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## Title word cross-reference

+ [FS82]. **\$103** [Lip83b]. **\$12.95** [Sch86].  $1s$  [ST89].  $2$  [Dod84, KMST86].  
**\$29.00** [Car85].  $2p$  [Lau88].  $2s$  [Lau88].  $3$  [Dod84]. **\$35.00** [Lip86].  $3d$   
[ST82, TSH81a].  $3\Pi$  [DBVMB84].  $3s$  [ST89, TSH81a].  $4$  [Dod84, FKS86].  
**\$45.00** [Gil87]. **\$46.95** [Gar82a]. **\$48.00** [Lil87]. **\$49.95** [Kro88].  $4f$  [ST82].  
**\$54.95** [Jur88].  $6$  [LHOM84]. **\$63.95** [Cra85]. **\$64.95** [Lip83a]. **\$79.95**  
[Wib86]. **\$85.00** [Boy86]. **\$9.00** [Ran86].  $[l, m, n]$  [Dod84]. +  
[CDL89, DD81, FS89, FS82, GLLOB88, Iku85, Kim85, RFLC89, TMOW85].  
++ [NRR82]. - [DD81, HPR80, JDS89, JI81, MV87, SK86].  $^1$  [BBJ88, MV87].  
 $^{13}$  [CW80, CZ88].  $^1\Sigma$  [MV87].  $^3$  [PD83].  $^{31}$  [DCNG85].  $^4$  [EGM+89].  $^{77}$   
[CGN87].  $^\alpha$  [KYJ88].  $^+$  [FS82]. *exp* [THW80]. *HFS* [THW80]. *Phe* [LDP80].  $^1$   
[PD83].  $^2$  [Ada89, BMLR88, BG86, BTS+83, BHR+86, Car82, CDL89,  
CvRS81, Cla81, CDL+87, CE87, CMRW86, Del87, DTPR85, DBVMB84,  
DbCV+86, FS89, FS82, FKS85, FKS86, GBT82, GDO89, GHT87, Hin80,

HPR80, Iku85, JDS89, KT88, KHRvH87, KvRS89, Klo83, LB87, LS87a, LS87b, LP88, LR87, Lop89, MV87, MTN87, NRS84, NR80, PKB88, PD83, PMZ86, RAS85, RRI88, Sax85, TG83, TW81, WKP+80].  $\frac{+}{2}$  [FKS85].  $\frac{-}{2}$  [CMRW86, Lop89].  $2n$  [LHOM84].  $2v$  [MTN87].  $3$  [Ada89, Bai84, BHR+86, Del87, Del89, FWB85, FS89, FS82, GBT82, Iku85, KvRS89, KPRT81, KPE+84, LS87b, NRS84, Ran83, Sie85, SK86, TMOW85, WKP+80].  $3v$  [SN87].  $4$  [BMLR88, CvRSKJ81, CvRS81, FS82, KvRS89, KSL87, LR87, NR80, RAS85, Sax85, SK89, ST80, WKP+80].  $\frac{2+}{4-n}$  [FKS86].  $5$  [WKP+80, YJ86].  $6$  [GDO89, Hin80, Sax85, SKJ88].  $60$  [BL88].  $7$  [GDO89].  $7^-$  [ROK86].  $8$  [Bai84, FS82, GDO89].  $9$  [GDO89].  $\alpha$  [THW80].  $MeH$  [EGM+89].  $N$  [VSS84, CDL89, CMRW86, Del87, Del89, FKS86, LHOM84, LB89b, MFG89c].  $\frac{+1}{n+1}$  [Del87].  $\alpha$  [FSH+84, HML83, KT88, LMW85, Lew87, LH85, PPV83, RP80, THW80, TW81, VCZB89].  $\alpha_{ta}$  [TW81].  $\beta$  [BTG81b, FSH+84, GBT80, Lew87, RP80, SMOT85].  $c$  [CP81].  $\cdot$  [Del87, FS82, TMOW85].  $\cdot_2$  [Ran83].  $\cdot_3$  [Ran83].  $\chi$  [Sen87].  $\cos \varphi$  [Sch89].  $d$  [CE87].  $FC = SCe$  [Mas88].  $HC = SCe$  [Mas88].  $l, m, n$  [Dod84].  $\log P$  [Lew89].  $N$  [BTRT88, HSS83, AP80, JdKdWB87, LCY82, SSSA82, TM84].  $n = 0$  [FKS86].  $n = 3$  [LHOM84].  $n \rightarrow \pi$  [Del81c].  $n \rightarrow \pi^*$  [Del81a].  $\nu$  [Lew87].  $\omega$  [ZW83a].  $p$  [Per84].  $p < 0$  [Per84].  $\pi$  [AG88b, Gre84, HAKW87, KM85, LCY82].  $\pi^*$  [Lew87, TM84].  $\pi^* \leftarrow n$  [SM80].  $\pi^* \leftarrow \pi$  [SM80].  $\rho^{1/2}$  [Mar87].  $\rightarrow$  [FS82, GBT82].  $\rightleftharpoons$  [GT84, PMZ86].  $S$  [Bra89, BW81].  $sd$  [SMKH87a].  $\sigma$  [Cla83, WB80].  $spd$  [SMKH87b].  $\varphi$  [Sen87].

\* [Cla83, ST89].

- [Bur80b, FSH+84, PPV83, RP80, VM86, ST89]. **-accepting** [KM85]. **-acetyl-N-methylphenylalaninamide** [KYJ88]. **-alkanes** [LCY82]. **-alkyl** [LCY82]. **-azabicyclane** [FSH+84]. **-bond** [Gre84]. **-butane** [AP80]. **-carboline** [SMOT85]. **-catechin** [VM86]. **-chymotrypsin** [VCZB89]. **-cis-1** [BW81]. **-electronic** [HAKW87]. **-epicatechin** [VM86]. **-Factors** [KMST86]. **-hydroxyacrolein** [BTG81b, GBT80]. **-Li** [MV87]. **-methylpyrazole** [CSCD+89]. **-MP** [SMKH87a, SMKH87b]. **-nitrosamine** [HSS83]. **-nitrosamines** [BTRT88]. **-nonane** [SSSA82]. **-nonbonded** [LCY82]. **-nonclassical** [WB80]. **-phellandrene** [PPV83, RP80]. **-substituted** [HML83, LH85]. **-SW** [TW81]. **-symmetric** [FWB85]. **-terminal** [CP81]. **-type** [ST89].

/2 [DS80]. /3 [HSW82, LHC84, MSSS80, MSS82, VVVG81]. /BW [TW82]. /CI [ZBR80].

1 [GDO89, RP80, STH82, Tat85]. **1-Methylcyclohexyl** [VMNGTVM86]. **11** [Coo77]. **164** [KW86]. **1983** [Str85]. **1984** [Ano83a]. **1986** [Ano86j]. **19XX**

[Ran86].

**2** [AF83, BP87b, ČHS84, Lew89, VSS84, WP82]. **2-** [LV82, Top87, VFM<sup>+</sup>89]. **2-aza-1** [BGT84]. **2-C** [GDO89]. **2-Dimethylcyclopentyl** [VMNGTVM86]. **2-Disilylethane** [PUNC86]. **2-dithiete** [God87]. **2-methylpropanoic** [SKE<sup>+</sup>84]. **2-propen-1-imine** [PKB88]. **2-pyrimidyl** [BL81]. **205** [ABE<sup>+</sup>85, BP87b, GM86, LGB<sup>+</sup>89, LW88, RD87]. **21G** [ST89, VLG89]. **2H** [DLMR85]. **2H-pyran-2-ones** [DLMR85]. **2nd** [Str85].

**3** [BSSW88, CZ88, GDO89, HHK<sup>+</sup>86, RP80, ST89, TSH81b, Top87, VMNGTVM86, VFM<sup>+</sup>89]. **3-** [VFM<sup>+</sup>89]. **3-21** [CCSvRS83]. **3-21G** [ST89]. **3-butadiene** [BW81, BCB82, BGT84, RP80]. **3-diaza-1** [BGT84]. **3-dichloropropane** [HW88]. **3-hydroxypyridine** [LV82]. **3-Phenylpiperidine** [Fro86]. **3-Phenylpyrrolidine** [Fro86]. **3-triazole** [CSCD<sup>+</sup>89]. **31** [NRR82]. **31G** [HR87]. **3G** [HR85, PH83].

**4** [TSH81b]. **4-** [Tos84]. **4-21G** [VLG89]. **4-fluorophenyl** [GG89]. **4-Hydroxyuracil** [Zie83]. **4-methylhistamine** [Top87]. **4-monosubstituted** [Del81a, VFM<sup>+</sup>89]. **4-R-pyrimidine** [Del81e].

**5** [ČHS84, Tat85]. **5-C** [GDO89]. **5-Dihetero-Spiro** [IL86]. **5-dimethoxytetrahydrofuran** [DPSF<sup>+</sup>88]. **5.2** [CCV89]. **54/5** [Tat85]. **548pp** [Wib86].

**6** [NRR82]. **6-31** [MK85a, NRR82]. **6-31G** [HR87]. **6-dialkylcyclooctatetraenes** [Tos84]. **6/1** [Ran86]. **64-bit** [HD88]. **64/5** [Tat85]. **64/6** [Tat85]. **6th** [Ano86i].

**7** [GDO89]. **7-C** [GDO89]. **7-Norbornadienyllithium** [LB86]. **74/6** [Tat85]. **74/7** [Tat85].

**8** [Ano88c]. **8-azapurine** [SOR87]. **82** [RD87].

**9-Dimethyl-1** [IL86].

= [BG86, Del87, Del89, FS89, MFG89c, PMZ86, THW80].

**Ab-initio** [KHRvH87, LCY82, GT82, MC88]. **absorption** [BCT83, HW82, KJ85]. **Academy** [Lil87]. **Acceleration** [KS82, PR84, Pul82]. **accepting** [KM85]. **acceptor** [GRS88]. **accuracy** [BC89, HRKW89]. **accurate** [DK84, DK85, HE85, MFG89c, MFG89b, Sen87, Ada89]. **acetyl** [FM87, KYJ88, KPE<sup>+</sup>84]. **acetyl-alanine-proline-alanine** [FM87]. **Acetylcholine** [MC88]. **acetylene** [PFRS82]. **acetylenes** [AP87].

**acetylenic** [HMA82]. **acid** [BTG80, BTG81b, BHR<sup>+</sup>86, FS89, GBT82, GT82, LS89a, LSROT80, LCL84, LKL87, OC88, SKE<sup>+</sup>84, ZP84]. **acidities** [Iku84, JI81]. **acidity** [SMF89]. **Acids** [De 86a, AH85, LZP84, MKSW83, MK84b, NK86, Rue87, SMF89, WKNC86]. **Acrolein** [BTG81b]. **across** [BSSW88]. **acrylic** [Rue87]. **active** [FK84, VV88]. **Activity** [GC86, FSH<sup>+</sup>84, GPC88, KK85, KR88, PPV83, RP80, Tin81]. **acyclic** [MSS82]. **add** [CBR87]. **addition** [BW81, CDL<sup>+</sup>87, SWM83]. **additional** [TSH81a]. **additions** [CDL<sup>+</sup>87]. **adjacent** [WM88]. **adjusting** [CPV84]. **Adrenergic** [Ano88c, SDKM87]. **adsorption** [BFAG81, CPV84]. **Advance** [KO86]. **advances** [CP87a]. **affinities** [BNR86, DM86a, Del85, Del86, FS83, HL83, Kal87, KKR<sup>+</sup>82, OUV84, RS85, SAV88, VFM<sup>+</sup>89]. **affinity** [MFG89a]. **Ag** [Klo83]. **AgH** [Klo83, KSB85]. **Agonists** [Ano88c, SDKM87]. **AH** [Del87, Del87, Del89, MFG89c]. **aid** [CL85]. **aided** [Boy86, Tri84]. **al** [Lip83b]. **ala** [RMB86]. **alanine** [FM87]. **Alder** [LHC84]. **alditols** [Bur80b]. **algebra** [Tri87, Tri88]. **algebraic** [FE87]. **Algorithm** [HG89, WG87, Bak86, Bak87, BG88, Bal82a, Ber83, BHW87, Cri89, Kar86, KE89, KS82, KCF84, LM89, Lin88, LV88, Mas88, Mat88, MBB85, MSKT87, RLR89]. **algorithms** [Cra85, GS87a, HB89, Rap84, RLR88, STZ88, BMB85a, PPT<sup>+</sup>80]. **AIH** [BMLR88]. **aliphatic** [BSM83]. **alkali** [GSB85, MK85b]. **alkanes** [FWS89, LCY82, MSSS80]. **alkenes** [VVVG81]. **alkyl** [AG88a, Kao88, LCY82, Tai81]. **alkyl-silanes** [AG88a]. **alkylamines** [GCW88]. **alkylation** [RS85]. **alkylbenzenes** [GCW88]. **alkyldisilanes** [PUC89]. **allenes** [AP87]. **Allinger** [Lip83a]. **allowed** [BW81]. **allylamine** [KS84]. **allylic** [Rit86]. **AIO** [RRI88]. **alternative** [Sil81]. **aluminum** [DGW<sup>+</sup>81, JI88, JSKI88]. **AM1** [HT88, BSSW88, CDL89, Fab88, SMF89, VFM<sup>+</sup>89]. **AMBER** [WK81]. **amenable** [KSS83, KVV<sup>+</sup>84, KSB84, SSSA82, SVS<sup>+</sup>81, SKV<sup>+</sup>85, SKE<sup>+</sup>84, VSS82]. **American** [Lip83a]. **amide** [OLBM83, RK81]. **amidine** [ZPCR82, ZPPC83, ZP84]. **amidinium** [EW87]. **amine** [BN85]. **amines** [GT82, GT83]. **amino** [Kao88, LS89a, AH85]. **ammonia** [BG81a, BG82b, BG82c, KTVRS86, LSROT80, OLBM83]. **Ammonia-Glycine** [OLBM83]. **amplitude** [Mar87]. **amplitudes** [VVVG81]. **Analgesics** [Fro86]. **analog** [TS83]. **analyses** [Kel80a]. **Analysis** [Ano88c, HAKW87, Bac89, BP82, CMR88, Cri82, Cri84, CP87b, CL85, DA83, Dod84, FGR89, HH80, HS82, HE85, IÖ84, KS84, KSS83, KVV<sup>+</sup>84, KSB84, NLB85, OE89, PKB88, PPT<sup>+</sup>80, RB87, SDKM87, SRKT87, SVS<sup>+</sup>81, SKV<sup>+</sup>85, SPBO87, SK85, SMF89, VCZB89, VU83, VU84, VM86, Gar82a]. **Analytic** [KBS88]. **Analytical** [Tay84, WM89, Bak87, LDM89]. **angle** [BA82, TMrGM88]. **angles** [BN85]. **anharmonic** [BTG80, BTG82, DbCV<sup>+</sup>86, HE85, ZP89]. **anion** [AB83, BP81, CCSvRS83, SCCvRS82]. **anionic** [DM86a, WB80]. **anions** [GB83, HPR80, HML83, LB86, SCCvRS82]. **Anisotropic** [WM87]. **Annals**

[Lil87]. **Annino** [Gil87]. **Announcement**  
 [Ano82a, Ano84a, Ano85a, Ano85b, Ano87a, Ano87b, Ano87c, Ano87d,  
 Ano88a, Ano88b, Ano89a, Ano89b, Kin83, Ano86i, Ano89l].  
**Announcements** [San82]. **anomeric** [ASFW89, NLA84]. **antibiotics**  
 [SOR86a, SOR86b, SORT86]. **antibiotics-toyocamycin** [SOR86a].  
**antisymmetric** [ZP89]. **applicability** [GTB81, VVVG81, HB82].  
**Application** [Ano88c, BS89, JS87, JI87, JS88, JI88, KSI88, NRS84, SI88,  
 Tri87, CUCP89, DCG81, JT80, KBS88, LH87, Mey80b, NLB85, PS87,  
 SDKM87, Tri88, Wen82, CS80, DbCV<sup>+</sup>86, DPSF<sup>+</sup>88, HE85, HLH83, KR88,  
 LS87b, Lin88, LR87, VDD86, ZR81, ZP89]. **Applications**  
 [Bur80b, KHS86, MS88, BR85, Gil87, Kin87, RD87, RB87, SNR83, SDB87,  
 Tay84, vdGB84, BL88, KT88, SK86, Ste89b, Lil87]. **applied** [HO83, Kim85].  
**appraisal** [HP84a]. **Approach** [Ano88c, IL86, AFK82, BG87, BG82a,  
 BMT81, CP89a, Cio87, DBVMB84, Fuj87, Gla89, HPR80, KPRT81, KR88,  
 LH87, OE89, PR80, SDKM87, SMOT85, SRPY88, Sil81, SK84a, FA86].  
**Approaches** [AGL82, AH84, BR87]. **approx** [Boy86]. **approximate**  
 [ZW83b, FB89, Wen82]. **approximation**  
 [AP87, FT89, Kar87, RDAF83, RPAF83, Van88]. **approximations**  
 [Sen87, TM85]. **aqueous** [DD81, GLOB88, JMB87, KS82, Rue87]. **Archives**  
 [vRS86]. **area** [Mey86, Mey88]. **areas** [Mey86]. **Arg** [CP81]. **aromatic**  
 [AL87, HAKW87, JH83, KR88, LTLA87]. **arrangements** [KNS86, KNS89].  
**array** [BW83, EM84, PPT<sup>+</sup>80, RDW88]. **aryl** [GCW88]. **aryl-alkylamines**  
 [GCW88]. **aspects** [GF87, RPAF83, SSSA82, SF85]. **assess** [ZW83b].  
**assessment** [BMG84, GSH88]. **assisted** [DA83, Lil87, OMK<sup>+</sup>88, WK81].  
**association** [Ran86, SMOT85, BG81b, BG81a, BG82b, BG82c].  
**associations** [NF84, SF86]. **Atom**  
 [IvRS85, SLR<sup>+</sup>86, Cha83, CPH85, LDM89, LLSC85, ST89, SK85, WKNC86].  
**Atom-Atom** [SLR<sup>+</sup>86]. **Atomic**  
 [BR89, CF87, DM86b, GC86, GPC88, THW80, BW89, CP89a, CW81,  
 FVV85, JB85, LV88, Mul88a, Mul88b, Ran80, Wil88]. **atoms**  
 [ASS<sup>+</sup>85, AKRA84, BMB85a, BkBT82, DVA83, FB89, Gla89, NF84, RA87,  
 SMKH87a, SMKH87b, SF86, TH80, TSH81b]. **attached**  
 [BD84, KW86, LA85]. **attenuation** [Ehr84]. **augmented**  
 [CCSvRS83, Cre82a, SCCvRS82, SCvRSH87]. **AuH** [KSB85]. **autocatalytic**  
 [GHF87]. **Automatic** [RDW88]. **automating** [BBJ88]. **automorphisms**  
 [STZ88]. **average** [BkBT82]. **avoiding** [Mom81]. **axial** [ST82]. **aza** [BGT84].  
**azabicyclane** [FSH<sup>+</sup>84]. **azapurine** [SOR87]. **azines** [SAV88].  
**azoxyalkanes** [Bys83].

**B** [Cra85, DBVMB84, GDO89, Kro88, PD83, CvRS81, De 86b]. **B-DNA**  
 [De 86b]. **Babu** [Lil87]. **bacterial** [Tin81]. **Balaban** [Ano86b, Ano86b].  
**balance** [MH83]. **band** [LS84]. **bare** [Mey88]. **Bargon** [Jor81]. **barrelene**  
 [SAF88]. **barrier** [Ham87, Hin80]. **Barriers**  
 [WM88, ADY89, AM88b, BMLR88, BW81, KJ82, PUC89]. **base**

[Aid88, GT82, SRKT87, SK85]. **based**  
 [BMB85a, BMB85b, Dyk88, MBB84, RKM<sup>+</sup>85, RLR88, THW80]. **bases**  
 [ARS85, Del84, Del85, Del86, FS83, FS89, RS85, vRS86]. **basic**  
 [GS87b, Kel80a]. **basicities** [SAV88]. **Basis** [Del85, Del86, Del87, FB89,  
 HRKW89, LS87a, LS87b, LBM89, MSC<sup>+</sup>88, AKRA84, ARS85, Bau84, BP81,  
 CM89, CCSvRS83, Cre82a, Del84, DHK89, DH86, DH87a, DH87b, DH88,  
 FA86, FVV85, GT84, Gro87, HR87, MK85a, MFG89c, MFG89b, MTN87,  
 MR80, MH83, NRS84, NRR82, OTW81, PH83, RAS85, RA87, ST89, SHK83,  
 SCCvRS82, SCvRSH87, SMG87, SGW83, TKK<sup>+</sup>81, WP83, WM88, YNAK88,  
 ZW83a, ZW84, AKRA84, Mag84, MFG89b]. **basis-set** [MH83, AKRA84].  
**bay** [BKKB80, KSJT83]. **BCN** [GT84]. **Be** [WKP<sup>+</sup>80]. **behavior**  
 [BMLR88, DPSF<sup>+</sup>88, SK84b]. **Belousov** [ZR81]. **bending** [LPB84, MHA89].  
**Benedek** [Boy86]. **benzaldehyde** [SM80]. **Benzene**  
 [AL87, PL87, BTG85, DHP83, Lin88, RRH86]. **Benzene-benzene** [PL87].  
**benzenes** [BPP82, Kel80b, KPRT81]. **benzenoid**  
 [BKKB80, Bro83, BCC87, KSJT83]. **benzenoids** [RHP89]. **benzo**  
 [FMTS84]. **benzo-derivatives** [FMTS84]. **benzocyclobutenes** [Kel82].  
**benzoic** [Rue87, SMF89]. **Benzophenone** [PW81]. **benzylic** [LUNV85].  
**BeO** [NRS84]. **berislaviceva** [Ran86]. **Beryllohydrides** [CPTC84]. **best**  
 [Lau88]. **between** [Bau84, BTG82, CDL<sup>+</sup>87, De 86a, De 86b, DLMR85,  
 FM87, HPR80, KDEHK89, LSROT80, Lew87, MK85a, MH83, Tos84]. **BH**  
 [BMLR88, KPRT81]. **bias** [Gar89]. **bibliographies** [vRS86]. **bicarbonate**  
 [GBT82]. **bicyclic** [Bur80b, EW87, Sau89]. **Bicyclo**  
 [ACvRS81, Ōsa82, ST80]. **bifluorenylidene** [FSST82]. **bimolecular** [Del89].  
**binding**  
 [BP81, BC89, Cri87, GC85, Hil80a, Hil80b, KCF84, MK85b, De 86a, De 86b].  
**biochemical** [Gol87, KBS88, ZD87]. **biological**  
 [JG89, SMOT85, SNR83, TMOW85, WG89]. **biologically** [FK84, VV88].  
**biopolymers** [AVF84]. **biphenyl** [HR85, HR87]. **Bis** [BL81]. **bit** [HD88].  
**Bivariate** [Sil89]. **BLMO** [ZW84]. **blocker** [SHDP89]. **blocks** [NSKNK87].  
**BNC** [GT84]. **body** [BMLR88, BG82a]. **Boltzmann** [DM89]. **Bond**  
 [Bai86, BE87, AG88a, BTG81a, BTG82, BGT84, Del81b, Del81c, Del81d,  
 Del81e, Del83, Del87, Gre84, HRKW89, Iku84, Jug84, KPE<sup>+</sup>84, LSROT80,  
 LD87, MK85a, MFG89c, MFG89b, NSGK<sup>+</sup>81, NR80, OLBM83, SAP88, Wil88].  
**bond-polarization** [MFG89b]. **bonded**  
 [Aid88, Dyk88, HPR80, KSL87, LSROT80, TMOW85]. **bonding**  
 [AG88b, AKI88, BTG81a, BG81b, BG81a, BG82b, BG82c, DS80, Gol87,  
 Gre84, Kin87, MKSW83, NRM85]. **bonds**  
 [Cla81, Cla82, Cla83, Fab88, LCY82, PS87, SSSA82, WW81, WM88, ZD87].  
**Book**  
 [Boy86, Car85, Cra85, Gar82b, Gar82a, Gil87, Jor81, Jur88, Kro88, Lil87,  
 Lip83b, Lip83a, Lip86, Ran86, Sch86, vRS86, Str85, Tri82, Wer82, Wib86].  
**boranes** [Kin87]. **Born** [Ehr86, GS85]. **Bornanylidene** [FSST82]. **boron**  
 [DGW<sup>+</sup>81]. **Boston** [Sch86]. **bound** [PASTB87]. **boundary** [Ehr81, Ehr84].

**branched** [Lip87]. **branching** [BG88, CRR85, MSSS80]. **bridgehead** [WP82]. **bridging** [YJ86]. **Brigada** [Ran86]. **bromine** [BE87, DH83]. **Brown** [Sch86]. **Brownian** [GM86]. **build** [GS87a]. **build-up** [GS87a]. **building** [NSKNK87, WK81]. **Burkert** [Lip83a]. **Burns** [ZW84]. **but-3-enoic** [LCL84]. **butadiene** [ACvRS81, BW81, BCB82, BGT84, RP80]. **butanal** [KVV<sup>+</sup>84]. **Butane** [PUNC86, AP80]. **butanoic** [SKE<sup>+</sup>84]. **butylene** [Rit86]. **butylethylene** [FST81].

**C** [FS82, Gar82a, GDO89, KPE<sup>+</sup>84, VM86, BL88, BTG82, BGT84, CvRSKJ81, CW80, CZ88, CvRS81, FWB85, FS82, FKS85, FKS86, GDO89, HHK<sup>+</sup>86, Kao88, LHOM84, MTN87, ST80, SN87, VM86]. **C1** [SAP88]. **C2** [SAP88]. **Ca** [STH81a]. **Cahn** [Mey80b]. **calculate** [BKL87]. **calculated** [BF82, BC83, BTG85, BTG86, FS82, GL88, GL89, HL83, LS89a, MSSS80, MSS82, MH83, OUV84, TM85, WP82, ZW83a, ZW84]. **Calculating** [EM84, GSH88, Cri89, KCF84, Lin88, Mul88a, Mul88b]. **Calculation** [BkBT82, DFC<sup>+</sup>84, FWS89, IFvRSS87, KI81, PV82a, RLR88, BR87, Bau84, Ber83, BN85, Bre81, BA82, Cha83, CW80, CP81, DS87, Dyk88, Fuj87, Gal82, HW82, HG89, HLH83, Lew89, MFG89c, MM87, MR80, NSGK<sup>+</sup>81, NN87, PLFL85, PR84, RLR89, STH81b, SAS87, TKI89, TW81, WG87, BC89, HSW82]. **calculational** [STYA87]. **Calculations** [AB83, Ano88c, ASFW89, DM86b, FBBA86, IL86, OG86, YE89, AGL82, AH84, AH85, AG88b, AS88, Ada89, ABP80, ASS<sup>+</sup>85, AFK82, AVBF84, ARS85, BT81, BR89, BKC86, BTG81b, BG80, BTRT88, BL81, BSSW88, BBO<sup>+</sup>83, Bur80b, Bur80a, Cao89, CF83, CZ88, CM89, CCSvRS83, Cre82a, Cre82b, CG86a, CT87, CL85, CE87, DGW<sup>+</sup>81, DTPR85, DM83, DR83, DH83, EWM85, Fab88, FBKK85, FGR89, FWB85, FS83, GT84, GHT87, Gol87, GHHS85, GL87, HHK<sup>+</sup>86, HLG88, HW88, Hur88, Iku84, Jaf88, JdKdWB87, Kar81, KHRvH87, Klo83, KKR<sup>+</sup>82, KSB85, LRP87, LCC87, LBM89, LMW85, Lew87, LGB<sup>+</sup>89, MK85a, Mag84, MK84a, Mey84, MH83, MSČ<sup>+</sup>88, MM83, MM89, PW82, PW81, PL87, RAS85, RV85, SMKH87a, SMKH87b, SDKM87, SAV88, Sax85, SKJ88, SK89, Sch88, SL81]. **calculations** [ST87, SK85, SHK83, SBS82, SCCvRS82, SCP82, SDB87, Str85, THW80, Van88, VDD86, Ver82, WP83, YNAK88, ZD87, AF83, DHS84, FA86, TMOW85, Lip86, Wer82]. **calicene** [HSEČ83]. **CAMSEQ** [GCW88]. **Canada** [Ano86j]. **Canadian** [Ano86j]. **cancer** [BT80a, BT80b]. **canonical** [BMB85a, KDEHK89]. **carbamate** [LKL87]. **carbamic** [BHR<sup>+</sup>86]. **carbanions** [LUNV85]. **carbocation** [HSW82]. **carbocations** [HLH83]. **carbocycles** [AYS80]. **Carbocations** [CvRSKJ81]. **carbohydrate** [Bur80b]. **carbohydrates** [JT80]. **carboline** [SMOT85]. **carbon** [FS83, MM89, PSSS80]. **carbonic** [BHR<sup>+</sup>86, GBT82]. **carbonions** [WP83]. **carbonyl** [ASS<sup>+</sup>85, BTG81a, MR83]. **carbonyls** [BG82a]. **carborane** [GDO89]. **Carboranes** [OG86]. **carboxylate** [BP81]. **carcinogenesis** [BTRT88]. **carcinogenic** [BKKB80]. **Carlo** [Che89, Gar89, GLOB88, JMB87, KS82, MC88, OC88, RMB86, RPV87, ZR81]. **carrying**

[SK86]. **Cartesian** [Ess83]. **case** [PW81]. **CASSCF** [Tay84].  
**catacondensed** [RHP89]. **catalysis** [FWS89, Per84]. **catalyzed** [OLBM83].  
**catechin** [VM86]. **catenated** [Bai84]. **Cation**  
[VMNGTVM86, BCB82, BP81, CF83, Cla81, FS83, HL83]. **cationic** [WB80].  
**cations** [CSCD<sup>+</sup>89, Cla83, FS82, HHK<sup>+</sup>86, Kim85]. **Causality** [KK85].  
**Cavity** [Ehr81, Ehr84, PASTB87]. **CC** [HRKW89, SSSA82]. **CCHHCNH**  
[PKB88]. **Cd** [Gro87, STH82]. **CDC** [RD87]. **cellular** [KJ85]. **center**  
[PW82, PKD88, RLR88, RLR89]. **centers** [VDD86]. **Centrifugal** [LH87].  
**certain** [BKKB80, Ran86]. **CF** [GHT87]. **CH** [FS89, FS82, NR80, PMZ86,  
TMOW85, KvRS89, KPRT81, KPE<sup>+</sup>84, SK86, TG83, KPE<sup>+</sup>84, WW81].  
**chain** [CU89, CS82, SSSA82, LS89b]. **chains** [FWS89, KB84a, Mom81].  
**chalcogenides** [GT83]. **channel** [Kim85, VU83, VU84]. **Character**  
[SN87, LB89b]. **Characteristic**  
[Bal85, Bal84, Bal88, HO83, HAKW87, HB89, Ran82]. **Characteristics**  
[Aid88, CPTC84, RFP86]. **Characterization**  
[YF86, AM88a, BKKB80, Ran80, SWM83]. **Characters** [ZP89]. **Charge**  
[AH85, AG88b, AS88, Ehr86, AGL82, AH84, BT80a, BT80b, BR89, CW81,  
EH83, Hil80b, HK88, JFG89, KI81, Mez87b, PASTB87, PHG89]. **charged**  
[Del89]. **Charges** [DM86b, CF87, HLG88, Mul88a, Mul88b, SK84a, TM84].  
**CHARMM** [BBO<sup>+</sup>83]. **CHCOO** [JDS89]. **chelate** [Ham87]. **Chem**  
[Ano88c]. **Chemical**  
[CG86b, Kin87, Lip83a, AJMM88, BMB85a, BMB85b, Bal84, BT80a, BT80b,  
BTRT88, BKT82, Boy86, CW80, CZ88, CM89, GHF87, Gre84, Hil80a, Hil80b,  
Jur88, Kel80a, Lip86, MBB84, MBB85, Mil87, NSKNK87, PS87, RKM<sup>+</sup>85,  
RB85, Ran83, ROK86, Rap84, RDW88, Rou87, SK84b, Tin81, ZR81].  
**chemisorption** [LP88]. **Chemistry**  
[Ano86b, Ano86j, Ano89c, BD84, Bur80b, Fra87, Gar82a, Lip86, SNR83,  
Sch86, vRS86, See81, Sil81, STZ88, Tri87, Ano86i, Jor81, Gar82b, Lip83b].  
**chemists** [Ran86, Ano86k, Str85]. **Chemometrics** [Kro88]. **Chichester**  
[Wer82]. **chiral** [LDP<sup>+</sup>87, LDL<sup>+</sup>88, LBZ89]. **chirality** [Ōsa82]. **chlorine**  
[Cla83, DR83, JS87, MSS82]. **chloroalkanes** [VVVG81]. **Chlorosilanes**  
[CUCP89]. **CHOH** [LS87b]. **choice** [MŠ<sup>+</sup>88]. **chromatography**  
[LDP<sup>+</sup>87, LBZ89]. **chymotrypsin** [VCZB89]. **CI** [CP87a, CP80, FBKK85,  
HW82, KHRvH87, LCC87, PMZ86, SKJ88, SK89, Wen82]. **CIPSI** [CP87a].  
**cis** [BW81, BTG80, DVA83, DPSF<sup>+</sup>88, KJ85]. **cis-** [BTG80, DPSF<sup>+</sup>88].  
**cis-diamminedichloroplatinum** [KJ85]. **Cl**  
[CvRS81, Del89, FS89, SK86, NR80, STH81b, SCvRSH87]. **Clarendon**  
[Str85]. **Clark** [Lip86]. **classes** [NF84, Ran86, SF86]. **Classical**  
[Dod84, FE87, HB82, KW86, RH87]. **classification**  
[BKT82, BCC87, RDW88]. **cleft** [LZ89]. **Clementi** [ZW84]. **closed**  
[HHK<sup>+</sup>86, RA87]. **closed-** [HHK<sup>+</sup>86]. **closed-shell** [RA87]. **Cluster**  
[NLB85, Ada89, Kal87]. **clustering** [Iku85, Jur88]. **clusters**  
[BL88, BG82c, CDL89, CMRW86, Dyk88, FBKK85, GLOB88, JSKI88,  
LP88, LYH87, WKP<sup>+</sup>80]. **CN** [FS89, RK81]. **CNDO**



[BP87a, CP89a, DS80, Lew89, MR83, TW82, WP83, ZBR80]. **CNDO/2** [Lew89]. **CNDO/force** [MR83]. **CNH** [PKB88]. **CNO** [KHRvH87]. **CO** [GBT82, Sch86, BHR<sup>+</sup>86, Iku85, ST80]. **Coast** [Ano83a]. **code** [KW86]. **coding** [BMB85b, BKT82]. **coefficient** [KNS85]. **Coefficients** [GC86, KI81]. **collisions** [ST87]. **color** [BR85, EB87]. **colorings** [LB89a]. **Column** [LDP<sup>+</sup>87]. **Combination** [BKL87]. **combinational** [Cra85]. **Combinatorial** [STZ88, KCF84]. **Combined** [MFG89c, MFG89b, Kar87, SK86]. **Compact** [AKRA84, ARS85, RAS85, Cio87]. **Comparative** [JB85, DS80, GCW88, MTN87, SM80, MK85b]. **compared** [EIO85]. **Comparison** [HTT88, JBFR86, MK85a, PUNC86, Top87, ZW83a, ZW84, BTG81b, CDL<sup>+</sup>87, DM89, FGR89, Gla89, KPRT81, Kin87, KSS83, KPE<sup>+</sup>84, KSB84, PHG89, WB80, GHT87]. **compatible** [ČHS84]. **complex** [CPTC84, DBVMB84, FM87, OTW81, SK86, TMOW85, YJ86]. **complexation** [DAU88]. **complexes** [BMLR88, Del81b, Del81c, Del81e, Del83, Del87, Del89, Gen87, GRS88, HS82, JI81, KM85, Lin88, Ved88]. **compliance** [MR83]. **Component** [De 86a, SK85]. **Components** [SLR<sup>+</sup>86]. **compounds** [AG88b, AF83, BS89, BTG81a, CMR88, CMR89, DGW<sup>+</sup>81, DH83, DHS84, DH86, DH87a, DH87b, DH88, DLMR85, FSL84, GHHS85, GL88, GL89, HHR87, JS87, JI87, JS88, JI88, KTvRS86, KPE<sup>+</sup>84, KR88, MK85a, Mag84, MSS82, MS88, PH83, TLA89]. **compression** [HD88]. **Comput** [Ano88c]. **Computation** [KF88, Mor85, RDK83, BPP82, Hur88, KE89, KSHD88, KDEHK89, Mey88, MT82, Sen87, WD88, ZM88]. **Computational** [Ano86b, Ano86j, CG89, GF87, God87, HB89, LV82, SF85, TMOW85, DCG81, FT89, Gil84, GRS88, Lip86, Mey80b, SRKT87, RPAF83, SK84b, Gar82a, Jor81]. **computationally** [CPV84]. **computations** [GL88, GL89]. **computed** [Del84, Del85, Del86, Del87, XB86]. **Computer** [Ano86b, BFB85, Bal82b, Bal83, Bal84, BR85, Bal88, BL88, Cio87, CG86b, DA83, KSJT83, KMS<sup>+</sup>87, Lil87, LB89b, LB89a, OMK<sup>+</sup>88, PLFL85, RB85, TG86, BKKB80, KBS88, RKM<sup>+</sup>85, RMB86, SAS87, TS83, Tri87, vGBC<sup>+</sup>84, Gil87, Boy86, Ran86]. **Computer-assisted** [DA83, Lil87]. **computer-oriented** [SAS87]. **computerized** [Tin81]. **computers** [BD82, CBR87, Gar82b]. **computing** [KNS85, SK84a, TTZWGQKC81]. **concentration** [TTZWGQKC81]. **concept** [JFG89]. **Condon** [DK85]. **Conference** [Ano86j]. **Configuration** [Wen82, Ada89]. **Configurational** [SRKT87, BMG84]. **Conformation** [BP82, FSH<sup>+</sup>84, HLPT82, HPW82, LS89b, SRPY88, Tai81, TMrGM88]. **Conformational** [Ano88c, CvRS81, CP81, Cri82, Cri84, CL85, DPCS80, EIO85, FMTS84, FSH<sup>+</sup>84, Fro86, GCW88, HW88, IL86, KS84, OE89, PPT<sup>+</sup>80, RMB86, VM86, YJ86, ZPPC82, BSSW88, BA82, CMR88, CP87b, DPSF<sup>+</sup>88, Dod84, FGR89, Ham87, LS89a, LDP80, LS88, MR80, NLB85, OTPH87, Ōsa82, RFP86, SDKM87, SKV<sup>+</sup>85, SKE<sup>+</sup>84, VVVG81, VV88, VU83, WG87, Wer82, Bur80b, KSS83, KVV<sup>+</sup>84, KSB84, Mey81, SVS<sup>+</sup>81, Ska83]. **conformations**

[BHW87, Che89, Cri89, Fab88, FSL84, GS87a, HR87, JMB87, PR84, Sau89, Sch88, ZPCR82]. **conformers**  
 [DCG81, FWS89, FWB85, FK84, GBT80, GBT82, Iku85]. **Congress**  
 [Ano86i, Ano86k]. **conical** [LR87]. **conjugate**  
 [DM89, Iku84, WMHJ88, BW81]. **conjugated**  
 [AH84, AS88, Fab88, Kao88, LA85, RP80, VV88]. **connectivities**  
 [BMB85a, BMB85b, MBB84, MBB85, RKM<sup>+</sup>85]. **connectivity** [TKI89].  
**Consecutive** [GHF87]. **consequences** [PR80]. **consideration** [BCT83].  
**consistency** [CT87]. **consistent** [BD82, BL81, DCG81, HHR87, LBM89].  
**constant** [BTG81a, Hur88, MR83, SF85, Tay87]. **constants**  
 [BP87a, BTG81b, BTG82, CGN87, DA83, DVA83, DCNG85, EGM<sup>+</sup>89,  
 GBT82, KBS88, LA85, MAR<sup>+</sup>84, PV82a, SAS87, XB86, ZP89].  
**constitutional** [Bur80b]. **constrained** [BK86, VK80]. **Constraints**  
 [Dil86, AM88b, BHW87, Cri89, Dil87, HT82, TMrGM88]. **Construction**  
 [Lau88, Mom81, MSKT87, RHP89, LS87a]. **containing**  
 [ASS<sup>+</sup>85, ASFW89, BTG82, DGW<sup>+</sup>81, DM83, DR83, DH83, DHS84,  
 HHK<sup>+</sup>86, JH83, Kao88, STH81b, TKK<sup>+</sup>81, Ver82]. **Continuum**  
 [Ehr89, FT89, PASTB87]. **contour** [GDP<sup>+</sup>85, LS84]. **contours**  
 [MKS87, MK84b]. **contracted**  
 [AKRA84, STH81a, STH81b, STH82, TH80, TSH81a, TSH81b, Tat85].  
**Contraction** [DHK89]. **contribution** [FT89, WD88]. **contributions**  
 [BMLR88]. **conventional** [EM84]. **Converged** [ST87]. **convergence**  
 [Bra89, KS82, MF85, Mit88, PR84, Pul82]. **converging** [WMHJ88].  
**converting** [Wib84]. **convolutionally** [Szö87]. **COO** [JDS89]. **COOH**  
 [JDS89]. **Cooper** [Car85, Str85, Tri82]. **Cooperative** [KSL87]. **coordinate**  
 [CL85, LS88]. **coordinates** [Ess83, HLH83, KJLW84, LV88]. **coplanar**  
 [BL81]. **core** [MR80]. **Correct** [OTPH87]. **Correction**  
 [Ano88c, GL89, Gol87, OTW81]. **Corrections** [Ehr86, CT87, LD87, RV85].  
**correlated** [LD87, NRR82]. **Correlation**  
 [SMF89, Ada89, BW89, CPTC84, Cre82b, Del84, Del85, Del86, Del87, GT84,  
 HLH82, Tin81, WD88, WM88, Lew87, Lew89, MH83]. **corresponding**  
 [LV82]. **counterpoise** [LD87]. **Counting** [Bro83]. **Coupled**  
 [Ada89, BG87, SBS82, Kal87, TDK83, WP83]. **coupled-cluster** [Kal87].  
**coupling** [CGN87, DA83, DVA83, DCNG85, EGM<sup>+</sup>89, PW81]. **couplings**  
 [DVA83]. **CpGpCp** [YJ86]. **CpGpCp-pentapeptide** [YJ86]. **Cr** [RAS85].  
**Crambin** [LGB<sup>+</sup>89]. **CRAY** [BP87b]. **Crick** [Aid88]. **Crippen** [Wer82].  
**criterion** [ZW83b]. **Critical** [KPE<sup>+</sup>84, BE87, Gla89]. **croatia** [Ran86].  
**cross** [Mey86]. **cross-sectional** [Mey86]. **crossing** [LR87]. **crosslinked**  
 [KNS86, KNS89]. **crown** [DAU88]. **crystal** [HW80, MB84, PR84]. **crystals**  
 [AL87]. **curve** [SAS87]. **curved** [Dar89]. **curves** [Szö87]. **cutoff** [Kar87].  
**Cyanide** [vRSSRH86]. **Cyanide/Isocyanide** [vRSSRH86]. **cyanobenzene**  
 [BTG85]. **Cyber** [RD87, ABE<sup>+</sup>85, BP87b, LGB<sup>+</sup>89, LW88, GM86].  
**Cyber-205** [GM86]. **cycle** [SK84b]. **Cycles** [Ano86b, BFB85]. **cyclic**  
 [HW80, KSL87, VSS82, ZBR80, CMR89]. **cycloalkanes** [LHOM84, MSSS80].

cyclobutene [BCB82]. cyclobutenes [Kel82]. cyclodextrin [VCZB89]. cycloheptane [IO84]. cycloheptasulfur [LRP87]. cyclohexane [EIO85, KMS85]. cyclohexasulfur [LRP87]. cyclononane [FGR89]. cyclooctane [IO84]. cyclooctasulfur [LRP87]. cyclopentadienes [Kel80b]. cyclopentadienyl [Kel80b]. cyclopentenyl [GHHS85]. cyclopropyl [HML83, LH85]. cyclosporin [PHG89]. cytosine [Del83, PV82b].

**D** [Gil87, Kro88, Str85]. **Damping** [CU89]. **Danuher** [Ano88c]. **data** [BF82, BC89, BBJ88, Cre82a, Cre82b, HD88, KSB84, KJ85, Mor85, PPT<sup>+</sup>80, vRS86, Sch88, Sil85, SS84]. **databases** [RDW88]. **decane** [Ösa82]. **decanes** [Bur80b]. **decarboxylation** [LCL84, Rue87]. **decay** [SS84, Szö87]. **decomposition** [FBD80, HB82, KHRvH87]. **Dedication** [Ano86a]. **defects** [BG82a, SDL82]. **defined** [Gla89]. **deformation** [CE87, Kar87, LTLA87]. **Degenerate** [KvRS89]. **degree** [KR87]. **dense** [CM89]. **densities** [CE87]. **density** [AVF84, Bac89, BW89, EH83, Gla89, HAKW87, Jug84, KI81, Mar87, MSG80, OTW81, RB87]. **Deorthogonalization** [CP89a]. **deoxyribose** [SPBO87]. **dependence** [Del84, HRKW89, Ehr84]. **deprotonated** [ZPPC82, ZPCR82]. **derivative** [Bra89, MHA89, PHG89]. **derivatives** [BC83, FSST82, FMTS84, FS89, FK84, GHHS85, Kao88, WM89]. **derived** [BR89, BTG81b, CF87, KJ85, TMrGM88]. **described** [Bau84]. **description** [BMB85a, BMB85b, LPB84, LWD82, MBB84, MBB85, PASTB87, PS87, RKM<sup>+</sup>85, ZD87]. **design** [Fuj87, HBK80, LDP<sup>+</sup>87, Cra85]. **designs** [Sil89]. **detailed** [CF87]. **detection** [BFF86]. **determinants** [SS84]. **Determination** [BFAG81, CRR85, CP87b, LCL84, OC88, SWM83, TMrGM88, BHW87, DM86a, MFG89b, SHDP89]. **determined** [BPP82]. **determining** [BBJ88, DE83]. **deuterium** [AF83, HLH83]. **Development** [YNAK88, LPB84, Ran86, SHK83, CUCP89]. **developments** [DCG81]. **deviation** [ZW83b]. **Dewar** [Kel80b]. **diabatic** [BMR87]. **diacetals** [Bur80b]. **diagnostic** [Ran80]. **diagonalization** [BR87]. **diagrams** [GDP<sup>+</sup>85]. **dialkylcyclooctatetraenes** [Tos84]. **diamine** [Ham87]. **diaminomethylene** [ASFW89]. **diamminedichloroplatinum** [KJ85]. **dianions** [WP83]. **diatomic** [BE87, DK84, DHK89, KDKC83, KKE88]. **diaza** [BGT84]. **dication** [PFRS82]. **Dications** [FKS86]. **dichloropropane** [HW88]. **dielectric** [Ehr84, Ehr89]. **dielectrics** [Ehr81]. **Diels** [LHC84]. **dienes** [RP80]. **difference** [DM89, KPE<sup>+</sup>84, KKE88, MM83]. **different** [Bau84, GT84]. **differential** [Gar89]. **differentiating** [Sch89]. **diffuse** [CCSvRS83, SCCvRS82, SCvRSH87]. **diffusion** [AS81, Gar89, Per84, RPV87]. **diffusion-limited** [AS81]. **Digital** [TS83]. **Dihetero** [IL86]. **dihydrofolate** [Gre85]. **dihydroxycarbene** [FBD80]. **dilute** [GLOB88]. **Dimensional** [GC86, IL86, AM88b, GPC88, GDP<sup>+</sup>85, KSI88, SI88, SDL82, SK84b]. **dimensions** [LW88]. **dimer** [Has84]. **dimerization** [VU83]. **dimers** [BG82b, VM86, ZP84]. **dimethoxytetrahydrofuran** [DPSF<sup>+</sup>88]. **Dimethyl** [IL86, KMS85, OE89]. **dimethyl-** [OE89]. **Dimethylcyclopentyl**

[VMNGTVM86]. **dimethylheptanes** [CL85]. **dimethylphosphate** [JMB87]. **Diophantine** [Bur82]. **dipeptide** [RMB86]. **Diphenyl** [TKK<sup>+</sup>81]. **diphenylmethyl** [AB83]. **dipolar** [AP85]. **Dipole** [BC83, Ehr89, HE88, Wil88]. **diradicals** [LCY82]. **direct** [AFK82, FWB85, HA89, KKR<sup>+</sup>82, LV88, RPAF83]. **Directed** [GC86, Bal88, GPC88, LS89b]. **directing** [TM84]. **directly** [HPR80]. **Discrete** [Fra87]. **Discrimination** [RRG<sup>+</sup>84, BMT81]. **disiloxane** [GL87]. **Disilylethane** [PUNC86]. **dispersion** [FT89, KSJ82]. **dissociation** [FS82, MK85a, MFG89c, MFG89b]. **distance** [Ber83, BHW87, LMV86, MSKT87, TMrGM88, Wer82]. **distorted** [Szö87]. **distortions** [LH87]. **distributed** [PHG89]. **Distribution** [Ehr86, Hil80b, HK88, PASTB87, RB87, TTZWGQKC81]. **distributions** [BW89, GDP<sup>+</sup>85, Mez87b, NLB85]. **disubstituted** [KPRT81, PR80]. **disulfide** [BL81, KNS86, KNS89, BL81]. **disulfide-crosslinked** [KNS86, KNS89]. **dithiete** [God87]. **dithioglyoxal** [God87]. **Divinylketone** [Ska83]. **DNA** [Aid88, Dar89, De 86b, SRKT87]. **docking** [Kar86, PLFL85]. **donor** [GRS88]. **donor-acceptor** [GRS88]. **Dopaminergic** [Ano88c, SDKM87]. **double** [BFAG81, Gre83, WM88, ZP84]. **double-layer** [BFAG81]. **double-stranded** [Gre83]. **Doublet** [RRI88]. **doubly** [JG89]. **doubly-extended-guanidine** [JG89]. **Driver** [Gil87]. **driving** [BA82]. **Drug** [Ano88c, BC89, Cra85, SDKM87]. **during** [CS82, SOR87]. **dynamic** [Mit88]. **dynamical** [Fra87]. **Dynamics** [GM86, HB82, IL86, SLC86, BBO<sup>+</sup>83, CU89, FM87, Fuj87, GHF87, GCW88, HLC88, NKC85, NK86, SHDP89, TJ86, YE89].

### easily

[KSS83, KVV<sup>+</sup>84, KSB84, SSSA82, SVS<sup>+</sup>81, SKV<sup>+</sup>85, SKE<sup>+</sup>84, VSS82]. **economical** [NRR82]. **Ed** [Jor81, Gar82b, Str85]. **edge** [Bal88, HB89, LB89a]. **edge-weighted** [Bal88, HB89]. **Edited** [Lil87]. **editor** [DMB88]. **Effect** [DPSF<sup>+</sup>88, HLH82, ASS<sup>+</sup>85, ASFW89, BTG85, BTG86, BW89, FSH<sup>+</sup>84, GS85, GT84, GL87, Kim85, NLA84, TSH81a, TM84, WM88]. **effective** [KSB85]. **Effects** [FOSV86, RS85, AH84, AF83, AKRA84, BTS<sup>+</sup>83, BCT83, CS82, DVA83, Del81e, Del85, Del86, Del87, Ehr81, Ehr84, EH83, HPR80, HLH83, JI81, KPRT81, KSL87, KSJ82, Mag84, MSČ<sup>+</sup>88, MM89, PR80, Rit86, SSSA82, SMF89, SMG87, WB80, BTRT88]. **Efficient** [CCSvRS83, Dyk88, KO86, ČFHS85, FBBA86, Mas88, OTPH87, PR87, SL81, Sen87]. **eigenvalue** [DK84, HT82, KDKC83, KKE88, Mas88]. **eigenvalues** [DK88, Gal82, NN87]. **eigenvectors** [Gal82, SN87]. **elastase** [FM87, Fuj87]. **elastin** [CU89]. **electric** [WP83, ZM88]. **electrical** [BFAG81, WW81]. **electrically** [Dyk88]. **electrochemiluminescence** [AS81]. **electrocyclic** [Kel80a]. **electrode** [BFAG81]. **Electron** [AVF84, CPTC84, Cla82, GRS88, OTW81, Bac89, BNR86, BW89, ČHS84, CvRS81, Cla81, Cla83, CS80, DCG81, GDP<sup>+</sup>85, GT84, HLH82, KF88, KKR<sup>+</sup>82, LCC87, MM87, PW82, RLR88, RLR89, RB87, RDK83, WM88, ZW83a, ZW84, Kal87].

**electronegative** [ASS<sup>+</sup>85]. **electronegativity** [LDM89]. **Electronic** [KS83, KJ82, LYH87, PPV83, SM80, ABE<sup>+</sup>85, AVBF84, BT80a, BT80b, BE87, BKL87, Gor88, HAKW87, Lew87, NVGB81, PW82, RP80, SSSA82, SMG87, TM84, WD88]. **electrophiles** [FS89]. **Electrostatic** [Ehr86, HLG88, PASTB87, CF87, CW81, EM84, GSH88, LDP80, LZP84, MK84b, NSGK<sup>+</sup>81, PHG89, PR80, SK84a, Wil88, ZP85]. **element** [KSI88, MK85a, SI88]. **elemental** [WKP<sup>+</sup>80]. **elements** [Bal83, CPTC84, CCSvRS83, DbCV<sup>+</sup>86, DH86, Gro87, KDEHK89, MHA89, PKD88, SCvRSH87, SGW83]. **Elizabeth** [Ano88c]. **ellipsoid** [BHW87]. **Elsevier** [Lip83b]. **embedding** [Cri82, Cri84, CP87b, Cri89]. **emission** [BCT83]. **Empirical** [NK86, PW82, BG81b, BG81a, BG82b, CP87b, RPV87, SDB87, VDD86]. **employing** [WM89]. **emulation** [TS83]. **Enantioselectivity** [LBZ89]. **ended** [BD82]. **energetic** [CPTC84, SPBO87]. **Energetics** [GB83, SLB83, HW88, KC87, OTPH87, VU83, VU84]. **Energies** [Ehr86, AYS80, Bys83, CvRSKJ81, CP89b, Cre82a, Cre82b, Del84, Del87, Del89, DFC<sup>+</sup>84, GTB81, Gre85, IvRS85, Iku84, Iku85, JDS89, KTVRS86, LD87, MK85a, MFG89c, MFG89b, MR80, NR80, TW82, VSS82, VVVG81, WP82, Wib84, WM88]. **Energy** [Ano88c, DM86b, FA86, SK85, SLR<sup>+</sup>86, YF86, BMLR88, BHW87, BSSW88, BBO<sup>+</sup>83, Car82, CDL89, CP81, Cri82, Cri84, CP87b, Del84, DPCS80, FWS89, FST81, FSST82, FT89, FKS85, GBT80, GBT82, GS87a, Ham87, Has84, HHR87, IÖ84, KSHD88, KSJ82, LDM89, Lip86, LDL<sup>+</sup>88, Lop89, MHA89, MT82, NK86, Ösa82, PLFL85, PR87, RDAF83, SDKM87, SOR86a, SOR86b, SORT86, SOR87, SPBO87, SO87, Sch88, ST87, SHK83, Tay84, TM85, TMrGM88, VK80, VSSS84, WG87, WM89, WMHJ88, WD88, WK81, WSP88, MK84a]. **Energy-optimized** [FA86]. **enethiol** [BSM83]. **engineering** [Gil87, Wen82]. **England** [Jur88]. **enoic** [LCL84]. **enol** [BT80b]. **enthalpies** [Bys83, IvRS85, IFvRSS87, Wib84]. **Enumeration** [BCC87, KHS86, KMST86, Cio87, Häs87, KSJT83, KMS<sup>+</sup>87, OTPH87, TKI89]. **environment** [Ran80]. **enzyme** [FM87, TTZWGQKC81]. **enzyme-ligand** [FM87]. **EPEN** [BG82b]. **epicatechin** [VM86]. **equal** [Dod84]. **Equation** [Ehr86, CPV84, DK84, DM89, GS85, GF87, KSI88, NN87, SI88]. **equations** [BG87, BR87, KKE88, KBS88, MSG80, RFLC89, Tri87]. **equilibria** [Bur80b, Mey81]. **equilibrium** [CG89, Sch82b, Tos84]. **equivalence** [BFF86]. **equivalents** [IvRS85, Wib84]. **Ermiler** [GTB81]. **Erratum** [Ano86b, DH88]. **error** [GSH88, MFG89b, MH83, RPV87]. **errors** [MSSS80, OTW81, TM85, ZW83b]. **essential** [Fab88]. **ester** [KSS83, SVS<sup>+</sup>81]. **estimates** [VSS82]. **estimation** [GTB81, HK88, Cre82a]. **ether** [Bur80a]. **ethers** [DAU88]. **ethyl** [Bur80a, FS83, HB82, KSB84]. **ethyl-cation** [FS83]. **Ethylene** [FKS86, CF83, CDL<sup>+</sup>87, SBS82]. **ethylenes** [FSST82]. **ethylmethyamine** [ABP80]. **Ethylmethylsilane** [PUNC86]. **evaluating** [FBBA86, MR83, Sch89]. **Evaluation** [FT89, MSSS80, MSS82, OUV84, BNR86, BCT83, JBFR86, Kar81, KR88,

Ran82, Sch82a, SCvRSH87, Szö87, GRS88, MKSW83, MK84b]. **evaluations** [EM84]. **Examination** [ZP84]. **example** [RFLC89]. **examples** [Coo77]. **exchange** [KvRS89, SK86]. **excitations** [Wen82]. **excited** [Cha83, Del81a, Del81c, DFC<sup>+</sup>84, JH83, MM87, SM80]. **excluded** [HG89]. **exclusion** [SLB83]. **expansion** [CP89b, NF84, PKD88, SF86]. **expansions** [LZP84, ZP85]. **expectation** [ZW83a, ZW84]. **experiment** [KSS83, KVV<sup>+</sup>84, KSB84, SSSA82, SVS<sup>+</sup>81, SKV<sup>+</sup>85, SKE<sup>+</sup>84, VSS82]. **Experimental** [SK84b, BHW87, Sil89]. **experimentally** [ACvRS81]. **Explorations** [LDL<sup>+</sup>88]. **exponents** [ZW84]. **expressions** [FVV85, Sch89]. **Extended** [DH88, WP83, BMB85a, BMB85b, BP81, GS85, JG89, Kin87, KSL87, Koz87, MBB84, MBB85, RKM<sup>+</sup>85, WG89, DH86, DH87a, DH87b]. **extended-guanidine** [WG89]. **extension** [CU89]. **external** [Lin88]. **Extrapolation** [Gar89, MSG80].

**F** [CvRS81, DD81, Del89, FKS85, FKS86, MFG89c, CCSvRS83, HPR80, JDS89, KT88]. **Factors** [KMST86, DK85]. **family** [Mil87]. **Fast** [BC87, CBR87, Mat88, SCP82, Ber83, Kar86, LV88, TTZWGQKC81]. **Faster** [MM83]. **FCH** [JDS89]. **Fe** [GLLOB88]. **feasible** [GC85]. **features** [KSS83, KVV<sup>+</sup>84, KSB84, LUNV85, LB86, SSSA82, SVS<sup>+</sup>81, SKV<sup>+</sup>85, SKE<sup>+</sup>84, VSS82]. **Feldmann** [Lil87]. **fenchylidene** [FSST82]. **Ference** [Boy86]. **ferrous** [HS82]. **FH** [Del87]. **Fibonacci** [EB87]. **field** [AP87, BD82, BL81, CUCP89, CCV89, EIO85, GG89, HP84b, HHR87, LBM89, RFP86, Ska83, WP82, WKNC86]. **fields** [BTG80, HP84a, MF85, WM89]. **fifth** [Gro87]. **Filip** [Ano86b]. **films** [LP88]. **Finding** [Ano86b, BFB85, BMB85a]. **finite** [DM89, KSI88, MM83, SI88]. **finite-difference** [MM83]. **finite-element** [KSI88, SI88]. **First** [MHA89, Ada89, CCSvRS83, DHK89, DH87a, DH88, FBBA86, GHF87, KTVRS86, KBS88, MK85a, PH83, SHK83, SCCvRS82, Tri87]. **first-** [FBBA86, PH83]. **first-order** [Ada89, GHF87, KBS88, SHK83]. **first-row** [CCSvRS83, DHK89, DH87a, DH88, KTVRS86, SCCvRS82]. **Fischer** [CS82]. **fitted** [NRS84]. **fitting** [Dar89, LMV86, LV88, SAS87]. **five** [DA83, DVA83, DPSF<sup>+</sup>88, Ham87, Hil80a, Hil80b]. **five-membered** [DA83, DVA83, DPSF<sup>+</sup>88, Ham87, Hil80a, Hil80b]. **flexibility** [RMB86]. **Flexible** [Ano88c, GC85, Kar86, LMV86, PR84, SDKM87]. **floating** [HL83, Hur88, KW86]. **Florida** [Ano83a]. **fluoride** [Has84]. **fluorides** [MR83]. **fluorinated** [BPP82, Mey80a]. **Fluorine** [FKS86, ASS<sup>+</sup>85, Rit86]. **Fluorine-Substituted** [FKS86]. **fluorobenzene** [BTG85]. **fluorophenyl** [GG89]. **fluorophosphine** [SMG87]. **fluxional** [BMLR88]. **Fock** [LMW85, Cre82a, GTB81, Kar81, LB87, MSG80, RFLC89, RDAF83, RPAF83, TDK83, WP83]. **FOGO** [HL83]. **Force** [BL81, GG89, AP87, BP87a, BTG80, BTG81b, BTG81a, BTG82, CUCP89, CCV89, EIO85, GBT82, HP84a, HP84b, HHR87, Hur88, LA85, MF85, PV82a, RFP86, Ska83, WM89, WP82, WKNC86, XB86, ZP89]. **force-field** [HP84b, RFP86]. **formaldehyde** [HE85, HE88, SWM83]. **formalism**

[BMR87, NRM85, SDL82]. **formamide**  
 [BT80b, WSP88, ZPPC82, ZPPC83, ZP84]. **formamidic** [ZP84]. **formate**  
 [KSB84]. **formation** [BTRT88, BHR<sup>+</sup>86, Bys83, Cre82b, HSW82, HSS83,  
 IvRS85, OLBM83, SAS87, Wib84, YJ86]. **formic** [BTG81b]. **formulae**  
 [DS87]. **formulas** [HO83]. **formulation** [Fra82, TW82]. **formyl**  
 [EH83, MR83]. **Fortran** [LW88]. **Forty** [Ano89c]. **four**  
 [AYS80, Lau88, SKJ88]. **four-membered** [AYS80]. **fourfold** [Wen82].  
**Fourier** [CP89b]. **Fourier-series** [CP89b]. **fourth** [DH86, SGW83].  
**fourth-row** [DH86, SGW83]. **FPS** [HD88]. **fragment** [Che89, FSL84].  
**fragments** [Kao88, NSGK<sup>+</sup>81, NSKNK87, SS81]. **Franck** [DK85]. **free**  
 [FWS89, RMB86]. **freedom** [KR87]. **frequencies**  
 [BTG80, HLH82, HLH83, RK81, SBS82]. **full** [Dil87, HRKW89]. **function**  
 [AP80, CCSvRS83, CP87b, HHR87, LPB84, MFG89c, MFG89b, SAS87,  
 SCCvRS82, SCvRSH87, VDD86, WG87]. **function-augmented**  
 [CCSvRS83, SCCvRS82, SCvRSH87]. **functionalized** [Mey84]. **Functions**  
 [PUNC86, ABP80, BTG85, BTG86, Bur80a, CE87, Ehr89, FB89, GSB85,  
 GL87, Hur88, JFG89, KDEHK89, MK85a, MR83, NK86, PW82, Sen87,  
 TSH81a, TM85, ZW83a]. **fundamental** [BTG80]. **Furan** [TLA89]. **Fusenes**  
 [KHS86].

**G** [NRR82, Str85, Wer82, CCSvRS83]. **G\*** [MK85a]. **Ga** [STH82]. **GaH**  
 [BMLR88]. **gallamine** [SHDP89]. **Gas**  
 [RRH86, FS82, LCL84, LLC85, SK86, VFM<sup>+</sup>89]. **Gas-phase**  
 [RRH86, FS82, LCL84, LLC85]. **gaseous** [GB83]. **gases** [Boy86]. **Gaussian**  
 [AKRA84, Bre81, DHK89, Gro87, LPB84, MR80, MH83, NRS84, RA87,  
 RD87, ST89, STH81a, STH81b, STH82, ST82, SGW83, TH80, TSH81a,  
 TSH81b, Tat85]. **Gaussian-type**  
 [AKRA84, Bre81, STH81a, STH81b, STH82, TH80, TSH81a, TSH81b, Tat85].  
**Ge** [Hin80]. **gearing** [Iro80]. **geminals** [PS87]. **General**  
 [FVV85, Lin88, AS88, AM88b, CRR85, CCV89, Ess83, TJ86, WK81, RKM<sup>+</sup>85].  
**Generalized** [KJ87, NRM85, Bai86]. **generated** [FSL84]. **generates**  
 [Mar87]. **generating** [Sch88]. **generation**  
 [BKKB80, Bal82a, Bal82b, Bal83, Bal84, BR85, Bal88, BL88, KSJT83,  
 KMS<sup>+</sup>87, LB89b, LB89a, RB85, Ran86, HBK80]. **generators** [RWKH87].  
**Generic** [MB84]. **geometric** [Cri89, DHP83, Ess83, KNS86, KNS89].  
**geometrical** [BTG85, BTG86]. **Geometrically** [GC85]. **geometries**  
 [CG89, SKV<sup>+</sup>85, Sch82b, vdGB84, Gre85, VVVG81]. **Geometry**  
 [Del84, FST81, FSST82, KJLW84, Bak87, BTG80, BSSW88, GBT80, GBT82,  
 Gre84, HL83, MH83, MŠ<sup>+</sup>88, OC88, Sil81, Ska83, VLG89, Wer82]. **germyl**  
 [MAR<sup>+</sup>84]. **glucose** [BP87a]. **Gly** [YJ86]. **glycine**  
 [DCG81, KSS83, SVS<sup>+</sup>81, OLBM83]. **glycolipids** [SRPY88]. **glyoxals**  
 [BT80b]. **Golender** [Cra85]. **Gradient**  
 [FA86, DM89, HRKW89, VLG89, WMHJ88]. **gradient-optimized** [VLG89].  
**gradients** [Bak87, Tay84]. **gramicidin** [Kim85, VU84, VU83]. **Graph**

[BKKB80, BKT82, CG86b, RWKH87, BMB85a, HB87, Kin87, KR87, KR88, MBB84, OMK<sup>+</sup>88, CG86b]. **graph-theoretical** [Kin87]. **graphics** [PLFL85].

**Graphite** [SA80]. **Graphs**

[Ano86b, BFB85, Bal84, BR85, Bal88, BL88, DE83, EB87, HO83, HB89, LB89a, MBB84, Mil87, RB85, Ran83, ROK86, Sim87, STZ88]. **Green**

[SDL82]. **Ground** [DM83, DR83, DH83, DHS84, BG80, Del81a, DTPR85, Has84, LR87, Ska83, WSP88, Del81b]. **ground-state** [WSP88, Del81b].

**Group** [Dil86, Wib84, ASFW89, AJMM88, BG82a, BE87, DH86, EH83, EGM<sup>+</sup>89, GG89, Kin87, LA85, SGW83, Tri84, Mez87b]. **groups**

[BTG82, HPR80, Iro80, KPRT81, KSL87, LDP80, LB89b, LB89a]. **growth**

[CS82, Fra87]. **GTO** [FA86, FB89]. **GTOs** [TSH81a]. **guanidine**

[JG89, WG89]. **Guanidinium** [JG89, WG89, SS81]. **Guanidinium-Type**

[JG89, WG89]. **guide** [Lip86]. **Guidelines** [SHK83].

**H** [BBJ88, CDL89, Cla81, CMRW86, DTPR85, FS82, FKS85, FKS86, GBT82, GDO89, Hin80, LS87a, LHOM84, Lop89, Sax85, SKJ88, SK89, Sch86, ST80, TMOW85, Ada89, BG86, BTG82, BHR<sup>+</sup>86, CvRSKJ81, CDL89, GBT82, HHK<sup>+</sup>86, Iku85, KvRS89, LS87b, NRS84, PKB88, ZD87]. **H-bonds**

[ZD87]. **halide** [GB83, GSB85]. **halides**

[CDL<sup>+</sup>87, GT83, MAR<sup>+</sup>84, Mey80a, Mey81]. **Haloalkanes** [HLG88].

**halogen** [AKRA84]. **haloperidol** [VLG89]. **Hamiltonian** [GHF87].

**Hammond** [AM88b]. **handbook** [Lip86]. **harmonic** [BTG80, BTG82].

**Hartree** [Cre82a, GTB81, Kar81, LB87, LMW85, MSG80, RFLC89, RDAF83, RPAF83, TDK83, WP83]. **HCl** [CDL<sup>+</sup>87, NRS84]. **HCN** [GT84].

**head** [VU83]. **head-to-head** [VU83]. **heats** [Cre82b, HSW82, SAF88].

**Hehre** [Wib86]. **HeLi** [MTN87]. **helical** [AVBF84, VU84]. **helices** [Sch88].

**Helix** [VU83]. **hemoglobin** [Che89]. **hemoglobin-fragment** [Che89].

**Hertfordshire** [Jur88]. **Hessian** [WG87]. **hetero** [DVA83, LHC84].

**hetero-Diels** [LHC84]. **heterocycles** [Hil80a, Hil80b]. **heterographs**

[Bal88]. **hexachloride** [DHP83]. **hexamethylbenzene** [Iro80]. **HF**

[CDL<sup>+</sup>87, LS87a, Ada89, KvRS89, Lop89, NRS84, ST87]. **Hg**

[SMKH87a, SMKH87b]. **hidden** [MK84b]. **hierarchically**

[BMB85a, BMB85b, MBB84, MBB85, RKM<sup>+</sup>85]. **high** [DK84, DK85].

**higher** [KSI88, ZP89]. **Highly** [DK85, RDW88, DK84]. **Hill** [CPV84].

**histamine** [Top87]. **HNC** [GT84]. **HOC**

[BMB85a, BMB85b, MBB84, MBB85, RKM<sup>+</sup>85]. **hole** [KKR<sup>+</sup>82].

**homoaromaticity** [WB80]. **HONDO** [ČHS84]. **HOO** [DS80]. **HOR'** [JI81].

**HOS** [DS80]. **HSO** [DS80]. **HSS** [DS80]. **Hückel** [Kin87]. **Hwan** [Ano88c].

**HXCHY** [PMZ86]. **hybrid** [Lau88]. **hydrated** [GB83]. **Hydration**

[GLOB88, KC87, BP81, BTRT88, Del81d, JMB87, KS82]. **hydrazide**

[HH80]. **hydrides** [BE87, CPTC84, Del89, KKR<sup>+</sup>82]. **hydrocarbon**

[CS82, SSSA82]. **hydrocarbon-chain** [CS82]. **hydrocarbons**

[ASS<sup>+</sup>85, BKKB80, Bro83, BCC87, CW80, CZ88, HRKW89, HAKW87,

IFvRSS87, KSJT83, Mey84, Sau89, VSS82]. **Hydrogen**



[AKI88, Aid88, BTG81a, BG81b, BG81a, BG82b, BG82c, CDL<sup>+</sup>87, Del81b, Del81c, Del81d, Del81e, Del83, Del87, Gol87, Iku84, KvRS89, KSL87, LSROT80, LLC85, LLSC85, LD87, TMOW85, WM87]. **hydrogen-bonded** [Aid88, LSROT80]. **hydrogen-hydrogen** [WM87]. **hydrogenation** [IFvRSS87, SAF88]. **hydrolysis** [KJ85, LKL87]. **hydrophobic** [GPC88, Lew89, KS82]. **Hydrophobicity** [GC86]. **hydroxyacrolein** [BTG81b, GBT80]. **hydroxyl** [EWM85]. **hydroxypyridine** [LV82]. **Hydroxyuracil** [Zie83]. **Hylleraas** [LCC87]. **hyperchaos** [RH87]. **hyperpolarizabilities** [FBBA86]. **hypersurfaces** [BSSW88, KSHD88].

**I/O** [HD88]. **icosahedral** [Kin87]. **identification** [BKKB80, KSJT83]. **iduronate** [RFP86]. **II** [KJ85, BHR<sup>+</sup>86, BT80a, BkBT82, CMR89, Cla82, Cre82b, CE87, De 86b, Dil87, FB89, FSST82, HB82, Hil80a, Jaf88, Kel80b, KM85, Koz87, LS89b, LSROT80, LDP80, MFG89b, MK85b, MSSS80, MBB85, MH83, RAS85, RPAF83, SMKH87b, Ste89b, VU84]. **iii** [BHR<sup>+</sup>86, AH85, BMB85b, CCSvRS83, Cla83, GPC88, Kel82, LS89c, MSS82, Mey80a, Mey86, NN87, SBS82, TH80]. **Ile** [CP81]. **Illman** [Kro88]. **illustrated** [FBKK85]. **imidazole** [EWM85]. **imine** [PKB88]. **imines** [HHR87]. **imino** [Del84]. **Implementation** [ABE<sup>+</sup>85, RD87, RKM<sup>+</sup>85, vdGB84]. **implications** [JG89, WG89, FWS89, FS89]. **importance** [CT87, LS89c, MR80]. **importance-sampling** [LS89c]. **important** [YJ86]. **imposition** [HT82]. **Improved** [HD88, Pul82, RLR89, DR86, LWD82, Sch82a, PASTB87]. **Improvement** [Gol87]. **Improvements** [HA89]. **Improving** [LMV86, Kar81, Mit88]. **INA** [Ran86]. **including** [BTG85, BTG86, BCT83]. **inclusion** [KJ87, Wen82]. **independent** [FBBA86]. **index** [CRR85]. **indexes** [TKI89]. **indices** [MBB84, Mil87, RRG<sup>+</sup>84, Rou87]. **INDO** [BG80, CW80, DS80]. **INDO-type** [BG80]. **inductive** [BCT83]. **infinitely** [HAKW87]. **influence** [BTG81a, BC89]. **information** [BMT81, Jur88, RRG<sup>+</sup>84]. **infrared** [WW81]. **Ingold** [Mey80b]. **inhibitor** [Fuj87]. **inhibitors** [Gre85]. **inhomogeneous** [ZR81]. **Initial** [FSL84]. **Initio** [OG86, PUNC86, Wib86, Aid88, ADY89, ABP80, ASS<sup>+</sup>85, AFK82, AVBF84, BT81, BMLR88, BR89, BP81, BG86, BTG80, BTG81b, BTG81a, BTG82, BTS<sup>+</sup>83, BPP82, BN85, BCT83, BTRT88, Bre81, BSM83, Bur80a, Cao89, CvRS81, Cre82a, Cre82b, CE87, DM86a, Del81a, Del89, DTPR85, EWM85, FKS85, GBT80, GBT82, GDO89, GT82, GT83, GT84, GHT87, GL87, GL88, GL89, HW82, HR85, HR87, HRKW89, HE85, HSS83, HSEČ83, HT88, HE88, IvRS85, Iku84, JI81, JFG89, KS84, Kar81, KB84a, KB84b, KHRvH87, KvRS89, KSS83, KPE<sup>+</sup>84, KVV<sup>+</sup>84, KSB84, KSL87, Koz87, LSROT80, LCY82, LH87, MC88, MFG89c, MFG89a, MV87, MTN87, MH83, MSČ<sup>+</sup>88, OLBM83, PKB88, PHG89, PUC89, STH81b, SS81, SSSA82, SVS<sup>+</sup>81, SKV<sup>+</sup>85, vRS86, SAP88, SAF88, SKE<sup>+</sup>84, SK86, Str85]. **initio** [TG83, Top87, VSS82, Van88, Wib84, WSP88, ZPCR82, ZPPC83, ZD87]. **Inn** [Ano83a]. **Innate** [KR87]. **inner** [TKK<sup>+</sup>81]. **inner-shell** [TKK<sup>+</sup>81].

**inorganic** [DH86, DH87a, DH87b, DH88, PH83]. **instabilities** [LB87].  
**instability** [RRI88]. **Institute** [Ano86j]. **instruction** [Tri84]. **Integral**  
 [HD88, ČHS84, Kar81, Van88, Koz87]. **Integrals**  
 [KO86, DS87, FVV85, KF88, LCC87, PW82, RLR88, RLR89, RDK83, SL81].  
**Integrated** [CS80]. **integration** [Gla89, SL81]. **intensities**  
 [HE88, SBS82, WW81]. **Interaction** [De 86a, De 86b, SOR86a, SOR86b,  
 SORT86, SOR87, SLR<sup>+</sup>86, Ada89, BT80b, BTS<sup>+</sup>83, Bre81, CF83, EW87,  
 Gre83, KTVRS86, KPRT81, LV82, LD87, MV87, PASTB87, SHK83, Wen82].  
**Interactions**  
 [MKS87, MK84b, BT80a, BT80b, Fra82, GPC88, GRS88, HLG88, KMS85,  
 LS87a, LS87b, LCY82, PL87, PR80, SRKT87, SK85, WK81, WM87, HPR80].  
**interactive** [AP85, Kar86, Ved88]. **intercalation** [SLB83]. **interconversion**  
 [Ham87]. **interconversions** [BA82]. **interest** [Gol87]. **interface** [BFAG81].  
**Intermediate** [KYJ88, GHF87, Sie85]. **intermediates** [HMA82].  
**Intermolecular**  
 [SLR<sup>+</sup>86, BKC86, BG82c, DT88, Dyk88, Gen87, GRS88, SHK83].  
**internal** [CU89, Hin80, KJ82, LS88, Ran83]. **International** [Ano86i].  
**interpolation** [Sil89]. **interpretation** [Gre84]. **Interscience** [Tri82].  
**intersections** [LR87]. **intrachain** [OTPH87]. **Intramolecular**  
 [BTS<sup>+</sup>83, BTG81a, KMS85]. **introduced** [TSH81a]. **Introduction**  
 [Coo80, Mez87a, Gar82a, Tri82]. **invariant** [KTVRS86]. **invariants**  
 [OMK<sup>+</sup>88]. **inverse** [Häs87]. **inversion** [ADY89, Ōsa82, SF85].  
**investigation** [AP85, FKS85, GTB81, GHT87, Sie85]. **Investigations**  
 [FKS86, BT80a, BT80b, GS85, RRH86, SKE<sup>+</sup>84]. **involved** [BTRT88].  
**involving** [BHR<sup>+</sup>86, EGM<sup>+</sup>89, KvRS89, KSL87, ST80, Sil81, ZP84]. **iodine**  
 [DHS84]. **ion**  
 [Del86, Del87, EW87, Ehr89, GBT82, KKR<sup>+</sup>82, MK85b, NRS84]. **ion-fitted**  
 [NRS84]. **ionic** [BG80]. **ionization** [GT83, Gre85, KKR<sup>+</sup>82, TKK<sup>+</sup>81].  
**ionophore** [MK84a]. **ions** [Bai84, CE87, Iku84, Kel80b, KS83]. **IR** [SBS82].  
**Ishtar** [AP85]. **iso** [Rit86]. **iso-butylene** [Rit86]. **isocyanate** [LLC85].  
**isoelectronic** [KPRT81, PMZ86]. **isoelectronically** [Kel80b, Kel82].  
**Isomer** [BMT81, Häs87]. **Isomeric** [KvRS80, DPCS80, RRG<sup>+</sup>84].  
**isomerizations** [Kel80b]. **isomers**  
 [CvRSKJ81, DHP83, GDO89, GHT87, HT88, Kel80b, KMS85, SKJ88, TG83].  
**isomorphisms** [STZ88]. **isopotential** [NSGK<sup>+</sup>81]. **isopropyl**  
 [HML83, KSB84, LH85]. **Isotope** [AF83, HLH83]. **isotropic** [LPB84].  
**Iterative** [Gal82, Per84]. **IV**  
 [BT81, AS88, BT80b, KKR<sup>+</sup>82, TDK83, TSH81a]. **IX**  
 [MK84b, ROK86, Tat85].  
**J** [Ano88c, EGM<sup>+</sup>89, Jor81, Lil87, Ran86, Sch86, Wib86]. **Jahn** [LR87].  
**James** [Car85, Tri82]. **John** [Boy86, Cra85, Lip86, Wib86]. **Jones** [DK88].  
**Jorgensen** [BG82c]. **Journal** [Ano86b]. **June** [Ano86j].

**Kern** [GTB81]. **Ki** [Ano88c]. **Ki-Hwan** [Ano88c]. **Kim** [Ano88c]. **kinetic** [TS83, Tri87]. **kinetics** [KBS88, ZR81]. **king** [BR85]. **Kirkwood** [BC83]. **Knop** [Ran86]. **knowledge** [Wen82]. **Koopmans** [BG82a, GT83]. **Kowalski** [Kro88].

**L** [Kro88, Lip83b, Lip83a, Str85, Wib86]. **laboratory** [Coo77, Car85]. **Lagrange** [Dil87, vdGB84]. **language** [KBS88]. **Laplace** [SF85]. **large** [Bro83, CG86a, Gal82, HB82, HG89, HAKW87, Kar81, LM89, Mul88a, Mul88b, PR87, Ran82, Van88, YNAK88]. **large-molecule** [HB82]. **lattice** [AP85]. **lattices** [BR85, RB85]. **layer** [BFAG81]. **LCAO** [ARS85, FA86, RAS85]. **LCAO-LSD** [ARS85, RAS85]. **least** [Lau88, LV88, SAS87]. **least-squares** [Lau88, LV88, SAS87]. **length** [BTG81a, BTG82, Gre84, KPE<sup>+</sup>84]. **lengths** [HRKW89]. **Lennard** [DK88]. **Lennard-Jones** [DK88]. **Letchworth** [Jur88]. **Letter** [DMB88]. **Leu** [CP81]. **level** [CG89, Mit88, VLG89]. **levels** [DK84, DK85, DK88]. **Li** [MFG89c, MV87, CCSvRS83, DD81, Kal87, KT88, TH80, Tat85]. **librational** [Lin88, VU84]. **LICAO** [AFK82]. **lifetime** [PD83]. **ligand** [FM87, GC85, KCF84]. **ligands** [KM85]. **light** [CPTC84]. **like** [PR87]. **Lilly** [Ano88c]. **limit** [Cre82a, GTB81, SK84b]. **limited** [AS81]. **Linear** [HB87, BKT82, CMR88, FWS89, HT82, WP83]. **Linearized** [Cri89, DM89]. **lines** [MK84b]. **linked** [VM86]. **liquids** [Boy86]. **list** [YE89]. **literature** [vRS86]. **Lithium** [vRSSRH86, BE87, Cha83, Del86, FBKK85, HL83, KTvRS86, KvRS89]. **lithium-hydrogen** [KvRS89]. **Little** [Sch86]. **lobe** [NRS84, ST82]. **Localized** [Hil80a, KM85, TW82, PS87, SDL82]. **Locally** [CM89]. **Location** [De 86a, De 86b, Bak86, BG88]. **log** [Bra89]. **log-derivative** [Bra89]. **Logic** [Cra85]. **lone** [KKR<sup>+</sup>82, LWD82, WM89]. **lone-pair** [WM89]. **Long** [EGM<sup>+</sup>89, FWS89, SSSA82]. **long-chain** [SSSA82]. **Long-Range** [EGM<sup>+</sup>89]. **loops** [KNS86, KNS89]. **Low** [FOSV86]. **Low-Lying** [FOSV86]. **lowest** [SM80]. **LSD** [ARS85, RAS85]. **lumiflavin** [SMOT85]. **Lying** [FOSV86]. **Lykos** [Gar82b].

**M** [Kro88, Wer82]. **machine** [BFF86]. **macrocyclic** [FSL84]. **macromolecular** [BBO<sup>+</sup>83, LV88, PV82a, vGBC<sup>+</sup>84, Lil87]. **Macromolecules** [De 86a, De 86b, GM86, BK86, Kar86, Kar87, VK80]. **Madelung** [Tay87]. **magnesium** [JI88]. **Main** [SLR<sup>+</sup>86, BE87, DH86, SGW83]. **main-group** [DH86]. **major** [BFF86, TMrGM88]. **maleic** [HH80]. **malformin** [HLPT82]. **maneuver** [Kar86]. **manipulating** [vdGB84]. **manipulation** [FE87]. **many** [BG82a, BMLR88]. **many-body** [BG82a, BMLR88]. **Mapping** [Ano88c, Kel80a, Kel80b, Kel82, SDKM87]. **maps** [NSGK<sup>+</sup>81]. **March** [Ano83a]. **Martin** [Ano88c]. **master** [GF87]. **Masthead** [Ano80a, Ano80b, Ano80c, Ano80d, Ano81a, Ano81b, Ano81c, Ano81d, Ano82b, Ano82c, Ano82d, Ano82e, Ano83b, Ano83c, Ano83d, Ano83e,

Ano84b, Ano84c, Ano84d, Ano84e, Ano84f, Ano84g, Ano85c, Ano85d, Ano85e, Ano85f, Ano85g, Ano85h, Ano86c, Ano86d, Ano86e, Ano86f, Ano86g, Ano86h, Ano87e, Ano87f, Ano87g, Ano87h, Ano87i, Ano87j, Ano87k, Ano88d, Ano88e, Ano88f, Ano88g, Ano88h, Ano88i, Ano88j, Ano88k, Ano89d, Ano89e, Ano89f, Ano89g, Ano89h, Ano89i, Ano89j]. **matching** [HO83, HB89, RB85, RHP89]. **Mathematical** [Ano86j, MBB85]. **mathematics** [SK84b]. **matrices** [LMV86, LM89]. **Matrix** [DbCV<sup>+</sup>86, KHS86, BR87, BP87b, Ber83, Bra89, BC87, Cao89, Cri89, Dil87, Gal82, KDEHK89, LM89, MSG80, MHA89, MSKT87, PKD88, SDL82]. **matrix-vector** [LM89]. **MAXI** [Tat85]. **MAXI-1** [Tat85]. **MAXI-5** [Tat85]. **MC** [Rap84, SKJ88, SK89]. **MCD** [KJ85]. **MCSCF** [Tay84, YNAK88]. **means** [DA83, Fuj87, SMOT85, VFM<sup>+</sup>89]. **Measure** [GC86]. **mechanical** [Bur82, EW87, FGR89, Mey84, MF85, SK86, Tos84]. **Mechanics** [Dil86, IL86, SJ86, AGL82, AH84, AH85, AG88b, AS88, AG88a, AF83, AL87, BR85, BMG84, BW83, Bur80b, Bys83, CMR88, CMR89, DAU88, DHP83, Dil87, FGR89, FWB85, GS87b, GHHS85, GL88, GL89, HLG88, HB82, HP84b, IÖ84, JT80, Kar87, LGB<sup>+</sup>89, LA85, LTLA87, MK84a, MK85b, Mey80a, Mey81, Mey86, Mey88, MM89, NLA84, OE89, PL87, PR87, SHDP89, SRPY88, SA80, TLA89, TMrGM88, Tri88, VDD86, Ved88, VCZB89, vdGB84, Lip83a]. **mechanics-NMR** [SRPY88]. **mechanism** [BTRT88, BKT82, DLMR85, Ham87, HSS83, Rue87, ZPPC83]. **Mechanisms** [Ösa82, KvRS89]. **mediated** [DVA83, ZPPC83]. **medium** [FWS89, SMOT85]. **medium-size** [SMOT85]. **Meeting** [Ano89j]. **membered** [ADY89, AYS80, DA83, DVA83, DPSF<sup>+</sup>88, Ham87, Hil80a, Hil80b, TSH81a]. **memory** [BD82]. **Menschutkin** [VSSS84]. **Metabolic** [TG86]. **metabolism** [BTRT88]. **metacyclophanes** [JdKdWB87]. **Metal** [NR80, BG80, BG82a, FB89, KM85, MS88, SMKH87a, SMKH87b, TSH81b, VDD86]. **metallation** [KvRS89]. **metalloproteins** [VDD86]. **metals** [DH87a, DH87b, PH83, DH88]. **metathesis** [GHHS85]. **methane** [Gil84, KS82]. **methanes** [PR80]. **methanimine** [PKB88]. **methanol** [BG81b, BG82b, BG82c, Iku84, JI81]. **Method** [KHS86, KO86, SJ86, AS88, Ada89, BD82, BFF86, BHW87, BC83, BA82, CP87a, CG86a, Dar89, Dil87, DCG81, FGR89, FBBA86, HA89, HLH83, JBFR86, Kal87, KT88, KSI88, KI81, KNS85, KDEHK89, LCC87, Lew89, LWD82, Mit88, MS88, Mul88a, Mul88b, OMK<sup>+</sup>88, PW81, PR87, RDK83, SI88, Sch82a, SO87, SAS87, Sil85, SK86, SMF89, STYA87, SS84, Szö87, TDK83, TTZWGQKC81, VK80, VVVG81, WMHJ88, vdGB84, ARS85, Bai86, GSH88, SDB87, Ste89a]. **Methods** [CP89b, BS89, BP82, Bra89, Bur82, BKL87, DM89, DS80, FBBA86, GCW88, HTT88, HT88, HW88, Jor81, Kin87, Lau88, MV87, MR83, RB87, SPBO87, Ste89a, Ste89b, Top87]. **methyl** [Bur80a, EGM<sup>+</sup>89, FS83, Gil84, GT82, GT83, Has84, Iro80, KSS83, KPE<sup>+</sup>84, LKL87, LA85, OE89, SVS<sup>+</sup>81, SCCvRS82, MAR<sup>+</sup>84]. **methy-** [OE89].

**methyl-and** [FS83]. **methyl-CH** [KPE<sup>+</sup>84]. **methylamine** [BG82b]. **methylbutanoate** [SKV<sup>+</sup>85]. **Methylcyclohexyl** [VMNGTVM86]. **Methylene** [FOSV86, BW81]. **methylhistamine** [Top87]. **methyloxiranes** [DPCS80]. **methylphenylalaninamide** [KYJ88]. **methylpropanoic** [SKE<sup>+</sup>84]. **methylpyrazole** [CSCD<sup>+</sup>89]. **metric** [Cri89]. **Metropolis** [KS82]. **Microcomputer** [Tri84, Sch86]. **Microcomputer-aided** [Tri84]. **Microscopic** [Kim85]. **MIDI** [STH82, TSH81b]. **MIDI-1** [STH82]. **MIDI-3** [TSH81b]. **MIDI-4** [TSH81b]. **mimics** [VCZB89]. **MINDO** [BSSW88, CZ88, HHK<sup>+</sup>86, HSW82, LHC84, MSSS80, MSS82, Top87, VVVG81, VMNGTVM86, VFM<sup>+</sup>89]. **MINDO/3** [BSSW88, CZ88, HHK<sup>+</sup>86, Top87, VMNGTVM86, VFM<sup>+</sup>89]. **MINI** [STH82, TSH81b]. **MINI-1** [STH82]. **MINI-3** [TSH81b]. **MINI-4** [TSH81b]. **minicomputer** [Coo77, Car85]. **minicomputers** [See81]. **Minimal** [TKK<sup>+</sup>81, RPD<sup>+</sup>86]. **minimization** [BHW87, BBO<sup>+</sup>83, BK86, Dil87, GS87a, Ham87, LS89c, MK84a, NK86, PLFL85, PR87, RDAF83, RPAF83, SO87, TMrGM88, VK80, WMHJ88]. **minimum** [LS88, ZW84]. **mixed** [BG82b]. **MM** [AF83, WP82]. **MM2** [HLG88, LGB<sup>+</sup>89, TLA89, AP87, AKI88, CUCP89, GCW88, PL87, PUNC86, PUC89]. **MM2/MMP2** [PL87]. **MM3** [AL87]. **MMP2** [OE89, STYA87]. **MNDO** [Bai84, BF82, BSSW88, DGW<sup>+</sup>81, DM83, DR83, DH83, DFC<sup>+</sup>84, DHS84, DR86, FS83, FS89, GBP85, GRS88, GHT87, Gol87, HHK<sup>+</sup>86, JdKdWB87, OUV84, Top87, Ver82, VSSS84, VFM<sup>+</sup>89]. **MNDOC** [CT87]. **MO** [AFK82, BT81, EWM85, GDO89, HTT88, Iku84, Jaf88, LSROT80, LCL84, RBEV80, Gro87, NR80]. **Mo-Cd** [Gro87]. **mode** [HLH83]. **Model** [AS81, De 86b, KW86, SMKH87a, SMKH87b, AM88a, CW81, FT89, HHR87, Kel80a, Klo83, LP88, LR87, MS88, OLBM83, PR80, SLB83, WK81].

**modeling** [EW87, Lil87, LS88, LYH87, OTPH87, Rou87, TMOW85, WK81, GPC88].

**models** [BR89, BC89, Boy86, Cri87, EM84, Ehr84, Fra87, KvRS89, PHG89, STZ88, Wil88, Rue87]. **modes** [BC89, GC85, Gor88, WM89]. **modification** [Sil81]. **Modifications** [ST89]. **Modified** [CZ88, CP80, FBKK85, LWD82].

**modular** [Sch88]. **MOL** [Lew87]. **molar** [Lew89]. **Molecular** [BMG84, BW83, BP81, Bys83, Cao89, CMR88, CMR89, Del81b, Del81c, Del81d, Del81e, Del83, Dil86, DH86, DH87a, DH87b, Ehr86, FGR89, FM87, GS87b, GHHS85, GL88, Hil80b, HP84b, IL86, Kar87, KMS85, KO86, LRP87, Lew87, LGB<sup>+</sup>89, MAR<sup>+</sup>84, Mey80a, Mey81, Mey86, Mey88, NF84, OTPH87, PH83, SJ86, Sim87, SLC86, SF86, TDK83, Wib86, AGL82, AH84, AH85, AG88b, AS88, AG88a, Aid88, ADY89, AF83, AL87, AKRA84, ASFW89, AM88a, AJMM88, BNR86, BMB85b, BG87, BR87, BD82, BGT84, BCT83, BSSW88, Bur80b, CRR85, CHS84, CW81, Cri89, DAU88, DE83, DHP83, Del89, Dil87, EM84, Ess83, FSL84, FS89, Fra82, FBBA86, Fuj87, GTB81, Gor88, GCW88, HR85, HR87, HRKW89, HH80, HS82, HP84a, HLG88, HLC88, HB87, Hil80a].

**molecular** [IÖ84, Jaf88, JT80, JBFR86, KS84, KM85, KVV<sup>+</sup>84, KSB84, LCC87, LS87a, LS87b, LMV86, LA85, LTLA87, LZ89, LBZ89, LS88, MK84a,

MK85b, Mey84, MF85, MH83, Mez87b, MM83, MSKT87, MM89, NSKNK87, NKC85, NLA84, OE89, OTW81, PL87, PR87, RRI88, SMKH87a, SMKH87b, SHDP89, SMOT85, SRPY88, SVS<sup>+</sup>81, SK86, SN87, SA80, STZ88, SDB87, Str85, TLA89, TKI89, TJ86, TM85, TMrGM88, TW82, VSS82, VVVG81, VDD86, Ved88, VCZB89, WP83, Wil88, ZM88, ZW83a, ZW84, vdGB84, DH88, FWB85, GL89, KKR<sup>+</sup>82, LCL84, SKV<sup>+</sup>85, Ska83, YE89, Lip83a]. **molecular-mechanical** [MF85]. **molecule** [ACvRS81, Ber83, BFF86, DAU88, DTPR85, GC85, HB82, Iku84, KDKC83, Lin88, TW81, Ved88]. **Molecules** [Ano88c, De 86a, De 86b, ASS<sup>+</sup>85, AL87, Bai84, Bal83, BFAG81, BP82, BkBT82, BG86, BTG82, BW89, Bre81, BG82c, CvRS81, CS80, CG86a, DM86a, DM83, DR83, DH83, DHS84, DHK89, Dod84, Fab88, GSH88, Gla89, GSB85, HG89, JB85, KT88, Kar81, Kel80b, Kel82, Koz87, Lew87, LR87, Lip87, LH87, Mag84, MFG89c, MTN87, MAR<sup>+</sup>84, Mey86, Mey88, MKSW83, MK84b, Mul88a, Mul88b, PR84, PR87, Ran82, STH81b, SDKM87, SK84a, TKK<sup>+</sup>81, Van88, Ver82, WK81, ZP89, Ran86]. **Møller** [WD88]. **MOM** [ZW83a, ZW84]. **moments** [Bau84, GF87, HE88]. **MOMM** [BKL87]. **mono** [PR80]. **mono-** [PR80]. **monocenter** [FVV85]. **monohydrate** [OC88]. **monomethylammonium** [Gre83]. **monopole** [LZP84, ZP85]. **monoprotonated** [EWM85]. **monosubstituted** [Del81a, VFM<sup>+</sup>89, BTG81a]. **monotone** [Per84]. **Monte** [Che89, Gar89, GLOB88, JMB87, KS82, MC88, OC88, RMB86, RPV87, ZR81]. **Morse** [DbCV<sup>+</sup>86]. **Motion** [SLC86, KJ87]. **MP** [ČHS84, SMKH87a, SMKH87b]. **MP2** [MV87]. **MRD** [KHRvH87]. **MRDCI** [RV85]. **MSX** [KT88]. **MT** [KT88]. **MT-MSX** [KT88]. **Muller** [Ran86]. **Multicollinearity** [SNR83]. **multiconfigurational** [RPD<sup>+</sup>86]. **multidimensional** [LDL<sup>+</sup>88]. **multiexponential** [SS84]. **multiphoton** [BG87]. **Multiple** [RFLC89, LS88, MSG80]. **multiplication** [BC87, LM89]. **multiplicative** [Van88]. **multiplier** [Dil87, vdGB84]. **multiply** [CBR87]. **multipole** [PHG89, Wil88]. **multireference** [Ada89, CP87a, FBKK85]. **MuMATH** [Tri87, Tri88]. **mutagenesis** [Tin81]. **mutagenicity** [KR88]. **myelin** [GS87b].

**N** [Del89, GHT87, LB87, Ran86, TKK<sup>+</sup>81, TG83, BTG82, BTS<sup>+</sup>83, BGT84, CvRS81, HHK<sup>+</sup>86, Iku85, KT88, Kao88, KYJ88, TW81]. **Na-Cl** [SCvRSH87]. **NaBH** [BMLR88]. **naming** [Cio87]. **naphthalene** [DHP83, HW82]. **nature** [OTW81, WW81]. **NCN** [ASFW89]. **NCN-containing** [ASFW89]. **NCOCH** [FS82]. **NDDO** [ZW83a, ZW84]. **near** [BFF86]. **NeI** [DBVMB84]. **neighbor** [SLB83]. **neighbors** [YE89, vGBC<sup>+</sup>84]. **net** [CW81]. **networks** [HAKW87]. **neuromuscular** [SHDP89]. **neurotensin** [CP81]. **neutral** [BFAG81, DAU88, DM86a, Del89, FS83, SK85, ZPPC82, ZPCR82]. **neutrals** [HPR80]. **Newton** [Dil87, PR87, SO87]. **Newton-like** [PR87]. **NG** [ZW83a]. **NH** [Del87, HPR80, LS87b, PMZ86, TMOW85, Ada89, BHR<sup>+</sup>86, Del89, KvrS89, KPRT81, NRS84]. **NHF** [LS87b]. **NHOH** [LS87b]. **Ni** [RAS85]. **nitric** [LSROT80, Sie85]. **nitrobenzene** [KHRvH87]. **Nitrogen**

[ADY89, Del85, Del86, FS83, JH83, LB87, MSS82, RS85]. **nitrophenols** [NVGB81]. **nitrosamine** [HSS83]. **nitrosamines** [BTRT88]. **nitrosation** [RRH86]. **nitrosomethanol** [HT88]. **NMR** [BBJ88, SRPY88, TMrGM88]. **NMR-derived** [TMrGM88]. **NO** [FS82, CE87, Sie85]. **Noggle** [Sch86]. **non** [Dil87]. **non-full-matrix** [Dil87]. **nonan** [Osa82]. **nonan-9-one** [Osa82]. **nonane** [SSSA82]. **Nonbonded** [WM87, LCY82]. **nonclassical** [WB80]. **nonelectrocyclic** [BCB82]. **Nonempirical** [SLR<sup>+</sup>86]. **Nonequivalence** [DVA83]. **nonfused** [KR88]. **nonlinear** [AP87, FBBA86, WP83]. **nonplanar** [KNS89, PV82b]. **Nonrelativistic** [Klo83]. **nonrigid** [Bal83]. **nonstrained** [HRKW89]. **norbornadiene** [GHHS85]. **Norbornadienyllithium** [LB86]. **normal** [CL85, HLH83, Mag84, WM89]. **normal-mode** [HLH83]. **Norman** [Lip83a]. **Norris** [Gar82a]. **notations** [HB87]. **Note** [Gor88, LA85, MSG80, Sen87]. **novel** [KR88]. **nuclear** [Bal82a, Bal82b, KJ87]. **Nucleic** [De 86a, FS89, LZP84, MKSW83, MK84b, NK86, WKNC86]. **nucleophiles** [FS89]. **nucleoside** [SOR86a, SOR86b, SORT86]. **Number** [Ano86b, FWS89, MFG89a, ZP89]. **numbering** [BMB85a]. **Numerical** [BSSW88, NN87, Gar82a, KDEHK89, Jaf88]. **numerically** [RV85]. **Numerov** [Bra89].

**O** [BG86, BTS<sup>+</sup>83, CDL89, CvRS81, CMRW86, Del89, GBT82, HPR80, LS87a, NR80, AG88a, Ada89, BTG82, BHR<sup>+</sup>86, CvRS81, CMRW86, HHK<sup>+</sup>86, HD88, KvRS89, Lop89, NRS84, PMZ86, KPE<sup>+</sup>84]. **objective** [SAS87]. **objects** [Sim87]. **obtained** [GHHS85]. **obtaining** [HO83]. **OCS** [Car82]. **octahedral** [Kin87]. **octalene** [FMST84]. **Offcenter** [Ehr86]. **OH** [Del87, FS89, TMOW85, BTG82, CP81, HPR80, KSL87]. **OHF** [LS87b]. **olefin** [GHHS85]. **olefins** [CDL<sup>+</sup>87, Mey80a, WP82]. **oligonucleotides** [Gre83]. **Olti** [Boy86]. **One** [PKD88, AM88b, GHF87, KSI88, KF88, Osa82, RLR88, RLR89, SDL82, ZW83a, ZW84]. **One-center** [PKD88]. **one-dimensional** [AM88b, KSI88]. **one-electron** [RLR88, RLR89, ZW83a, ZW84]. **ones** [DLMR85]. **Onsager** [Ehr81]. **Open** [Kal87, BD82, HHK<sup>+</sup>86, HTT88]. **open-ended** [BD82]. **Open-shell** [Kal87, HHK<sup>+</sup>86, HTT88]. **opening** [Kel82]. **Operational** [Sil85]. **Operator** [HO83]. **operators** [Jaf88, Jug84]. **opiates** [FSH<sup>+</sup>84, FK84]. **Opioid** [Fro86]. **optical** [PPV83, RP80]. **Optimization** [Bai86, Sch82b, Ste89a, Ste89b, Bak87, CG89, HR85, HR87, HL83, HHR87, KJLW84, MH83]. **optimizations** [HRKW89]. **Optimized** [LZP84, OG86, Szö87, ZP85, BSSW88, CW80, FA86, VLG89]. **orbit** [Bre81, KF88, KSJ82, PW81]. **Orbital** [Cha83, CPH85, HPH83, Kel80a, Kel80b, Kel82, LDM89, Wib86, Aid88, ADY89, BW81, Bau84, BD82, BGT84, BSSW88, Del81b, Del81c, Del81d, Del81e, Del83, Del89, DH86, DH87a, DH87b, DH88, FS89, HL83, KS84, KM85, LCL84, Lew87, PH83, PR80, STH81a, STH81b, STH82, Str85, TH80, TSH81a, TSH81b, TW82, ZD87, Kel80b, Kel82]. **orbital/bond** [ZD87].

**orbitals** [Ada89, CP80, FBKK85, FVV85, Hil80a, Jaf88, Lau88, ST82, Tat85]. **orbits** [BMB85a]. **order** [Ada89, CP87a, FBBA86, FC88, GHF87, Gre84, Jug84, KSI88, KBS88, Per84, SHK83, Tri87, WD88]. **ordered** [BMB85a, BMB85b, MBB84, MBB85, RKM<sup>+</sup>85]. **ordering** [MBB84]. **Organic** [Ano86k, Bal85, Dod84, Lip83b, LB86, Mey80a, Mey81, Mey86]. **organomagnesium** [DLMR85]. **organometallic** [DH86, DH87a, DH87b, DH88, PH83]. **organosilicon** [GL88, GL89]. **orientational** [BCT83]. **oriented** [SAS87]. **originals** [CP89a]. **origins** [BW81]. **ortho** [MFG89a]. **ortho-substituted** [MFG89a]. **orthonormal** [Lau88]. **oscillator** [DbCV<sup>+</sup>86, SK84b]. **oscillatory** [SL81]. **other** [BL88, Lew87]. **out-of-plane** [BN85, LTLA87]. **overall** [ZW83b]. **overcrowded** [FSST82]. **overlap** [DS87, Gal82]. **Oxford** [Str85]. **oxidation** [Sie85]. **oxide** [Sie85, SBS82, SMG87]. **oxides** [BT81]. **oxime** [VV88]. **oximes** [HHR87]. **oxirane** [FS89]. **oxyacids** [BT81]. **oxyanions** [BT81]. **oxygen** [ASS<sup>+</sup>85, CF83, Del85, Del86, FS83, MSS82, RS85]. **oxygenated** [BS89]. **ozone** [KvRS80, LH87].

**P** [Ano86b, Del89, DCNG85, Wib86, DCNG85, ROK86, TKK<sup>+</sup>81]. **p-Tolylsulfonyl-Sulfilimine** [TKK<sup>+</sup>81]. **package** [NSKNK87]. **packing** [HH80, HS82]. **pages** [Lip83a]. **pair** [BG82c, SMOT85, WM89]. **pairs** [Aid88, DCG81, KKR<sup>+</sup>82, LWD82, SRKT87]. **Palm** [Ano83a]. **pancreatic** [FM87, Fuj87]. **Parallel** [See81, WD88, GDP<sup>+</sup>85, NKC85, RDW88]. **parameter** [Lew89]. **parameterization** [GG89, HP84b]. **Parameters** [GC86, BFAG81, BTG85, BTG86, CUCP89, DR86, Ess83, GPC88, GL88, GL89, LMW85, NF84, SF86, Ste89a, Ste89b]. **parametric** [Ösa82]. **Parametrization** [CMR88]. **parent** [MFG89b]. **Part** [ARS85, RAS85]. **partial** [HLG88]. **partition** [KI81, KNS85, GC86]. **PASCAL** [Tri82, Co080]. **path** [BCB82, CF83]. **paths** [BG88, FBD80]. **pathway** [KHRvH87]. **pathways** [VSS84]. **Pattern** [LS89a, LS89b, LS89c, OMK<sup>+</sup>88]. **Paul** [Boy86]. **PCILO** [BP82, LWD82]. **PDP** [Coo77]. **PDP-11** [Coo77]. **1** [Ran86]. **2** [DS80]. **3** [HSW82, LHC84, MSS80, MSS82, VVVG81]. **5** [Tat85]. **6** [Tat85]. **7** [Tat85]. **bond-orbital** [ZD87]. **BW** [TW82]. **CI** [ZBR80]. **force** [MR83]. **Isocyanide** [vRSSRH86]. **MMP2** [PL87]. **topology-allowed** [BW81]. **penetration** [PW82]. **pentapeptide** [CP81, YJ86]. **pentenone** [ST80]. **PEOE** [HLG88]. **peptide** [OLBM83]. **peptides** [AH85, LGB<sup>+</sup>89]. **perception** [Mat88]. **percolation** [Fra87]. **performance** [Mag84, SCvRSH87]. **performic** [BTG81b]. **pericyclic** [BW81]. **periodic** [Bal85, NLB85, SL81]. **permeable** [Per84]. **permethylcyclohexane** [EIO85]. **peroxides** [CMR88, CMR89]. **perpendicular** [HR85, HR87]. **personal** [Gil87, Gar82b]. **perspective** [GDP<sup>+</sup>85]. **PERTURB** [FE87]. **perturbation** [CP87a, FE87, FBBA86, FC88, RV85, WP83]. **perturbed** [TDK83]. **Peter** [Gar82b]. **Ph** [FS89]. **pharmacological** [FSH<sup>+</sup>84]. **phase** [FS82, LCL84, LLC85, LDP<sup>+</sup>87, LDL<sup>+</sup>88, RRH86, Sen87, SK86, VVVG81, VFM<sup>+</sup>89]. **phellandrene** [PPV83, RP80]. **phenomena** [Rou87]. **phenyl**



[PL87]. **phenyl-phenyl** [PL87]. **Phenylpiperidine** [Fro86].  
**Phenylpyrrolidine** [Fro86]. **phosphaalkenes** [Bac89]. **phosphaalkynes**  
[Bac89]. **phosphate** [LDP80]. **phosphine** [SMG87]. **phosphines**  
[Bac89, GT82, GT83]. **phospholipid** [KC87]. **phosphorus**  
[JS88, Mag84, Cla83]. **photography** [HPH83]. **physical** [KMS<sup>+</sup>87, Sch86].  
**Physicochemical** [GC86, GPC88]. **Pictorial** [GDP<sup>+</sup>85]. **Pitfalls** [BA82].  
**pithomycolide** [HPW82]. **Planar**  
[PV82b, BTG82, GBT80, GBT82, HR85, HR87]. **plane** [BN85, LTLA87].  
**planes** [GDP<sup>+</sup>85]. **Plenum** [Jor81]. **Plesset** [WD88]. **Point**  
[KW86, PHG89]. **points** [BG88, BE87, KSHD88, Lop89]. **Poisson** [DM89].  
**Polar** [De 86a, De 86b]. **polarizabilities** [Lew89]. **polarizability** [BC83].  
**Polarization** [LD87, BTG85, BTG86, GL87, MFG89c, MFG89b]. **polarized**  
[BP81, LMW85]. **Polyatomic** [HE85, Bre81, MAR<sup>+</sup>84]. **polycyclic**  
[HAKW87]. **polyenes** [ZBR80]. **polyethers** [SK86]. **polyethylene** [KB84a].  
**polyhex** [HO83]. **Polyhexes** [KMST86, Cio87]. **polymer** [Lip87]. **polymers**  
[AVF84, AVBF84, Bal85, BKL87, KB84a, KB84b, OTPH87]. **polymethylene**  
[LCY82]. **polyminals** [RB85]. **polynomial** [HAKW87, Ran82, RHP89].  
**polynomials** [Bal84, BR85, Bal85, Bal88, EB87, HO83, HB89]. **polynuclear**  
[Bro83]. **polynucleotide** [Sch88]. **polyoxyethylene** [BMG84].  
**Polyoxymethylene** [KB84b]. **Polypentapeptide** [CU89]. **polypeptide**  
[BHW87, BBJ88]. **polypeptides** [BR89, HP84a, ZP85]. **Polypyrene**  
[KHS86]. **Pople** [Wib86]. **population** [BS89]. **populations** [CS80, Gla89].  
**porcine** [FM87, Fuj87]. **porphyrin** [HS82]. **portion** [LPB84]. **positive**  
[Del87]. **possessing** [GHF87]. **possibility** [Kar81]. **Possible**  
[Ano86b, BFB85, Sie85]. **postulate** [AM88b]. **potent** [SHDP89]. **Potential**  
[GSB85, PUNC86, YF86, ABP80, AP80, BP81, BG81b, BG81a, BG82b,  
Bur80a, Car82, CDL89, CW81, DK88, EM84, FKS85, GSH88, Has84, HHR87,  
KB84a, KSHD88, Klo83, KSB85, KJ87, LDP80, LPB84, Lin88, LDL<sup>+</sup>88,  
Lop89, Mar87, MC88, MS88, MR83, PHG89, SMOT85, SPBO87, SO87,  
Sch88, ST80, VDD86, VSS84, Wil88, WSP88, ZM88]. **Potentials**  
[SLR<sup>+</sup>86, BKC86, BG82c, CF87, DTPR85, DbCV<sup>+</sup>86, Dyk88, Gen87, GT83,  
KKR<sup>+</sup>82, LDP80, SMKH87a, SMKH87b, TKK<sup>+</sup>81]. **powerful** [SO87, See81].  
**powers** [ZP89]. **pp** [Ano86b, Boy86, Car85, Cra85, Gar82a, Jur88, Kro88,  
Lil87, Lip86, Ran86, Sch86]. **pp**. [Gar82b, Gil87, Jor81, Wer82]. **practical**  
[Lip86]. **PRDDO** [TM85]. **precision** [HRKW89]. **predicted** [HW88].  
**predicting** [GS87a]. **Prediction**  
[HW80, Gre84, LS89a, LS89b, LS89c, SAV88]. **predissociation** [DBVMB84].  
**Preface** [Ano84h]. **preferences** [CvRS81, GCW88, Ska83]. **Preferred**  
[De 86a, De 86b, Fab88, SAV88]. **Preliminary** [Ano86i]. **Prelog** [Mey80b].  
**preparation** [STH81a, STH81b, STH82, TH80, TSH81a, TSH81b, Tat85].  
**presence** [Kim85]. **presentation** [MKS83, MK84b]. **Press** [Jur88, Wer82].  
**Price** [Car85, Gar82a, Lil87, Lip83b, Lip86, Wib86, Ran86, Sch86].  
**primitives** [ST89]. **Principles** [AFK82, RKM<sup>+</sup>85]. **Pro** [CP81].  
**probabilities** [LS89a]. **probability** [LS89b]. **probability-directed** [LS89b].

**probe** [GRS88]. **probes** [Kar86]. **Probing** [ASFW89]. **problem** [Häs87, KDKC83, KKE88, LS88, MM87]. **problems** [HT82, Mas88, Per84, Sil81]. **procedure** [CP80, FBKK85, GTB81, GS87a, LS89b, LS89c, Mit88, RPAF83]. **procedures** [BMB85a, BMB85b, HP84b, MBB84, MBB85, RKM<sup>+</sup>85, Rap84]. **process** [BBJ88]. **processes** [BG87]. **processing** [PPT<sup>+</sup>80, See81]. **processor** [BD84, BW83, KW86, RDW88]. **Processors** [Bai86, EM84, HD88]. **prodine** [FK84]. **produced** [KJ85]. **product** [BP87b]. **products** [GHHS85]. **Program** [Ano86b, ABE<sup>+</sup>85, BFB85, BBO<sup>+</sup>83, ČHS84, ČFHS85, FE87, Koz87, LS84, PR84, TKI89, TJ86, Tin81, Ved88, WK81, YNAK88, DA83]. **programs** [Boy86]. **Progress** [Lip83b]. **projection** [Gla89, Jaf88]. **prolate** [Ehr84]. **Proleterskih** [Ran86]. **proline** [FM87]. **Prolog** [TKI89]. **proofs** [MBB85]. **propadienone** [Tay84]. **propagation** [LW88, MH83]. **propanal** [KVV<sup>+</sup>84]. **Propanic** [EGM<sup>+</sup>89]. **propanoate** [KSS83]. **propanoic** [SKE<sup>+</sup>84]. **propanol** [Bur80a]. **Propellanes** [Dod84]. **propen** [PKB88]. **Properties** [GM86, JH83, LSROT80, AVF84, AKRA84, BP81, BkBT82, BF82, BW89, BKL87, DE83, DH86, DH87a, DH87b, DH88, EIO85, FSH<sup>+</sup>84, GT82, JSKI88, LZP84, Lew87, MH83, MM83, PH83, Ran83, ROK86, SPBO87, ZP85, Fro86]. **proposed** [DLMR85, HSS83]. **propylamine** [ABP80, SAP88]. **Propylsilane** [PUNC86]. **protein** [CP87b, GS87a, GS87b, LS89a, LS89b, LS89c, LGB<sup>+</sup>89, Ved88]. **proteins** [KNS86, KNS89, PPT<sup>+</sup>80, WG87, WKNC86, ZP85]. **Proton** [HL83, CDL89, DA83, DVA83, DM86a, Del85, EGM<sup>+</sup>89, FS83, KKR<sup>+</sup>82, MFG89a, OUV84, RS85, SAV88, TMOW85, VFM<sup>+</sup>89, ZP84]. **proton-proton** [EGM<sup>+</sup>89]. **protonated** [CDL89, FS89, KvRS80, ZPPC82, ZPCR82]. **protonation** [Del84, LHOM84, SAV88, SK86]. **pseudoatoms** [WM89]. **pseudoenergy** [SRPY88]. **Pseudopotential** [Sax85, BMLR88, NRS84, PKD88, RBEV80]. **pseudorotation** [DA83, Tri88]. **PSEUROT** [DA83]. **pteridines** [Gre85]. **published** [Lip83a]. **purpose** [CCV89, FE87, TJ86]. **PXYH** [BG86]. **pyran** [DLMR85]. **pyridine** [BTG86, Gen87]. **pyridines** [MFG89a, VFM<sup>+</sup>89]. **pyridones** [LV82]. **pyrimidine** [Del81e]. **pyrimidines** [Del81a]. **pyrimidyl** [BL81]. **pyrrolopyrimidine** [SOR86a, SOR86b, SORT86].

**quadratic** [Kar87, MR83]. **quadrature** [RDK83]. **quadrupolar** [AP85]. **Quadrupole** [DM86b]. **qualitative** [KR88]. **quality** [FB89, ZW83b]. **Quantitative** [GC86, AP85, GPC88]. **Quantum** [Ano86i, BD84, BT80a, BT80b, EW87, Tri88, Ano89c, Bur82, FGR89, Gar89, NSKNK87, NRM85, Rap84, SHDP89, vRS86, See81, SK86, Tos84]. **quantum-mechanical** [FGR89]. **Quasi** [SDL82]. **Quasi-one-dimensional** [SDL82]. **quasiclassical** [DBVMB84]. **Quasiperiodization** [RH87]. **quasirelativistic** [Klo83].

**R** [Gil87, KT88, Kro88, Ran86, Wib86, Del81e]. **racemization** [FWB85]. **radial** [Ehr89, LPB84]. **radiative** [PD83]. **radical** [BCB82, CF83, Cla81, Cla83, EWM85, Gil84, HB82, RFLC89]. **radicals** [BF82, DS80, LCY82, LH85]. **Radom** [Lip83b, Wib86]. **Raman** [SBS82]. **Random** [Ran80]. **Range** [EGM<sup>+</sup>89]. **Raphson** [Dil87]. **Rapid** [De 86a, De 86b, HG89, HK88, WG87]. **rapidly** [WMHJ88]. **rate** [Bra89, KBS88, SF85]. **rates** [MM89]. **rationalized** [MM89]. **Reaction** [CF83, AM88b, BG88, DLMR85, GBT82, Gil84, HB82, HMA82, HBK80, LHC84, LLC85, LLSC85, MM89, Per84, SK86, TTZWGQKC81, VSSS84, ZR81]. **Reactions** [BHR<sup>+</sup>86, AJMM88, BW81, BTRT88, BKT82, EWM85, FS89, GHF87, GT84, KvRS89, Kel80a, OLBM83, VSSS84, ST80]. **reactivity** [JB85, LCL84, NVGB81]. **real** [FVV85, Gal82, PLFL85]. **real-time** [PLFL85]. **Rearrangement** [VMNGTVM86, FBD80]. **reassessment** [GTB81]. **Rebek** [LZ89]. **Receptor** [Ano88c, GC85, SDKM87]. **recipe** [Sch89]. **recognition** [LS89a, LS89b, LS89c, LZ89, LBZ89, MBB84, OMK<sup>+</sup>88, VCZB89]. **recurrence** [RLR88]. **recurrence-based** [RLR88]. **Recursion** [DS87, HO83]. **redistribution** [OTW81]. **reduced** [HD88, ZW83b]. **reductase** [Gre85]. **reduction** [Gre85]. **reequilibrium** [Mor85]. **reference** [MSC<sup>+</sup>88]. **Refined** [HR87]. **Refinement** [Dil86, WK81]. **Regional** [YF86]. **regions** [BKKB80, KSJT83]. **regioselectivity** [AJMM88, FS89]. **regular** [KB84a]. **Reinforcement** [WB80]. **related** [AVF84, Koz87, TLA89]. **relating** [IvRS85, Tin81]. **relation** [BT80a, BT80b]. **relationship** [BTG82, Gre84, KR88, WW81]. **Relationships** [GC86, GPC88]. **Relative** [OG86, CPTC84, GHT87, Iku85, JI81, MR80, SAV88, TG83, WM88, ZW83b]. **Relativistic** [KSB85, LBM89]. **relaxation** [AP85, Cha83, CPH85, DM89]. **relevant** [BTRT88]. **Reliable** [RA87, Mul88b]. **Remarkable** [vRSSRH86]. **remarkably** [KTvRS86]. **Remarks** [IO<sup>+</sup>84, Mey84, HAKW87]. **removal** [MK84b]. **renormalized** [Bra89]. **Representation** [CW81, Wil88, Ehr84, GDP<sup>+</sup>85, HP84a, KE89, LDM89, LZP84, LTLA87, ZP85]. **representations** [MR80, ZP89]. **repulsion** [FVV85, PW82, RDK83]. **Research** [Jur88, Ran86, Wer82, Tri84]. **resonance** [BR87, Bro83, JG89, MT82, WG89, AH84]. **Resort** [Ano83a]. **Restricted** [RDAF83, RPAF83, GTB81]. **resulting** [FS82]. **Results** [PUNC86, DK84, GDO89, HE85, SDL82]. **Review** [Boy86, Car85, Cra85, Gar82b, Gar82a, Gil87, Jor81, Jur88, Kro88, Lil87, Lip83b, Lip83a, Lip86, Ran86, Sch86, vRS86, Str85, Tri82, Wer82, Wib86]. **Revised** [GS87a]. **revisited** [CP87a, Zie83]. **RHF** [ZW83a, ZW84]. **ribbon** [Dar89]. **Richard** [Lil87]. **Richards** [Str85]. **rigid** [Lin88, Dil86]. **rigorous** [ZM88]. **ring** [AYS80, Kel82, KR88, LB87, Mat88, RFP86, Tri88]. **rings** [ADY89, AL87, DA83, DVA83, DPSF<sup>+</sup>88, Ham87, JH83, LTLA87]. **RIPS** [FGR89]. **RN** [Gro87]. **RO** [JI81]. **role** [CE87, Gor88, YJ86]. **Rosenblit** [Cra85]. **rotamers** [PKB88]. **Rotation** [BGT84, SAP88, DK84, DK85, Fab88, Hin80, KJ82, LS84, PUC89, Ran83, WM88, KDKC83]. **Rotational**

[PUNC86, SLC86, ABP80, Bur80a, FSL84, FWB85, HE85, HT88, ST87].

**rotor** [SN87]. **row**

[CCSvRS83, DHK89, DH86, DH87a, DH87b, DH88, FB89, Gro87, KTVRS86, MK85a, Mag84, PH83, SCCvRS82, SCvRSH87, SGW83, TH80]. **rules**

[Mey80b]. **Rydberg** [Cha83, CPH85]. **Rys** [RDK83].

**S** [Ano86b, BG86, Del89, LB89b, MV87, TKK<sup>+</sup>81, BT81, Bai84, KSL87, LB87, TKK<sup>+</sup>81, VSS84]. **S-Diphenyl-N** [TKK<sup>+</sup>81]. **sampling** [Gar89, LS89c]. **Sanathanan** [Ano88c]. **Sangivamycin** [SORT86]. **Sanibel** [Ano83a]. **Saskatoon** [Ano86j]. **Satellite** [Ano86j]. **Saturated** [MSS82]. **saxitoxin** [SS81]. **scalar** [CBR87]. **scaled** [Cri84]. **scaling** [HLC88]. **scattering** [BR87]. **SCF** [AFK82, BTG81b, Cha83, Cre82a, CG86a, EWM85, GDO89, GT82, GT83, HA89, KKR<sup>+</sup>82, KSB85, LSROT80, MV87, MM87, Mit88, PMZ86, Pul82, Rap84, RBEV80, SKJ88, SK89, TW81]. **SCF-MO** [RBEV80]. **schemes** [TMOW85]. **Schleyer** [Wib86]. **Schrödinger** [Cre82b, KSI88, NN87, SI88]. **Sciences** [Lil87]. **Scientific** [Gil87]. **scientists** [Coo80, Tri82]. **SCL** [Cla82]. **SDRE** [ZW83b]. **Se** [CGN87, CGN87]. **search** [LS89b, Sau89, vRS86, STZ88]. **searching** [LS88, vGBC<sup>+</sup>84]. **second** [CP87a, DH87b, FB89, FBBA86, FC88, Mag84, MHA89, PH83, SCvRSH87, WD88, TH80]. **second-order** [FBBA86, FC88, WD88]. **second-row** [DH87b, Mag84, PH83, TH80]. **secondary** [BBJ88, HLH83]. **section** [Kar81]. **sectional** [Mey86]. **Segment** [De 86b]. **selected** [BTG81b, GBT82, RV85]. **Selection** [KO86]. **selections** [LBM89]. **Selectivity** [CS82]. **self** [BD82, BL81, DCG81, LBM89, Mom81]. **self-avoiding** [Mom81]. **self-consistent** [BD82, BL81, DCG81, LBM89]. **Semi** [SDB87]. **Semi-empirical** [SDB87]. **semianalytic** [TTZWGQKC81]. **semiclassical** [Sen87]. **Semiempirical** [PW81, CT87, CG89, Fra82, HTT88, HT88, PW82, SMOT85, SCP82, Ste89a, Ste89b]. **sense** [VU83]. **sensitivity** [BSSW88]. **separate** [BCT83, EM84]. **sequence** [LS89a]. **sequences** [HBK80, JBFR86]. **series** [Cha83, CPH85, CP89b, JG89, KR88, PMZ86, WG89]. **set** [AKRA84, BP81, CCSvRS83, Del84, Del85, Del86, Del87, DR86, FB89, GDP<sup>+</sup>85, HR87, HRKW89, Lau88, LBM89, Mag84, MFG89b, MH83, MSČ<sup>+</sup>88, NRR82, OTW81, ST89, SMKH87a, SMKH87b, SMG87, WM88]. **sets** [AKRA84, ARS85, CM89, CCSvRS83, Cre82a, DHK89, DH86, DH87a, DH87b, DH88, FA86, GT84, Gro87, KBS88, LS87a, LS87b, LV88, MK85a, MFG89c, MFG89b, MTN87, MR80, MH83, PH83, RAS85, RA87, STH81a, STH81b, STH82, SHK83, SCCvRS82, SCvRSH87, SGW83, TH80, TSH81a, TSH81b, Tri87, YNAK88, ZW84]. **several** [BT80b, HW88, MTN87]. **Shape** [AM88a, AJMM88, Mey86, Mey88, Mez87b]. **Sharaf** [Kro88]. **shell** [HHK<sup>+</sup>86, HTT88, Kal87, MR80, RA87, TKK<sup>+</sup>81]. **Sheraton** [Ano83a]. **shift** [CZ88, CM89, Mit88, PMZ86]. **shifts** [CW80]. **short** [Kar87]. **Si** [AG88a, Sax85, SKJ88, SK89]. **sigma** [GBP85]. **significance** [Tri87]. **SiH** [TG83]. **silaallenes** [KJ82]. **silanes** [AG88a]. **silica** [LYH87]. **silicon** [JI88, JSKI88, Ver82, AG88b]. **silicon-containing** [Ver82]. **silyl**

[GT82, GT83, MAR<sup>+</sup>84]. **similarity**  
 [AJMM88, HB87, JBFR86, MBB84, Jur88]. **Simple** [KNS85, NSGK<sup>+</sup>81, PUC89, CZ88, CS80, FT89, FS89, MAR<sup>+</sup>84, Mul88b, SDB87, KM85].  
**simplex** [CW80]. **Simulation** [GM86, Lip87, LW88, TG86, BD82, FM87, GLOB88, MC88, OC88, RMB86, TJ86, ZR81]. **simulations**  
 [Che89, HLC88, KS82, RPV87, SK86, WKNC86, YE89, vGBC<sup>+</sup>84]. **SINDO1**  
 [JS87, JI87, JS88, JI88]. **single** [Fab88, SSSA82]. **Singlet**  
 [FOSV86, Car82, SM80, MM87]. **site** [BC89, Cri87, GC85]. **Sites**  
 [De 86a, De 86b, MB84, MKSW83, SAV88]. **six** [GBT80, KBS88, TSH81a].  
**six-membered** [TSH81a]. **sixteen** [VM86]. **sixth** [Gro87]. **size**  
 [CT87, FB89, SMOT85]. **size-consistency** [CT87]. **skeleton** [ROK86].  
**Slater** [LMW85, ZW84]. **Small** [De 86a, De 86b, HHR87, WKP<sup>+</sup>80, BP82, BD82, BG82c, DM86a, JSKI88, Lew87, MR80, Ved88]. **small-molecule**  
 [Ved88]. **smooth** [Dar89]. **SMP** [KBS88]. **SNH** [RFLC89]. **Society** [Lip83a].  
**sodium** [JS87]. **software** [NSKNK87]. **solids** [Mor85]. **solute** [PASTB87].  
**solutes** [BCT83]. **solution** [BFAG81, DD81, Ehr89, GSH88, GLOB88, KYJ88, Mey81, Per84, Rue87, SRPY88, TS83, TMrGM88, BR87]. **solutions**  
 [KS82, KBS88, MSG80, RFLC89]. **solvated** [Kim85]. **Solvation**  
 [DM86b, Ehr86, FT89, JDS89]. **Solvent** [Ehr84, GS85, BCT83, MB84, JI81].  
**Solvent-effect** [GS85]. **solvents** [Lew87]. **Solving** [DM89, Mas88].  
**Solvolysis** [MM89]. **Some**  
 [RB87, AYS80, AM88a, BS89, BPP82, CL85, Del85, Del86, GTB81, HS82, MAR<sup>+</sup>84, SNR83, SDB87, VSS82, WP83, WP82, ZBR80, HAKW87, SDL82].  
**Space** [DVA83, Sil81, CGN87, DCNG85, LS88, RMB86, Sim87]. **sparse**  
 [BP87b]. **Spatial** [KNS86, KNS89, CS80]. **Spatially** [BK86]. **special** [FE87].  
**special-purpose** [FE87]. **species** [Bal82a, Bal82b, KJ85]. **specific** [Fuj87].  
**specificity** [Lil87, SRKT87]. **spectra**  
 [BL88, MSČ<sup>+</sup>88, NVGB81, SBS82, XB86]. **spectral** [KJ85]. **Spectroscopic**  
 [ZBR80, KPE<sup>+</sup>84, KSB84]. **spectrum** [HW82]. **Spherically** [ST82].  
**spheroidal** [Ehr84]. **Spin**  
 [KSJ82, AP85, Bal82a, Bal82b, Bre81, DA83, DVA83, KF88, LMW85, PW81].  
**spin-lattice** [AP85]. **spin-orbit** [KF88]. **Spiro** [IL86]. **split** [HR87].  
**split-valence** [HR87]. **squares** [Lau88, LV88, SAS87]. **SS** [Cla82]. **SSH**  
 [Cla81]. **Stabilities** [OG86, GHT87, Iku85, TG83]. **stability**  
 [DCG81, PFRS82, RMB86]. **Stabilization**  
 [SCCVRS82, JG89, OTW81, WG89]. **stable** [WMHJ88]. **stacking**  
 [OTW81, SRKT87]. **Standard** [ZW83b, LR87]. **starting** [Sch88]. **state**  
 [BG80, Cha83, CG89, Del81b, DTPR85, DPCS80, GT84, Has84, LDM89, PD83, Ska83, WSP88]. **States** [FOSV86, Bak86, BR87, Bau84, BG80, Del81a, Del81c, DM83, DR83, DH83, DFC<sup>+</sup>84, DHS84, HAKW87, JH83, KKR<sup>+</sup>82, KJ82, LDP80, Lin88, LR87, MM87, Sch82a, SM80, VU84, ZP84]. **Stationary**  
 [Lop89, KSHD88, LDP<sup>+</sup>87, LDL<sup>+</sup>88]. **statistical** [Bal82a, Bal82b, BR85].  
**statistics** [BMG84]. **step** [Gar89, RPV87]. **stepwise** [SAF88].  
**stereochemical** [BMB85b]. **Stereodynamics** [FWB85]. **stereoregular**

[AVF84]. **Stereotopological** [Mil87]. **Steric** [MM89, MKSW83, MK84b]. **STO** [HR85, PH83, ZW83a]. **STO-3G** [HR85, PH83]. **Stochastic** [Sau89]. **storage** [HD88]. **STOS** [RLR88, RLR89]. **Strain** [Ham87, WP82, Bys83, VSS82]. **strained** [Dod84, VSS82]. **stranded** [Gre83]. **Strategies** [BP87b, CG89]. **Strategy** [YF86, NKC85, Sch88]. **stretching** [BTG81a, BTG82, MHA89, RK81]. **strictly** [PS87]. **strong** [LSROT80]. **Structural** [LUNV85, LB86, BF82, KSS83, KVV<sup>+</sup>84, KSB84, SSSA82, SVS<sup>+</sup>81, SKV<sup>+</sup>85, SPBO87, SKE<sup>+</sup>84, VSS82, PR80, SSSA82, SKE<sup>+</sup>84].

**Structure**  
 [GC86, JSKI88, vRSSRH86, ABE<sup>+</sup>85, AYS80, AVBF84, BMB85b, BMR87, BTS<sup>+</sup>83, BBJ88, DS80, GPC88, GT82, GB83, HW80, HAKW87, KK85, KR88, KS83, LS89a, LS89b, LS89c, Lil87, Lip86, LYH87, NVGB81, OMK<sup>+</sup>88, PW82, PSSH80, PFRS82, RDW88, RP80, RRI88, SVS<sup>+</sup>81, SWM83, SM80, Tin81]. **Structure-Activity** [GC86, GPC88]. **Structure-Directed** [GC86]. **Structures** [BPP82, OG86, ASS<sup>+</sup>85, BMB85a, BMB85b, Bal85, BE87, Bro83, CvRSKJ81, CG89, Del89, FS82, HR85, HR87, HRKW89, JT80, KvRS80, KC87, KYJ88, KVV<sup>+</sup>84, KSB84, KMS85, LV88, MSSS80, MSS82, MBB84, MBB85, PPT<sup>+</sup>80, PUC89, RKM<sup>+</sup>85, RRG<sup>+</sup>84, Sch82b, Sch88, SMG87, VSS82, VVVG81, WKP<sup>+</sup>80, WM88]. **studied** [Ösa82]. **Studies** [BG81b, BG81a, BG82b, BG82c, DLMR85, Jur88, Wer82, AJMM88, BP81, BG86, Bys83, CDL89, CMRW86, FMTS84, God87, Gre85, HMA82, HSS83, HSEČ83, JI81, JB85, Kao88, KB84a, KB84b, KM85, KSS83, KVV<sup>+</sup>84, KSB84, KK85, KR88, KSL87, LCY82, LLSC85, LKL87, LDP<sup>+</sup>87, LZ89, LBZ89, Lip87, MK85b, MTN87, OMK<sup>+</sup>88, PUC89, RMB86, SHDP89, SOR86a, SOR86b, SORT86, SOR87, SSSA82, SVS<sup>+</sup>81, SKV<sup>+</sup>85, SKE<sup>+</sup>84, VSS82, VVVG81, WSP88]. **Study**  
 [SMOT85, VMNGTVM86, AG88a, Aid88, ADY89, Bai84, BMLR88, BTG80, BTG81a, BTG82, BTS<sup>+</sup>83, BGT84, BSM83, Che89, CF87, CDL<sup>+</sup>87, DAU88, DS80, DHP83, Del81a, Del89, EIO85, FBD80, FS89, Fra82, FK84, Gen87, GBT80, GBT82, Gil84, GS87b, GT82, GT83, Gre83, GCW88, Ham87, HT88, HML83, Iku85, JDS89, JMB87, KS84, KvRS80, Kin87, LV82, LSROT80, LCL84, LHC84, LHOM84, LLC85, LH85, LUNV85, MFG89a, MV87, MTN87, OLBM83, PMZ86, PHG89, RFP86, RBEV80, RPV87, Rue87, SS81, SSSA82, SAP88, SAF88, SM80, SMG87, SK84b, TLA89, TKK<sup>+</sup>81, TG83, Top87, Tos84, VV88, VSSS84, VFM<sup>+</sup>89, YJ86, ZPPC82, ZPCR82, ZPPC83, ZBR80, CvRS81]. **Subgraph** [KHS86, TKI89]. **subject** [Cri89]. **submatrix** [LM89]. **subroutines** [CBR87]. **Substituent**  
 [EH83, FOSV86, Mag84, Ehr84, HPR80, KPRT81, PR80, SMF89, Del81e]. **substituents** [BTG81a, DPSF<sup>+</sup>88, KPRT81, SCCvRS82]. **Substituted** [FKS86, HML83, Kel80b, Kel82, LH85, MFG89a]. **substitution** [Rit86]. **substrate** [TTZWGQKC81]. **substrates** [Gre85, MM89]. **substructures** [BFF86]. **sulfamates** [OMK<sup>+</sup>88]. **sulfide** [SBS82]. **Sulfilimine** [TKK<sup>+</sup>81]. **sulfoxides** [Tai81]. **sulfur**  
 [Bai84, DM83, DR86, LB87, Mag84, MSS82, ST89, TKK<sup>+</sup>81].

**sulfur-nitrogen** [LB87]. **sulphur** [JI87]. **supercomputer** [WG87].  
**superiority** [SCCVRS82]. **supermatrix** [Cao89]. **supermolecular** [KE89].  
**superposition** [AKRA84, MFG89b, OTW81]. **Surface**  
 [LP88, BMR87, Car82, CDL89, Has84, LDL<sup>+</sup>88, Lop89, Mey88, MK84b,  
 PASTB87, ST80, WSP88, Mey86]. **Surfaces**  
 [YF86, AM88a, DPCS80, FKS85, IO84, KE89, KJ87, Osa82, VSS84].  
**survey** [Kel80b, Kel82]. **susceptibilities** [WP83]. **SW** [TW81]. **symbolic**  
 [KBS88, Tri88]. **symmetric** [FWB85, LB89b, ST82, ZP89]. **symmetrical**  
 [ZP89]. **Symmetry**  
 [KO86, Ran83, ROK86, Bal83, BW81, Cao89, ČHS84, DE83, FSL84, HLH83,  
 Jaf88, KJLW84, Mez87b, SN87, TDK83, Tay84, Cao89]. **Symmetry-matrix**  
 [Cao89]. **symmetry-supermatrix** [Cao89]. **symmetry/topology** [BW81].  
**symmetry/topology-allowed** [BW81]. **Symposium**  
 [Ano83a, Ano86j, Ano86j]. **syn** [VV88]. **syn-oxime** [VV88]. **synthesis**  
 [CS82, HBK80]. **System**  
 [CG86b, ABE<sup>+</sup>85, AP85, LA85, MTN87, SK89, SL81, Tri87, Tri88].  
**Systematic** [HBK80, SDKM87, TM85, CP80, STH81a, STH81b, STH82,  
 TH80, TSH81a, TSH81b, Tat85, Ano88c]. **Systems**  
 [KW86, AH84, AS88, ASFW89, BL88, Ehr89, Gal82, HTT88, Kao88, Kel80a,  
 KSL87, Koz87, LB87, LSROT80, RK81, SDL82, SK86, SN87, SDB87, TS83,  
 TMOW85, Tri88, TTZWGQKC81, vGBC<sup>+</sup>84, Jur88]. **Szymnsky** [Ran86].

**T** [Ano86b, LR87]. **T.-S** [Ano86b]. **tables** [LB89b, SN87]. **taste** [OMK<sup>+</sup>88].  
**tautomer** [Gre85]. **tautomerism**  
 [BSM83, CSCD<sup>+</sup>89, ROK86, Top87, Zie83, ZPPC83]. **tautomers** [BT80b].  
**Te** [RBEV80]. **technique**  
 [BD82, DE83, Gar89, HO83, Kel80a, LMV86, Per84, RPD<sup>+</sup>86]. **techniques**  
 [SL81, TS83, RDAF83]. **technologists** [Ran86]. **Teller** [LR87]. **tempered**  
 [DHK89]. **ten** [KKR<sup>+</sup>82]. **ten-electron** [KKR<sup>+</sup>82]. **terminal** [CP81]. **terms**  
 [FC88, GF87]. **tert** [FST81]. **tertiary** [MM89]. **test** [Bur82, PW81]. **testing**  
 [KKE88]. **tests** [LS87a, RAS85]. **tetra** [FST81]. **tetra-tert-butylethylene**  
 [FST81]. **tetrachloride** [DHP83]. **tetrahydroborate** [BMLR88]. **tetramer**  
 [KSL87]. **tetraoxabicyclo** [Bur80b]. **tetrapeptide** [HW80]. **tetrodotoxin**  
 [SS81]. **th** [Per84]. **their** [BR85, CSCD<sup>+</sup>89, CE87, FK84, GTB81, Hur88,  
 Iku85, Kao88, KPRT81, KS83, LDP80, PUC89, Ran80, VSS82, WK81].  
**theorem** [GT83]. **theoretic** [RRG<sup>+</sup>84]. **Theoretical**  
 [Ano86k, CDL<sup>+</sup>87, CMRW86, FKS86, Gen87, Gre85, HMA82, Iku85, Kao88,  
 LLC85, LLSC85, LKL87, LPB84, LZ89, LBZ89, Rue87, SAV88, VU83, VU84,  
 VFM<sup>+</sup>89, BKKB80, BKT82, Cre82b, FBD80, Gre83, HT88, HPR80, HML83,  
 HLH82, JDS89, KvRS80, KPRT81, Kin87, LHOM84, LH85, Lip83b, LUNV85,  
 OMK<sup>+</sup>88, PR80, TW81, WB80, LDP<sup>+</sup>87, RRH86]. **Theoretically** [KJ85].  
**Theory**  
 [CG86b, KKR<sup>+</sup>82, PD83, BT80a, BT80b, Boy86, Del81b, Del81c, Del81d,  
 Del81e, Del83, DH86, DH87a, DH87b, DH88, Ehr81, FE87, FC88, Gla89, Kin87,

KR88, LCL84, Mez87b, NRM85, PH83, RV85, Tri84, WP83, PW81, Wib86].  
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 [Cre82a, Cre82b]. **Thermodynamical** [BF82]. **thermodynamics** [Boy86].  
**these** [ZP84]. **thin** [LP88]. **thiocarbonyls** [BSM83]. **thioketone** [BSM83].  
**thioformic** [BTG80]. **Thiophene** [TLA89]. **third** [DH86]. **third-** [DH86].  
**Three** [Cla81, Cla82, Cla83, GC86, IL86, ADY89, GBT82, GPC88, GDP<sup>+</sup>85,  
 LW88, PKB88]. **Three-Dimensional** [GC86, IL86, GDP<sup>+</sup>85].  
**Three-Electron** [Cla82, Cla83]. **three-membered** [ADY89]. **threefold**  
 [Wen82]. **through-bonds** [LCY82]. **Through-Space**  
 [DVA83, CGN87, DCNG85]. **Tim** [Lip86]. **Time**  
 [RPV87, FBBA86, Gar89, PLFL85]. **time-independent** [FBBA86].  
**time-step** [Gar89]. **toluene** [XB86]. **Tolylsulfonyl** [TKK<sup>+</sup>81]. **Tool**  
 [CG86b, GRS88, HK88, See81]. **Topological** [Bac89, IL86, BMT81, BW89,  
 Kel80a, MBB84, MT82, RRG<sup>+</sup>84, Rou87, Sim87, BMB85b]. **Topology**  
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**torsional** [AP80, CP89b, IÖ84, LA85, MHA89, Ösa82, KB84a]. **total**  
 [TM85, Cre82b]. **toyocamycin** [SOR86a]. **trajectories** [BSSW88, SDB87].  
**trajectory** [KW86]. **trans** [BTG80, BL81, DPSF<sup>+</sup>88]. **trans-2** [DPSF<sup>+</sup>88].  
**trans-thioformic** [BTG80]. **transannular** [EW87]. **transcription**  
 [SOR87]. **Transfer**  
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 [NSKNK87]. **transform** [SF85]. **Transformation**  
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 BG80, CG89, DH87a, DH87b, DH88, FB89, GT84, HE88, KM85, MS88,  
 PH83, SMKH87a, SMKH87b, Sch82a, Sch82b, SWM83, TSH81b, ZP84].  
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**transmembrane** [Kim85, VU83, VU84]. **transmission** [CGN87, DCNG85].  
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 KDKC83, Koz87, NLA84, Sil85, SA80, Tay84]. **tree** [CRR85, LS88]. **trees**  
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**Triplet** [FOSV86, CF83, DPCS80, HW82]. **triplet-state** [DPCS80]. **Tripos**  
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 [SOR86b]. **twisted** [HR85, HR87]. **Two** [BR87, ČHS84, KF88, LV88, MM87,  
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 [JG89, WG89, Aid88, AKRA84, Bre81, Mas88, ST89, STH81a, STH81b,  
 STH82, TH80, TSH81a, TSH81b, Tat85, BG80]. **Tyr** [CP81]. **tyrocidine**  
 [TMrGM88].

**UF** [KS83]. **UH** [KS83]. **UHF** [BF82]. **Ulrich** [Lip83a]. **UMP** [MK85a].



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**V** [Cra85, Ran86, Wib86, AG88b, MBB84, Mey81, Mey88, Ran83, STH81a]. **vacuo** [SHDP89]. **Valence** [Bai86, CvRS81, HR87, Jug84, JFG89, LDM89, LRP87, MR80, NRM85, ROK86, ZD87]. **valence-orbital** [ZD87]. **valence-orbital/bond-orbital** [ZD87]. **valences** [JB85]. **valency** [Mag84]. **Validation** [CCV89]. **Validity** [AM88b]. **valinomycin** [MK84a, MK85b]. **value** [Gre84, Ran80]. **values** [GBP85, ZW83a, ZW84, NF84, SF86]. **vapor** [VVVG81]. **various** [BS89, BG80, BTRT88, LDP80]. **VAX** [CBR87]. **Vector** [Bai86, BP87b, CBR87, EM84, LM89]. **vector-scalar-multiply-and-add** [CBR87]. **Vectorization** [GM86, KW86, Rap84]. **Vectorizing** [TJ86, BP87b]. **VEH** [BKL87]. **velocity** [HLC88]. **Venkataraman** [Lil87]. **Versus** [ST89, Ada89, FB89]. **very** [Kar87, LM89]. **VI** [BT81, KB84a, STH81b]. **via** [DVA83, HLG88]. **viable** [ACvRS81]. **vibration** [DK84, DK85, KDKC83]. **Vibrational** [DK88, DBVMB84, BTG80, Gor88, HE85, HLH82, HLH83, HE88, Lin88, MAR<sup>+</sup>84, MSČ<sup>+</sup>88, PKB88, Ska83, SBS82, VVVG81, XB86]. **vibrations** [LPB84, PV82b]. **vibronic** [LS84]. **vicinal** [DVA83]. **view** [GDP<sup>+</sup>85]. **VII** [KB84b, MKSW83, TSH81b]. **VIII** [BG82a, BTRT88, RKM<sup>+</sup>85, STH82]. **vinyllic** [Rit86]. **violuric** [OC88]. **virtual** [CP80, FBKK85]. **voltage** [Kim85]. **Volume** [Ano86b, HG89, Lip83b]. **volumes** [KE89]. **Voronoi** [BC89, Cri87].

**W** [Car85, Ran86, Str85, Tri82, Wib86, Gro87]. **W-RN** [Gro87]. **Waals** [AL87, DTPR85, DBVMB84, MTN87]. **walks** [Ran80]. **Water** [De 86a, De 86b, BG82b, BG82c, CDL89, Del81b, Del81e, Gen87, GLLOB88, Iku84, JI81, KTVRS86, KYJ88, KSL87, LV82, LLC85, Lin88, MC88, OC88, RMB86, SWM83, YJ86, ZPPC83, Del81c, Del83]. **Water-cytosine** [Del83]. **water-mediated** [ZPPC83]. **water-pyridine** [Gen87]. **Watson** [Aid88]. **Watson-Crick** [Aid88]. **wave** [FB89, JFG89, KDEHK89, LW88, TM85]. **wave-propagation** [LW88]. **wavefunctions** [Bre81, NRR82, ZW83b]. **weakly** [Dyk88]. **weighted** [Bal88, HB89, SAS87, ZW83a]. **weights**

[Bal82a, Bal82b]. **well** [DHK89]. **well-tempered** [DHK89]. **which** [Mar87]. **Wiener** [CRR85]. **Wiley** [Boy86, Car85, Cra85, Gar82b, Gar82a, Gil87, Kro88, Lip86, Tri82, Wib86]. **Wiley-Interscience** [Tri82]. **Willett** [Jur88]. **within** [AP87, BG82b, BG82c, Ehr81, TM85, TW82]. **without** [Bak87, Mez87b]. **World** [Ano86k].

**X** [BG86, CvRS81, FS89, FS82, MV87, TW81, HPR80, Iku85, KPE<sup>+</sup>84, PMZ86, THW80]. **XCHCH** [FS89]. **XCHYH** [PMZ86]. **XCL** [FS82]. **Xe** [SGW83]. **XeF** [KSJ82]. **XI** [MM89]. **xii** [Jur88]. **XMP** [BP87b]. **XXX** [Del83]. **XY** [Ran83, LR87, Ran83].

**years** [Ano89c]. **yeast** [LDP80]. **YETI** [Ved88]. **York** [Boy86, Car85, Cra85, Gar82b, Gar82a, Gil87, Jor81, Kro88, Lil87, Lip83b, Lip86, Tri82, Wer82, Wib86]. **YU** [Ran86]. **YU-41000** [Ran86]. **Yugoslavia** [Ran86]. **Yvonne** [Ano88c].

**Zagreb** [Ran86]. **Zero** [KO86, SS84]. **Zhabotinskii** [ZR81]. **zipper** [HMA82]. **Zn** [ARS85]. **ZnCl** [LP88]. **ZnS** [LP88].

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