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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]. 3II [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, GLL0B88, Iku85, Kim85, RFLC89, TMOW85].
++ [NRR82]. - [DD81, HPR80, JDS89, JI81, MV87, SK86]. ¹ [BBJ88, MV87].
¹³ [CW80, CZ88]. ¹Σ [MV87]. ³ [PD83]. ³¹ [DCNG85]. ⁴ [EGM⁺89]. ⁷⁷
[CGN87]. ^α [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 3^{-} [ROK86]. 8 [Bai84, FS82, GDO89]. 9 [GDO89]. α [THW80]. MeH [EGM+89]. N [VSS84, CDL89, CMRW86, Del87, Del89, FKS86, LHOM84, LB89b, MFG89c]. $\frac{+1}{n+1}$ [Del87]. α [FSH+84, HML83, KT88, LMW85, Lew87, LH85, PPV83, NR80, THW80, TW81, VCZB89]. α_{ta} [TW81]. β [BTG81b, FSH+84, GBT80, Lew87, RP80, SMOT85]. c [CP81]. \cdot [Del87, FS82, TMOW85]. $\cdot 2$ [Ran83]. $\cdot 3$ [Ran83]. χ [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]. ν [Lew87]. ω [ZW83a]. p [Per84]. $p < 0$ [Per84]. π [AG88b, Gre84, HAKW87, KM85, LCY82]. π^* [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]. σ [Cla83, WB80]. spd [SMKH87b]. φ [Sen87].

* [Cla83, 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⁺89]. **2-aza-1** [BGT84]. **2-C** [GDO89]. **2-Dimethylcyclopentyl** [VMNGTVM86]. **2-Disilylethane** [PUNC86]. **2-dithiete** [God87]. **2-methylpropanoic** [SKE⁺84]. **2-propen-1-imine** [PKB88]. **2-pyrimidyl** [BL81]. **205** [ABE⁺85, BP87b, GM86, LGB⁺89, LW88, RD87]. **21G** [ST89, VLG89]. **2H** [DLMR85]. **2H-pyran-2-ones** [DLMR85]. **2nd** [Str85].

3 [BSSW88, CZ88, GDO89, HHK⁺86, RP80, ST89, TSH81b, Top87, VMNGTVM86, VFM⁺89]. **3-** [VFM⁺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⁺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⁺89]. **4-R-pyrimidine** [Del81e].

5 [ČHS84, Tat85]. **5-C** [GDO89]. **5-Dihetero-Spiro** [IL86]. **5-dimethoxytetrahydrofuran** [DPSF⁺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⁺84]. **acetyl-alanine-proline-alanine** [FM87]. **Acetylcholine** [MC88]. **acetylene** [PFRS82]. **acetylenes** [AP87]. **acetylenic** [HMA82]. **acid** [BTG80, BTG81b, BHR⁺86, FS89, GBT82, GT82, LS89a, LSROT80, LCL84, LKL87, OC88, SKE⁺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⁺84, GPC88, KK85, KR88, PPV83, RP80, Tin81]. **acyclic**
 [MSS82]. **add** [CBR87]. **addition** [BW81, CDL⁺87, SWM83]. **additional**
 [TSH81a]. **additions** [CDL⁺87]. **adjacent** [WM88]. **adjusting** [CPV84].
Adrenergic [Ano88c, SDKM87]. **adsorption** [BFAG81, CPV84]. **Advance**
 [KO86]. **advances** [CP87a]. **affinities** [BNR86, DM86a, Del85, Del86, FS83,
 HL83, Kal87, KKR⁺82, OUV84, RS85, SAV88, VFM⁺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⁺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⁺81, JI88, JSKI88]. **AM1**
 [HT88, BSSW88, CDL89, Fab88, SMF89, VFM⁺89]. **AMBER** [WK81].
amenable
 [KSS83, KVV⁺84, KSB84, SSSA82, SVS⁺81, SKV⁺85, SKE⁺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⁺84, KSB84,
 NLB85, OE89, PKB88, PPT⁺80, RB87, SDKM87, SRKT87, SVS⁺81,
 SKV⁺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⁺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⁺86, DPSF⁺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⁺80, RDW88]. **aryl** [GCW88]. **aryl-alkylamines**
[GCW88]. **aspects** [GF87, RPAF83, SSSA82, SF85]. **assess** [ZW83b].
assessment [BMG84, GSH88]. **assisted** [DA83, Lil87, OMK⁺88, WK81].
association [Ran86, SMOT85, BG81b, BG81a, BG82b, BG82c].
associations [NF84, SF86]. **Atom**
[IvRS85, SLR⁺86, Cha83, CPH85, LDM89, LLSC85, ST89, SK85, WKNC86].
Atom-Atom [SLR⁺86]. **Atomic**
[BR89, CF87, DM86b, GC86, GPC88, THW80, BW89, CP89a, CW81,
FVV85, JB85, LV88, Mul88a, Mul88b, Ran80, Wil88]. **atoms**
[ASS⁺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⁺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⁺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⁺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⁺81, WP83, WM88, YNAK88, ZW83a, ZW84, AKRA84, Mag84, MFG89b]. **basis-set** [MH83, AKRA84]. **bay** [BKKB80, KSJT83]. **BCN** [GT84]. **Be** [WKP⁺80]. **behavior** [BMLR88, DPSF⁺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⁺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⁺84, LSROT80, LD87, MK85a, MFG89c, MFG89b, NSGK⁺81, NR80, OLBM83, SAP88, Wil88]. **bond-orbital** [ZD87]. **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⁺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⁺84]. **Butane** [PUNC86, AP80]. **butanoic** [SKE⁺84].
butylene [Rit86]. **butylethylene** [FST81]. **BW** [TW82].

C [FS82, Gar82a, GDO89, KPE⁺84, VM86, BL88, BTG82, BGT84, CvRSKJ81, CW80, CZ88, CvRS81, FWB85, FS82, FKS85, FKS86, GDO89, HHK⁺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⁺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⁺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⁺85, AFK82, AVBF84, ARS85, BT81, BR89, BKC86, BTG81b, BG80, BTRT88, BL81, BSSW88, BBO⁺83, Bur80b, Bur80a, Cao89, CF83, CZ88, CM89, CCSvRS83, Cre82a, Cre82b, CG86a, CT87, CL85, CE87, DGW⁺81, DTPR85, DM83, DR83, DH83, EWM85, Fab88, FBKK85, FGR89, FWB85, FS83, GT84, GHT87, Gol87, GHHS85, GL87, HHK⁺86, HLG88, HW88, Hur88, Iku84, Jaf88, JdKdWB87, Kar81, KHRvH87, Klo83, KKR⁺82, KSB85, LRP87, LCC87, LBM89, LMW85, Lew87, LGB⁺89, MK85a, Mag84, MK84a, Mey84, MH83, MSČ⁺88, MM83, MM89, PW82, PW81, PL87, RAS85, RV85, SMK87a, SMK87b, 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⁺86]. **carbanions** [LUNV85]. **carbocation** [HSW82]. **carbocations** [HLH83]. **carbocycles** [AYS80]. **Carbodications** [CvRSKJ81]. **carbohydrate** [Bur80b]. **carbohydrates** [JT80]. **carboline** [SMOT85]. **carbon** [FS83, MM89, PSSS80]. **carbonic** [BHR⁺86, GBT82]. **carbonions** [WP83]. **carbonyl** [ASS⁺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⁺89, Cla83, FS82, HHK⁺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⁺84, SK86, TG83, KPE⁺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⁺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⁺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⁺87, LDL⁺88, LBZ89]. **chirality** [Osa82]. **chlorine** [Cla83, DR83, JS87, MSS82]. **chloroalkanes** [VVVG81]. **Chlorosilanes** [CUCP89]. **CHOH** [LS87b]. **choice** [MSC⁺88]. **chromatography** [LDP⁺87, LBZ89]. **chymotrypsin** [VCZB89]. **CI** [CP87a, CP80, FBKK85, HW82, KHRvH87, LCC87, PMZ86, SKJ88, SK89, Wen82, ZBR80]. **CIPSI** [CP87a]. **cis** [BW81, BTG80, DVA83, DPSF⁺88, KJ85]. **cis-** [BTG80, DPSF⁺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⁺86, RA87]. **closed-** [HHK⁺86]. **closed-shell** [RA87]. **Cluster** [NLB85, Ada89, Kal87]. **clustering** [Iku85, Jur88]. **clusters** [BL88, BG82c, CDL89, CMRW86, Dyk88, FBKK85, GLOB88, JSKI88, LP88, LYH87, WKP⁺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⁺86, Iku85, ST80]. **Coast** [Ano83a]. **code** [KW86]. **coding** [BMB85b, BKT82]. **coefficient** [KNS85]. **Coefficients** [GC86, KI81]. **collisions** [ST87]. **color** [BR85, EB87]. **colorings** [LB89a]. **Column** [LDP⁺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⁺87, DM89, FGR89, Gla89, KPRT81, Kin87, KSS83, KPE⁺84, KSB84, PHG89, WB80, GHT87]. **compatible** [ČHS84]. **complex** [CPTC84, DBVMB84, FM87, OTW81, SK86, TMOW85, YJ86]. **complexes** [DAU88]. **complexes** [BMLR88, Del81b, Del81c, Del81e, Del83, Del87, Del89, Gen87, GRS88, HS82, JI81, KM85, Lin88, Ved88]. **compliance** [MR83]. **Component** [De 86a, SK85]. **Components** [SLR⁺86]. **compounds** [AG88b, AF83, BS89, BTG81a, CMR88, CMR89, DGW⁺81, DH83, DHS84, DH86, DH87a, DH87b, DH88, DLMR85, FSL84, GHHS85, GL88, GL89, HHR87, JS87, JI87, JS88, JI88, KTvRS86, KPE⁺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⁺87, Lil87, LB89b, LB89a, OMK⁺88, PLFL85, RB85, TG86, BKKB80, KBS88, RKM⁺85, RMB86, SAS87, TS83, Tri87, vGBC⁺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⁺84, HLP82, HPW82, LS89b, SRPY88, Tai81, TMrGM88]. **Conformational** [Ano88c, CvRS81, CP81, Cri82, Cri84, CL85, DPCS80, EIO85, FMTS84, FSH⁺84, Fro86, GCW88, HW88, IL86, KS84, OE89, PPT⁺80, RMB86, VM86, YJ86, ZPPC82, BSSW88, BA82, CMR88, CP87b, DPSF⁺88, Dod84, FGR89, Ham87, LS89a, LDP80, LS88, MR80, NLB85, OTPH87, Ōsa82, RFP86, SDKM87, SKV⁺85, SKE⁺84, VVVG81, VV88, VU83, WG87, Wer82, Bur80b, KSS83, KVV⁺84, KSB84, Mey81, SVS⁺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⁺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⁺89,
 GBT82, KBS88, LA85, MAR⁺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⁺85, ASFW89, BTG82, DGW⁺81, DM83, DR83, DH83, DHS84,
 HHK⁺86, JH83, Kao88, STH81b, TKK⁺81, Ver82]. **Continuum**
 [Ehr89, FT89, PASTB87]. **contour** [GDP⁺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⁺89, PW81]. **couplings**
 [DVA83]. **CpGpCp** [YJ86]. **CpGpCp-pentapeptide** [YJ86]. **Cr** [RAS85].
Crambin [LGB⁺89]. **CRAY** [BP87b]. **Crick** [Aid88]. **Crippen** [Wer82].
criterion [ZW83b]. **Critical** [KPE⁺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⁺85, BP87b, LGB⁺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 [IÖ84]. **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⁺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, FMST84, FS89, FK84, GHHS85, Kao88, WM89]. **derived** [BR89, BTG81b, CF87, KJ85, TMrGM88]. **described** [Bau84]. **description** [BMB85a, BMB85b, LPB84, LWD82, MBB84, MBB85, PASTB87, PS87, RKM⁺85, ZD87]. **design** [Fuj87, HBK80, LDP⁺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⁺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⁺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⁺85, KSI88, SI88, SDL82, SK84b]. **dimensions** [LW88]. **dimer** [Has84]. **dimerization** [VU83]. **dimers** [BG82b, VM86, ZP84]. **dimethoxytetrahydrofuran** [DPSF⁺88]. **Dimethyl** [IL86, KMS85, OE89]. **dimethyl-** [OE89]. **Dimethylcyclopentyl** [VMNGTVM86]. **dimethylheptanes** [CL85]. **dimethylphosphate** [JMB87]. **Diophantine** [Bur82]. **dipeptide** [RMB86]. **Diphenyl** [TKK⁺81].

diphenylmethyl [AB83]. **dipolar** [AP85]. **Dipole** [BC83, Ehr89, HE88, Wil88]. **diradicals** [LCY82]. **direct** [AFK82, FWB85, HA89, KKR⁺82, LV88, RPAF83]. **Directed** [GC86, Bal88, GPC88, LS89b]. **directing** [TM84]. **directly** [HPR80]. **Discrete** [Fra87]. **Discrimination** [RRG⁺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⁺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⁺83, CU89, FM87, Fuj87, GHF87, GCW88, HLC88, NKC85, NK86, SHDP89, TJ86, YE89].

easily

[KSS83, KVV⁺84, KSB84, SSSA82, SVS⁺81, SKV⁺85, SKE⁺84, VSS82]. **economical** [NRR82]. **Ed** [Jor81, Gar82b, Str85]. **edge** [Bal88, HB89, LB89a]. **edge-weighted** [Bal88, HB89]. **Edited** [Lil87]. **editor** [DMB88]. **Effect** [DPSF⁺88, HLH82, ASS⁺85, ASFW89, BTG85, BTG86, BW89, FSH⁺84, GS85, GT84, GL87, Kim85, NLA84, TSH81a, TM84, WM88]. **effective** [KSB85]. **Effects** [FOSV86, RS85, AH84, AF83, AKRA84, BTS⁺83, BCT83, CS82, DVA83, Del81e, Del85, Del86, Del87, Ehr81, Ehr84, EH83, HPR80, HLH83, JI81, KPRT81, KSL87, KSJ82, Mag84, MSČ⁺88, MM89, PR80, Rit86, SSSA82, SMF89, SMG87, WB80, BTRT88]. **Efficient** [CCSVRS83, Dyk88, KO86, ČFHS85, FBBA86, Mas88, OPH87, 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⁺85, GT84, HLH82, KF88, KKR⁺82, LCC87, MM87, PW82, RLR88, RLR89, RB87, RDK83, WM88, ZW83a, ZW84, Kal87]. **electronegative** [ASS⁺85]. **electronegativity** [LDM89]. **Electronic** [KS83, KJ82, LYH87, PPV83, SM80, ABE⁺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⁺81, PHG89, PR80, SK84a, Wil88, ZP85]. **element** [KSI88, MK85a, SI88]. **elemental** [WKP⁺80]. **elements** [Bal83, CPTC84, CCSvRS83, DbCV⁺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⁺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⁺86, YF86, BMLR88, BHW87, BSSW88, BBO⁺83, Car82, CDL89, CP81, Cri82, Cri84, CP87b, Del84, DPCS80, FWS89, FST81, FSST82, FT89, FKS85, GBT80, GBT82, GS87a, Ham87, Has84, HHR87, IO84, KSHD88, KSJ82, LDM89, Lip86, LDL⁺88, Lop89, MHA89, MT82, NK86, Osa82, 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⁺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]. **Ermler** [GTB81]. **Erratum** [Ano86b, DH88]. **error** [GSH88, MFG89b, MH83, RPV87]. **errors** [MSSS80, OTW81, TM85, ZW83b]. **essential** [Fab88]. **ester** [KSS83, SVS⁺81]. **estimates** [VSS82]. **estimation** [GTB81, HK88, Cre82a]. **ether** [Bur80a]. **ethers** [DAU88]. **ethyl** [Bur80a, FS83, HB82, KSB84]. **ethyl-cation** [FS83]. **Ethylene** [FKS86, CF83, CDL⁺87, SBS82]. **ethylenes** [FSST82]. **ethylmethylanine** [ABP80]. **Ethylmethyilsilane** [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⁺84, JH83, MM87, SM80]. **excluded** [HG89]. **exclusion** [SLB83]. **expansion** [CP89b, NF84, PKD88, SF86]. **expansions** [LZP84, ZP85]. **expectation** [ZW83a, ZW84]. **experiment** [KSS83, KVV⁺84, KSB84, SSSA82, SVS⁺81, SKV⁺85, SKE⁺84, VSS82]. **Experimental** [SK84b, BHW87, Sil89]. **experimentally** [ACvRS81]. **Explorations** [LDL⁺88]. **exponents** [ZW84]. **expressions** [FVV85, Sch89]. **Extended** [DH88, WP83, BMB85a, BMB85b, BP81, GS85, JG89, Kin87, KSL87, Koz87, MBB84, MBB85, RKM⁺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⁺84, KSB84, LUNV85, LB86, SSSA82, SVS⁺81, SKV⁺85, SKE⁺84, VSS82]. **Feldmann** [Lil87]. **fenchylidene** [FSST82]. **Ference** [Boy86]. **ferrous** [HS82]. **FH** [Del87]. **Fibonacci** [EB87]. **field** [AP87, BD82, BL81, CUCP89, 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⁺88, Ham87, Hil80a, Hil80b]. **five-membered** [DA83, DVA83, DPSF⁺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⁺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, MR83, 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⁺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⁺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⁺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⁺85]. **Generalized** [KJ87, NRM85, Bai86]. **generated** [FSL84]. **generates** [Mar87]. **generating** [Sch88]. **generation** [BKKB80, Bal82a, Bal82b, Bal83, Bal84, BR85, Bal88, BL88, KSJT83, KMS⁺87, LB89b, LB89a, RB85, Ran86, HBK80]. **generators** [RWKH87]. **Generic** [MB84]. **geometric** [Cri89, DHP83, Ess83, KNS86, KNS89]. **geometrical** [BTG85, BTG86]. **Geometrically** [GC85]. **geometries** [CG89, SKV⁺85, Sch82b, vdGB84, Gre85, VVVG81]. **Geometry** [Del84, FST81, FSST82, KJLW84, Bak87, BTG80, BSSW88, GBT80, GBT82, Gre84, HL83, MH83, MSČ⁺88, OC88, Sil81, Ska83, VLG89, Wer82]. **germyl** [MAR⁺84]. **glucose** [BP87a]. **Gly** [YJ86]. **glycine** [DCG81, KSS83, SVS⁺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⁺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⁺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⁺86, CvRSKJ81, CDL89, GBT82, HHK⁺86, Iku85, KvRS89, LS87b, NRS84, PKB88, ZD87]. **H-bonds** [ZD87]. **halide** [GB83, GSB85]. **halides** [CDL⁺87, GT83, MAR⁺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⁺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⁺87, LS87a, Ada89, KvRS89, Lop89, NRS84, ST87]. **Hg** [SMKH87a, SMKH87b]. **hidden** [MK84b]. **hierarchically** [BMB85a, BMB85b, MBB84, MBB85, RKM⁺85]. **high** [DK84, DK85]. **higher** [KSI88, ZP89]. **Highly** [DK85, RDW88, DK84]. **Hill** [CPV84]. **histamine** [Top87]. **HNC** [GT84]. **HOC** [BMB85a, BMB85b, MBB84, MBB85, RKM⁺85]. **hole** [KKR⁺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** [GLLOB88, KC87, BP81, BTRT88, Del81d, JMB87, KS82]. **hydrazide** [HH80]. **hydrides** [BE87, CPTC84, Del89, KKR⁺82]. **hydrocarbon** [CS82, SSSA82]. **hydrocarbon-chain** [CS82]. **hydrocarbons** [ASS⁺85, BKKB80, Bro83, BCC87, CW80, CZ88, HRKW89, HAKW87, IFvRSS87, KSJT83, Mey84, Sau89, VSS82]. **Hydrogen** [AKI88, Aid88, BTG81a, BG81b, BG81a, BG82b, BG82c, CDL⁺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⁺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, SMK87b, Ste89b, VU84]. **iii** [BHR⁺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⁺85, RD87, RKM⁺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⁺84, Rou87]. **INDO** [BG80, CW80, DS80]. **INDO-type** [BG80]. **inductive** [BCT83]. **infinitely** [HAKW87]. **influence** [BTG81a, BC89]. **information** [BMT81, Jur88, RRG⁺84]. **infrared** [WW81]. **Ingold** [Mey80b]. **inhibitor** [Fuj87]. **inhibitors** [Gre85]. **inhomogeneous** [ZR81]. **Initial** [FSL84]. **Initio** [OG86, PUNC86, Wib86, Aid88, ADY89, ABP80, ASS⁺85, AFK82, AVBF84, BT81, BMLR88, BR89, BP81, BG86, BTG80, BTG81b, BTG81a, BTG82, BTS⁺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⁺84, KVV⁺84, KSB84, KSL87, Koz87, LSROT80, LCY82, LH87, MC88, MFG89c, MFG89a, MV87, MTN87, MH83, MSČ⁺88, OLBM83, PKB88, PHG89, PUC89, STH81b, SS81, SSSA82, SVS⁺81, SKV⁺85, vRS86, SAP88, SAF88, SKE⁺84, SK86, Str85]. **initio** [TG83, Top87, VSS82, Van88, Wib84, WSP88, ZPCR82, ZPPC83, ZD87]. **Inn** [Ano83a]. **Innate** [KR87]. **inner** [TKK⁺81]. **inner-shell** [TKK⁺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⁺86, Ada89, BT80b, BTS⁺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⁺86, BKC86, BG82c, DTPR85, Dyk88, Gen87, GRS88, SHK83].
internal [CU89, Hin80, KJ82, LS88, Ran83]. **International** [Ano86i].
interpolation [Sil89]. **interpretation** [Gre84]. **Interscience** [Tri82].
intersections [LR87]. **intrachain** [OTPH87]. **Intramolecular**
 [BTS⁺83, BTG81a, KMS85]. **introduced** [TSH81a]. **Introduction**
 [Coo80, Mez87a, Gar82a, Tri82]. **invariant** [KTVRS86]. **invariants**
 [OMK⁺88]. **inverse** [Häs87]. **inversion** [ADY89, Ösa82, SF85].
investigation [AP85, FKS85, GTB81, GHT87, Sie85]. **Investigations**
 [FKS86, BT80a, BT80b, GS85, RRH86, SKE⁺84]. **involved** [BTRT88].
involving [BHR⁺86, EGM⁺89, KvRS89, KSL87, ST80, Sil81, ZP84]. **iodine**
 [DHS84]. **ion**
 [Del86, Del87, EW87, Ehr89, GBT82, KKR⁺82, MK85b, NRS84]. **ion-fitted**
 [NRS84]. **ionic** [BG80]. **ionization** [GT83, Gre85, KKR⁺82, TKK⁺81].
ionophore [MK84a]. **ions** [Bai84, CE87, Iku84, Kel80b, KS83]. **IR** [SBS82].
Ishtar [AP85]. **iso** [Rit86]. **iso-butylene** [Rit86]. **isocyanate** [LLC85].
Isocyanide [vRSSRH86]. **isoelectronic** [KPRT81, PMZ86].
isoelectronically [Kel80b, Kel82]. **Isomer** [BMT81, Häs87]. **Isomeric**
 [KvRS80, DPCS80, RRG⁺84]. **isomerizations** [Kel80b]. **isomers**
 [CvRSKJ81, DHP83, GDO89, GHT87, HT88, Kel80b, KMS85, SKJ88, TG83].
isomorphisms [STZ88]. **isopotential** [NSGK⁺81]. **isopropyl**
 [HML83, KSB84, LH85]. **Isotope** [AF83, HLH83]. **isotropic** [LPB84].
Iterative [Gal82, Per84]. **IV**
 [BT81, AS88, BT80b, KKR⁺82, TDK83, TSH81a]. **IX**
 [MK84b, ROK86, Tat85].

J [Ano88c, EGM⁺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⁺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⁺82, LWD82, WM89]. **lone-pair** [WM89]. **Long** [EGM⁺89, FWS89, SSSA82]. **long-chain** [SSSA82]. **Long-Range** [EGM⁺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⁺83, LV88, PV82a, vGBC⁺84, Lil87]. **Macromolecules** [De 86a, De 86b, GM86, BK86, Kar86, Kar87, VK80]. **Madelung** [Tay87]. **magnesium** [JI88]. **Main** [SLR⁺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⁺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⁺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⁺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⁺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** [Ano89]. **membered** [ADY89, AYS80, DA83, DVA83, DPSF⁺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⁺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⁺89, FS83, Gil84, GT82, GT83, Has84, Iro80, KSS83, KPE⁺84, LKL87, LA85, OE89, SVS⁺81, SCCvRS82, MAR⁺84]. **methyl-** [OE89]. **methyl-and** [FS83]. **methyl-CH** [KPE⁺84]. **methylamine** [BG82b]. **methylbutanoate** [SKV⁺85]. **Methylcyclohexyl** [VMNGTVM86].

Methylene [FOSV86, BW81]. **methylhistamine** [Top87]. **methyloxiranes** [DPCS80]. **methylphenylalaninamide** [KYJ88]. **methylpropanoic** [SKE⁺84]. **methypyrazole** [CSCD⁺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⁺86, HSW82, LHC84, MSSS80, MSS82, Top87, VVVG81, VMNGTVM86, VFM⁺89]. **MINDO/3** [BSSW88, CZ88, HHK⁺86, Top87, VMNGTVM86, VFM⁺89]. **MINI** [STH82, TSH81b]. **MINI-1** [STH82]. **MINI-3** [TSH81b]. **MINI-4** [TSH81b]. **minicomputer** [Coo77, Car85]. **minicomputers** [See81]. **Minimal** [TKK⁺81, RPD⁺86]. **minimization** [BHW87, BBO⁺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⁺89, TLA89, AP87, AKI88, CUCP89, GCW88, PL87, PUNC86, PUC89]. **MM2/MMP2** [PL87]. **MM3** [AL87]. **MMP2** [OE89, PL87, STYA87]. **MNDO** [Bai84, BF82, BSSW88, DGW⁺81, DM83, DR83, DL83, DFC⁺84, DHS84, DR86, FS83, FS89, GBP85, GRS88, GHT87, Gol87, HHK⁺86, JdKdWB87, OUV84, Top87, Ver82, VSSS84, VFM⁺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⁺89, MAR⁺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⁺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⁺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⁺82, LCL84, SKV⁺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⁺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⁺84, Mey86, Mey88, MKSW83, MK84b, Mul88a, Mul88b, PR84, PR87, Ran82, STH81b, SDKM87, SK84a, TKK⁺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]. **monoprotated** [EWM85]. **monosubstituted** [Del81a, VFM⁺89, BTG81a]. **monotone** [Per84]. **Monte** [Che89, Gar89, GLOB88, JMB87, KS82, MC88, OC88, RMB86, RPV87, ZR81]. **Morse** [DbCV⁺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⁺86]. **multidimensional** [LDL⁺88]. **multiexponential** [SS84]. **multiphoton** [BG87]. **Multiple** [RFLC89, LS88, MSG80]. **multiplication** [BC87, LM89]. **multiplicative** [Van88]. **multiplier** [Dil87, vdGB84]. **multiply** [CBR87]. **multiple** [PHG89, Wil88]. **multireference** [Ada89, CP87a, FBKK85]. **MuMATH** [Tri87, Tri88]. **mutagenesis** [Tin81]. **mutagenicity** [KR88]. **myelin** [GS87b].

N [Del89, GHT87, LB87, Ran86, TKK⁺81, TG83, BTG82, BTS⁺83, BGT84, CvRS81, HHK⁺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⁺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⁺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** [Ösa82]. **nonan-9-one** [Ösa82]. **nonane** [SSSA82]. **Nonbonded** [WM87, LCY82]. **nonclassical** [WB80]. **nonelectrocyclic** [BCB82]. **Nonempirical** [SLR⁺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⁺83, CDL89, CvRS81, CMRW86, Del89, GBT82, HPR80, LS87a, NR80, AG88a, Ada89, BTG82, BHR⁺86, CvRS81, CMRW86, HHK⁺86, HD88, KvRS89, Lop89, NRS84, PMZ86, KPE⁺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⁺87, Mey80a, WP82]. **oligonucleotides** [Gre83]. **Olti** [Boy86]. **One** [PKD88, AM88b, GHF87, KSI88, KF88, Ösa82, 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⁺86, HTT88]. **open-ended** [BD82]. **Open-shell** [Kal87, HHK⁺86, HTT88]. **opening** [Kel82]. **Operational** [Sil85]. **Operator** [HO83]. **operators** [Jaf88, Jug84]. **opiates** [FSH⁺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⁺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⁺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⁺85, CF83, Del85, Del86, FS83, MSS82, RS85]. **oxygenated** [BS89]. **ozone** [KvRS80, LH87].

P [Ano86b, Del89, DCNG85, Wib86, DCNG85, ROK86, TKK⁺81]. **p-Tolylsulfonyl-Sulfilimine** [TKK⁺81]. **package** [NSKNK87]. **packing** [HH80, HS82]. **pages** [Lip83a]. **pair** [BG82c, SMOT85, WM89]. **pairs** [Aid88, DCG81, KKR⁺82, LWD82, SRKT87]. **Palm** [Ano83a]. **pancreatic** [FM87, Fuj87]. **Parallel** [See81, WD88, GDP⁺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** [VSSS84]. **Pattern** [LS89a, LS89b, LS89c, OMK⁺88]. **Paul** [Boy86]. **PCILO** [BP82, LWD82]. **PDP** [Coo77]. **PDP-11** [Coo77]. **penetration** [PW82]. **pentapeptide** [CP81, YJ86]. **pentenone** [ST80]. **PEOE** [HLG88]. **peptide** [OLBM83]. **peptides** [AH85, LGB⁺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⁺85]. **PERTURB** [FE87]. **perturbation** [CP87a, FE87, FBBA86, FC88, RV85, WP83]. **perturbed** [TDK83]. **Peter** [Gar82b]. **Ph** [FS89]. **pharmacological** [FSH⁺84]. **phase** [FS82, LCL84, LLC85, LDP⁺87, LDL⁺88, RRH86, Sen87, SK86, VVVG81, VFM⁺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⁺87, Sch86]. **Physicochemical** [GC86, GPC88]. **Pictorial** [GDP⁺85]. **Pitfalls** [BA82]. **pithomycolide** [HPW82]. **Planar** [PV82b, BTG82, GBT80, GBT82, HR85, HR87]. **plane** [BN85, LTLA87]. **planes** [GDP⁺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⁺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]. **polymimials** [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⁺88, Lop89, Mar87, MC88, MS88, MR83, PHG89, SMOT85, SPBO87, SO87, Sch88, ST80, VDD86, VSS84, Wil88, WSP88, ZM88]. **Potentials** [SLR⁺86, BKC86, BG82c, CF87, DTPR85, DbCV⁺86, Dyk88, Gen87, GT83, KKR⁺82, LDP80, SMKH87a, SMKH87b, TKK⁺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⁺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⁺85, Rap84].
process [BBJ88]. **processes** [BG87]. **processing** [PPT⁺80, See81].
processor [BD84, BW83, KW86, RDW88]. **Processors**
 [Bai86, EM84, HD88]. **prodine** [FK84]. **produced** [KJ85]. **product**
 [BP87b]. **products** [GHHS85]. **Program**
 [Ano86b, ABE⁺85, BFB85, BBO⁺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⁺84].
Propanic [EGM⁺89]. **propanoate** [KSS83]. **propanoic** [SKE⁺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⁺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⁺89, Ved88]. **proteins**
 [KNS86, KNS89, PPT⁺80, WG87, WKNC86, ZP85]. **Proton**
 [HL83, CDL89, DA83, DVA83, DM86a, Del85, EGM⁺89, FS83, KKR⁺82,
 MFG89a, OUV84, RS85, SAV88, TMOW85, VFM⁺89, ZP84].
proton-proton [EGM⁺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⁺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⁺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⁺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⁺88, VCZB89]. **recurrence** [RLR88]. **recurrence-based** [RLR88]. **Recursion** [DS87, HO83]. **redistribution** [OTW81]. **reduced** [HD88, ZW83b]. **reductase** [Gre85]. **reduction** [Gre85]. **reequilibration** [Mor85]. **reference** [MSC⁺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** [IÖ84, Mey84, HAKW87]. **removal** [MK84b]. **renormalized** [Bra89]. **Representation** [CW81, Wil88, Ehr84, GDP⁺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⁺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+81, BT81, Bai84, KSL87, LB87, TKK+81, VSS84]. **S-Diphenyl-N** [TKK+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+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+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+85, HR87, HRKW89, Lau88, LBM89, Mag84, MFG89b, MH83, MSČ+88, NRR82, OTW81, ST89, SMK87a, SMK87b, 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+86, HTT88, Kal87, MR80, RA87, TKK+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+84]. **similarity** [AJMM88, HB87, JBFR86, MBB84, Jur88]. **Simple** [KNS85, NSGK+81, PUC89, CZ88, CS80, FT89, FS89, MAR+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⁺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⁺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⁺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, MS⁺88, NVGB81, SBS82, XB86]. **spectral** [KJ85]. **Spectroscopic**
 [ZBR80, KPE⁺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⁺84, DHS84, HAKW87, JH83, KKR⁺82,
 KJ82, LDP80, Lin88, LR87, MM87, Sch82a, SM80, VU84, ZP84]. **Stationary**
 [Lop89, KSHD88, LDP⁺87, LDL⁺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⁺84, KSB84, SSSA82, SVS⁺81, SKV⁺85, SPBO87, SKE⁺84, VSS82, PR80, SSSA82, SKE⁺84].

Structure
 [GC86, JSKI88, vRSSRH86, ABE⁺85, AYS80, AVBF84, BMB85b, BMR87, BTS⁺83, BBJ88, DS80, GPC88, GT82, GB83, HW80, HAKW87, KK85, KR88, KS83, LS89a, LS89b, LS89c, Lil87, Lip86, LYH87, NVGB81, OMK⁺88, PW82, PSSS80, PFRS82, RDW88, RP80, RRI88, SVS⁺81, SWM83, SM80, Tin81].

Structure-Activity [GC86, GPC88]. **Structure-Directed** [GC86].

Structures [BPP82, OG86, ASS⁺85, BMB85a, BMB85b, Bal85, BE87, Bro83, CvRSKJ81, CG89, Del89, FS82, HR85, HR87, HRKW89, JT80, KvRS80, KC87, KYJ88, KVV⁺84, KSB84, KMS85, LV88, MSSS80, MSS82, MBB84, MBB85, PPT⁺80, PUC89, RKM⁺85, RRG⁺84, Sch82b, Sch88, SMG87, VSS82, VVVG81, WKP⁺80, WM88]. **studied** [Osa82]. **Studies** [BG81b, BG81a, BG82b, BG82c, DLMR85, Jur88, Wer82, AJMM88, BP81, BG86, Bys83, CDL89, CMRW86, FMTS84, God87, Gre85, HMA82, HSS83, HSEC83, JI81, JB85, Kao88, KB84a, KB84b, KM85, KSS83, KVV⁺84, KSB84, KK85, KR88, KSL87, LCY82, LLSC85, LKL87, LDP⁺87, LZ89, LBZ89, Lip87, MK85b, MTN87, OMK⁺88, PUC89, RMB86, SHDP89, SOR86a, SOR86b, SORT86, SOR87, SSSA82, SVS⁺81, SKV⁺85, SKE⁺84, VSS82, VVVG81, WSP88]. **Study** [SMOT85, VMNGTVM86, AG88a, Aid88, ADY89, Bai84, BMLR88, BTG80, BTG81a, BTG82, BTS⁺83, BGT84, BSM83, Che89, CF87, CDL⁺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, OLB83, PMZ86, PHG89, RFP86, RBEV80, RPV87, Rue87, SS81, SSSA82, SAP88, SAF88, SM80, SMG87, SK84b, TLA89, TKK⁺81, TG83, Top87, Tos84, VV88, VSSS84, VFM⁺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⁺88, KPRT81, SCCvRS82]. **Substituted** [FKS86, HML83, Kel80b, Kel82, LH85, MFG89a]. **substitution** [Rit86]. **substrate** [TTZWGQKC81]. **substrates** [Gre85, MM89]. **substructures** [BFF86]. **sulfamates** [OMK⁺88]. **sulfide** [SBS82]. **Sulfilimine** [TKK⁺81]. **sulfoxides** [Tai81]. **sulfur** [Bai84, DM83, DR86, LB87, Mag84, MSS82, ST89, TKK⁺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⁺88, Lop89, Mey88, MK84b,

PASTB87, ST80, WSP88, Mey86]. **Surfaces**
 [YF86, AM88a, DPCS80, FKS85, IÖ84, KE89, KJ87, Ōsa82, 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⁺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⁺84, Jur88]. **Szymnsky** [Ran86].

T [Ano86b, LR87]. **T.-S** [Ano86b]. **tables** [LB89b, SN87]. **taste** [OMK⁺88].
tautomer [Gre85]. **tautomerism**
 [BSM83, CSCD⁺89, ROK86, Top87, Zie83, ZPPC83]. **tautomers** [BT80b].
Te [RBEV80]. **technique**
 [BD82, DE83, Gar89, HO83, Kel80a, LMV86, Per84, RPD⁺86]. **techniques**
 [SL81, TS83, RDAF83]. **technologists** [Ran86]. **Teller** [LR87]. **tempered**
 [DHK89]. **ten** [KKR⁺82]. **ten-electron** [KKR⁺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⁺89, CE87, FK84, GTB81, Hur88,
 Iku85, Kao88, KPRT81, KS83, LDP80, PUC89, Ran80, VSS82, WK81].
theorem [GT83]. **theoretic** [RRG⁺84]. **Theoretical**
 [Ano86k, CDL⁺87, CMRW86, FKS86, Gen87, Gre85, HMA82, Iku85, Kao88,
 LLC85, LLSC85, LKL87, LPB84, LZ89, LBZ89, Rue87, SAV88, VU83, VU84,
 VFM⁺89, BKKB80, BKT82, Cre82b, FBD80, Gre83, HT88, HPR80, HML83,
 HLH82, JDS89, KvRS80, KPRT81, Kin87, LHOM84, LH85, Lip83b, LUNV85,
 OMK⁺88, PR80, TW81, WB80, LDP⁺87, RRH86]. **Theoretically** [KJ85].
Theory
 [CG86b, KKR⁺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].
thermal [Kel80a, Kel80b, Kel82, Rue87, SF85]. **Thermochemical**
 [Cre82a, Cre82b]. **Thermodynamical** [BF82]. **thermodynamics** [Boy86].
these [ZP84]. **thin** [LP88]. **thiocarbonyls** [BSM83]. **thioketone** [BSM83].

thiolformic [BTG80]. **Thiophene** [TLA89]. **third** [DH86]. **third-** [DH86].
Three [Cla81, Cla82, Cla83, GC86, IL86, ADY89, GBT82, GPC88, GDP⁺85, LW88, PKB88]. **Three-Dimensional** [GC86, IL86, GDP⁺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⁺81]. **Tool** [CG86b, GRS88, HK88, See81]. **Topological** [Bac89, IL86, BMT81, BW89, Kel80a, MBB84, MT82, RRG⁺84, Rou87, Sim87, BMB85b]. **Topology** [LR87, Kel80a, Kel80b, Kel82, Kin87]. **topology-allowed** [BW81]. **torsion** [BA82, LS84, TMrGM88]. **torsional** [AP80, CP89b, IÖ84, LA85, MHA89, Ösa82, KB84a]. **total** [TM85, Cre82b].
toyocamycin [SOR86a]. **trajectories** [BSSW88, SDB87]. **trajectory** [KW86]. **trans** [BTG80, BL81, DPSF⁺88]. **trans-2** [DPSF⁺88].
trans-thiolformic [BTG80]. **transannular** [EW87]. **transcription** [SOR87]. **Transfer** [KHS86, BT80a, BT80b, CDL89, LLSC85, ST87, TMOW85, ZP84].
Transfer-Matrix [KHS86]. **transferability** [SSSA82]. **transferable** [NSKNK87]. **transform** [SF85]. **Transformation** [TG86, ČHS84, Ess83, GF87, Koz87]. **Transition** [BMR87, Bak86, Bau84, BG80, CG89, DH87a, DH87b, DH88, FB89, GT84, HE88, KM85, MS88, PH83, SMKH87a, SMKH87b, Sch82a, Sch82b, SWM83, TSH81b, ZP84].
transition-state [CG89]. **transitions** [BCT83, Gor88, TM84].
transmembrane [Kim85, VU83, VU84]. **transmission** [CGN87, DCNG85].
Transport [GM86]. **Treatment** [Jaf88, SLC86, SS84, GBP85, Jug84, KDKC83, Koz87, NLA84, Sil85, SA80, Tay84]. **tree** [CRR85, LS88]. **trees** [KMS⁺87]. **trialene** [ACvRS81]. **triazole** [CSCD⁺89]. **tricarboneyls** [BG80].
triethylamine [FWB85]. **trimethylisochromanes** [OE89]. **Trinajstic** [Ran86]. **trinucleotide** [YJ86]. **trioxide** [PSSS80]. **Tripeptide** [LS89a].
Triplet [FOSV86, CF83, DPCS80, HW82]. **triplet-state** [DPCS80]. **Tripos** [CCV89]. **tRNA** [LDP80]. **Tropsch** [CS82]. **truncated** [SO87]. **Tubercidin** [SOR86b]. **twisted** [HR85, HR87]. **Two** [BR87, ČHS84, KF88, LV88, MM87, Ösa82, PW82, RLR88, RLR89, SI88, SN87, SK84b, LCC87]. **two-center** [PW82, RLR88, RLR89]. **two-dimensional** [SI88, SK84b]. **two-electron** [ČHS84, MM87, LCC87]. **two-parametric** [Ösa82]. **Type** [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].
UMP2 [ČFHS85]. **unbranched** [RHP89]. **uncatalyzed** [OLBM83].
uncomplexed [MK84a]. **unconventional** [CG86a]. **Undecanes** [IL86].
undecapeptide [PHG89]. **unified** [Jug84]. **unimolecular**

[FS82, HB82, SF85]. **Unique**
 [BMB85a, BMB85b, MBB84, MBB85, RKM⁺85]. **Units** [De 86a].
unrestricted [MSG80, RFLC89]. **unsaturated** [AYS80]. **unsymmetrical**
 [Kel80b, Kel82]. **unweighted** [ZW83a]. **upon** [HT82, RS85]. **Uracil**
 [Zie83, Del81b, Del81d, Del81c]. **urea** [BHR⁺86]. **Use** [ČHS84, Dil86, BA82,
 Dil87, GS85, Hur88, Kar87, KR88, MR83, RV85, TSH81a, Top87]. **used**
 [LDP⁺87]. **Useful** [CG86b]. **Usefulness** [FBKK85]. **using**
 [Bre81, BG81b, BG81a, BG82b, BG82c, Cio87, Coo77, DFC⁺84, FGR89,
 Gen87, GCW88, HLH83, KS82, KJLW84, KO86, KBS88, LMV86, LGB⁺89,
 LW88, MR80, OMK⁺88, PR84, RDW88, RRG⁺84, RLR88, Rou87, RDK83,
 TMrGM88, TW81, WP83, ZW83a, ZW84]. **utilizing** [NSKNK87].

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⁺84, MŠ⁺88, PKB88, Ska83, SBS82, VVVG81, XB86]. **vibrations**
 [LPB84, PV82b]. **vibronic** [LS84]. **vicinal** [DVA83]. **view** [GDP⁺85]. **VII**
 [KB84b, MKSW83, TSH81b]. **VIII** [BG82a, BTRT88, RKM⁺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, GLOB88,
 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]. **Willet** [Jur88]. **within** [AP87, BG82b, BG82c, Ehr81, TM85, TW82]. **without** [Bak87, Mez87b]. **World** [Ano86k].

X [BG86, CvRS81, FS89, FS82, MV87, TW81, HPR80, Iku85, KPE⁺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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