVGB97, KSY97, Koh95, KD95, KG99, Kut94, KL97c, LL94b, Lef99, LP96, Lin97, LD94, Löw90c, LZ92, Löw96c, Löw99, LLBM+95, LAS+95, LJN+98, Mar95b, Mar98a, MO98, MHM95b, MC97a, MC97b]. **Theory** [Mat99, MV99, Mun92, NOYY94, NYY96, Nag94, Nag98a, NU95, NMKP94, NV94a, Oli99, PV99, PP98a, PEBS97, PLA98, PM93, Deu97, QS98, RDF98, RL95, RB95, RH96b, RZ96, RPB+97, Rin94, SSK+92, SPH98, Sah95a, SD97, SZ96, SZ97a, Sch93, Scu95, SB96, SG98, SAFK97, SN98, SAS99, STY+98, ŠH96, Su93, Suk94, Suk95, SPL97, SV95, TKNI96, Tac96, TMP97, TC98a, TG95, The97, The98, Tob99, VDBPR97a, VVS94, Wal94, Wan94, WL99, Wen98, Wło95, WWM+98, jYL94, YCML91, ZLHZ94, vDvLR99, Ågr91, Ada90, Ada91b, Ada94, Ada96a, Ali99, AC95, Ano90g, Ano90i, Ano92l, Ave89, BZ90, BAR94, BX94, BSP98, BAL95, BDPS97, Cal93, CT95, CWZ98b, CCS98, Cha96, Cha92, Che92, CLGW95, Cim96, CA91, CEM+96, Csi77, Cze99, DDA92]. **theory** [DA91, DP96, EDH+92, EKI94, EZ92, Fau92, Fer92, För92a, FS99, GJPF92, GNF90, GL95, GP91b, GK91, GZSvD99, GW91, Gut99a, HW84, HW87b, HW92, HW94, HW96, HW00, HW04, Hal93, HR99, HC91, HC96a, HC96b, HC96c, HC96d, HLJ96, HZ92, IL95, Ish92, Jac92, JH92, Jur99d, Jur99c, KSF91, Kla93, KMP+90, KM90b, KCLI95, KL90, KLM91, KL92a, KK92b, Kum93b, Kum93a, KP90, LC90, LK99, LM93, Lin96a, LBL98, LZ91, Löw91a, Löw91b, Löw91c, Löw91d, Löw92b, Löw92c, Löw92d, Löw92a, Löw92h, Löw93a, Löw93b, Löw94b, Löw95c, Löw95f, Löw95d, Löw95b, Löw96a, Löw96b, LTY90, Mar92a, MS91, Mar92b, Mar95a, MHN98, Mar99a, MVS97, MHM95a, MUMH97, Mat96, MM99b, McW90, McW99, MB93, MCA92, MRT95, Mon93, Mon94, MAAP90, MRD92, MD92c, Nal95b, OKY+99]. **theory** [OGK90, Ort91, Ort92, Ort93, Ort95, Ort97, PL93, PV91, PY89, Par90b, PMDM97, PZDM97, PMDM98, PZDM98, PP90, PG96, Pet92, PS95, Pop90, Qui02, RVP92, Rig92, SH90a, SS99a, SB92a, SP95, Sem96a, SOK+98, SNNY99, SS91, SC99, Suh92, Suh93, SO97, SNH99, SBZ92b, SB92b, SJR91, TNSM99, TMA97, Tet93, TC98c, TGDS97, Tri96, VDBPR97b, VVO98,

VDL95, VCMLL90, WB93, WMZ98, Yor95, ZC99, ZP90, ZYZ90, ZY94, Zie96, ZJ89, ZJ93, ZJ96, ZJ02, ZPBC97, LP98, Brä98b, Cal90b, Ano92k, Brä95, Brä98b, Gre98, Jør92, Cal90f]. **Theory-Based** [BDG96]. **therapeutic** [WWFR99]. **There** [KJ95, Ada90]. **Thermal** [BMK96, KW92, LMR94, RW92, Tob99, KPW+95]. **thermally** [OS90]. **Thermochemical** [Bec94, HPSC97]. **Thermochemistry** [GBL97]. **Thermodynamic** [VH96, Chu99]. **Thermodynamics** [FD96a, FDD95, Gar95, Mic96a]. **Thermolysis** [ZH99a]. **Thiamin** [FB96, FVN98]. **Thiazole** [MH98]. **Thickness** [MPV94, Boe92]. **Thin** [MPV94, Bat92, Boe92, MV90]. **think** [Ber96c]. **thioacetone** [SSM90]. **Thioanisole** [DZOR98]. **thiocyanate** [Pro94]. **thioformacetal** [BV93]. **thioformaldehyde** [GH96b]. **thioguanine** [RBB+94]. **Thiooxamides** [KM90a]. **Thiophene** [BSB94, SL98, BL92a]. **Thiophene-** [SL98]. **thiophenes** [EVSN92]. **Third** [BSB94, DM94b, LFS94, NK96a, Suh93, SPL97, VFHL93, ZO95, CJM+91, DCK92, Kor90, Ort97, PWL98]. **Third-Order** [BSB94, LFS94, SPL97, VFHL93, ZO95, Suh93, DCK92, Ort97]. **Thirty** [Nal95b]. **Thomas** [Csa92, Csa96, GC91, MK97a, MHN98, ZP92b]. **Three** [ABB93, ANB96, Art98, DM96, DTM96, GBL97, HS91, Hoo94, KFS92, KJ95, PM95, PPP97, Pie93, SPH98, Sta95, Sta96a, Sta96b, Sta98d, Sta98e, VDD96, WD95, WD97, Bud92, BFW92, DS99, DCK92, GSPSM93, GDF92, ITT+94, Kin99, KE90, LL99, MBG90, MVHV96, MS92, MSC92, NM91, RA91, Sta98b, NM96]. **Three-** [GBL97, PM95, PPP97, GDF92, MS92]. **Three-Body** [KFS92, Pie93, WD95, WD97, KE90, MVHV96]. **Three-Center** [HS91, KJ95, SPH98, RA91]. **Three-Dimensional** [Art98, DM96, Sta96a, Sta95, Sta96b, Sta98d, Sta98e, DS99, LL99, MSC92, Sta98b]. **Three-Dimensional-Doped** [DTM96]. **three-electron** [Bud92, BFW92, Kin99, NM96]. **Three-Level** [ABB93, ANB96, DCK92, GSPSM93, NM91]. **three-stranded** [ITT+94]. **threonylcarbonyl** [SSM+99]. **threshold** [CB96a]. **thromboxane** [ARBB95]. **thylakoid** [DS99]. **Thymine** [AKD96, LF90]. **Ti** [SGB97, SGB98, BRS95, GFY+99, SG97, WY99]. **TI-doped** [BRS95]. **TiCH** [SG97]. **TiCO** [hJH97, SG97]. **Tight** [LRM96, MAD98, TR94, GL92]. **Tight-Binding** [LRM96, MAD98, TR94, GL92]. **Time** [ABB93, AL98, AM97, CT96, CSP98, CJH98, CCE+93, DD95, DD98b, Gör98, HGC93, LM91, MS97a, MS97b, Mey94, Mey97, Mic96b, RB95, RJ97, RW98, SB95a, SB98, TC98a, TC98c, TCM98, YB99, YBM97, BFL91, BMA99, CCS98, CÅ92a, FMR91, HZ93, Hag95, Lin94, PL91, PG96, Rod91, RMF90, YCML91, SB92a]. **Time-Averaged** [CJH98]. **Time-Dependent** [AM97, CT96, CSP98, DD98b, Gör98, RB95, RW98, SB95a, TC98a, TCM98, DD95, TC98c, YB99, BFL91, BMA99, CCS98, FMR91, PG96, Rod91, RMF90, SB92a]. **Time-Evolution** [Mic96b, RJ97]. **Time-Independent** [MS97a, MS97b, SB98]. **Time-resolved** [LM91, PL91, YCML91]. **Time-Reversal** [Mey97]. **Time-Varying** [ABB93]. **times** [Hag92]. **Tin**

[LEG+94, RRC94]. **Tin-Encapsulated** [LEG+94]. **TiO** [HSLL92, PSBL98, SAB+97, SCS98, SX96]. **tip** [LMC97b]. **tip-Al** [LMC97b]. **TiS** [MCA95a]. **Titanium** [BLE96, HLS94]. **Titanium/Oxygen** [BLE96]. **Title** [Ano90-29]. **TlBa** [Min96]. **Tokyo** [Str93]. **Toluene** [NM95]. **Toluene-** [NM95]. **Tool** [HNB92, SRM98, Wen96a, BAR94, CE90, Kry96, SP95, Tri96, Wen96b]. **Tools** [Lio92, Val96, Har91, Mez90, WM92]. **Top** [HHHP99, PEBS97, YLD97]. **Topic** [PDC96]. **Topics** [Lun92]. **Topographical** [SG94]. **topoisomerase** [JDB99]. **Topological** [HSES94, LLL91, MESH93, ZLHZ94, ZM96, VD90, HGP+92, OS95]. **Topologies** [BKLV94]. **Topology** [Sch97, SRM98, SHC+98, AM90b, BFL91]. **Torsion** [VBUS99]. **Torsional** [GW98b, MJLL99, YY96, MSS99b, SLL+91, VVO98]. **Total** [CM94, GZDZ97, IY99, Ort92, VV95, AH92a, Csa90a, Csa91, DWM90, GL92, GH92, LH94, LFD99]. **total-energy** [GL92]. **Totally** [IP93]. **toxicological** [BTKVG99]. **trace** [GHB+99]. **Traces** [PRTV97, Val96]. **Track** [BJ92, WA94]. **tracts** [LSGS91]. **trajectories** [Art93, CSG99, KLW92]. **trans** [KBT94, YAD92, CAM+97, CPA98, DY96, FF96, JZ95a, MI93, PRB96, ŠG96a, Sta98e, Suh92, TYTY91, VZ93, WBH90, WL90, YITY93, MZ95]. **trans}-2** [CAM+97]. **trans}-effect** [ŠG96a]. **trans}-Nitric** [JZ95a]. **trans}-pinocarveol** [PRB96]. **trans}-Polyacetylene** [MI93, VZ93, DY96, Sta98e, TYTY91, WL90, YITY93]. **Transannular** [CG97b, DS96]. **transcriptase** [DZB92b]. **Transfer** [ATI97, BLBP97, BCS96, BAD99, CAK+96, CLSI94, CR93, DTM96, Del96, GL98, HP98, Mik94, Nal94, PK90, RML97, SBM97, Spr96, Sta98a, Sur95, WPB98, BZ90, BOA95, BADM97, BKY99, BCY95, CDB90, CMSF93, Cul91, DM97b, DSW93, EMS90, EBMS92, FMR91, Gao93, GZSvD99, GBS99, HE90, KK99b, KS95a, LBBK91, LB93, LKM99, LS92b, MM91, MKK96, Nal98, OKY+99, Pal92b, PMO90, PC91, PBR96, RBB+94, RMF90, SY91, Sta98b, WG99, WI96, ZBL99]. **Transferability** [FSVZ97, GS91, MM98]. **Transfers** [GBS93b, DS92]. **Transform** [ABLA97, HS92e, KM97, Mez97b, MK98b, CM99, CP92, KKK90, KK91, KK92a, Kin93, Kin94, MK95, MK96, Rod91, RW98]. **Transformation** [AH97, BA93, Gho95, LLBM+95, SF95b, Boe97, Fan90, GV92, LBL98, PV91, PMDM97, PZDM97, PMDM98, PZDM98, Úle92, Wen93]. **Transformations** [HM97a, Lef97, LBPL97, LBKLC98, LBLKC98, LR94, Löw96c, SPH98, Wen96a, BA92, Cio90a, Löw92h, Pau92, Wen96b]. **Transforming** [ITK91]. **Transforms** [FD93, MK97b, Ced94]. **Transient** [FSF96, TMM97]. **Transition** [ART94a, ADPS98, BA97a, BC97a, BTN98, BK98, CLZ95, CAK+96, CJA94, DHL+94, DMFR93, Dun99, Gre94, HHPT91, JK90, LRM97, MTD93, MBA94, MR94, NYY96, OYNY98, PAT93, RW92, SZ97a, SPS96b, SDE94, Sim93b, SGB97, SGB98, STM96a, SDG97, Tit93, YLLJ96, ACZ91, And93a, BBSS96, BRL92, BUZ94, BCLS94, BDK90, Boe93, Bro95a, Bro96, BPVP92, CLZ99,

CKM91, DV96, FZZ92, GZSvD99, KSF91, Ken93, LU92a, Mar99b, MSMR99, MAC96, MS93a, MLK94, MCCF95, Nor91, PO91, PSO90, PTL90, PZA92, ROL+90, SHB+96, STM96b, SC99, TKO+92, TTOY93, Van96, WS92, ZBL99]. **Transition-Element** [SGB97, SGB98]. **Transition-Metal** [BA97a, BC97a, MBA94, STM96a, Bro95a, Bro96, CKM91, MSMR99, Nor91, PZA92, STM96b, SC99, Van96, ZBL99]. **Transition-State** [NYY96, RW92, SDG97, OYNY98, BBSS96]. **Transitional** [Luo95]. **Transitions** [Art97, BM96, JI95, MPR97, MSS99a, Mor94, NMN+97, NMN+98, PSD97, TD96a, Art96, Dun96b, LMMK93, LM95, MBG90, MLB92, MKDL93, MCL95, Rep96, RBB+94, SMM+90, Sme92, WSM+94, YBZ92]. **Translated** [Brä95]. **Translation** [ČHMA95, MRC99]. **Translational** [Jou97, TW90, TW92]. **transmission** [DRGC90, Hag99b, TWK+92]. **transpolyacetylene** [DYD96]. **Transport** [Ara94, DY96, DP93, DM96, DS99, Ino96, Khu92, Mar94c, MK96]. **Trapped** [RM99]. **Trapping** [KSKJ94]. **traversal** [HZ93]. **treat** [Mar99a]. **treated** [LK90]. **Treating** [May98, US96]. **Treatment** [AMRT94, AEAO99, BMA93, BLBP97, BXZ95, Bla96, BP93e, GY95, HAEMA92, Kry93, LCLO95, MM94, MH98, SKTN97, Sch95c, TNM98, VBUS99, AHM97, CF93, FL91, FR98, Hir92, KRZ91, KY91a, KSK+99, MD94, MD95, NSTFC94, NKS+96, SS98, ST91, TFYY91, TTM99]. **Treatments** [MCM98, SPM+96]. **Tree** [JM96b, JGP91]. **tree-search** [JGP91]. **Trees** [JM96b, TMH94]. **Trends** [MM95, SL98, Tay91]. **Triads** [SBM97]. **Trial** [Gui98]. **Trianion** [Kup98]. **Triatom** [AS96]. **Triatomic** [NFVM94, RABZ94, Su93, BZMR92, HZF+91, MIW91, ST91, Sut99a, MKDL93]. **triatomics** [Pet92, TS92]. **Triazole** [PGS97]. **tribute** [Ano96-58]. **tricyclic** [CMA+99]. **Tricyclo** [Lu99, XSA+92]. **Tricyclohexane** [Gal96]. **Tricyclopentane** [Gal96]. **tridiagonal** [NZ92]. **triexcited** [ČPV90, LP98]. **trifluoromethyl** [KH97]. **Trifluoromethylvinyl** [KH97]. **Triggered** [PW97]. **triglycerides** [CDM+94]. **Trimer** [CCB+97, Fou94, GW98b]. **trinitroimidazole** [CP99b]. **trioxane** [BJM+94]. **Tripeptide** [MK98a]. **Triphenylphosphino** [Boč96]. **Triple** [CS98, PG94, WB93]. **Triple-Excitation** [CS98]. **Triple-Zeta** [PG94]. **Triples** [HKC96, NU95, WB94]. **Triplet** [BS94, CG97a, GV93, HHKM95, Jur97c, KBBK90, STMR97, Gut99b, KD92, LM91, LS93b, SC98b]. **Triplet-singlet** [KBBK90]. **triplex** [PWL98]. **Triply** [PTP95, RSD97, HOF+97]. **TRIPOS** [WHF92]. **Trisnitroxymetaphenylene** [TD96b]. **tromsø** [Fuk90, Löw90d]. **tropolone** [WBS99]. **Trotter** [Lun91]. **Trp** [LU92b]. **Truncated** [Sad97]. **tryptamine** [DB93]. **Tryptamines** [HAEMA92]. **TST** [JC90]. **TTF** [Sta98b]. **TTF-2** [Sta98b]. **TTF-DCNQI** [Sta98b]. **TTF-TCNQ** [Sta98b]. **Tungsten** [DFDK99, FDD95, LMC97b, LFD99]. **Tunnel** [EMS90]. **Tunneling** [BSS96, BCS96, CR93, Hag98, NBS95, SB97b, SC94, CMG92, DVL+91, EBMS92, Hag92, HZ93, Hag94, VBD+98]. **Turkey** [Yur95]. **turn** [SJB90]. **Twentieth** [JPP87, Cal90c]. **twist** [RK96]. **twisted** [MFCA94]. **Twisting** [MZ93, MGK99]. **Two**

[Bal90, BBC+94, BMK96, BGS98, Chr94, Chr97, DTA+96, De 97, DP97, DQB97, FK94, FS95c, FWT+96, GJP91, GY95, HBL99, Har98a, HO94, HS92e, IY99, IP94, LS93a, LMR94, LR94, MT90b, MBA97, MRL99, NMM97, NPL90, NYLBNSB97, Pan95, PSO90, PM95, PMN+92, Pie93, PAT93, RML97, RDK97, SB97b, SSD96, Taş96a, TE96, TZ97b, Val96, VBUS99, WG95, WFK97, YO92, ZWZ96b, vvBS96, ASM91, BSS97a, Bud92, BFW92, BMA99, BG98b, BG98c, CB99, Cio90b, CE90, Dav90, DWB98, DW90, Fan90, FR98, GP91a, GDYY97, GDF92, HR99, HW91, ITT+94, Jon93, KG92, KLW92, KM99b, KTCN93, LLL91, LDJH92, LDHJ92, LM92, MHN98, MBG90, MA99a, MS92, MGLBP95, MD93b, NM91, NM94, NV97a, PTL90, PZ91, RDK02, SB95b, SB92b, TGS99]. **two** [Tit96, WDS97, YKN+99]. **two-**
[Bud92, BFW92, ITT+94, MS92, NM91]. **Two-Body** [FS95c, YKN+99]. **Two-Center** [GY95, HO94, HS92e, IY99, LR94, MBA97, Pan95, MT90b, Bud92, BFW92, Cio90b, DW90, Jon93, MGLBP95]. **Two-Component** [HBL99, vvBS96]. **two-coordinated** [ASM91]. **Two-Dimensional** [BBC+94, FWT+96, Har98a, LS93a, SB97b, SSD96, TE96, VBUS99, WG95, YO92, GDF92, HR99, LLL91, LM92, NV97a, SB95b]. **Two-Electron** [BGS98, De 97, NMM97, RDK97, GJP91, CB99, Dav90, FR98, GP91a, KG92, KM99b, KTCN93, RDK02]. **Two-Particle** [ZWZ96b, NM94]. **Two-Particle-Hole** [DP97]. **Two-photon** [PSO90]. **Two-Point** [LMR94]. **two-proton** [MA99a]. **Two-Row** [WFK97]. **two-shell** [BG98b, BG98c]. **Two-Site** [RML97]. **two-state** [BMA99]. **two-step** [Tit96]. **two-valence** [MBG90]. **Two-Well** [Taş96a]. **two/one** [BSS97a]. **two/one-component** [BSS97a]. **Type**
[AM98b, BR94, BFH96, BEJ98, BGS98, CB93a, DTS97, DQB97, FFD98, GY95, GİA96, Gus98, GOAY98, HO94, HS91, HS92e, Ish96, JZ95a, JZ95b, Jur96a, Jur97c, KL97a, MBA97, PR97, SZ97a, Sim97, Sur95, Wil96, Boe96, BJA99, BDPS97, Bud92, BFW92, CS99, Ell91, EJ93, FDC92, FM92b, GS92b, HBJ+92, HS92f, JL91, JE90, JEB92, Jon92b, Jon93, Jon97, KKT97, MHS95, NMCK92, RAA94, SMM+90, SH90b, VL91, XYC98, ZZ93, ZFZ92]. **type-IV** [FDC92]. **Types** [Chr94]. **typical** [RRC94]. **Tyr** [LU92b, TWK+92]. **tyrosine** [KÅ99].

U [MECE97, Tit92]. **UB** [Loh91]. **UBC** [Loh91]. **ubiquinone** [CMSF93]. **UC** [Loh91]. **UF** [DN96]. **UFe** [MECE97]. **UHF** [NM96]. **UK** [Str93]. **ultimate** [WP90]. **ultime** [GK90b]. **ultra** [Boe92]. **ultra-thin** [Boe92]. **Ultrafast** [ESTM95, YCML91, Kra96]. **Ultrahigh** [SS97a]. **Ultrasharp** [FSHC99]. **Ultrashort** [MY99]. **ultrathin** [AST95, WTSN94]. **Ultraviolet** [MK97b]. **Unambiguous** [BCL98]. **uncoupled** [CMA93]. **Uncoupling** [MÅ99b]. **Uncovering** [Chu99]. **undergo** [MJLL99]. **underlying** [MM93]. **Understanding** [Kor95, OSA+97, SRW96, Jak93, MS93a, NOY98]. **Unexpected** [GMMH97]. **unfolded** [GSM+92]. **unfolding** [Chu99]. **Uniaxial** [LMAK93]. **Unification** [BCD95]. **Unified** [CG96, GY95, Kel97]. **uniformly** [HFM91, MFH91]. **Unimolecular**

[KW92, MR94, RZ96, AKCS91]. **Union** [Kra96]. **Unique** [FCMB99]. **Uniqueness** [AFTM95a, AFTM95b, AFO+97, AFTM98, Fuk95, AFZ+99]. **Unit** [PFMC97, ZYY95]. **Unitary** [JPJ95, LP98, Löw96c, MK98a, YPC97, Cam92, Ell92, JH92, KSS92, Löw92h, ZYZ90]. **Unitary-group-based** [LP98]. **Units** [DTM96, SST93, TMDB98, SST94]. **Universal** [GSD97, JM93a, JM95, JG95, JGR98, JMR98, MSD95, JM96a]. **University** [Brä95, Cal90f, Cal93, Deu96, Jør92, Kla93, Lin93, Lin96a, Mic96a, Str93]. **unknown** [TGDS97]. **unlike** [Sco90]. **unrelaxed** [PNB94]. **Unrestricted** [CCC93, PGH95, KLO+98, YITY93]. **Unsaturated** [GBL97, LFD94, Sak98, DHDP92]. **unstable** [HS95]. **until** [Cle92a]. **unusual** [Cio93, RA91]. **upon** [JCA97, MBA94, RC92b, RWT91]. **Upper** [AR99b, Fer90, HMLK98, TVP93, Taş96a, Žit94, AR99a, LK94]. **Upper-** [HMLK98]. **UPt** [Loh91]. **Uracil** [BP93e, PCE95, Les91]. **uranium** [BJA99, Loh91]. **Urea** [CXL97, ADB95]. **Urea-Nitrate** [CXL97]. **urocanic** [LHNK99]. **Use** [BK96, BTKVG99, Bro93, CDD+99, Her97, LV97, MG93a, MS97a, NM95, PG94, RW98, Ryc94, SM98, SMO+96, VES+99, BC97b, CB91, DRGC90, JEB92, MHK95, SPS96a, Van96, WBP91, ZWD98a, ZWD98b]. **Used** [CL94, PTC94, ML99, ZFZ92]. **Usefulness** [KKM99]. **Using** [AL98, Amo96, Art98, BB97b, BL92b, CM96a, CJA94, CMFA93, CTG97, CA97, DE92, EMMS97, FCVL98, FFD98, GD96, GT93, GİA96, GOAY98, HS92b, Jon94, Jur96b, Jur97c, Jur97e, KSG93, KSR95, Kin96, KD95, KLLI97, KO95, KMM96, LKBJ97, LTP96, LR94, MSD95, MRB+96, MAD98, MAI95, MM98, NK96a, Oli99, PM95, PVLG93, PHH94, PMN+92, PR97, RL95, RP98a, ROSM96, SS92b, SD97, SBD+92, SAL+94, TNS+94, Tos95, WHF92, WR96, AR92, ACB+99, ANB94, ACAT92, ACHT95, Ali99, BZ92, BZMR92, Boe95, Boe97, CÅ92a, CP92, Cor92, Csa92, DGMW90, DSS90, DO90, EZ92, EJ93, FL91, FJR96, HC96d, HS92c, HS99, HZF+91, HS92d, HW91, Ish92, ITK91, JL91, JE90, KK99a, KLO+98, KKNY99, KE90, KYW95, KM90c, LP97d, LLB99, LS92b, MHS95, MSMR99]. **using** [MVHV96, MK90, MM94, MR92a, MP91, MRD92, PMDM97, PZDM97, PMDM98, PZDM98, RTS91, Rod91, RBB+94, Sem94, ST97, SSC92, SN90a, Sme92, Tal93, TP94, Tho96, Tom91, TMD96, VA90, VCMLL90, WG99, WDS97, YBZ92, ZZW94]. **Utilization** [BG98a]. **Utopia** [VD95]. **UV** [FLWZ90, KJL96].

V [Ano92l, Brä98a, Brä98c, Cal90a, NM95, REU+91, ABCM93, AFZ+99, BMP93, DTM96, GC91, KSSG95, KL92a, Ney95b, Pal98, SD98, SES93, Wil90]. **V-VII** [BMP93]. **vacancies** [SAB+97]. **Vacancy** [FD96b, SPFL93]. **vacuo}** [AGAP98]. **Val** [LU92b]. **Valence** [BDH+97, BvL96, CWZ98a, Cul95, DC97, FLRV97, FDF97, GLBM96, Har96, Har97a, JM93a, JM95, JG95, JGR98, JF92, KFS92, KGC+96, KZVGB97, LP92, LP96, MF96, McW90, NFVM94, NMM97, PS93, Par97, Rin94, RL92, Rot96, SR96, SBD+92, TC98b, WWM+98, DDC95, DHDP92, For92b, HBJ+92, HSES94, JM96a, KJL96, KT95, MBG90, McW99, MAAP90, NM94, NM96, Rin96, SCJK90, SLDB91, TGS99, WG99, YJL92, Rot97, Sta98d].

Valence-Bond
[Cul95, KGC+96, KZVGB97, SBD+92, For92b, McW99, SLDB91, WG99].
Valence-Shell [KFS92, SR96]. **Valence-split** [Sta98d]. **Valence-Universal**
[JM93a, JM95, JG95, JGR98, JM96a]. **Valencies** [CPTR96, ETV94].
Valency [SGK+95, SG90]. **Valent** [CC96]. **valid** [Sch94]. **Validity**
[Ada96b, Csa96]. **Valproic** [CLR+93]. **Valpromide** [TBBE97, TBBE98].
Valuable [HNB92]. **Value** [JM93b, EMP92]. **Values**
[KS98, NS93b, Núñ95a, Sie93, Jon93, JJ96]. **Vanadate** [KW98]. **vanadium**
[GWB97]. **Vapor** [CL95]. **Variable** [AH97, ST96a, VJ95, VJ97].
Variable-Step [ST96a]. **variables** [YG90]. **variants** [FV96, KRRB99].
Variation [DDD93, DC95, KG92, LG92]. **Variation-Iteration** [DDD93].
Variational [CG95, CT96, CMCR96, CJA94, CJH98, CTG97, CLKMTA95,
HZF+91, HW91, Rot96, Ryc94, TMSI98, Tit93, TŚP97, WN90, Wło94, ZB92,
ACAT92, CZ93, Csa90a, Csa90b, CK91, Fer91, FR98, KDB90, KS92, LV97,
MRD92, Rot97, SGGC99, TTM99, Wil99a, BBMM99]. **variety**
[LS92b, ZW96a]. **Various** [BLRD92, BAK96a, DP93, IAN+94, JM95,
Löw93d, BHGC99, CLGW95, DSS90, JM96a, WW97, WP90]. **Varying**
[ABB93, DPP+94, PB95a, Hag95]. **VB**
[CTG97, KSR95, LP97d, MZ95, Oli99]. **VBSCF** [CWZ98b, DV99]. **VCO**
[hJH97]. **Vector** [FCVL98, PZA92]. **Vectors** [Alt96]. **Verlag**
[Brä95, Brä96b, Brä96c, Car96, Dun96b, Sjö96, Str91]. **Version**
[Amo96, Fue98, LLBM+95, CGMG92, LBL98]. **Versus**
[Cha97, SBIP97a, EMP92, MCB99, MCCF95, OCK99, PZDM97, PZDM98].
Vertex [MD93c]. **Vertex-Alternation** [MD93c]. **vertical** [MHY98, ZM95].
Very [DKWM97, DKM97, Koh95, MLT+96, SPOAS97, Sul97, DKM96,
NSTFC94, New97]. **VI** [TGDS97, CF99, ERC91]. **VI.** [LRM97]. **Via**
[CR93, AKS+90, AFTM95a, AFTM95b, AFO+97, AFTM98, AFZ+99, CSZ97,
DM97a, GGSA98, JBT+95, KM97, LZ96, LKMCVT95, LKMCVT96, Mar95a,
MK95, MK96, MK97b, MK98a, Sah95a, SN99, SD98, SE95b, SE97, FF96].
Vibration [GSSD+96, LT99, TL98, VJ97, CTF92, FR93a, ST91, TS92].
vibration-rotation [ST91]. **Vibrational**
[AML+95, AMD+97, ABDM94, BKWL97, BZMR92, Bau97, BCMÖ97, Cha97,
FSHC99, GDID98, GH99, Hea97, Her98, Hua92, JDJP99, JAG95, Kal90,
KVB97, KC98a, KLC98a, KC98b, KC97, KMM96, KL97c, LKMCVT95,
LKMCVT96, Pal93b, RABZ94, SM96b, STMR97, TLC98, TT98, VX99,
VJ95, WD91, YBM97, Ali99, AH92a, BFL91, ČDM91, FLHT90, FB90, FL95,
GZDZ97, HS99, HZF+91, Kar90, KLC98b, KL92b, LTY90, MHL94, McH91,
NL96b, OSS95, RCWN94, SE92, SBZ92b, TLTL92, TBP99, WBS99, Zha92b].
Vibrational-Rotational [LKMCVT96]. **Vibrationally** [DDH+96, BJ92].
Vibrations [CG96, Her93a, Her93b, HP97, JBT+95, Sch95b, Sch95c, GT97,
LF99, MG97, MRBM91, PCB92, Sch95a, SZCO99, TG96]. **Vibronic**
[CC97a, GS90b, xLTY92, PSD97, CSG99, Tac92]. **View**
[Par94a, Kel97, KDB90]. **Viewpoint** [DB99, ZM97, KM90b]. **Views**
[Mon99c]. **VIF** [Sin92]. **VII** [BMP93, DS99, LP96, PVLG93]. **vinelandii**

[SZ98]. **Vinyl** [ADPS98, Mor97a]. **Vinylamine** [ADPS98]. **vinylpyridines** [AEHM91]. **violating** [SB92b]. **Virial** [KBA96, LCB98, Nag94, Pop98, GSM90, GS92a, GS92b, SN90b]. **virial-type** [GS92b]. **Viridis** [CMSF93]. **Virtual** [Coo96, MR92b, RSGC96, RS98, WZW96, BBK90, MPP92, Pau92, Was91]. **Vision** [PS92a]. **Visualization** [PJ96, YKN$^+$99]. **Vitae** [Ano91z, Ano91-27, Cle92b]. **vitro** [Bha99]. **VO** [Bro95a]. **void** [BB93]. **Vol** [Ano92j, Eri92, Lun91, Lun92, Mon94, Ano93h, Mon93, Tri96]. **voltage** [MD93b]. **Volume** [Ano95-47, Ano96-59, Ano96-60, Ano96-61, Ano96-62, Ano97p, Ano97q, Ano97r, Ano97s, Ano98q, Ano98r, Ano98s, Ano98t, Ano98u, Ano99q, Ano99r, Art98, Cal90f, DFDK99, PP98b, Art94b]. **Volume-Dependent** [DFDK99]. **volumes** [PS92c]. **Voronoi** [PS92c]. **VPA** [BBE95]. **VPGG** [LCP$^+$91]. **vs** [ÅGL97, Boe96, KM92, KD98, RK95, SCA93, Sur97]. **VSCC** [SR96].

W [Brä95, Cal93, Str93, KO95]. **Waals** [AMRT94, Dob98, GZDZ97, HBL99, Lin91, LAS$^+$95, RAM91, RP98b, SDP$^+$95, XY98, ZRNZ97]. **Wagging** [VBUS99]. **walk** [CE90]. **walking** [SN90a]. **Walks** [BKM93, CDG04]. **wall** [KSH92]. **Walls** [LKFF98]. **Wannier** [ITK91, Tac94]. **Water** [AMRT94, AMT$^+$99, AR96, BTTS97, BSP97, BMK96, ESP98, GW98b, JCÁ96, Kry98, Mez94a, NS97a, NS97b, SPC96, TNM98, TNS$^+$94, ZL98, ACB$^+$99, BHL$^+$99, BPVP92, CLOFR98, CBL95, Cor92, Ell91, GSPSM93, GGHP94, HS92a, Hua92, KS94c, KY91b, LADV92, MD94, MD95, MRBM91, SM92a, TW90, TW92, YSJ94, ROL$^+$90, SOK$^+$98]. **Water-Assisted** [BTTS97]. **Water-Carbon** [AMRT94]. **Watson** [FL95, ZL98]. **Waugh** [XYC98]. **Waugh-type** [XYC98]. **Wave** [AC97, BDT96, BBC$^+$96b, BK94b, BGS98, CWZ98a, CC98, CZ94b, CB96a, CPTR96, CTG97, DLV95, DKWM97, DKM97, GVC96, Gui98, Hoo94, Kry95, Kut94, LB98, Maz98, Moi97, MV99, NP96a, Núñ95a, Núñ95b, Núñ97, Oht98, OK96, Pen93, Pen96, SN98, TKMA92, TM93, TT98, AA92, BBS91, BS91a, BCC99, Bar90, BUZ94, BE93, BGS97, BYGA99, CC91a, DBLV94, DKM96, DBM99, FG99, GL99, HK95a, Hos97, HYS91, KE90, KKWT99, KT95, LP97d, LV97, LDJH92, LDHJ92, MD99, Mez90, MPSLB91, PY92, PL91, PDO92, Res99, Sch92c, Sch94, SG90, Sir99, Sme92, SKRK90, TWK98, VA90, Wil99b, YKN$^+$99, YG90, AS93]. **Wave-Function** [BBC$^+$96b, Kry95, SN98, CB96a, CC91a, Sme92]. **wave-packet** [PL91]. **wavefunctions** [Cio93, HS92c, TH90]. **Wavelet** [FD93]. **Wavelets** [Cal96b]. **wavepacket** [BFV$^+$93]. **wavepackets** [NNY$^+$96, NKS$^+$96]. **Waves** [Sur97, BK97, LB96b, Lin92, TBW90]. **Way** [Gin96a, KC98a, KLC98a, KC98b, PJ96, VdV96, KLC98b, Löw90d]. **Ways** [ZZZY96]. **Weak** [Pal95, SE93b, SL93]. **Weakly** [Fer95, EE91]. **weight** [KÅ99]. **weighted** [BRV99]. **Weizsäcker** [RDY95]. **Well** [PB95a, Taş96a, MCB99]. **well-depth** [MCB99]. **Wells** [PB95a, LTSL96]. **Werner** [BDPS97]. **Werner-type** [BDPS97]. **Weyl** [LP92]. **WF** [Gut99b].

Wheeler [CGMG92]. **Wheland** [EMMK94]. **Which** [Reg92]. **While** [MZ95]. **Whose** [JM96b]. **widths** [GZDZ97, MTTS93]. **Wiener** [Luk92, SYZ96]. **Wigner** [Ell92, Lai94, MYPL90, SD96a, SIM93a, Wen98, WI98, WN90]. **Wigner-Based** [Wen98]. **Wigner-like** [WI98]. **Wiley** [Cal90g]. **William** [Ano91z, Ano91-27]. **Wires** [BW97]. **Wirzba** [Kar93]. **withdrawing** [LRR92]. **Within** [Aqu95, DD98b, Gin95, Hag97, MR99, Sah95a, SV95, VDBPR97a, A.95, AGNS92, AO93, DDG93, DM92, KLC98b, KSH92, MCT99, Min90b, RWT92, Røe91, RK92, VDBPR97b]. **Without** [CM94, Mar98b, Maz98, STY$^+$98, SNNY99]. **WKB** [And93a, SR99]. **WO** [SL97, SL97]. **Wolf** [Brä95, Brä98b]. **Wolfgang** [Brä96c]. **Woodward** [SS92g]. **words** [Löw91e]. **Work** [Sah95a, Sah95b]. **Working** [NS93a]. **Works** [BPE97]. **Workshop** [Kar93, RS97a, Ano96-31]. **Workstations** [VHFL93]. **wrong** [Klo90]. **Wurtzite** [RAA94]. **Wurtzite-type** [RAA94]. **Wyatt** [Deu98a].

X [BL99, BP93b, GARC97, JH90, Kor90, LDP93, LSC98, LCS98, Mic96a, NL96a, STMR97, SES93, VABM94, YZX96, Str92, ÅGL97, ACHT95, BKS97, DD96, DC97, Deu96, FV96, GGHP94, HMGP93, HHPT91, Kar96, LH94, LP99, Mar98a, Moc99, NÅJ91, NÅJ92, NMCK92, PVČ$^+$90, RSCP91, RA96, SL93, SST93, SST94, TNS$^+$94, WS94b, Brä98c]. **X-Alpha** [HHPT91]. **X-NO** [HMGP93]. **X-Ray** [ÅGL97, DC97, Mar98a, TNS$^+$94, ACHT95, BKS97, DD96, GGHP94, WS94b, Brä98c]. **Xe** [EKI94, Ish92, JM99, KKWT99, RP98b, SCL96]. **Xe-NMR** [SCL96]. **XeF** [MSD95]. **Xenon** [SM95]. **XH** [BL99, EMS92]. **XII** [Mor93a]. **XIII** [GS90b]. **xiv** [Str91, PFMC97]. **XPS** [BL98, DHDP92, DO90]. **xvi** [Str92]. **XXVI** [Mat96]. **XY** [GARC97, GARC97, STMR97]. **xylose** [FNSV99]. **XYSO** [GKKM96]. **XYZPO** [GKKM96].

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Z [Cal90d, Deu98a, Kor90, HRH99]. **Z-1** [HRH99]. **Zagreb** [Cal90d]. **Zahradník** [Ano90y, Ano90-28]. **Zajonc** [Deu98b]. **ZDO** [Boč90]. **Zeeman** [BLG95]. **Zeolite** [LV98, NNMH96, MBML91, PB95b]. **Zeolite/Adsorbate** [NNMH96]. **Zeolites** [KD98, SPG97, SHC$^+$98]. **zeolitic** [LADV92]. **zero** [AH92a, MD93b, ROL$^+$90]. **zero-field** [ROL$^+$90]. **zero-point** [AH92a]. **zero-voltage** [MD93b]. **Zeroth** [Sie93]. **zervamicin** [HMK96]. **Zeta** [KZ99, PG94, TKSH93]. **Zeta-Function** [KZ99]. **ZH** [Kor90]. **Zhang** [Deu98a]. **Ziegler** [Nov92, Sak97]. **Ziegler-Natta** [Sak97]. **Zimm** [Jac92]. **Zimmerman** [Zho94]. **Zinc** [Ryd94, LMMK93]. **Zinn** [Kum93a]. **Zinn-Justin** [Kum93a]. **zippers** [SKM99]. **Zn**

[IK97]. **ZnO** [MAL93, MALT96, MLT98, NF92, SBD+92]. **ZnS** [MW92, MW92, SZ97b]. **ZnSe** [MW92, MW92, Por98, Wil90]. **Zr** [Bec97a, Cun92, CC96]. **ZrO** [ABCM93]. **ZrSiO** [ABCM93]. **Zwitterionic** [PLV92].

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Anonymous:1992:Mr

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Anonymous:1992:Mw

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Anonymous:1992:Mx

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Anonymous:1995:Mf

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