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## Title word cross-reference

10 [FK91]. 12 [FK91]. **$120.00** [Gol92]. **$142.00** [Dun90]. **$152** [Dav97]. $1 \rightarrow 4$ [GZL+94]. 2 [KMM99, SCMV97]. 3 [AT93]. **$34.95** [Gar90]. **$35.00** [Mez91]. 4 [JFR92a, JFR92b, KMM99, KHG96, SCMV97]. $4 \leq n \leq 8$ [KT91]. 5 [KHG96]. **$55.00** [Var92]. 6 [FK91, KMM99, SCMV97]. **$65.00** [Klo92]. **$72.00** [Ran92]. [$n$] [BRLD92]. $^{+}$ [Cha92, CLS+97, GS90d, GCG97, GLLOB91, JKS93, Lóp95b, LDMS99, Mar98, PFFF97, PGBM97, Sie96]. $^{+}_{13}$ [GYT+98]. $^{-}$ [GS90d, MI99, Sie96]. $^{1}$ [CGBC96, CÉC97]. $^{11}$ [WHM+96]. $^{13}$ [KMM99, Wib99]. $^{15}$ [GM98a]. $^{19}$ [KMM99]. $^{2+}$ [GWHD99, GLLOB91, Gre95, GSK95, GG96, Mar98, TRG99]. $^{2-}$ [SHM99]. $^{3}$ [CGBC96, CLS+97, GdAG+98, TK94]. $^{\alpha}$ [HMČ91, Kik96, Kik99]. $^{cdot,2+}$ [GCG97]. $_{1}$ [AVC93, AVP93, CGBC96, GdAG+98, MR93, MRG97]. $_{10}$ [MFG91]. $_{12}$ [FM99]. $_{1A}$ [AT93]. $_{2}$ [AS98a, Arn94, AHLR+91, BSvRS95, BADP92, BvH+92, BSN99, BBS96,

**/empirical** [YM98].

**0-947143-84-5** [Ran92].

**1** [GdAG+98, MRG97, RM94, VHV90, YBD+94, YTRB97]. **1-amino-3-propenal** [FA99]. **1-butene** [PG91]. **1-chlorosilatrane** [CH96b]. **1-difluoro-4** [LCA94]. **1-fluorosilatrane** [CH94]. **1-methyl-dihydronicotinamide** [CG90]. **1-Palmitoyl-2-linoleoyl-phosphatidylcholines** [LH96]. **1-X-3-M-bicyclo** [GdAG+98]. **10-diazabicyclo** [SHHČ90]. **10-dihydroanthracene** [SR92]. **10-dihydrophenanthrene** [SR92]. **10-electron** [WAM93]. **10-vertex** [ZBM91]. **10.1002** [Ano15]. **10.1002/** [Ano15]. **1096-987X** [Ano15]. **12-dihydropleiadene** [SR92]. **12-vertex** [ZBM91]. **15** [Ano97]. **16-tetraoxa-1** [SHHČ90]. **18-crown-6** [LHBF93, SK92b]. **1988** [Chr90]. **1a** [CLQSS98]. **1s** [CDG+99].

**2** [Ano15, Bic99, CG90, LS98, SBM97]. **2-** [SK91, VFM+90, WJL+96, WJV+96]. **2-benzodioxaphosphorin** [KTS92]. **2-D** [SHCY93]. **2-dimensional** [RPGS97]. **2-dinitrosoethylenes** [SCP92]. **2-dioxin** [FLHP97, PFLH93]. **2-dithiin** [FLPH98, PFLH93]. **2-ethanediol** [RBSB96]. **2-hydroxypyridine** [RGK93]. **2-hydroxypyridine/2-pyridone** [RGK93]. **2-K** [Ano15]. **2-methylbutyronitrile** [CC91b]. **2-phenyl** [WMM+95]. **2-pyridone** [RGK93, BA94]. **2-sulfides** [KTS92]. **2-trifluoromethylphenol** [KKCH96]. **20-hydroxy-4** [SHHČ90]. **21G** [FG96]. **21SP** [MHB97]. **22SP** [MHB97]. **272** [MRG97]. **2A** [HEN+94].

**3** [ST92, FDMB92, KHF91, Kas90, MFG91, Tay99, VFM+90]. **3-** [SK91, VFM+90]. **3-21G** [FG96]. **3-21SP** [MHB97]. **3-amino-1** [IMP91]. **3-aminotropanes** [LSDB99]. **3-azabicyclo** [SMS98]. **3'-azido-3'-deoxythymidine** [ST92]. **3-benzazepines** [AVP93]. **3-butadiene** [JZ96, LV90]. **3-c** [CLQSS98]. **3-diamines** [LSDB99]. **3-diaza-1** [JZ96]. **3-dihydro-1** [FLHP97, FLPH98]. **3-diox-4-ene** [FLHP97]. **3-dioxanes** [HCK95]. **3-dioxin** [FLHP97]. **3-dipolar** [CN98, MP98, SSQ92]. **3-dipoles** [MM94a]. **3-dithiin** [FLPH98]. **3-methyl-1-butene** [PG91]. **3-methyl-1-pentyne** [CC91b]. **3-methylindole** [WLKJ92]. **3-shifts** [IBKvRS92]. **3-substituted-1-methyl-1** [BHK+91]. **3-triphenyl-1-propyl** [IMP91]. **3.0.CO** [Ano15]. **3.2** [MR92]. **3.2/CHARMm(R)** [MR92]. **31** [MR93, RM94]. **31-8959** [MR93, RM94]. **31g*** [CNOJ93, OJL93, FW93a]. **3D** [AC94, Cri99, HGB93].

**4-22SP** [MHB97]. **4-amino-4-oxo-2-butenoic** [Kat90a]. **4-bis** [WJL+96, WJV+96]. **4-dihydro-1** [FLHP97, FLPH98]. **4-dihydro-1a** [CLQSS98]. **4-dihydropyridines** [BHK+91]. **4-dimethoxyphenyl** [WJL+96]. **4-dimethylcycloheptane** [LCA94]. **4-dioxene** [FLHP97].

**4-dioxin** [FLHP97]. **4-dithiin** [FLPH98]. **4-fluorophenyl** [Fro93]. **4-monosubstituted** [SK91, VFM+90]. **4-substituted** [AHLR+91].

**5** [AT93]. **5-cyclooctadiene** [RD97]. **5-Dimethoxy-1** [WJL+96]. **5-distyrylpyrazine** [ENHE98]. **5-HT** [AT93]. **5-tri-** [OC98]. **5-trimethoxyphenyl** [WJV+96]. **5.1** [GPPS91]. **5.21** [GPPS91]. **500-ps** [SYHW99].

**6** [OJL93]. **6-31g*** [FW93a]. **6-31G*-based** [OJL93]. **6-31g*-derived** [CNOJ93]. **6-dihydro-1** [FLHP97, FLPH98, PFLH93].

**7** [Zho97]. **7-tetrahydroazepines** [AVC93].

**8-methyl-N5-deazapterin** [CG96]. **8-methylpterin** [CG96]. **86th** [EHNW96]. **87** [Fro91, Tay99]. **87-118** [GS90c]. **87-16-12049-3** [Tay99]. **8959** [MR93, RM94].

**9-deazaguanine** [KG99]. **987X** [Ano15].

**=** [AS98a, BSvRS95, BT92, FBTD92, GS90d, JFR92b, Lóp95b, SHM99, SM91, ZY96].

**A*** [LP90]. **A-DNA** [BB98a]. **Ab-initio** [GCRSAIVB99, KHA90]. **Ability** [JS93, Wib99]. **absence** [YBD+94]. **absolute** [Åqv96, SCC93]. **absorption** [Che95a]. **accelerator** [TMK+99]. **acceptance** [SN90]. **acceptor** [GC98]. **acceptor-substituted** [GC98]. **acceptors** [NPLT97]. **accessibility** [YB95a]. **accessible** [CS95, FB98, FS97, GŌ95, Her97, PCG+92, SNS95, Wan91, WL91a, WWSS98a, WWSS98b, WSS99c, ZKSB93]. **Accompanying** [Ish98a]. **account** [ZS99]. **Accuracy** [CNOJ93, AS97, BNDS97, DM91, Gen99, HW97, HK95, SW96a, RSOF96]. **Accurate** [CB96, DP95, Mar97a, Mar97b, Mar98, MHB97, KUT+97, KK92, MFG91, OL90, PFM91, PN95, SSRO92, TKTN99, Tav96, WF94]. **acetamide** [CK91]. **acetate** [LYH+95]. **acetic** [MvEP+98, PRRD98]. **acetyl** [HMČ91, SVS+97]. **acetylacetone** [HR97, SHCR97]. **acetylalanylglycine** [SJDW90]. **acetylaminofluorene** [FW91]. **acetylene** [LSSvRS96]. **achieved** [BNDS97]. **acid** [ALPH91, AGP91, BF96, DW98, HOL98, HMČ91, Kat90a, LDVP91, MP98, MvEP+98, NBG93, PRRD98, PFM91, RC95, RTGJ98, SV94, SCZC99, TGW96]. **acid-catalyzed** [Kat90a]. **acidic** [GHS97]. **acidities** [Kas90, WCK96]. **acidity** [KHF90, KF94, LS96]. **acids** [ASM+92, BB98a, BKK+96, CBIT94, GK90, KHF90, Kat90a, Kik99, NTK96, NS98, PC93, Smi99]. **across** [CA95]. **acrylamide** [BB96a]. **acryloyl** [BADP92]. **actinide** [SHM99]. **action** [MSSS95, SSM96]. **activation** [CY98, Vya97]. **active** [CT97, CG96, FA99, GBE92, HK90, SWS+90, SBS99]. **active-site** [CG96]. **activity** [AT93, KF94, RdBN90, Ric91]. **acyclic**

MFG91, OL90, RC93, SUG92, SMF91, VFM+90, WF94, Wel90].
**AM1-calculated** [GMO93]. **AM1/MST** [LBO94]. **AMBER**
[Can93, DK93, HKŠ+97, HA95, SL95]. **AMBER4** [VM95]. **AMBERCUBE**
[DK93]. **ameliorate** [SLPP97]. **amide** [KB92, MR93, SJDW90]. **amides**
[BB96a, DH95, GM99, LA91, MHJ+98]. **amiloride** [VPV91]. **amine**
[GBT97]. **amines** [LCD+97, SUG92]. **amino** [BB96a, BF96, DW98, FA99,
GK90, HMČ91, IMP91, Kat90a, Kik99, NTK96, NS98, PFM91, Smi99].
**aminotropanes** [LSDB99]. **ammonia** [KS96]. **ammonium** [LCD+97].
**among** [CSC96, GPF97, PPK92]. **amorphous**
[CJC+93, CTJ+94, CJC+96, DH99]. **AMPAC** [LW92]. **amplitude** [SG95].
**AMSA** [SUG92]. **AMSOL** [HL96a]. **analog** [Fro93]. **analogs**
[BH91b, Can93, PRRD98, Sul95]. **analogue** [CG90]. **analogues**
[DRF92, HS95a]. **analyses** [KTT94, KTT95]. **Analysis**
[BC95, BBR98, BGZP97, CDG+96, Cso93, FD94, MJ93, Mer92, SSQ92,
VCLB92, AT93, AGN+90, AVC93, AJB96, AHLR+91, Art94, ARLG+94,
BPS93, BB98a, BB96a, BF96, BKL+90, BW90, BR97, BJK95, Bro99,
CGdAC91, CEÁ92, CT97, DNC96, DRF92, DZ97, FBTD92, FGG+92, FRC91,
FPR97, FCS98, Fro93, GM98a, Gen99, fGGG94, Gio98, Gla90, GSB99, GW98c,
GSK95, HS93a, HKK91, HH99b, HCCC99, IMP91, ISH98b, JB95, JVB95,
Jem97, KT91, KZ99, KG91, KPI95, KCK98, KHL96, KRB+92, KRB+95,
KTS92, LPD90, LP90, LK92, LSDB99, LFB96, LBA+99, MvRSL+97, Mar90,
MNVM97, MM97, MFG97, MR93, MRG97, PSY+99, Pet93, PD99, Ran91,
RM94, RD97, RPR+98, ST92, SSD93, SD90, SM94, SB98b, SR94b, Sul95,
SSO94, SSRS94, SSR94, SSR95, SFB91, TKF92, TGW96, TLBP99]. **analysis**
[VTR+94, VSF97, WSV92, WCMS91, WJV+96, YC95, ZHSB92, dANS+96,
dVA92, MSSS95, VGN+92]. **Analytic** [Jon91, DKK+93, EA93, SG95].
**Analytical** [CMC96, Pac93, PT96, ŽRK+95, EKS97, FB98, GŌ95, MK92,
PCG+92, Pet94, WS99a, WS99b, YB95a]. **analyzing** [HH99a, JMH96]. **AnF**
[SHM99]. **angle** [BBvG95, CNS96, KG91, LPK99, SF92, TGW96]. **angles**
[BK96, GH98, GS90a, LA90, SG95, Tav96, WTLC93]. **angular** [ZS95].
**anharmonicities** [HI98]. **anharmonicity** [VHV99]. **aniline** [AYC94].
**anilines** [KHF90]. **anion** [FSCS99, LH99, O'm99]. **anions**
[DBS91, ENvRS94, LK90]. **anisole** [MV91]. **anisotropic** [WAW+97].
**Anisotropy** [ST94]. **annealed** [AW90, SSD93]. **annealing**
[BM99, CE96, EHNW96, GW95, LSR97, MPBM98, NVS91, Nil91, Sno92,
WP97, WCMS91, YTT97]. **Announcement** [Ano90a, Ano90b, Ano92a,
Ano93a, Ano94a, Ano94b, Ano94c, Ano94d, Ano95a, Ano95b, Ano96a].
**Announcements** [Ano91a, Ano91b, Ano93b, Ano94e]. **Anomalous**
[GvRSvEH+93]. **anomeric** [Arn94, FRC91, FVR92, KA96a, KHA90].
**anomers** [BSC+98, DDV93]. **anthracycline** [SSM96]. **anti** [FHT99].
**antialiasing** [BNDS97]. **antibiotics** [FDMB92, FDMB93]. **any** [SSRO92].
**apically** [GS90d]. **apicophilicity** [WZG+93]. **apparent** [CT95, CTC95].
**Applicability** [GML94, MRM97]. **applicable** [She90]. **Application**
[BP94, CCJ+99, CCBK95, CHSK96, HEN+94, KF94, LJ92, RPGS97, SKA93,

SS93, WMM+95, ACD99, AKF93, BMW+90, BMD99, Ber97b, BRH90, CPR90, DH95, EKS97, FR90, FW92, FSI95, GGP96, HB91, KT93b, LPD90, LFB96, MK97a, NVK+97, PL94, SHM99, VWGF95, AW90, BBH99, CFK97, CT99, CBSR99, CG94, GVH94, GP94, GK90, GW95, HY96, JCV+93, Kik96, KJ97, KG99, LKLB+99, MN95, PNJS93, PKN+95, Pet95, RGK93, RTSM93, SMM97, TEdV90, VRBE93, YTRB97, ZS99, ZM90]. **Applications** [Nil91, TKSM96, VVSV96, WCMS91, ATK94, BDKJL95, DZSB94, GBW98, JM90, Klo92, SJ95, YTT97, AJ99b, BK97a, FRZ93, HK90, LLD98, PS92, WLKJ92, WS93]. **applied** [BMN99, DKL90, FPL95, GH98, ST91, SW93a, SHCR97, TEHL93]. **Approach** [CN98, AD90, BBR96, BDH+94, BCG97, BFST93, BWS+95, BP93b, CZM98, CC91a, CE96, CS96, DF96, DF97, DM91, DH99, ES99, Flo92, FW93a, GGK98, Gri90, HO93, HY96, JJTP93, JAdV96, Jur96, KW91b, KPI95, LL94, Lim97, ORK+91, PS97, PP98, RM91, RCAA99, SB99b, SBK97, SC95, SKM94, SSRS94, TLBP99, TP93, TS99a, WP97, YM98, YH93, ZYY95b, Zho93, ZL94, ŽRK+95]. **Approaches** [WH95, ALO94, BT96, BKMH97, BKL+90, BBS96, CKP96, ELA+95, GCT96, MRM97, NVS91, FM91]. **Approaching** [NBB+99]. **Approximate** [KKJ97, WSS99a, dlVM91, ABBC99a, ABBC99b, AGM91, WSS99b, ZG92, ML92]. **approximately** [ZS99]. **approximation** [ACD97, FRSNS92, FTA91, FM91, HHC90, LM93, NBB+99, PG98, PS91, PS92, PT99, RHK90, RHKK90, Tru91]. **approximations** [BBS96, AJ99a]. **AQUARIUS2** [PMRG93]. **aqueous** [CG93, CT92, CG94, CG97, CG99, Gao97, GK93, Mar90, NBS94, PPAS+99, Pra93, TYMS98, UF93]. **arbitrarily** [TG98]. **arbitrary** [JCV+93, Phi90, TAC98, Vya97, YH93]. **architecture** [RBE98]. **area** [BG96a, BG96b, ELA+95, GÖ95, Her97, LM93, NBS94, STPA91, VB93, WL91a]. **areas** [FB98, Her93, PCG+92, SNS95, WWSS98b, WSS99c, WWSS98a]. **argon** [NQ99, Pul97]. **ARGOS** [SM90]. **aromatic** [BCF+92, LDJ+97, NPLT97, PNJS93, PMHRG97, SUG92, Sun94]. **aromaticity** [FM99]. **aromatics** [PBS97]. **Artificial** [TYRD92, CS94, FPL95, LPD90]. **aryl** [FHT99, KHF91]. **ASC** [CT95]. **ascent** [HKK91]. **ascorbic** [ALPH91]. **aspects** [CG90, DBS96, Pet94, SN99]. **aspirin** [PRR+99]. **assemblies** [ELA+95, Tel90]. **Assessing** [VHKB98, VHD+98]. **Assessment** [VRBE93, AS97, CSC96, OM96, BG96a, SW96a]. **assignment** [BGBW97, CCN90, ORK+91]. **assisted** [LL94, VP92]. **association** [RTSM93]. **asymmetric** [GML94]. **Asymmetrization** [GC98]. **Asymmetry** [MS98]. **atmosphere** [AIDAVB98]. **atmospheric** [GCRSAIVB99]. **Atom** [KVL91, BW90, BR97, DFTRJ97, DK97, GDK92, HREK98, LKSS91b, ML91, ORK+91, SKA93, SB99a, ST94, ZA94, ZKA94]. **atom-centered** [BW90, DK97]. **atom-type** [ORK+91]. **Atomic** [BMK90, DM94, Din91a, DJ92, GM99, Pac95, SH98, WF94, ACD97, AGM91, BSS90, BRC94, BCG97, CDR+95, CDG+99, ČTS98, Din91b, DH95, DJ93, FR94b, FS94, FCCG96,

NVER97, Par99, RLG98, SBM97, STB+94, SS95, SG95, TRG99, WCK96]. **Beyond** [KT93a, DK97, HKŠ+97]. **Bezier** [TS99a]. **BH** [MQS+97]. **Bi** [BT92, Ste91]. **biased** [KG93]. **bicyclic** [AW90]. **bicyclo** [GdAG+98]. **bidentate** [TRG99]. **Bidirectional** [KLR96]. **bielectronic** [CDR+95]. **bifunctional** [VCLB92]. **bilayer** [CCJ+99]. **bilayers** [TM95]. **bimolecular** [Lóp95a, Lóp95b, MGLL99]. **binding** [Åqv96, APC98, BPZL96, BG99, BSL91, CS95, Cri95, CG96, GSB99, GJL+90, Gre95, GG96, KSB+93, MLA+99, MGH+98, PBS97, RM94, SQ95, SW96a, SN91, SB99b, SR90, TRG99, Van97]. **biochemical** [Mul91, SACKH95]. **biologic** [DDV93]. **biological** [CG90, DDLV95, DVL90, TKTN99, WNW91, ZKSB93]. **biologically** [BHK+91, Gre95, GG96]. **biomacromolecular** [SKT94]. **biomaterials** [PC94b]. **biomolecular** [DZSB94, JLW99, Mar90, SKT93, ZM92]. **biomolecules** [GS93, KWWS91, KRB+92, ZM90, ZS93]. **bioorganic** [MRG+90]. **biopolymer** [Elv91]. **biopolymers** [CCBK95]. **biorthogonal** [MM94b, MM94a]. **biphenyl** [LH99]. **bis** [GWHD99, VW96, WJL+96, WJV+96]. **Bleep** [MLAT99, MLA+99]. **blocked** [PFM91]. **blockers** [Fro93]. **Bloembergen** [Kar99]. **BO** [IBKvRS92]. **boat** [HCK95]. **bodies** [FS98a, FS00, WM95]. **body** [KL91, Kna92, MPJ98, MPJC98, ZvN93]. **Boltzmann** [AS97, Bru93, BNDS97, CF97a, CF97b, HL96a, HS93c, HS95b, LDM92b, NH91, RM91, Sha91, SQ95, SW96a, SMM97, TG98, ZYY95b, ZPV+96]. **Bond** [WB91, ACK+96, BPS93, BW91a, BFST93, BKMH97, BBH99, CW91, Che95b, CTJ+94, DH94, EGH+93, Fag91, GH98, GdAG+98, GW98b, GHT98, GMY97, GM99, HD92, Jai90, JB98, LPK99, MM94b, MM94a, McD97, MP90, OL93a, Pao90, PHG94, RR92, SR94b, TK94, TNS97b, VF92, WP96, ZRVD93, LA90]. **bond-charge** [BBH99]. **bond-length** [PHG94]. **bonded** [AG90, Art94, TEdV90, VHV90, Zho93]. **Bonding** [LM96, AS98a, CDG+96, FF93, JG93b, JS93, KWWS91, KKCH96, LA98, LKC+98, LPT97, Mag95, NPLT97, PSY+99, SHHČ90, UVRCR92, VRC92, ZM92, PD99]. **bonds** [AJ97, CBSR99, FVR92, FS94, GM90, KPSM98, LBA+99, PD99, RBSB96, Rod94, TLBP99, vDvdRvD92]. **Book** [Chr90, Dav97, Dun90, Gar90, Gol92, Klo92, Mez91, Ran92, Tay99, Var92, Zho97]. **Boolean** [LM93]. **boranes** [IBKvRS92, ZBM91, TLBP99]. **Born** [BG93, NBS94]. **Born/surface** [NBS94]. **boron** [GM98a, WHM+96]. **boronic** [CBIT94]. **both** [DDV93]. **bound** [DV97, Lóp95a, Lóp95b, YBD+94]. **boundary** [BWS+95, ÇHP91, DM91, EJ95, För92, FUS+94, PN95, Pur98, SKT93, VS97, WWXS97, YKU96, YL90, ZV96]. **bounded** [DF96]. **bovine** [Kik96, PS92]. **Bowl** [SD98, FM99]. **Bowl-shaped** [SD98, FM99]. **box** [Bek97]. **Boys** [BP93b]. **Br** [AS98a, SI93, HK95]. **bracing** [LL94]. **bradykinin** [SSD93]. **Breit** [SCMV97]. **Broken** [RCAA99]. **Brönsted** [BKK+96]. **Brownian** [Elv91, SMA92, SWOW97]. **Broyden** [AB98b]. **BSSE** [PS98, VVM93]. **Buckingham** [ZY96]. **Buckminsterfullerene** [BMP+91]. **build** [PT98].

**Building** [YTRB97, PAS90]. **Bulk** [CW93, ACB97, NBB+99]. **bulky** [PSK98]. **butadiene** [JZ96, LV90]. **butanal** [LP92]. **butene** [PG91]. **butenoic** [Kat90a]. **butyl** [BH98a, Ove91]. **bz** [GWHD99].

**C** [CÉC97, GCRSAIVB99, GdAG+98, GCG97, JFR92b, MFG91, TDFdC91, ZY96, CLQSS98, AOYŌ96, DJ94, FM99, Fro91, GCRSAIVB99, GdAG+98, HDA93, IBKvRS92, KMM99, Kik96, Kik99, KG99, LSSvRS96, MFG91, PT99, SA99, vRSD92, SD98, SC91, TDFdC91, Wib99, YSJ95, ZY96, TDFdC91]. **C-** [HDA93]. **C-NMR** [Wib99]. **C-terminal** [YSJ95]. **C1** [SI93]. **C13** [CBSR99]. **C14** [CBSR99]. **C15** [CBSR99]. **Ca** [FR94b, GG96, Mar98]. **cadmium** [HM90]. **cage** [LKSS91a]. **cages** [LKSS91b]. **calcium** [CHPK91, SN91]. **calculate** [BB96b, Gri90, PL94]. **Calculated** [SCP92, AJB96, DM90, DJ93, GMO93, GPPS91, GLoNP96, HBLL98, HYA92, KHF90, KHF91, Kas90, LSCA98, MGLL99, Nic97, REA+98, SC94, SKK+93]. **calculates** [AFK+95]. **Calculating** [DM90, ZYY95a, ATS90, CR95, HVM99, KPR91, Mul91, Net94, PZBM98, Pur98, RC95, SKT94, SNS95, VDF+97, WL91a, WO97]. **Calculation** [Åqv96, BF96, BB98b, DZ97, ER95, GH97, Her93, KOH97, KOH98, KKE93, KSD90, Mit98a, Phi90, RE99, SQ95, SACKH95, ADG99, AC94, ACRC97, BSS90, BG96a, BG96b, CPJ98, CMC92, CGBC96, CD97, CBSR99, Cul92, DKBS97, EA93, Fag91, FW92, FW93a, FB98, FS97, GJR91, GPF97, HGC+95, HG93, HW97, KW91b, Kul90, LV90, LDM92a, Mar98, MVS92, MSDC94, Mez92, Mit94, NIS98, NL91, Pet94, RK97, RCAA99, SW96a, SOL97, SMF91, SC95, SKM94, TKTN99, VSF97, WHHP97, WWF95, YG92a, vDvdRvD92, MLA+99]. **Calculations** [CMS91, AGN+90, AMY98, ALYT90, ASM+92, AF93, AF94, AYC94, Ano97, AL98, BLO94, BFH94, BCFM98, Bec99a, BFST93, BB96a, BJ94, Bog99, BB95, BW91b, BNDS97, BLF95, BRH90, CLCL96, CW97, CDG+99, CHPK91, CBWF98, CBIT94, CT99, CRME93, CKP96, CW93, Cso93, CG94, CG99, DPK94, DH90a, DB98, DJ92, DBT98, Ear93, EGH+93, FGBH90, FA94, Fel96, FR90, FK91, FGG+92, FPSK92, FM99, FDMB92, FDMB93, FLHP97, FPC91, GBE97, GC97, GMY97, HK90, HS99, Hil97, HHC90, HWH+91, HA95, IRRR93, Jai90, JP92a, JP92b, JFKK94, JK98, JG91, JFR92a, JFR92b, KSP90, KZ99, KMO92, KHB92, KK91, KRB+92, KRB+95, KPV96, KTS92, LCW93, LSR97, LMRRL98, LCD+97, LA94, LSFFM+95, LO98, LDM92a, LW92, MM93, MNVM97, MRW91, MSB95, MSB96, MM91, Mit98a]. **calculations** [MPJ98, MPJC98, MTR90, NCA96, NLA96, NA96, NSA+97, OS98, OBL95, PLY98, Pea94, PR95, PC94a, PFLH93, PK91, PN95, RG99, RC93, RPW98, RCv96, RCvRS97b, RCvRS97a, RvRS98, RSOF96, RLA+98, RHKK90, RSK92, SN90, SD90, SJDW90, SHM99, SKA93, SS93, SN99, SLH96, SKT93, SR94b, SS95, SRI92, SCRI93, SCMV97, TP93, TA94, TNS97a, UF93, VRV99, VÅJ94, VVSV96, Van99, VW96, VFK92, VW91, VES+99, VA98, VHV90, WM95, WZG+93, WF94, WP96, WSS99c, WH95, WJL+96, Wun92, ZA94, ZKA94, ZL94, ZM99, DBS91]. **calix** [VW96]. **cam**}

[DvRSH94]. **CNDO** [BMD99]. **CNDO/S** [BMD99]. **CO** [VHV90, Dav97, GBT97, BJ94, MRW91, Cha92]. **coarse** [LMFA92]. **coarse-grain** [LMFA92]. **cobalt** [UVRCR92]. **cobra** [SYHW99]. **cocaine** [Fro93, VL90, WNW91]. **code** [Ear90, LWNS95, MKF+97, RBC+98]. **codes** [DVJ+95a, DVJ+95b, FV98, IG94]. **coefficient** [KW91b]. **coefficients** [BH91b, Gen99, MN92]. **Collective** [GPB+97, TS99a]. **Collective-variable** [GPB+97]. **collision** [BB96b]. **collisional** [LB96]. **COLUMBUS** [DLS+97]. **column** [BR97]. **combination** [DS90, DRP98, HH99b, KV93]. **combinations** [Flo92, WSS99a]. **Combinatorial** [TSZ90, GM98b]. **Combined** [BMW+90, LS94, Rau96, YM98, BT96, BvGMP97, CCJ+99, CG90, CG98, ER95, FBK90, FG96, FUS+94, PPAS+99, GG96, SR92]. **Combining** [EKS97, WH93, ZS93, WS99a]. **CoMFA** [YC95]. **Comment** [SC99]. **Comments** [Bal91a, DHHY90, Ste90, DW98, Hol93]. **commonly** [KNST96]. **Compact** [BC90, HS99]. **Comparative** [AGN+90, AVA93, GG96, HL96a, KF99, LIO90, PS98, AT93, Che95b, EPBD95, FSCS99, KHL96, NVS91, SR94b, YC95]. **Comparing** [FPRD99, GW98c]. **Comparison** [ALO94, AVP93, BP93b, Fag91, FGG+92, For91, GHS97, HVM99, HKŠ+97, KVKK93, KCK98, MSZ96, NBS94, OJL93, PFFF97, RC95, ST91, SS98b, SW93a, SR98, VVM93, VW91, WR93, WO97, Wib99, BP93a, Bak93, BC96, BKL+90, DHHY90, FGBH90, FRR90, GWHD99, GGP96, GPPS91, GLoNP96, HL96b, JU91, KS96, KHL96, LHBF93, Luk94, MFG91, MJFT96, MLA+99, RK97, Ric91, RK99, RMS93, SSD93, STB+94, SLH96, Ste90, TS99a, TEHL93, VDF+97, WSV92, WCK96, AS97, BL91, FW93a, FV98, HVvRS93, HW97, Her97, JB95, JVB95, JLW99, Kna92, NSA+97, PK95, SUG92, Sul95, TRG99, WHM+96, WWF95]. **comparisons** [FZL97, HO97]. **compartmentalization** [SOL90]. **Compatibility** [RW99]. **complement** [SSRO92]. **complementarity** [MV91]. **complete** [WAM91, ZPV+96]. **completeness** [BKL+90]. **complex** [ACD99, Büh99, CFK97, CLQSS98, CR95, CG94, DKJ96, KTT94, KTT95, MGLL99, MP90, NBG93, PDPM97, Yos90, ZS99, ZHSB92]. **complexation** [VHWC98]. **complexes** [Bér97a, BF91, BBS96, CDG+96, CHPK91, CA95, CY98, FR90, GGK98, GMY97, GSK95, GMO93, Had98, KT93b, KTT94, KTT95, LHBF93, MM93, Mag95, MKF+97, MV91, PKCM99, RCAA99, SCZC99, SH91, SR90, SSO94, TRG99, VW96, VHWC98, VHV90, ZY96]. **component** [HBLL98, HNS+97, MPJ98, MPJC98, SSR94, SSR95, SFB91, TEdV90, VES+99]. **components** [Gao97, SWOW97]. **composed** [CDG+99]. **composite** [Bec99a]. **composition** [BW91a]. **compound** [FDMB92, GSB99, PSK98]. **compounds** [AF94, Ano97, BCMZ99, BCF+92, BH98b, BBH99, DDV93, DDLV95, DVL90, ER95, FA94, FRC91, FM94, FSCS99, GPSS93, HDA93, JFR92a, JFR92b, KSP90, LA90, LJ92, LDJ92, LDJ+97, MHJ+98, MNVM97, Mar98, MSB95, MSB96, PK95, RdBN90, RR92, Rod94, SHM99, SI93, SW93a, SR94b, SUG92, TA98, TYMS98, VF92, VW91, WZG+93, WO97]. **Comprehensive** [PSY+99, MTRJ95]. **compression** [FW93b, She90, SCC93]. **compuational**

[For91]. **Comput** [Ano97]. **Computation** [COR99, GS93, TEdV91, TRLRB96, BMD99, CS94, FOCB96, GM90, GŌ95, Klo97, MD95, MOSD97, MGPR90, Ove91, PaST94, Ran91, RM91, RK99, SAF93, Sun94, Tav96, VT91, WWSS98a, WWSS98b, WHHP97]. **Computational** [Ano15, BSGB98, CY98, DKL90, LSDB99, MM93, PC94b, Rog90, Rog94, Rog03, Rou90, TNKM91, WP96, Zho97, Bog99, BSL91, Chr90, EA93, Fel96, FTA91, FTW+96, GSB99, Hal96d, HGK+96, MFG97, PC93, SSM96, SE94, SW93a, SR90, TYRD92, WJV+96, Ran92, Var92]. **computations** [ACFO91, FR94b, Gre95, KL91, KV93, RRR92, TRR+94, VS97]. **compute** [ALO94, BG93, OL90]. **computed** [BR97, Fro91, PE92]. **Computer** [Bal90, Bal91b, Bal93, LB90, TNKM91, DVJ+95a, DVJ+95b, Ear90, Elv91, HL96b, HEN+94, HR97, KW91b, KF94, KUT+97, LL94, Mez92, RPG+95, SLG93, VP92, VHV99]. **computer-aided** [VHV99]. **computer-assisted** [LL94, VP92]. **computers** [BBR96, BDKJL95, CS90, DK93, DPK94, FK95, HA93, LBI+97, MD95, MOSD97, MTBS91, RBC+98]. **Computing** [ABE+96, ZM90, Dum91, HB91, Ish98a, OS91, ZV96, STPA91]. **concentrations** [CR95]. **concepts** [Bic99, PM93, JM90, Klo92]. **concerning** [TMB93]. **concerted** [Bau90]. **Concise** [ABD90]. **concurrent** [CMC92]. **condensation** [DLM+98]. **condensed** [CBSB94]. **conditions** [ÇHP91, För92, MSZ96, SKT93, YKU96]. **configuration** [BBR98, CGBC96, DLS+97, DKH98, GBE97, PS96a, RBE98, RSK92, SWK99]. **configuration-selecting** [SWK99]. **configurational** [AGM91, CLO99, WJV+96]. **configurations** [Kri90, TvG94]. **Conformation** [CH88, JFKK94, TK94, ATK94, Cri92, GM90, HO93, HNS+97, HMČ91, JLW99, KD96, KPR91, MJ93, MM94c, WP97, Dun90]. **conformation-dependent** [GM90]. **Conformational** [AVC93, BCMZ99, BFST93, CT97, CSR92, CC91b, DRF92, FBTD92, Fro93, GJK+93, GW95, GK93, HS93a, HP94, HCCC99, JJTP93, KS96, KG91, KPI95, KTS92, LK92, LLD98, MNVM97, MR93, MRG97, Nic97, PG91, SSD93, SMM97, SM91, SW92, SW93b, Sul95, SK92b, SSO94, SSRS94, TGW96, TJP96, UF93, VGN+92, ZLM92, Art93, AW90, BPS93, BP93a, BKL+90, BW90, CHSK96, CÉC97, FGG+92, FRC91, FPR97, FCS98, GLP95, GS91, GBE92, GPPS91, GLoNP96, HN96, Hal99b, HKK91, HBR+99, IMP91, JLW97, KMKW98, KG99, Kuc96, LPD90, LP90, LSR97, LSDB99, LCA94, MK98, MK94, MJFT96, MJSV92, NBS94, NIS98, NWÅM95, PD92, RJP97, RD97, RPR+98, ST92, SB98b, STT95, SB99b, SACKH95, Sun94, SG95, VRC91, VRC92, VTR+94, VL90, WMM+95, Wan97, WHF97, WSV92, WCMS91]. **Conformational** [BP93a, BB96a, Cso93, Gio98, KG93, LSR97, PHG94]. **conformational-determining** [NWÅM95]. **conformationally** [KVL91, MKS90]. **conformations** [ALPH91, BK97a, BGZP97, BSV94, Dav93, FM94, GHR93, HCK95, KF99, LHBF93, Luk94, Mez98, Obe98, PS91, Par99, PMIB99, SSD93, SM94, Sno92, TEHL93, Wel90, vFB91]. **Conformers** [ZCP98, BSC+98, BB95, FLPH98, PFC96, PE92, Sau91, SJV93, WMM+95].

[CG97, CG99, FKN+93, Kar99, MRS98, RGK93, SHM95, TMCM+96]. **coupled-cluster** [RGK93]. **coupling** [BBR98, BSN99, CGdAC91, EGH+93, GdAG+98, RCAA99, TEdV90, VES+99]. **couplings** [O'm99, VRV99]. **covalent** [ER95, WB91]. **CP** [TEdV90]. **Cray** [SOCF98]. **Crick** [SCZC99]. **Crippen** [Dun90]. **criteria** [RWB99]. **criterion** [RBC+98, Yos90]. **Critical** [CEÁ92, EK97, SSV93, DV99, FB97, Gri90, HD92, MvRSL+97, MFG91, TEHL93]. **critical-point** [FB97]. **crossing** [AB97, FD91]. **crown** [LHBF93, SK92b]. **crown6** [VW96]. **cryptand** [AW90]. **cryptophane** [PKCM99, VHWC98]. **Crystal** [MvEP+98, YTT97, HDA93, KG92, KRL+93, KRM92, LOP+97, PRRD98, VK97, VTR+94, WS93, WPLC95, WJL+96, vEK99]. **crystalline** [DDV93, DVL90, EKS97, HYH+94, TM95, Dil95b]. **crystallography** [BSL91, SYHW99]. **crystals** [ACRC97, FCNSÁ98, KVKK93, LYH+95, SWAH91]. **Cs** [JLN98]. **Csonka** [Ano15]. **Cu** [SWS+90, SMA92, TKSM96]. **cube** [HTC98, HGB93]. **cubic** [ACRC97, ELA+95]. **Cumulative** [Pet93, SSRO92]. **curves** [BG93, PLB92, WB91]. **cutoff** [GZ95, SB94]. **CVFF** [HKŠ+97]. **cyanates** [LS98]. **cyanoketene** [CLQSS98]. **cyclic** [Che95b, CD97, HVvRS93, KG93, KHG96, MV91, NBB+99, PD92, PHG94, TA98]. **cyclization** [LK90]. **cycloaddition** [ARLG+94, NVER97, SSQ92]. **cycloadditions** [CN98, MP98]. **cycloalkanes** [Cri92, WA99]. **cycloalkene** [SJV93]. **cyclodextrin** [BPZL96, WSV92]. **cyclohexaglycine** [BB95]. **cyclohexanetriol** [BPZL96]. **cyclooctadiene** [RD97]. **cyclooctane** [RPR+98]. **cyclopentadienyl** [RvRS98]. **cyclopentane** [CHSK96, Jai90]. **cyclopentenes** [Bal98]. **cyclopropeniumyldiazonium** [Gla90]. **cytochrome** [BO93, HL96a, Kat93]. **cytosine** [RTGJ98, SLH96].

**D** [AT93, AVC93, AVP93, BO93, Ear90, GH98, MNVM97, MK94, NL91, SHCY93]. **D-CICADA** [MK94]. **D-norcamphor** [BO93]. **data** [Als95, BG93, BB98a, FSW96, FM94, GSB99, Hal96d, HGB93, HBR+99, KFML99, LHBF93, LOP+97, MTH94, MM97, Mer92, MLA+99, NL98, PGAL93, RGK93, SAdV97, She90, SC95, SYHW99, VTR+94, WAW+97, YB94, YB95b]. **database** [EK97, MK97a, AGN+90, LHBF93]. **databases** [Fel96]. **David** [Dav97]. **Davidson** [Cis93, VVSV96, vLP90]. **Davydov** [För92]. **DD** [BSL91]. **DD-peptidase** [BSL91]. **DDRP** [DBS93]. **dead** [GM98b]. **dead-end** [GM98b]. **deaminase** [HK90]. **deazaguanine** [KG99]. **deazapterin** [CG96]. **debate** [Ove91]. **deca** [KG91]. **deca-alanine** [KG91]. **decahydroisoquinoline** [MR93]. **decarboxylation** [NBG93]. **decaying** [LP99]. **Decomposition** [KTT94, KTT95, ABBC99b, BBR96, DH90b, LZZ98, WAW+97, YB94]. **Decoupling** [BBS96]. **dediazoniation** [Gla90]. **dedicated** [CGBC96]. **deduced** [Pac95]. **deduction** [Cri95]. **defined** [DBS96]. **defining** [PP98]. **DefPol** [PT98, PTCB99]. **degenerate** [Ber97b, GML94]. **degradable** [PC94b]. **degradation** [PC93]. **degrees** [Bér97a, DMB91, SEJ95].

**Dispersion** [FTA91, LLB99]. **Display** [SR94a]. **disrotation** [MQS+97]. **dissociation** [Kri90]. **dissociative** [PLB92]. **dissolved** [DS92]. **Distance** [CH88, Bal90, GHR93, GHR94, JCV+93, PD92, Pet95, WSV92, PP97, Dun90]. **distances** [Kik96, Kik99]. **distinct** [GSB99]. **distorted** [ATK94]. **distortion** [KK92]. **Distributed** [RGK93, BDKJL95, CS90, DK93, Fer91, FK95, Lim97, LMCPP92, MD95, MOSD97, PFM91, WPLC95, CS96]. **distributed-memory** [CS90, DK93, LMCPP92, CS96]. **distribution** [ABD+98, CNS96, DA96, GZ95, HK92, Non97, RM91, SR94b, SKOR93, VGN+92, VSF97]. **distributions** [FS91, PFM91, RMS93, SK92a, YTRB97]. **distyrylpyrazine** [ENHE98]. **disubstitution** [WZG+93]. **disulfide** [GS97]. **dithiin** [FLPH98, PFLH93]. **Divide** [SHCY93, PLY98]. **Divide-and-conquer** [SHCY93, PLY98]. **DMA** [PSK98]. **DMA-DMPP** [PSK98]. **DMC** [MJSV92]. **DMPP** [PSK98]. **DNA** [BB98a, CDG+96, CCBK95, DZ97, FOCB96, FZL97, FW91, GPB+97, HNH+91, HKŠ+97, RTGJ98, SUG92, SWOW97, ZS99]. **DNAs** [SWOW97]. **Docking** [APC98, CFK97, JTM+95, ATK94, CA95, DV99, EK97, GSB99, GVD96, KG99, MK97a, MK98, MSK92, MGH+98, SKB92, TS99a, TS99b, VHKB98, VHD+98, Wan91, ZS99]. **Does** [vRSD92]. **DOI** [Ano15]. **domain** [WAW+97, YB94]. **Donald** [Var92]. **donor** [GC98]. **dopamine** [Fro93, GH98, UF93]. **dot** [ELA+95]. **double** [DNC96, ELA+95, GML94, JB98, RSK92, SWOW97]. **double-excitation** [RSK92]. **double-helix** [SWOW97]. **double-iterated** [DNC96]. **drive** [Jai90]. **driven** [RPG+95, WWZD92]. **droplet** [EJ95]. **Drug** [LJKL98, Tay99, CS94, Cri95, PM93]. **drug-design** [CS94]. **DSP** [ENHE98]. **dual** [AL98]. **dual-topology** [AL98]. **due** [SF92]. **Dunham** [Mit98a]. **during** [Dav94b, FS94, KHW+90, MS98]. **dye** [ENHE98]. **dyes** [Che95a]. **Dynamic** [YB95b, ACRC97, GVD96, MvRSL+97, PM93, RL95]. **dynamically** [DBS96, FB97]. **Dynamics** [GS90a, AFK+95, AW90, BBR96, BKLS95, BO93, BvGMP97, BSS97, BBS96, CCJ+99, CHSK96, CG96, CG98, DOO93, DDV93, DK93, DS92, DVL90, DBT98, DV97, EGH+93, EGHT97, Elv91, FSW96, FHB99, FBK90, För92, FW91, Gen99, GS90b, GMM95, GJD94, GT98, GS94c, GK93, HS93a, HS93b, Har93, HTC98, Her93, HYA92, HEN+94, HYH+94, HBR+99, JP92b, JVB95, JMH96, KR96, KLR96, KG91, KHW+90, Kna92, KID93, KUT+97, KVKK93, LK95, LPK99, LB96, LHBF93, LCA94, LLD98, LBI+97, LMCPP92, MV91, Maz97, MTBS91, MN95, MJSV92, NQ99, NSWP90, OS94, OL93a, OM96, OC98, PMIB99, PH96, PKCM99, PDPM97, RBC+98, SSD93, SAdV97, SN99, SS98b, SHCR97, Sha91, SWM90, SN91, SMA92, Ske91, SMM97, SB99a, SWOW97, SM90, SK92b, SYHW99, SG95, TMB93, TYMS98]. **dynamics** [TvG94, TMK+99, TWR+95, VDF+97, VWGF95, WWXS97, WSV92, WAW+97, WS98, YKU96, Yos94, Yos96, YB94, YB95b, ZS93]. **dynamics-based** [HBR+99]. **dynamics/Monte** [MJSV92, SMM97].

**E2** [Bic99]. **ECEPP** [RPG+95]. **Eckart** [AC94]. **Econometrics** [Gar90].

[ACB92, AS97, Bru93, CF97a, CF97b, DF97, DM91, HS93c, HS95b, LDM92b, Mit94, NH91, RM91, SOL90, SBA97, SW96a, TG98, ZYY95b, ZPV+96].
**equations**
[KTnH99, LMB96, Maz97, Pol90, Ram90, RPGS97, SBJ92, WS99b].
**equatorial** [CPJ98]. **equilibria** [CPJ98, Fab91, NBS94]. **equilibrium**
[CR95, LV90, MM95, PASF96, TRLRB96]. **equipartition** [HTC98].
**equivalent** [BR97, SC94, VK97]. **erased** [BW96]. **Errata** [KTT95, SSR95].
**Erratum** [Ano15, FS00, WWSS98a]. **Error**
[AFK+95, IC96, HVM99, WB91, KZ99]. **errors**
[AG90, BG96a, CMPT98, DB98, GPF97, RK97]. **essential** [VDF+97]. **ester**
[DLM+98, LMB99, LPT97]. **esters** [ASM+92, FBTD92, GM99]. **estimate**
[AVP93]. **estimated** [HI98]. **estimates** [RK97]. **Estimating**
[MAP97, SVM99, NBS94]. **Estimation**
[DJ93, CB96, DNC96, HK92, VTR+94]. **ethane** [HMG96, MS98].
**ethanediol** [RBSB96]. **ethanes** [CPS90]. **ethenol** [LDJ+97]. **ethenyl**
[WJL+96, WJV+96]. **ether** [LPT97]. **ethers** [BMJ90, VRC91, VRC92].
**ethyl** [EPBD95, FBTD92]. **ethylene** [BPS93, Fag91, JB98, LV90, MSSS95].
**ethylenes** [MP98]. **ethylenic** [JB98]. **ethylnitrene** [KW91a]. **Evaluating**
[BDKJL95]. **Evaluation**
[GJR91, GHT98, GMO93, ISH98b, JCV+93, LP95, MGPR90, Vya97, ACFO91, AFK+95, ABD90, BBR96, CDR+95, CS95, CTC95, DV99, EGHT97, EK97, Fer95, GP94, HA93, HW97, KW91b, KF94, Lim97, LWS+95, MSK92, MJSV92, NTK96, RKL93, TRG99, WCC91, YG92b, ZG92, Živ90].
**evaluations** [OJL93]. **Evans** [ABBC99a, ABBC99b]. **events** [SB98a].
**evidence** [LP92]. **evolution** [LMB96]. **Ewald** [CÇG97, DKBS97, KVKK93].
**Exact** [FB98, WS99b, BK97b]. **exactly** [GS97]. **examination**
[KWWS91, SHM95]. **example** [ACD99, DBS93, JZ96, HREK98]. **excess**
[SW96b]. **exchange**
[AB98a, FS98b, GW91, HVvRS93, HREK98, LP99, MQS+97, RCAA99].
**Excitation** [HT99a, BA94, Gri94, RSK92]. **excited**
[ČTS98, FA99, FRZ93, GWHD99, GJCC93, RSK92, WLKJ92].
**excited-state** [FA99, GWHD99]. **excluded** [Bla91, GŌ95, KPR91].
**excluding** [PaST94]. **Exhaustive** [BV97]. **existence** [SS95]. **Exo**
[CGdAC91]. **Exo-exo** [CGdAC91]. **expanded** [TSZ90]. **Expanding**
[LCA94]. **expansion** [Ish98a, MGPR90, PG98]. **Experiences** [DBS93].
**experiment** [JU91, NSA+97, Sul95, WWF95, Obe98]. **experimental**
[Hal96d, Her93, MLA+99, NL98, PK95, SUG92, SF96, Wib99]. **expert**
[CCN90]. **explicit** [ED99, JAdV96]. **Explicitly**
[ZA94, KA92, SKA93, ZKA94]. **Exploiting** [MRM97]. **exploratory**
[GS90b, KW91a]. **Exploring**
[Bec99b, Cri92, SMS98, JLW97, PFFF97, SBA97]. **exponential** [CDR+95].
**exponential-type** [CDR+95]. **exponentially** [LP99]. **exponents**
[CR95, GvRSvEH+93, Mag93b]. **expression** [MN92]. **expressions** [SF92].
**Extended** [HM90, ML92, BMN95, DJ94, EHNW96]. **Extension**

[LDJ92, LBAO96, MKF+97, PS97, WSS99c, Hal96d, Mar98, Ste91]. **Extensions** [HA95]. **extensive** [HK95]. **external** [Yos94]. **extraction** [VW96]. **extrapolation** [CW93]. **extraribosomal** [Dav94b].

**F** [AS98a, BSvRS95, BT92, Dun90, Jur96, SHM99, SI93, SM91, Tay99, DJ94, HDA93, KMM99]. **F-containing** [HDA93]. **Factors** [BSC+98, BPP90, BR97, GH97, WL91b, ZA94, BCF+92]. **Failure** [Wil94]. **FAMUSAMM** [EGHT97]. **Fan** [Ano97]. **Fast** [Als95, CÇG97, DJ94, FOCB96, HGB93, HC96, KUT+97, Pur98, RRR92, RK99, VK97, WSS99b, BCG97, BWS+95, BSS97, GGP96, SKT94, VS97, WF94, ZV96]. **Faster** [BR99, MK98]. **Fe** [GLLOB91]. **features** [Als95]. **FeCH** [VF92]. **FEP** [OJL93, VHWC98]. **Fermi** [PD99]. **few** [Mit94]. **Feynman** [HM92]. **field** [AT93, AGP91, ALY90, AF94, ACL96, Ano97, BMW+90, BCB+97, BPP90, BBH99, Can93, CPR90, CEÁ92, CHSK96, DFTRJ97, DDV93, DDLV95, DMV98, DVJ+95a, DVJ+95b, DVL90, Dil90, Dil95a, Dil95b, DW98, FRSNS92, FRC91, FR94a, FPR97, FZL97, FW92, FUS+94, FSI95, GH98, GZL+94, Gre95, Hal96a, Hal96b, Hal96c, HN96, Hal96d, HOL98, HGK+96, HA95, HH99b, JHB96, KLV94, KSB+93, KHL96, LV90, LYH+95, LCD+97, LA91, LA98, LOP+97, LPW+97, LKC+98, MHS+94, MHJ+98, McD97, MRM97, MKS90, MR92, MPJ98, MPJC98, OL93a, OM96, PK98, PGBM97, RG99, RSB96, RCv96, RCvRS97b, RCvRS97a, RRR92, SB99a, Sul95, Sun94, TRR+94, UF93, WH95, YC95, Yos94]. **fields** [CK91, Dil92, FSBMP99, GSW90, Hal99b, HGB93, HW97, Hil97, HA95, KE95, KVKK93, LDVP91, MHS+94, MHJ+98, PPK91, Pet93, RHN94, REA+98, SGB91, SCRI93, WS93, WFR99, vEK99]. **files** [ORK+91]. **filter** [DNC96]. **finding** [FPRD99, SB90, SA99]. **Finite** [BvGMP97, BNDS97, BSV94, YH93, ZPV+96, AC94, CW93, CF97a, CF97b, DM91, FR94b, FRZ93, LDM92b, MGPR90, NL91, NH91, Sha91, SW96a, ZYY95b, LDM92a]. **Finite-difference** [ZPV+96, LDM92b, Sha91, ZYY95b, LDM92a]. **finite-element** [CF97b]. **Finite-state** [BSV94]. **First** [FV98, Mil90, AJ99b, BW91a, CW91, CMC96, ENvRS94, HG93, Klo97, She90, dlVM91, ACD97, LS96]. **first-** [AJ99b]. **First-order** [FV98, Klo97, She90]. **first-row** [BW91a, CW91, dlVM91]. **fit** [FCCG96]. **fits** [TAC98]. **Fitted** [ACD99, BBH99, PS91, PS92, SACKH95]. **Fitting** [Ran93, ACD97, CBR97, HOL99, NVK+97, PGAL93, SW93b, MSDC94]. **five** [BW96, ENvRS94, PMHRG97]. **five-membered** [PMHRG97]. **fixed** [GS90a, GS90b, NM97, SCC93]. **FK506/rapamycin** [SSO94]. **FKBP** [CFK97, SSO94]. **FKBP-FK506** [SSO94]. **FKBP-FK506/rapamycin** [SSO94]. **FKBP-substrate** [CFK97]. **Fletcher** [AB98b]. **flexibility** [Art93, KPI95, ZS99]. **Flexible** [CA95, TS99a, APC98, Fer95, JTM+95, KG99, LK92, MK97a, MK98, MM97, MSZ96, SEJ95, SB99b, Tel90, TGW96, VHKB98, VHD+98, WCMS91]. **flexing** [KG93]. **Floating** [HM92]. **flow** [SR94a]. **fluctuation** [Kik99]. **fluctuations** [Art93]. **fluid** [FB97]. **fluids** [YB94]. **fluorescence** [PSK98].

[GM90, JDD97, JLN98]. **Genetic** [MS95, BP94, HS95a, HH99b, JLW97, JLW99, MJ93, MJFT96, MGH+98, NM97, Pul97, RWB99, JJTP93]. **geodesic** [Spa96]. **Geometric** [Pet95, VRC91]. **geometrical** [BM99, WCC91]. **geometrical-type** [WCC91]. **geometries** [Fro91, Hal96c, HN96, Hal99b, PASF96, SACKH95, TRLRB96, YH93, BRLD92]. **Geometry** [BH91a, Bak92, BCT98, Bér97a, CH88, DH95, PK91, Bak93, BMD99, BCT91, DJ94, Dun90, EPW97, fGGG94, GS90a, GS90b, GS97, Har99b, KKCH96, LSFFM+95, LZT91, MM95, MS95, Mit98b, MKS90, PS91, PS92, PD92, RRR92, SH91, SB92a, WSV92, O'm99]. **Geometry-dependent** [DH95]. **GEPOL** [PAS90, PaST94, STPA91]. **Gerald** [Klo92]. **GIAO** [WHHP97]. **glass** [OC98]. **Global** [AS98b, Art93, Har99b, NM97, CACD97, DV99, DS90, DRP98, FPRD99, KF99, KFML99, MS95, PP97, Sno92, SB99b, SBK97, DS90]. **globular** [DB98, GKS93, Yos94, Yos96]. **glucopyranose** [BSC+98]. **glucose** [DDV93, KVKK93, PE92]. **Glycerylphosphorylcholine** [SW92]. **glycine** [DKJ96, NSA+97, SS98b, WNW91, ZCP98]. **glycol** [Fag91]. **glycosidic** [DDLV95]. **glycyl** [SS98b]. **glyoxal** [AF94, Ano97]. **GMIPp** [HLO99]. **golden** [BBS96]. **Goldfarb** [AB98b]. **good** [AB98b, GKS93, GT98]. **Goodwin** [BB96b]. **Gordon** [AB98a]. **governed** [MGLL99]. **gradient** [Bec99b, BHE+93, FV98, HA93, HWH+91, MK97b, PG98, QHIH98, DKRK95]. **gradients** [BR99, FB98]. **grain** [LMFA92]. **grand** [HL96b]. **GRAPE** [HEN+94]. **GRAPE-2A** [HEN+94]. **Graph** [Rou90, TNKM91, Bal91a, DMB91, LK91, Ran92, Živ90]. **Graphical** [PP98]. **graphite** [SSF90]. **graphs** [Bal90, Bal91b, VT91]. **green** [ZvN93]. **Grid** [Bru93, Wan91, Bec99a, DM90, LWS+95, MSK92, OS98, PFC96]. **grid-based** [MSK92, OS98]. **grid-calculated** [DM90]. **Grid-search** [Wan91]. **GROMOS** [OM96]. **GROMOS96** [DMV98]. **groove** [ZS99]. **ground** [Cul92, FSCS99, FRZ93, GWHD99, GC98, GJCC93, RSK92, SKA93, WLKJ92, ZA94, ZKA94]. **ground-** [GWHD99]. **grounded** [Gre95]. **group** [BPS93, BT92, DvRSH94, ENvRS94, FM91, HS99, HK95, Mag95, MHS+94, MS98, MR93, SC94, WMM+95, Zho93, ZL94]. **groups** [Ear90, LB90, LDJ+97, LPT97, PGBM97, Ste98, WAM93, ZLM92]. **growth** [VGN+92]. **guanine** [RTGJ98]. **guanosine** [Can93, FW91]. **guest** [BF91, MV91, VHWC98]. **guests** [VHWC98]. **Guidelines** [Bog99, RG99]. **GVB** [Cul99, MKF+97].

**H** [BSvRS95, BKMH97, CLS+97, FM99, GMY97, IBKvRS92, JKS93, KG99, KHG96, Lóp95b, LSSvRS96, MI99, Mez91, Ran92, SM91, TDFdC91, VHV90, ZMC+97, KTS92, AG90, AC94, ACD99, AHLR+91, CLQSS98, Che95a, DJ94, DBS93, FLHP97, FLPH98, GvRSvEH+93, GMY97, GSW90, HDA93, LDMS99, Mag95, MRH99, MQS+97, NL91, PT99, RNDP98, RR92, SBM97, Sie96, TEdV90, VCLB92, ZMC+97]. **H-** [HDA93]. **h-1** [KTS92, FLHP97, FLPH98]. **H-azirine** [CLQSS98]. **H-bonded** [AG90]. **H-chromophores** [Che95a]. **H-phosphole** [SBM97]. **H/He** [GSW90].

**Hadamard** [Bal93]. **half** [OS91]. **half-projected** [OS91]. **halide** [LK90]. **halides** [MSSS95, SI93, SB98b, SB98c, VES+99]. **haloethanes** [SS97]. **halogen** [ZY96]. **halogenated** [PNJS93, PRRD98, WM93]. **Hamiltonian** [LO98, Maz97, PS97, ZL94]. **Hamiltonians** [OBL95]. **Hammett** [KHF90, KHF91]. **Hammett-type** [KHF90, KHF91]. **Handling** [EA93]. **hardness** [BSS90]. **Harmonic** [BJK95, JB95, JVB95, ZS99, AL98, BPP90, BNDS97, MTH94, RK99, SB92a, DDV93, DVL90]. **Hartree** [BLF95, CBWF98, CER94, HBLL98, HKŠ+97, JDD97, JLN98, Kar99, KZ99, KS96, LL92, NSA+97, OS91, Pac93, RW99, STB+94, SLG93, TKTN99]. **Hash** [IG94]. **Havel** [Dun90]. **HCl** [Lóp95b, HREK98, MSSS95]. **HCN** [MRH99]. **HCO** [PFC96]. **HCP** [GJCC93]. **headgroup** [SW92]. **Heats** [ASM+92, LSCA98, SC94, Fro91, HGC+95]. **heavy** [HBLL98, ML91]. **Heiles** [AC94]. **helical** [RM91]. **helices** [AJ97]. **helium** [KT93b, ZA94, ZKA94]. **helix** [SWOW97]. **Hellmann** [HM92]. **heneicosane** [SHHČ90]. **Henon** [AC94]. **heptaalanine** [VGN+92]. **Hessian** [AB98b, Bof94, BC95, HWH+91, Mit98b]. **heteroarotinoids** [WC90]. **heteroatomic** [KS91]. **Heteroatoms** [HK92]. **heterobinuclear** [RCAA99]. **heteroboranes** [ZBM91]. **heterocycles** [GBT97, NPLT97]. **heterocyclic** [Fab91, GH98, SW93a]. **heterodienophiles** [JZ96]. **hexacarbonyls** [Van97]. **hexafluorides** [Klo93]. **hexafluorodisilane** [CRP97]. **hexahydrated** [TRG99]. **hexamer** [BMD99]. **hexamethyldisilane** [CRP97]. **HF** [GS90d, Lóp95b, CW93, FW93a, McD96, MSSS95, YG92a]. **HF/6** [FW93a]. **HF/6-31g*** [FW93a]. **Hg** [FR94b, Ste91]. **HH** [FS98b]. **HIerarchical** [BGZP97]. **High** [AW90, Del96, FR94b, GMY97, Bec99a, BB96b, BW90, BR97, FTW+96, HGK+96, HEN+94, KK92, RC93, TMK+99]. **high-energy** [BR97]. **High-level** [GMY97]. **high-order** [Bec99a]. **high-performance** [FTW+96, HGK+96, HEN+94]. **High-precision** [FR94b]. **high-quality** [RC93]. **High-speed** [TMK+99]. **higher** [Ear90, GM90, GJR91, Ish98a]. **higher-symmetry** [Ear90]. **Highly** [KK92, SLG93, VM95]. **hindered** [For96, Tru91]. **hints** [DBS93]. **histamine** [AHLR+91, Sul95]. **histogram** [KRB+92, KRB+95]. **HIV** [MR93, MRG97, RM94, YBD+94, YTRB97]. **HIV-1** [MRG97, RM94, YBD+94, YTRB97]. **hoc** [MFG91]. **hole** [RMW91]. **holes** [PD99]. **homoaromaticity** [Hol93]. **homobinuclear** [RCAA99]. **homology** [DS90, DRP98]. **homolytic** [BFST93]. **homonuclear** [HK95]. **homopolar** [LBA+99]. **HONDO** [KD91]. **Hopfield** [KD96]. **Host** [MV91, BF91, VHWC98]. **Host-guest** [MV91, BF91]. **hosts** [BPZL96]. **HPC** [GJCC93]. **HPLC** [BR97]. **HT** [AT93]. **Hückel** [DJ94]. **human** [PS92, YSJ95]. **HUNTER** [WHF97]. **Hybrid** [CBSB94, FCS98, HY96, O'm99, Gao97, MJSV92, RW99, SLPP97]. **hybridization** [ML91]. **hydrated** [FSI95, KF99, SWOW97]. **Hydrating** [Dav94a]. **Hydration** [DBS91, SN90, SWM90, AGN+90, AS96, AS97, CNOJ93, CT99, ER95, FW92, GS93, HW97, HE99a, JN93, KOH97, Mar90, OJL93, TRLRB96, WL91b, Zau91, ZV96, SVM99]. **hydride** [CG90, CG98, JU91]. **hydride-ion** [CG90, CG98]. **hydrides** [LS96, WAM93].

[TA98]. **Incorporating** [Sha91, ZFYY95]. **Incorporation** [PHG94, Zau91, SH98]. **Increased** [BNDS97]. **increasing** [BM99]. **incremental** [FR90]. **increments** [BBH99]. **independence** [Bru93]. **independent** [ACB92, GM90]. **Index** [CS90, BP93a, KVL91, MK97b, TSZ90, VÅJ94]. **indexes** [BC93, Che99]. **Indexing** [AS99, YTT97]. **indices** [DMB91, PKRR97]. **indigoid** [Che95a]. **indirect** [TEdV90, VES+99]. **INDMOL** [SLG93]. **INDO** [NBB+99, SB95]. **induced** [CMPT98, KMM99, RMW91]. **inert** [AIDAVB98]. **Inexpensive** [HI98]. **infer** [VP94]. **Infia** [Bro99]. **Influence** [CPJ98, KS97, LMRRL98, Arn94, FDMB93, dVA92]. **infrared** [CJC+96, LA92, PK98, dANS+96]. **inhibition** [LK95]. **inhibitor** [Kik96, MRG97]. **inhibitors** [GBE92, HK90, HL96a, KG99, MR93, MRG97, Wel90, YTRB97]. **inhomogeneous** [Ram90]. **initial** [GCRSAIVB99, För92]. **Initio** [YG92a, ALPH91, AGN+90, AMY98, ALO94, AVA93, Arn94, ACRC97, BLO94, BFST93, BB96a, BL91, Bog99, BB95, BvH+92, BCT91, BT92, Cai94, CLCL96, CW97, CRP97, CG93, CH94, CH96b, CÉC97, CG90, DH90a, DKJ96, DW98, DBT98, Ear90, Ear93, EPW97, EGH+93, EKS97, Fag91, FF93, FRR90, FGG+92, FW93a, FLHP97, FLPH98, FG96, GH98, GCRSAIVB99, GPSS93, GM98a, GCT96, GS90d, GJCC93, GMY97, Gre95, GSK95, GG96, HKK+97, HOL98, HVvRS93, HS99, HKŠ+97, HA95, IBKvRS92, IRRR93, JFKK94, JG91, JZ96, KS91, KG92, Kar99, KRM92, Klo93, KA96a, KHB92, KB92, KCK98, KHA90, KHG96, KPSM98, KTS92, LL92, LKL95, LCD+97, LP92, LSFFM+95, LSSvRS96, LDMS99, LBAO96, MI99, MM95, MS98, MTRJ95, MRW91, MSB95, MSB96, MVS92, MSDC94, Mit98a, MKS90, NBS94]. **initio** [NWÅM95, NVER97, OL93a, PPK91, PSY+99, PFC96, PR95, PG91, PF99, PFLH93, PE92, PK95, Rau96, RCvRS97b, RCvRS97a, RvRS98, RCATD96, RPR+98, RMS93, RHK90, RHKK90, RK95, SB98a, SBM97, SD90, SC94, SLH96, SM91, SUG92, SLD+90, SOCF98, SCRI93, TKTN99, TEdV91, VCLB92, VK94, WZG+93, WO97, WL91b, WHM+96, WWF95, YM98, dANS+96, ASM+92, BCF+92, BSN99]. **initio-derived** [DW98]. **inorganic** [SH91]. **Insertion** [JB98]. **Insight** [Gao97]. **Institute** [Gar90]. **integer** [SCC93]. **Integral** [RPW98, FW93b, HWH+91, Ish98a, KMO92, LTHY96, Mor93, MN95, SBJ92, WHHP97, WCC91, YG92b]. **integrals** [ABD90, AD90, CW97, CDR+95, Flo92, JCV+93, Jon91, KA92, Ric93, RKL93, YG92b, YG92a, ZL94]. **integrate** [Pol90]. **integrated** [ATS90, MM95, McD96, MRG+90]. **Integrating** [Har99a]. **integration** [BRP92, CKP96, CG94, Del96, ELA+95, HW97, LMB96, MM91, SC95, ZS93]. **integrator** [Har93, LMB96]. **integrators** [ZS95]. **intelligence** [CS94, LPD90]. **Intensities** [LA92, LDVP91, McD96, PK98, dANS+96]. **Inter** [Kik96, BRLD92, JS93, KWWS91, Kik99]. **Inter-C** [Kik96, Kik99]. **inter-conversions** [BRLD92]. **interacting** [PS97]. **Interaction** [BDH+94, HNH+91, CGBC96, CG93, DLS+97, DKH98, DV97, EBD+99, GBE97, GSK95, GBT97, GW91, HVM99, Hal99b, HREK98, HKŠ+97,

[BP93a, Bec98, CBSR99, NTK96]. **marching** [CP98, HGB93]. **Mark** [Klo92]. **massively** [BBR96, DLS+97, HL96b, LBI+97, RBE98, SOCF98]. **master** [RPGS97]. **Masthead** [Ano90c, Ano90d, Ano90e, Ano90f, Ano90g, Ano90h, Ano90i, Ano90j, Ano90k, Ano90l, Ano91c, Ano91d, Ano91e, Ano91f, Ano91g, Ano91h, Ano91i, Ano91j, Ano91k, Ano91l, Ano92b, Ano92c, Ano92d, Ano92e, Ano92f, Ano92g, Ano92h, Ano92i, Ano92j, Ano92k, Ano93c, Ano93d, Ano93e, Ano93f, Ano93g, Ano93h, Ano93i, Ano93j, Ano93k, Ano93l, Ano93m, Ano93n, Ano94f, Ano94g, Ano94h, Ano94i, Ano94j, Ano94k, Ano94l, Ano94m, Ano94n, Ano94o, Ano94p, Ano94q, Ano95c, Ano95d, Ano95e, Ano95f, Ano95g, Ano95h, Ano95i, Ano95j, Ano95k, Ano95l, Ano95m, Ano95n, Ano96b, Ano96c, Ano96d, Ano96e, Ano96f, Ano96g, Ano96h, Ano96i, Ano96j, Ano96k, Ano96l, Ano96m, Ano96n, Ano96o, Ano96p]. **matching** [MRM97, PS96b, SHCY93]. **materials** [BR97, GC98]. **Mathematical** [Cas89, Gar90, Jem97, PPK91]. **matrices** [Bal93, BB98b, BC95, BB96b, CMC92, GM90, GHR93, Mit94]. **matrix** [BH91a, BC96, BB98a, Bof94, CT95, CLCL96, CW97, FTW+96, GHR94, KTK93, KV93, LMB96, LH99, Mil90, ZL94]. **matrix-inversion** [CT95]. **matter** [CBSB94]. **maxima** [Che95a]. **maximization** [CACD97]. **maximum** [JJ98]. **MC** [SS98a]. **McLafferty** [LP92]. **McMurchie** [Cis93]. **MCSCF** [LDJ+97, ML92, SSHB93, ZL94]. **MD** [DK93, LCA94, TMK+99, VHWC98]. **MD-FEP** [VHWC98]. **mean** [CKP96, FS97, GZ95, GS93, MLAT99, MLA+99]. **means** [Als95, SAdV97, SBJ92, VFM+90]. **measure** [Art93, Che95b, KRL+93]. **measures** [ACD97, ACDP98, ACD99, SA99, WM95]. **mechanical** [AGP91, ACFO91, AD90, BT96, BFH94, BvGMP97, Che95b, CG98, ER95, FCNSÁ98, FBK90, FG96, HCK95, JS93, JKS93, KMO92, KB92, LMA99, LS94, LW92, NL98, PSY+99, RD97, SHM95, TRR+94]. **mechanical/molecular** [FCNSÁ98]. **mechanics** [ALY90, ALYT90, AF93, AYC94, ACK+96, AF97, BFST93, BB96a, BK96, BBC+98, CPR90, CDG+99, CA93, CBIT94, CRP97, CK91, CT97, CC91b, CG97, CG99, DK97, FA94, FR90, FK91, FGG+92, FRC91, GGK98, GS90c, GCT96, Gre95, GG96, GBT97, GPPS91, GLoNP96, Har99a, HW97, HKK91, IMP91, KR96, KLV94, KRM92, KLR96, KHB92, LPK99, LA90, LH96, LBB94, LCD+97, LA92, LA94, LWS+95, MTH94, MM95, MV91, MSB95, MSB96, MRG+90, NBS94, NCA96, NLA96, NA96, Nic97, NWÅM95, NL98, OS98, OL93a, PPK91, PPK92, PK98, PGBM97, PG91, PB92, PPAS+99, RvRS98, RD97, SS93, SB98b, SB98c, SB92b, SL95, SR92, TH93, TRG99, TA94, TMCM+96, TNS97a, UF93, VWGF95, VRC91, VRC92, VFK92, Yos90, Zau91, Zim91]. **mechanics/grid** [LWS+95]. **mechanism** [AIDAVB98, HY96, IBKvRS92, LP92, PC94b, CLS+97]. **mechanisms** [AC92, ARLG+94, LMRRL98, vOC93]. **Mechanistic** [CG90, Bic99]. **mediated** [Kat93]. **medium** [GBT97]. **medium-sized** [GBT97]. **Medla** [WM95]. **melt** [WHM+96]. **membered** [AMY98, BKL+90, HKK+97, PMHRG97]. **membrane** [PMIB99].

BPZL96, BBC+98, BP94, ÇHP91, CHP90, CEÁ92, DP95, EHNW96, EPBD95, FZL97, FM91, GC97, Jen94, LP95, MRG+90, PFMI97, PF99, PMRG93, RSOF96, RL95, TRJ96, TS99b, WC90]. **Models** [Cas89, Sie96, BRP92, BMN99, CJC+93, CMPT98, Cri95, Gar90, GHS97, HK90, HVvRS93, JB95, LHL+95, LW92, Mag95, MK92, MSZ96, PFC96, PFM91, RC95, SC99, SLH96, SKOR93, TD95, TSZ90, WS99a, WO97, Wil94, WA99, WWF95]. **Modern** [Yar95, KLR96, Dav97]. **modes** [DOO93, DZ97, GW98c, KCK97, TRG99, ZS99]. **modification** [vLP90]. **modifications** [AJ99a, AJ99b, KRL+93, SMA92]. **Modified** [IRRR93, SAF93, AS99, DJ94, DW98, FW91, FS97, GLP95, KTnH99, Mar97a, Mar97b, Mar98, NM97, PNJS93, PKN+95, Rod94, TG98, WF94, WFR99, KLV94]. **modular** [TH93]. **Modulation** [BA94, AVP93]. **module** [DK93]. **molar** [WWF95]. **Molecular** [ALY90, ALYT90, AF93, AYC94, AF97, ACDP98, BBR96, BB96a, Bla91, BBC+98, BCF+92, BSL91, CLCL96, CW97, CP98, CBIT94, CH88, CG98, DS92, DMB91, FA94, FR90, FRC91, Fro91, GS90c, GMM95, GHR93, GBT97, HS93b, IMP91, LB96, LA90, LHBF93, LH96, LBB94, LJKL98, LBI+97, LMCPP92, LA94, NCA96, NLA96, NA96, NQ99, NSWP90, Obe98, OL93b, OC98, PKCM99, RvRS98, SBA97, SB98b, SB98c, SKB92, SB92b, Tay99, TYMS98, VHV99, Van97, VRC92, WC90, WLKJ92, YKU96, Yos90, vOC93, AM99, Aer95, AT93, AGP91, ALO93, AC92, ALO94, AVA93, ACK+96, AFK+95, AS98b, AHLR+91, Art93, AW90, BT96, BCB+97, BCT98, BKLS95, BO93, BDH+94, BRC94, Bec98, Bek97, BFST93, BvGMP97, BWS+95, Bic99, BSS97, BPZL96, BG96a, BG96b, BK96, BCT91, BV97]. **molecular** [BSB+97, BGZP97, BW90, BP94, BRH90, CZM98, CPR90, CDG+99, CHP90, CA93, Che95a, CC98, CCJ+99, CRP97, CK91, CACD97, CMS91, CMC96, CT97, CT92, CC91b, CH94, CH96b, CG96, CG97, CG99, DM94, DOO93, DDV93, DDLV95, DK93, DNC96, DVL90, DH90a, DV99, DK97, DA96, Dun90, Ear93, EGH+93, EGHT97, EA93, ELA+95, EPBD95, EK97, FSW96, FHB99, FCNSÁ98, FK91, FGG+92, FBK90, FW93a, FLHP97, FLPH98, FG96, FW91, FPC91, GGK98, GPSS93, Gen99, fGGG94, GS90b, GCT96, GC97, GC98, GGP96, Gre95, GG96, GJD94, GT98, GH97, GPPS91, GLoNP96, Hal96a, Hal96b, Hal96c, HN96, Hal96d, HS93a, Har93, Har99a, HTC98, HGB93, HW97, HE99b, Her93, Her97, HYA92, HBBF97, HEN+94, HYH+94, HšR95, HKK91, HCK95, IG94, JP92b, JVB95]. **molecular** [JM90, JG93a, JS93, KR96, KLV94, KRM92, KLR96, KWWS91, KHW+90, Klo92, KE95, KUT+97, KHB92, KB92, KVKK93, KKCH96, KKJ97, KHL96, KPR91, KTS92, LDVP91, LM93, LK95, LKL95, LPK99, LCA94, LLD98, LCD+97, LA92, LP95, LS94, LIO90, LO98, LWS+95, Mag93b, Mag93a, MK98, MTH94, Mar97a, Mar97b, Mar98, MI99, MM95, MV91, Maz97, MJ93, MSB95, MSB96, MK97b, ML91, MTBS91, MSDC94, MRM97, MM94c, Mit98b, MRG+90, MN95, MPBM98, Mul91, NBS94, NTK96, Nic97, NM97, NWÅM95, NL98, ORK+91, OS98, OS94, OL93a, OM96, PPK91, PPK92, PK98, PKRR97, PAS90, PaST94, PMIB99, PSY+99, PGBM97, PZBM98,

Pet95, PG91, PB92, PPAS+99, PS96b, PH96, PFLH93, PE92, PT98, PTCB99, PDPM97, RLG98, RC93, Ric91, RLA+98, RK99, RBC+98].
**molecular** [RD97, RMS93, RHK90, RHKK90, RSK92, RTSM93, RKL93, SSD93, SAdV97, SBB+93, SS93, SN99, SHCR97, Sha91, SWM90, SM94, SN91, STPA91, SB99a, SKOR93, SACKH95, SB90, SHM95, SKM94, SM90, SK92b, SYHW99, SL95, SR92, TH93, TMB93, Tav96, TRR+94, TRG99, TRJ96, TvG94, TMK+99, TMCM+96, TWR+95, TNS97a, TNS97b, UF93, VP94, VWGF95, VRC91, VFK92, VPV91, WAM91, Wan91, WWSS98a, WWSS98b, Wel90, WSV92, WA99, WPLC95, WAW+97, WKP+90, WNW91, YC95, YL90, YB94, YB95b, YTRB97, ZHSB92, ZM90, Zau91, ZYY95a, Zho93, ZL94, ZG92, Zim91, CBIT94, Hal96c, RJP97, SB98b].
**molecular-field** [MRM97]. **molecule** [AC94, Bro99, Kri90, NSA+97, RPR+98, TKTN99, TMCM+96, YB95a].
**molecules** [AS98a, ASM+92, BLO94, BP93a, BW91a, BKMH97, CNOJ93, CW91, CSC96, CACD97, Cul92, CG97, CG99, DF97, Din91a, Din91b, DJ94, EPW97, Fab91, FPL95, FW92, FRZ93, FS97, GM90, GJK+93, GP94, GW98c, Gri94, GSW90, HBLL98, HG93, HI98, Hea90, HK95, HMS93, JHB96, JJTP93, JTM+95, JS93, KG92, KD91, KJ97, KG93, KHA90, KSD90, LSCA98, LPD90, LL92, LKLB+99, MAP97, MK98, MHS+94, Mit98a, MRG+90, MPJC98, Net94, NVK+97, OJL93, PNJS93, PKN+95, PKRR97, PHG94, Phi90, PC94a, PD99, RCB99, RRR92, ST91, SC94, SR94a, SS98a, SNS95, SACKH95, SWAH91, TKF92, Tel90, TG98, TGW96, TJP96, WAM93, Wan97, WHF97, WS93, WCMS91, ZV96, vEK99]. **Møller** [BCFM98, Klo93, RPW98]. **MolSurf** [NS98]. **molybdenum** [Van97].
**moment** [LP95, McD96, SFB91]. **moments** [BRC94, Din91b, GM90, KE95, RSK92, SR98, SSRO92, SACKH95].
**momentum** [ZS95]. **Mono** [GSK95]. **Mono-** [GSK95]. **monodentate** [TRG99]. **monomer** [Kna92]. **monophosphate** [BB98a]. **monopole** [SKOR93]. **monopoles** [BW90]. **monosaccharides** [GZL+94].
**monosubstituted** [SK91, Van97, VFM+90]. **Monte** [Dum91, JJ98, JMH96, SS98b, BMJ90, CFK97, CE96, CCJ+99, CBSB94, CLO99, DBV98, DN92, DV97, ET98, FB97, FCS98, GLP95, GPB+97, GVH94, GLLOB91, GS94c, GBE92, HL96b, HNS+97, HHP91, JG93a, JN93, JLNTR93, JAdV96, KID93, Kul90, Mar90, MM97, MJSV92, NBS94, NVS91, PKRR97, PLB92, PHG94, RPG+95, SS98a, SMM97, TM95, TS99a, TMCM+96, VGN+92, vFB91]. **mori** [MN92]. **MORMIN** [PGAL93]. **Morse** [DKK+93, DKK95]. **most** [PP97, RTSM93]. **motion** [DOO93, DvRSH94, Maz97, Mil90]. **motions** [EPBD95, Gen99]. **MP2** [BvH+92, CW93, FV98, HA93, Lim97, MD95, PS98, VHV90]. **MP2-energy** [Lim97]. **MPGRAD** [HA93]. **MPSim** [LBI+97]. **MRCEPA** [VVSV96].
**MRCI** [VVSV96]. **MRD** [BW91a, Gri94, RHKK90]. **MSEED** [PCG+92].
**MST** [BLO94, CLO99, LBO94, LBAO96, OJL93, OBL95]. **MST-SCRF** [BLO94, LBO94]. **MST/SCRF** [LBAO96, OJL93, OBL95]. **Multi** [TG98, WHHP97]. **multi-Fock** [WHHP97]. **Multi-multigrid** [TG98].

SVS+97, SYHW99, VES+99, Wib99, WHM+96, WHHP97]. **NMR-derived** [SSD93]. **NO** [BL91, Tay99]. **non** [BRP92, BGZP97, LDM92b]. **non-HIerarchical** [BGZP97]. **non-linear** [LDM92b]. **non-stiff** [BRP92]. **nonadditive** [DK97]. **nonadditivity** [TRG99]. **nonan** [SMS98]. **nonan-9-one** [SMS98]. **nonbond** [SK95]. **nonbonded** [AFK+95, BPC91, GK93, KID93]. **nonbonding** [KMM99]. **nonclassical** [TLBP99]. **nonconjugated** [MSB95]. **nondegenerate** [BC93, GML94]. **nonempirical** [HKŠ+97, Ove91]. **nonidentity** [LKL95]. **Nonlinear** [RP99, AS99, HS95b, HOL99, KD91, KSD90, Ran93, ZYY95b, TLBP99]. **nonlinearized** [RM91]. **Nonlocal** [HGC+95]. **nonmagnetic** [EBD+99]. **nonoptimum** [Mag93b]. **nonorthogonal** [FM91]. **nonoverlapping** [KRL+93]. **nonpolar** [CKP96]. **nonproximate** [ČTS98]. **nonreactive** [SB98a]. **nonspherical** [Her97, HREK98]. **norbornane** [CGdAC91]. **norbornene** [CGdAC91]. **norcamphor** [BO93]. **Normal** [AC94, fGGG94, DZ97, GW98c, KCK97, ZS93, KG91]. **Normalization** [BB96b]. **note** [HHC90]. **Nova** [Ran92]. **novel** [DH90b, JLW97, TSZ90, WC90]. **novo** [PM93]. **Np** [SHM99]. **NPT** [JJ98]. **NT** [SW96b]. **nuclear** [BGBW97, CCN90, CRME93, CMC96, EPBD95, FGBH90, FSW96, For91, FM94, PGAL93, VRV99]. **nucleic** [BB98a, LDVP91, RC95, RTGJ98, SV94, SCZC99, TGW96]. **nucleophilic** [HKK+97, LS94]. **Nucleoside** [Wun92, VRBE93]. **nucleosides** [GLP95, VRBE93, Wun92]. **nucleotides** [PGBM97]. **nucleus** [McD97]. **number** [BMP+91, TSZ90]. **numbers** [Mar90, SCC93]. **Numerical** [BG96a, BG96b, CDR+95, CF97b, HO97, HS95b, SOL90, ACB92, ELA+95, För92, FPC91, HOL99, KTK93, KT93a, OS94, Pet94, RK97].

**O** [FBTD92, GS90d, GMY97, JKS93, KHA90, Lóp95b, LDMS99, MI99, Sie96, VHV90, BSN99, DJ94, GMY97, HDA93, Mag95, NL91, NQ99, PT99, RR92, Rod94, TK94, VCLB92, vDvdRvD92, SUG92]. **O-** [HDA93]. **o-AMSA** [SUG92]. **O-H** [VHV90, RR92]. **obeying** [LJ91]. **object** [SA99]. **Observations** [TMB93]. **obtain** [SSRO92]. **obtained** [LIO90, MM97, Mit98a, SAdV97]. **obtaining** [LJ91, MM91]. **OCN** [SAF93]. **OCN-containing** [SAF93]. **octane** [GHT98]. **octupole** [Din91b]. **OCXYCH** [Arn94]. **Off** [KID93, LOP+97, LPW+97, LKC+98]. **Off-lattice** [KID93, LOP+97, LPW+97, LKC+98]. **OH** [SHM99, Sie96, AIDAVB98, Luk94, vDvdRvD92]. **OH-propene** [AIDAVB98]. **OHF** [TEdV90]. **OHO** [VHV90]. **olefinic** [Sel90]. **oligoazine** [SE94]. **oligomeric** [fGGG94]. **oligomers** [RHN94, RCATD96, WJV+96]. **oligonucleotides** [GVH94]. **oligosaccharides** [DDLV95, ITP90, OM96]. **oncogenic** [YSJ95]. **One** [Kuc96, AD90, BBR98, CLQSS98, Cis93, FDMB92, JCV+93, Mit98b, SSM96, SMS98, VÅJ94, VHWC98, ARLG+94]. **One-** [Kuc96, SSM96]. **one-center** [Cis93]. **one-configuration-type** [BBR98]. **one-electron** [AD90, JCV+93]. **one-index** [VÅJ94]. **One-step** [ARLG+94]. **onto** [CBR97, JAdV96]. **open**

[ABD90, AD90, BCB+97, Cha92, ES99, LLB99, RCvRS97b]. **open-ended** [ABD90, AD90]. **open-shell** [BCB+97, LLB99]. **Operations** [Gar90]. **operator** [BBR98, LZT91]. **operators** [AD90, JCV+93, LL92]. **OPKINE** [PBRP91]. **OPLS** [BMJ90, DFTRJ97, HE99b, HKŠ+97, JN93, JLNTR93]. **OPLS-like** [HE99b]. **Oppenheimer** [BG93]. **optical** [KD91, KSD90, RP99]. **optima** [FPRD99]. **Optimal** [Mez97, RKL93, BWS+95, NSWP90, Ran91, TAC98, DF96]. **Optimization** [AKF93, BLO94, FG96, HH99b, MK97b, Ste91, WWSS98a, WSS99c, AS98b, BH91a, Bak92, BB93, Bak93, Bak97, BCT98, BMD99, Bér97a, BCT91, DV99, DJ94, EPW97, FSBMP99, FPL95, GM98b, Har99b, Hea90, KFML99, LSR97, LPW+97, LZT91, MM95, Mit98b, MPBM98, NM97, PKRR97, PP97, PK91, TEHL93, YM98, ZKA94, KT93b, WWSS98b]. **optimizationin** [RRR92]. **optimizations** [BvH+92, MS95, SH91]. **optimize** [PASF96]. **optimized** [BGZP97, FW92, LBO94, OBL95, SCRI93, CH96a]. **Optimizing** [ET98, AB97, AB98b, PPK92]. **Optimum** [Mag93b]. **option** [Hal99a]. **ORAC** [PDPM97]. **ORAL** [Zim91]. **orbit** [HBLL98, KMM99, LL92, VRV99]. **orbital** [AC92, BRC94, Bic99, CT92, CH94, CH96b, CG97, DM94, DH90a, FLHP97, FLPH98, GPSS93, Jur96, KWWS91, KTS92, LKL95, MI99, PNJS93, PKN+95, PSY+99, PFLH93, SRI92, SR92, VPV91, Wel90, vOC93]. **orbitals** [CDR+95, CDG+99, CC98, Ish98a, Jon91, KMM99, PF99, RLA+98, Zho93, ZL94, ZM99]. **orbiting** [DvRSH94]. **order** [ACD97, BW91a, Bec99a, Del96, FR94b, FV98, GW98b, Har99b, Ish98a, Klo97, NS95, Pao90, RPW98, She90, SG95]. **ordering** [KCK97]. **orders** [KK92]. **organic** [ASM+92, BMD99, BFST93, BBC+98, CNOJ93, CG97, DJ93, DN92, ER95, GC98, Gri90, HG93, HDA93, KG92, KJ97, LSCA98, LBAO96, MTRJ95, MRG+90, OC98, SC94, SACKH95, TYMS98]. **organization** [JMH96]. **organo** [LJ92]. **organo-transition** [LJ92]. **organolithium** [PK95]. **Organometallic** [Had98, JFR92a, JFR92b, SH91, VF92]. **orientation** [PS96b]. **orienting** [HP94]. **Origin** [LKC+98]. **Origins** [LS96]. **ortho** [OC98, SMF91]. **ortho-terphenyl** [OC98]. **Orthogonal** [Zho93]. **orthogonalized** [Ran93]. **other** [Bic99, Fro93, Hal99b, SCP92, SW93a, Tel90]. **out-of-plane** [LPK99, Mil90, TNS97a]. **outer** [CH96a]. **over-relaxation** [NH91]. **overall** [Tel90]. **overdamped** [GJD94]. **Overestimation** [TEdV90]. **Overhauser** [For91, FM94, PGAL93]. **overlap** [LTHY96]. **overlaps** [WSS99a]. **oxazole** [KS91, SW93a]. **oxidation** [BHK+91, GCRSAIVB99, SSV93, vOC93]. **oxide** [Rau96]. **oxo** [JFKK94, Kat90a]. **oxovanadium** [BH98b]. **oxyacids** [DJ93]. **oxyethylene** [DS92]. **oxygen** [BSGB98, LDJ+97, LPT97, NPLT97]. **oxygenated** [GS90d]. **oxymethylpyridines** [NWÅM95]. **oxyphosphoranes** [GS90d].

**P** [BT92, CLS+97, KTT94, KTT95, MRG97, Tay99, MR93, CLS+97, GS90d]. **P.C.** [Var92]. **P450** [HL96a, Kat93]. **P450-mediated** [Kat93]. **P450cam**

[BO93]. **pack** [vEK99]. **package** [SL95, TS99b, vEK99]. **packing** [CC91a, GS94a, GS94b]. **pair** [BMW+90, Cul92, GZ95, JZ96, LS98, RBC+98, SV94, SCZC99]. **pairing** [PD99]. **pairs** [Pra93, RC95]. **pairwise** [DH90b, WSS99a]. **palladium** [Sel90]. **Palmitoyl** [LH96]. **pancreatic** [Kik96, PS92]. **papain** [KR96]. **paperback** [Dav97, Dav97]. **paracyclophanes** [BRLD92]. **Parallel** [BCFM98, BHE+93, CBWF98, DKH98, GF96, LWNS95, Lim97, MD95, MOSD97, NIS98, Net94, NS95, PLY98, VT91, BBR96, Bec97, BDKJL95, CDG+96, CMC92, CS90, CS96, DLS+97, DPK94, FK95, GJL+90, HL96b, JP92a, JP92b, LBI+97, LMFA92, MTBS91, PH96, RGK93, RBC+98, RBE98, SS93, SLG93, SOCF98, SWK99, SL95, TMK+99, VM95, VA98, WHHP97, WH95, YB94, JP92a, JP92b]. **parallel-coordinates** [Bec97]. **Parallelization** [JG93a, KMO92, DK93, TA94]. **PARAM** [SLG93]. **paramagnetic** [Kar99]. **Parameter** [LFB96, BSV94, CA95, ISH98b]. **Parameterization** [Fer95, CT92, FSBMP99, FUS+94, GH98, Hal96a, LA90, LBB94, LFB96, NL98, SGB91, LPW+97]. **parameterized** [TRLRB96]. **parameters** [AJ99a, AGP91, ACFO91, AKF93, BLO94, BCB+97, Can93, FG96, GDK92, Hal96b, Hil97, HA95, HH99b, KT93b, KHB92, LOP+97, MTRJ95, MRH99, NWÅM95, Ran91, RSB96, SEJ95, SB95, Smi99, Ste91, SWAH91, SK95, VFK92, WH93, YM98, DDLV95, PT99]. **Parametrization** [DMV98, FR94a, HLO99, OM96, SN91, KVL91, LBAO96, NS98, OL93a, FRC91]. **Part** [Dav97, Dya98, VRC91]. **Partial** [GK90, Hea90, SWS+90, BT96, CNOJ93, PNJS93, PKN+95, SOL90, WLKJ92]. **particle** [Hil97, LW94]. **particles** [LLD98]. **particular** [YTT97]. **partition** [BH91b, KW91b, Tru91]. **Partitioning** [DOO93]. **passing** [VM95]. **Path** [Mor93, MN95, Bau90, DBS96, Mez92, PB92]. **paths** [HH99a, ZMC+97]. **pathway** [VP94, ZVP98]. **Pathways** [SR92, AJB96, Sau91, VP92]. **pattern** [CBR97, Mar90, SHCY93]. **Pauli** [Cha92]. **Pb** [JFR92b, Ste91]. **PC** [Rog90, Rog94, Rog03]. **PCs** [TRJ96]. **peak** [CCN90]. **PEFF** [Dil92]. **Penning** [CC98]. **penta** [TRG99]. **penta-** [TRG99]. **pentagon** [AOYŌ96]. **pentahalides** [BT92]. **pentanes** [GdAG+98]. **Pentium** [TRJ96]. **Pentium-based** [TRJ96]. **pentyne** [CC91b]. **peptidase** [BSL91]. **Peptide** [GVD96, PFC96, BPS93, BK97a, Bec97, Büh99, Dav94b, GS90c, HO93, HS95a, JLW97, KOH98, KFML99, MTRJ95, Par99, PMIB99, RK95, SS98b, WP97]. **peptides** [AC92, AS96, BCB+97, BM99, BMN99, Dav93, Dav94a, GS90a, GS90b, HYA92, KF99, MHJ+98, MM97, NTK96, SKOR93]. **Pepto** [CCN90]. **Performance** [BMN99, DNC96, HKŠ+97, SKT94, VA98, FTW+96, GM98b, Hal96a, HGK+96, HEN+94, RCB99, BBR96]. **pericyclic** [OS91]. **period** [LS96]. **periodic** [SKT93]. **periods** [ENvRS94]. **peroxides** [BFST93, CA93]. **peroxyl** [ARLAB99]. **perpendicular** [Din91a]. **perturbation** [CKP96, CG98, DPK94, ER95, FPSK92, HVM99, HK90, Klo97, MP90, NS95, RM94, RE99, Wun92, ZvN93]. **perturbations** [HE99a, SEJ95]. **Perturbative** [LLB99, ET98]. **perturbed** [DKK95]. **PES** [MK94]. **PESP** [Mar98]. **PF** [Cai94]. **PH** [GS90d, Mag95]. **pharmacophores** [SSM96].

[RLG98]. **probed** [EPBD95]. **Probing** [GBE92, Pea94]. **problem** [CE96, Cis93, DF96, Flo92, HO93, HO97, HT99b, KA96b, LK91, MFG91, MM94c, Pea94, RBSB96, SLPP97, Wan91, Zho93, ZL94]. **problems** [Bla91, CT95, MS95]. **procedure** [För92, LJ91, LLD98, PT98, PTCB99, SW93b]. **procedures** [CT95, MM97, She90, WR93]. **process** [EHNW96]. **processes** [LW92, TP93, TRLRB96, WMM+95]. **processing** [GJL+90, SS93, YG92b, YG92a]. **processor** [AFK+95, TMK+99]. **processors** [CDG+96, JP92a, JP92b]. **PRODEN** [ATS90]. **Prodock** [TS99b]. **produced** [FS91]. **product** [LB90]. **products** [FSW96, ZVP98]. **profiles** [MTRJ95, MRS98]. **Program** [HH99a, ATS90, BHE+93, Bro99, DLS+97, Dil92, Elv91, GW95, HA93, HGK+96, HHP91, JHB96, KLV94, KD91, LBI+97, MRM97, Nic97, PL94, PCG+92, PBRP91, PDPM97, RLA+98, SLG93, SM90, TH93, WHF97, vEK99, BMD99, BDKJL95, DBT98]. **programming** [GVD96, NSWP90, TH93]. **programs** [LCW93]. **progress** [SHM99]. **projected** [ATS90, OS91]. **Projection** [LZT91, AS99, GCG97, GW98c, SBS99]. **Promoting** [STT95]. **Propella** [GPK95]. **propenal** [FA99]. **propene** [AIDAVB98]. **proper** [Kri90, LMA99]. **properties** [AS98a, AGM91, BP93a, BFST93, CW93, DBS96, DA96, GM90, GWHD99, GCT96, GM99, Gri90, KD91, KS96, KSD90, Kut99, LV90, MvRSL+97, MVS92, NPLT97, Pac95, PSW96, RP99, SBA97, SR94b, SSRO92, SOL97, TKTN99, TEdV91, UVRCR92, Wel90, dVA92]. **property** [BSB+97, BR97, DJ92, DV97, Ran91, SV94]. **property-based** [DV97]. **proposed** [HO97, LDVP91, RMW91, VP93]. **propyl** [IMP91]. **protease** [MR93, MRG97, YBD+94, YTRB97]. **Protein** [DS90, DRP98, HT99b, JP92a, JP92b, ATK94, BFH94, Bec97, BF96, BG99, BSL91, BSV94, CDG+96, GS90c, GSB99, GJL+90, GK93, GF96, HO97, HYH+94, JB95, Kik99, Kna92, KID93, KUT+97, LOP+97, LPW+97, LKC+98, MKS97, MLAT99, MLA+99, Non97, RS92, Sno92, SG95, TS99b, TEHL93, VDF+97, Wan91, XWS92, YSJ95, Yos94, Yos96, ZFYY95, CHPK91]. **protein-DNA** [CDG+96]. **protein-folding** [Sno92]. **protein-structure** [LOP+97, LPW+97, LKC+98]. **proteinase** [RM94, SBS99]. **proteins** [ABE+96, AS99, AS96, BBR96, BCB+97, BMN99, CC91a, CE96, CCN90, CNS96, CCBK95, DB98, DP95, fGGG94, GKS93, GG91, GT98, JTM+95, JAdV96, Kik96, Kik99, KG91, KHW+90, LCW93, LA91, NTK96, PS92, PMRG93, SN91, VB93, WS99b]. **protocols** [REA+98]. **Proton** [PMHRG97, ACB97, BA94, CGdAC91, ČTS98, FS94, FA99, HR97, KS91, LMRRL98, RHKK90, STB+94, SHCR97, SK91, VFM+90, GHS97]. **proton-transfer** [LMRRL98]. **protonated** [LCD+97, NBG93, ZCP98]. **Protonation** [HOL98, RTGJ98, Wel90]. **prototypes** [GMY97]. **proximity** [SSV93]. **prudent** [HKK91]. **ps** [SYHW99, MKF+97]. **PS-GVB** [MKF+97]. **pseudo** [RL95]. **pseudo-diatomic** [RL95]. **pseudodiagonalization** [WHHP97]. **Pseudopotential** [KSP90, JFR92a, JFR92b, SS95, VSF97]. **pseudopotentials** [SRI92]. **pseudospectral** [BCFM98, CBWF98, KZ99].

[AC92, AJB96, AIDAVB98, ARLG+94, Bau90, CLS+97, DVJ+95a, DVJ+95b, DBS93, DBS96, FW92, FA99, FOA98, FUS+94, FSI95, GLLOB91, HOL98, HB91, IBKvRS92, JZ96, KCK97, LMB99, LV90, LS94, LSSvRS96, LDMS99, MGLL99, MRS98, NVER97, PLB92, PB92, RRR92, SBM97, SS97, VP92, VP93, VP94, Vas92, WO97, ZVP98]. **reaction-diffusion** [Vas92]. **reactions** [CG90, GCRSAIVB99, GHS97, JB98, JKN99, LKL95, LS98, LDJ+97, OS91, SMA92, SSV93, SWOW97, Vya97, ZMC+97]. **reactive** [SB98a, TRLRB96]. **reactivities** [BH98b]. **Reactivity** [BHK+91, SS97, Bic99, BSN99, Che99, ISH98b, JFKK94, LO98, OL93b, SSM96]. **real** [BC93, CMC92, Mit94, SCC93]. **realistic** [PDPM97]. **Realities** [Cas89, Gar90]. **realization** [WWZD92]. **Rearrangement** [CLQSS98, Bau90, HY96, LP92, RJP97]. **rearrangements** [KW91a]. **recently** [DHHY90, HO97, Ste90]. **receptor** [AT93, AVP93, AHLR+91, CA95, GH98, LK92, LWS+95, SQ95, ZS99]. **recipe** [Klo97]. **recognition** [CBR97, Mar90]. **Recommendations** [Pol93]. **Reconsideration** [SKK+93]. **reconstruction** [MKS97, RS92]. **recurrence** [RKL93]. **redox** [CG90, TYRD92]. **reduce** [DB98]. **Reduced** [TWR+95, AB97, BHK+91, BSV94, QHIH98]. **reduced-parameter** [BSV94]. **reduced-restricted-quasi-Newton** [AB97]. **reductase** [CG90, CG94, CG96, CG98, LK95, Wel90]. **reduction** [Bru93, WWSS98a, WWSS98b, fGGG94]. **reductive** [WM93]. **redundancies** [PPK92]. **redundant** [PASF96]. **reevaluation** [SSV93]. **Reference** [RLA+98, KTnH99, RSK92]. **refine** [MKS90]. **refinement** [Bec99a, GKM94, GF96, LFB96]. **Refinements** [FTA91]. **refining** [NWÅM95]. **reflection** [SA99]. **reflection-symmetric** [SA99]. **reformulation** [AB98b]. **regiochemistry** [CN98]. **region** [DH99]. **Regioselectivity** [NVER97]. **Registration** [PS96b]. **regressions** [Ran93]. **Regressive** [DMB91]. **regular** [GS94a]. **regularization** [SBJ92]. **related** [AF94, Ano97, Din91b, GS90d, Gri90, LPK99, LS98, Mag95, MHJ+98, MR93, MGPR90, RdBN90, SD98, SSV93, SB92b, WO97]. **relating** [Kna92]. **Relation** [McD97, SG95]. **relations** [MGH97, RKL93]. **relationship** [KF94, Pao90, Par99, Ran91]. **relationships** [DJ92, GLLOB91]. **Relative** [CGBC96, DN92, Pra93, BSC+98, BSvRS95, CK91, CG94, ER95, HCK95, LS96, RE99, SVM99, SCP92, SACKH95]. **Relativistic** [Dya98, ES99, HOL99, Kut99, PC94a, SCMV97, Van99, EBD+99, FV98, HKY98, Klo97, LL92, VES+99, SI93, Van97]. **relaxation** [NH91, SHCY93, WPLC95, ZRVD93]. **Relaxed** [ITP90]. **relevant** [Gre95, GG96, ZM92]. **Reliability** [SRI92, BKL+90, LIO90]. **Remarks** [CT95]. **renormalization** [CT95]. **Reorganization** [LH99]. **reparametrization** [MFG91]. **replace** [FK91]. **Replicated** [WAW+97, YB95b]. **Reply** [Ste90]. **represent** [Wil94]. **Representation** [TKF92, CZM98, CLO99, DH94, FS91, KKE93, LMB96, LBO94, Pac93, PSW96, Bér97a, TKSM96]. **representations** [BSV94, GKS93]. **representative** [CKP96]. **represented** [HH99a, WAM91]. **Representing**

[Bec97, BKMH97]. **reproduce** [Wib99]. **reproduced** [KD96]. **reproduces** [HCK95]. **repulsion** [CW97, Cha92, Cso93, FTA91, FS98b, FW93b, HREK98, Ish98a, Jon91, YG92a]. **repulsions** [ST94]. **required** [GM90]. **requirement** [fGGG94]. **rescaling** [HTC98]. **Research** [Dun90, Gar90, LJKL98, RG99, RPG+95, YTT97, Tay99]. **residence** [GS93]. **residue** [EHNW96, LOP+97, LPW+97, LKC+98, MRG97, PFM91]. **residues** [AGP91, BCB+97]. **resolution** [Cri99, RK99]. **Resonance** [CD97, BGBW97, CCN90, CRME93, EPBD95, FSW96, GW98a, GW98b, GBW98, LDVP91, PR95]. **RESP** [CCBK95]. **respect** [CMC96]. **response** [CT99, HE99a, VRV99, VÅJ94]. **restrained** [HE99a]. **restraints** [AL98, HE99b]. **restricted** [AB97, Bof94, LL92, LM96, PS96a, SLG93]. **restrictions** [BM99]. **results** [Bog99, BCF+92, FW93a, FV98, HKŠ+97, HOL99, KT93a, PT99, PK95, RG99, REA+98, RE99, SUG92, WJV+96, DJ94]. **retinal** [CBSR99]. **reuptake** [Fro93]. **Reversed** [RM94]. **Review** [Chr90, Dav97, Dun90, Dya98, Gar90, Gol92, Klo92, Mez91, Ran92, Tay99, Var92, Zho97]. **Reviews** [Zho97]. **revisited** [CD97]. **Rh** [BJ94]. **RHF** [MOSD97]. **rhinovirus** [YKU96]. **rhombic** [RP99]. **ribonuclease** [PS92]. **rich** [FHB99]. **rigid** [FS98a, FS00, fGGG94, GS97, Kna92, LP93, MK92, MSZ96, PS91, PS92]. **rigid-geometry** [GS97, PS91, PS92]. **ring** [Cso93, FGG+92, FDMB92, FD94, HKK+97, Jai90, LL94, MR93, Rau96, Sau91, SSM96, SR92, TP93, WO97]. **ring-bracing** [LL94]. **ring-form** [FD94]. **rings** [AMY98, KS91, PMHRG97, TGW96]. **RISM** [KOH97, KOH98]. **RKR** [DKK+93]. **Rn** [ACD99]. **RNA** [CCBK95, FCS98, GVH94]. **ro** [Net94, MR93, RM94]. **ro-vibrational** [Net94]. **robust** [HS95b, KOH97, MS95]. **rod** [RM91]. **rod-like** [RM91]. **Rogers** [Var92]. **role** [ARLG+94, Fel96, KMM99, TD95, AMY98]. **roll** [FS98a, FS00]. **rotamers** [KD96]. **rotating** [Phi90]. **rotation** [BADP92, CPS90, Fag91, FBTD92, MS98, Par99, RK99, TDFdC91, Tru91, MR93]. **Rotational** [CRP97, SSHB93, BB96a, Bro99, GCG97, KHB92, MTRJ95, PG91, Tel90, YKU96, ÇHP91]. **rotations** [ACD97, LM96]. **rotors** [For96]. **rouse** [Kna92]. **route** [BKMM99, DLM+98]. **routine** [BG93]. **Rouvray** [Ran92]. **rovibrational** [Mit98a]. **row** [AJ99b, BW91a, BC90, CW91, MHB97, SH91, dlVM91]. **rows** [SB95]. **RPA** [FKN+93]. **RRIGS** [AS97]. **Ru** [GWHD99]. **rule** [AOYŌ96, BBS96]. **rules** [Hal96d, WH93]. **rupture** [GHT98]. **ruthenium** [GWHD99]. **Rys** [ABD90].

**S** [Bic99, FBTD92, MI99, MRH99, RNDP98, Tay99, TDFdC91, BMD99, Jur96, LS98, Mag95, BF96]. **SA** [REA+98]. **saccharides** [LM96]. **saddle** [AB98b, QHIH98]. **salt** [KOH98]. **Sammon** [AS99]. **Sampling** [SS98b, AW90, BK97a, BW90, CSR92, GLP95, HP94, HNS+97, Kul90, PD92, PHG94, SMM97, SK92b]. **satisfying** [HM92]. **saturated** [ACL96, Dil90]. **saving** [vLP90]. **saxitoxin** [Pet95]. **Sb** [MTR90, Ste91]. **SCAAS** [LW92]. **SCAAS/AMPAC** [LW92]. **scalable** [DPK94, HGK+96, FTW+96]. **scale**

[AJ99a, AJ99b, GJ95, JG93b, KJ97, LJ92, LDJ92]. **single** [GVH94, HM92, SVM99, TK94, WJL+96]. **single-stranded** [GVH94]. **singlet** [KHF91, LDJ+97]. **singlet-triplet** [KHF91]. **singularities** [BK96, EA93, GŌ95]. **SiO** [AS98a, KHG96]. **Site** [WA99, Cri95, CG96, GBE92, KTnH99, SN91, SB99b]. **sites** [APC98, BG99, CS95, GSB99, HK90, KOH97, LK92, PMRG93, SBS99]. **six** [HVvRS93]. **six-center** [HVvRS93]. **Sixty** [LKSS91b]. **Sixty-atom** [LKSS91b]. **size** [Har99b, WTLC93, dVA92]. **sized** [GBT97]. **sizes** [COR99]. **skeletal** [Bér97a]. **Slater** [CDG+99, Jon91, Ric93, RLA+98]. **Slater-type** [CDG+99, Jon91, RLA+98]. **slow** [LMB99]. **SM3** [CT92]. **Small** [SG95, APC98, DF97, DBS91, DN92, GJK+93, JJTP93, KT91, LW94, Mag93a, OJL93, SACKH95, TP93, TJP96, WAM93, WO97, vEK99, MHB97, MPJC98]. **Small-amplitude** [SG95]. **smart** [SS98a]. **Smoothing** [PP97, BNDS97, DM91]. **Sn** [JFR92b, Ste91]. **soft** [Kul90]. **softness** [CN98]. **Software** [TS99b, MK94, MRG+90]. **solid** [Kul90, NQ99, Tav96, Vya97, WTLC93, FB97]. **solid-state** [Vya97]. **solids** [DKBS97, EBD+99, NBB+99, Ste98]. **soliton** [För92]. **solubilities** [Her93]. **solute** [BLO94, FS97, KOH97, Mez97, YB95a]. **solutes** [BCT91, DN92, LBAO96]. **Solution** [KR96, KTnH99, ACB92, BCT98, Bru93, CR95, CLO99, CF97b, CG94, CG97, DF96, DF97, DN92, FM94, Gao97, HYA92, HS93c, HS95b, KOH98, LB96, LS94, NBS94, PPAS+99, Pra93, RCB99, SOL90, SW96a, SYHW99, SBJ92, TYMS98, TG98, TRLRB96, UF93, VHWC98, Vas92, WCK96, YBD+94, ZPV+96]. **solutions** [AS97, Bla91, Cis93, CG93, DM91, JKN99, LW92, Mar90]. **solvated** [ARLAB99, LBO94, RRR92]. **Solvation** [KJ97, MRS98, REA+98, Smi99, Art94, CFK97, CT95, CBIT94, CK91, CMPT98, CT92, CG99, FTA91, HL96a, HY96, Her97, KOH98, LW94, LHL+95, LW92, PT98, Pur98, RE99, SH98, SK95, VWGF95, WWXS97, WWF95, dVA92, AVP93]. **solve** [NH91]. **Solvent** [CG96, MRH99, SJDW90, WCK96, ACB97, ARLG+94, BFH94, CTC95, CLO99, DF97, FRZ93, FDMB93, FS97, Gao97, GMM95, GŌ95, LDM92a, PSK98, PaST94, PLB92, PMRG93, PKCM99, SAdV97, Sha91, SNS95, SKK+93, VS97, WS99a, WWSS98a, WWSS98b, WSS99b, WSS99c, YB95a, ZKSB93]. **solvent-accessible** [FS97, GŌ95, WWSS98a, WWSS98b, WSS99c, ZKSB93]. **solvent-excluded** [GŌ95]. **solvent-excluding** [PaST94]. **solvent-inaccessible** [WSS99b]. **solvents** [LBAO96]. **solver** [HBBF97]. **Solving** [LDM92b, ZYY95b, Ram90, Wan91]. **Some** [SN99, Arn94, AGM91, BP98, BPC91, BPZL96, BH91b, BBS96, CKP96, FVR92, FR94a, GH98, IS91, KS91, RC95, SCP92, GS90c, Pet94]. **SONHICA** [BGZP97]. **Sons** [Dun90, Gar90, Klo92]. **sorption** [TYMS98]. **sp** [TK94]. **space** [BBR96, CLO99, Cri92, CÉC97, GLP95, GPF97, GS91, GBE92, JLW97, JLW99, KG91, KMKW98, KG93, LSR97, MJSV92, NM97, TGW96, vLP90, ZV96]. **Space-efficient** [ZV96]. **space-fixed** [NM97]. **space-saving** [vLP90]. **spaces** [FA99, PS96a]. **spanning** [BMP+91]. **sparse**

KW91b, KF94, LS98, LWNS95, LOP+97, LPW+97, LKC+98, Lóp95a, Lóp95b, MM93, MKF+97, MS95, MvEP+98, MTR90, ORK+91, PG98, PL94, RdBN90, Ran91, Ric91, vRSD92, SBB+93, SEJ95, TAC98, VK97, Van97, VTR+94, Yar95, YSJ95, YBD+94, ZM92, ZM99, vEK99, HBR+99, PSY+99].
**structure-activity** [Ric91]. **structure-property** [Ran91]. **structured** [YB94]. **Structures** [ENvRS94, RCATD96, TNKM91, AB98b, BCT98, BMD99, Bec97, Bof94, BC95, BvH+92, Che95a, CNS96, DvRSH94, ENHE98, EHNW96, GS94a, GC98, HBLL98, HDA93, KG92, KFML99, KA96a, MI99, MM95, NVS91, Obe98, PS91, PS92, PL94, PPK91, PRRD98, PD92, PE92, SCP92, SB98b, SC91, SB92b, Sun94, VP94, VK97, Wel90, WS93, WPLC95, VF92]. **studied** [BO93, HYH+94, KR96, SWM90, WJL+96, WJV+96]. **Studies** [AC92, Dun90, AF97, ACDP98, BRLD92, CRP97, CC91b, ENHE98, FW91, GPSS93, Gri94, Hal99a, HKK+97, HR97, JFR92a, JFR92b, Kat90b, KWWS91, Klo93, KCK97, KHA90, LK90, LKL95, LH96, LYH+95, LMA99, LO98, MKS90, O'm99, Ric91, SB98b, SB98c, SUG92, SF96, SB92b, TA98, VHWC98, VF92, Wel90, WC90, ZVP98, ZMC+97, vOC93, LCA94, SW93b]. **Study** [Kik99, SAdV97, ZM92, Zho93, ZL94, ACB97, ALPH91, AGN+90, AC92, AVA93, Arn94, BSGB98, BA94, BPZL96, BKMH97, BKL+90, BT92, BHK+91, BSN99, Büh99, Cai94, CLQSS98, CA93, Che95b, CKP96, CAC99, CLS+97, CH94, CER94, CH96b, CÉC97, CG90, CG98, CY98, DLM+98, DKJ96, DH90b, DKBS97, ER95, FF93, FVR92, FA99, FSCS99, FLPH98, FOA98, GCRSAIVB99, GJ95, GS90c, GS90d, GPK95, GJCC93, GJL+90, GHS97, GBT97, HL96a, HREK98, HLO99, HK95, HMČ91, HNH+91, IBKvRS92, JTM+95, Jur96, JZ96, KS91, KW91a, Kar99, Kat90a, Kat93, KMM99, KRM92, KF99, KF94, KA96a, KHB92, KKCH96, KHG96, LK95, LKL+97, LS98, LS94, LDJ+97, LSSvRS96, LDMS99, LIO90, MP98, MI99, MS98, MTRJ95, MV91, MSSS95, MP90, NVS91, NSA+97, NBB+99, NWÅM95, NBG93, NVER97, OL93a]. **study** [OL93b, PS98, PG91, PC93, PC94b, PFM91, PBS97, RdBN90, Rau96, RJP97, RCB99, RCATD96, RR92, Rod94, RK95, SSM96, SE94, SSHB93, SR94b, SLD+90, SSF90, SHHČ90, SVS+97, SSRS94, SR92, SK91, TM95, TYRD92, UVRCR92, Van97, VRC91, VRC92, VPV91, VCLB92, VKC96, VK94, VL90, VFM+90, WHM+96, WNW91, ZBM91, GJK+93, TJP96, TRLRB96].
**studying** [FR94a]. **subspace** [IC96, KTnH99]. **substances** [Gri90]. **substituent** [ISH98b, KHF90, KHF91, SLD+90, WTLC93, PC94b]. **substituents** [ENvRS94, SMF91]. **substituted** [AHLR+91, BCF+92, BHK+91, CPS90, GC98, JN93, JLNTR93, KHF90, MP98, PC93, TDFdC91, WM95, ZLM92]. **substitution** [ČTS98, GG91, HKK+97]. **Substrate** [BO93, CFK97, SMA92, WNW91]. **substrates** [CG90]. **substructures** [BV97]. **subsystems** [PS97]. **successive** [NH91]. **suggestion** [PM93]. **Suitability** [ALO93, SOL97]. **suited** [MFG91]. **sulfamates** [HA95]. **sulfated** [FPR97]. **sulfates** [HA95]. **sulfide** [Kat93]. **sulfides** [AF97, KTS92]. **sulfone** [GJ95]. **sulfones** [AF93]. **sulfur**

[PKN+95]. **sulfur-** [PKN+95]. **Sum** [For96]. **summation** [DKBS97, Pur98]. **sums** [CÇG97, KVKK93]. **Superacidity** [BKK+96]. **supercomputer** [SOCF98]. **supercritical** [MSZ96]. **superior** [Cul99]. **supermatrix** [CLCL96, CW97, YG92a]. **supermolecular** [Gre95]. **supermolecule** [GG96, HY96]. **supermolecule-polarizable** [HY96]. **superoxide** [SWM90, SWS+90, SMA92]. **Superposition** [NVK+97, AG90, HVM99, Kea90, WB91, CACD97]. **Supplementary** [Mag93b, Mag93a]. **support** [Fel96]. **supramolecular** [JMH96]. **surface** [BG96a, BG96b, BKMH97, BR97, CZM98, CT95, CP98, CS95, CLS+97, DvRSH94, DS90, EA93, ELA+95, FB98, FS97, GŌ95, Her93, Her97, HREK98, IBKvRS92, LM93, NBS94, PAS90, PaST94, PCG+92, SS98b, SNS95, SBS99, SVS+97, TA94, VB93, Wan91, WL91a, WWSS98a, WWSS98b, WSS99c, ZM90, ZYY95a]. **surface-derived** [SBS99]. **surfaces** [AVA93, AB97, AHLR+91, BW91a, Bec98, BJ94, BG99, CHP90, CMC96, DA96, FD91, HGB93, IRRR93, ITP90, Jen94, JAdV96, JKN99, LMA99, MTH94, PFMI97, PFFF97, PAS90, PaST94, PFC96, Pet94, PT98, QHIH98, RK99, SB98a, Sau91, STPA91, SB90, SC95, WAM93, WSS99a, ZHSB92, ZKSB93]. **Survey** [SHM99]. **switches** [AM99]. **sybyl** [GJK+93, TJP96, GPPS91]. **Symbolic** [Jem97, JK98, HB91]. **symmetric** [CMC92, KA96b, Mit94, Mit98b, SA99, SMS98]. **Symmetry** [Ste98, ÇHP91, CLCL96, CW97, Ear90, fGGG94, RCAA99, SA99, YKU96, ZL94, ZM99, CLCL96, CW97]. **symmetry-adaptation** [ZL94]. **Symmetry-matrix** [CLCL96, CW97]. **symmetry-supermatrix** [CLCL96, CW97]. **Symplectic** [ZS95]. **Symposium** [Tay99]. **Syn** [FHT99]. **Synergy** [BSL91]. **synthesis** [Dav94b]. **synthetic** [CT97]. **synthetical** [ZKSB93]. **System** [Gar90, BSN99, CCN90, CF97a, DN92, FF93, KKE93, LFB96, MRG+90, MR93, Ram90, SOL90, SBB+93, SE94, SB99a, TEdV90, Vas92]. **Systematic** [KMKW98, ZVP98, BT92, GS91, PFC96, dVA92, PS92]. **systems** [BFH94, BWS+95, BJK95, CHPK91, Cso93, DF96, EKS97, EA93, FB97, FHB99, FRSNS92, FGG+92, For96, GMY97, HVvRS93, Her97, IS91, JB95, JVB95, Jem97, Kar99, LMB96, LBI+97, Lóp95a, Lóp95b, LLB99, LBO94, MTRJ95, MSDC94, MFG97, Mor93, MPJ98, Mul91, MR93, MGPR90, PHG94, PH96, PDPM97, SSM96, Sel90, SAF93, SEJ95, SQ95, SM91, SCRI93, SKM94, TRR+94, TEdV91, TNS97b, WM95].

**T** [Dun90, Tay99]. **T1** [SI93]. **T3E** [SOCF98]. **T4** [EHNW96]. **tables** [HC96, LM93, LB90]. **Taiwan** [SYHW99]. **taken** [VSF97]. **Tanford** [ZFYY95]. **target** [SF96]. **Taunton** [Dun90]. **Tautomeric** [Fab91, CAC99]. **tautomerism** [Rau96, RGK93]. **tautomerization** [LKL+97]. **tautomers** [FD94]. **taxotere** [BMD99]. **Taylor** [BRP92]. **Te** [Ste91]. **Technical** [Gar90]. **technique** [Dav94a, FPL95, GS90b, Jai90, MGPR90, SJ95, TEdV90, TEdV91]. **Techniques** [Bak93, Dya98, SCC93, Bec99a, EKS97, FR94b, GBE92, KR96,

[BC93, DMB91, ZBM91]. **vertical** [Gri94]. **very** [LBI+97, LP93, TRR+94, ŽRK+95]. **VESPA** [BCG97]. **VI** [BW91a, Hal99a]. **via** [HE99a, LM93, NBB+99, PFC96, WR93, ZRVD93]. **Viability** [TRJ96]. **Vibrational** [DDV93, GW98c, MLBD92, SCZC99, AS98a, ACB92, AC94, BP98, BSB+97, BBS96, CJC+93, CMS91, CC91b, DDLV95, DVL90, DBT98, DV97, Hal96c, HI98, JHB96, KT91, KCK97, KCK98, McD96, NL91, Net94, NA96, PSY+99, RJP97, RCATD96, SC91, Sun94, Tru91, dANS+96, SB98c]. **vibrational-state-selected** [DBT98]. **vibrations** [GH97]. **vicinal** [CGdAC91]. **Vienna** [Gar90]. **VII** [Hal99b]. **VIII** [BHK+91, CW93]. **vinylcyclobutane** [Bau90]. **vinylcyclopropanes** [Bal98]. **vinylene** [WJV+96]. **Vinyloxyborane** [IBKvRS92]. **violation** [HTC98]. **virial** [BBvG95, LJ91]. **virions** [ÇHP91]. **virtual** [BP93b]. **Vis** [BMD99]. **vitamin** [MNVM97]. **Volume** [Zho97, Bla91, Chr90, ELA+95, GPF97, GŌ95, Gri90, KPR91, Pet95, STPA91]. **volume-based** [Pet95]. **volumes** [ABD+98, Pet94, WWF95]. **Voronoi** [GPF97]. **VRI** [Cri99]. **vs** [AGN+90, SSM96].

**W** [Var92]. **Waals** [WWSS98a, AHLR+91, BLO94, BR97, CÇG97, Hal96b, Hil97, LDG99, LLB99, Mar97b, Pet94, TEdV91, VHWC98, WH93, WWSS98b, Wil94]. **walks** [Bal91b, BW96]. **water** [BW91b, CG93, DKJ96, DN92, EGH+93, EJ95, FF93, Fer95, FS97, GZ95, GS93, GLLOB91, HS93b, JJ98, JKS93, KHW+90, KTnH99, Mez92, MK92, MSZ96, PMIB99, Sie96, SB99a, SK95, TRG99, TMCM+96, TRLRB96, VW96, VCLB92, Yos96]. **water/chloroform** [VW96]. **waters** [LLD98]. **Watson** [SCZC99]. **wave** [BBR98, CP92, FW93a, LJ91, Mag93b, Mag93a, Mar97a, Mar97b, Mar98, ML92, OL90, RMS93, WLKJ92]. **wavefunction** [LIO90]. **wavefunctions** [KKJ97, LIO90]. **weakly** [DV97, Lóp95a, Lóp95b]. **weighted** [KRB+92, KRB+95]. **weights** [LPW+97]. **well** [MFG91]. **wells** [GML94]. **WH** [HKY98]. **widely** [Hal99b]. **Wiener** [TSZ90]. **Wiley** [Dun90, Gar90, Gol92, Klo92, Mez91]. **Wilson** [Chr90]. **within** [LDG99, RHKK90, VP94]. **without** [CA95, KID93]. **WKB** [GML94]. **workstation** [BHE+93, HA93, SL95]. **workstations** [FKN+93, MK94]. **World** [Dav97]. **wreath** [LB90].

**X** [AS98a, BSvRS95, BT92, FBTD92, GdAG+98, Lóp95b, SHM99, SI93, SM91, TDFdC91, ZY96, Dun90, AS98a, BSvRS95, BSL91, Dav93, Dav94b, KRL+93, KHA90, PS91, PS92, SI93, SYHW99, WJL+96, WJV+96, ZMC+97, TDFdC91]. **X-PLOR** [Dav93]. **X-PLORing** [Dav94b]. **X-ray** [BSL91, KRL+93, PS91, PS92, SYHW99, WJL+96, WJV+96]. **XeF** [SCMV97]. **xenon** [Pul97, SCMV97]. **XH** [ZMC+97]. **XONO** [SM91]. **XSiO** [AS98a]. **XSSX** [BSvRS95]. **XVI** [PFC96]. **xvii** [Gar90].

**Yammp** [TH93]. **Yarkony** [Dav97]. **Yb** [FR94b]. **YO** [TDFdC91]. **York** [Chr90, Dun90, Gar90, Gol92, Klo92, Mez91, Ran92, Var92]. **yttrium** [HM90]. **Yukawa** [JCV+93].

**Z** [FW91, LPW+97]. **Z-DNA** [FW91]. **Z-score** [LPW+97]. **zeolite** [GHS97]. **zero** [LTHY96, SC95]. **zero-flux** [SC95]. **zero-overlap** [LTHY96]. **zinc** [KSP90, YBD+94]. **Zn** [Gre95, GSK95, GG96, Mar98, SWS+90, SMA92, Ste91, TRG99]. **Zupan** [Gol92]. **zwitterion** [DKJ96]. **zwitterion-water** [DKJ96].

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