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Title word cross-reference

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. 2 \[\text{[FKS85].}\] 2

[CMRW86, Lop89]. 2

n \[\text{[LHOM84].}\] 2

v \[\text{[MTN87].}\] 3 \[\text{[Ada89, Bai84, BHR86, Del87, Del89, FWB85, FS89, FS82, GBT82, Iku85, KvRS89, KPRT81, LS87b, NRS84, Ran83, Sie85, SK86, TMOW85, WKP+80].}\] 3

[SN87]. 4 \[\text{[BL88].}\] 4

n \[\text{[FKS86].}\] 5 \[\text{[WKP+80, YJ86].}\] 6 \[\text{[GDO89, Hin80, Sax85, SKJ88].}\] 6

2 \[\text{[BMLR88, CvRSKJ81, CvRS81, FS82, KvRS89, KSL87, LR87, NR80, RAS85, Sax85, SK89, ST80, WKP+80].}\] 2+

n \[\text{[Del87, FS82, TMOW85].}\] 2

3 \[\text{[Ran83].}\] 3

[Sen87]. cos \[\text{[Sch89].}\] d

CE87. FC = SCe \[\text{[Mas88].}\] HC = SCe \[\text{[Mas88].}\] l, m, n \[\text{[Dod84].}\] log P \[\text{[Lew87].}\] N \[\text{[BTRT88, HSS83, AP80, JdKdWB87, LCY82, SSSA82, TM84].}\] n = 0 \[\text{[FKS86].}\] n = 3 \[\text{[LHOM84].}\] n \rightarrow \pi \[\text{[Del81c].}\] n \rightarrow \pi^+ \[\text{[Del81a].}\] \nu \[\text{[Lew87].}\] \omega \[\text{[ZW83a].}\] p \[\text{[Per84].}\] p < 0 \[\text{[Per84].}\] \pi \[\text{[AG88b, Gre84, HAKW87, KM85, LCY82].}\] \pi^* \[\text{[Lew87, TM84].}\] \pi^* \leftarrow n \[\text{[SM80].}\] \pi^* \leftarrow \pi \[\text{[SM80].}\] \rho^{1/2} \[\text{[Mar87].}\] e \[\text{[FS82, GT82].}\] \rightleftarrows \[\text{[GT84, PMZ86].}\] S \[\text{[Bra89, BW81].}\] sd \[\text{[SMKH87a].}\] \sigma \[\text{[Cla83, WB80].}\] spd \[\text{[SMKH87b].}\] \varphi \[\text{[Sen87].}\]

* \[\text{[Cla83, ST89].}\]

-accepting \[\text{[KM85].}\] -acetyl-N-methylphenylalaninamide \[\text{[KYJ88].}\]

-alkanes \[\text{[LCY82].}\] -alkyl \[\text{[LCY82].}\] -azabicyclane \[\text{[FSH+84].}\] -bond \[\text{[Gre84].}\] -butane \[\text{[AP80].}\] -carboline \[\text{[SMOT85].}\] -catechin \[\text{[VM86].}\]

-chymotrypsin \[\text{[VCZB89].}\] -cis-1 \[\text{[BW81].}\] -electronic \[\text{[HAKW87].}\]

-epicatechin \[\text{[VM86].}\] -Factors \[\text{[KMST86].}\] -hydroxyacrolein \[\text{[BTG81b, GBT80].}\] -Li \[\text{[MV87].}\] -methylpyrazole \[\text{[CSCD+89].}\] -MP \[\text{[SMKH87a, SMKH87b].}\] -nitrosamine \[\text{[HSS83].}\] -nitrosamines \[\text{[BTRT88].}\]

-nonane \[\text{[SSSA82].}\] -nonbonded \[\text{[LCY82].}\] -nonclassical \[\text{[WB80].}\]

-phellandrene \[\text{[PV83, RP80].}\] -substituted \[\text{[HML83, LH85].}\] -SW \[\text{[TW81].}\] -symmetric \[\text{[FWB85].}\] -terminal \[\text{[CP81].}\] -type \[\text{[ST89].}\]

/2 \[\text{[DS80].}\] /3 \[\text{[HSW82, LHC84, MSS80, MSS82, VVVG81].}\] /BW \[\text{[TW82].}\] /CI \[\text{[ZBR80].}\]

1 \[\text{[GDO89, RP80, STH82, Tat85].}\] 1-Methylcyclohexyl \[\text{[VMNGTV86].}\] 11 \[\text{[Coo77].}\] 164 \[\text{[KW86].}\] 1983 \[\text{[Str85].}\] 1984 \[\text{[Ano83a].}\] 1986 \[\text{[Ano86].}\] 19XX \[\text{[Ran86].}\]

3 [BSSW88, CZ89, 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-ethyl-l-histamine [Top87].
4-methylhistamine [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, KY88, KPE+84]. acetyl-alanine-proline-alanine [FM87]. Acetylcholine [MC88]. acetylene [PFR82]. acetylenes [AP87]. acetylenic [HMA82]. acid [BTG80, BTG81b, BH8+86, FS89, GBT82, GT82, LS89a, LSROT80, LCL84, LKL87, OC88, SKE+84, ZP84]. acidities
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, DPF°88, HE85, HLH83, KR88, LS87b, Lin88, LR87, VDD86, ZR81, ZP89]. **Applications** [Bur80b, KHS86, MS88, BR85, Gil87, Kin87, RD87, RB87, SNR83, SDB87, Tay84, vGB84, BL88, KT88, SK86, Ste89b, Li87]. applied [HO83, Kim85].

**appraisal** [HP84a]. **Approach** [Ano88c, IL86, AFR82, BG87, BG82a, BMT81, CP89a, Cio87, DBVMB84, Fuj87, Gla89, HPR80, KPR81, KR88, LH87, OE89, PR80, SDKM87, SMOT85, SRPY88, Sil81, SK84a, FA86].


associations [NF84, SF86]. **Atom** [iVR85, SLR°86, Cha83, CPH85, LDM89, LLSC85, ST89, SK85, WKNC86]. **Atom-Atom** [SLR°86]. Atomic [BR89, CF87, DM86b, GC86, GPC88, THW80, BW89, CP89a, CW81, FV885, JB85, LV88, Mui88a, Mui88b, Ran80, Wl88]. atoms [ASS°85, AKRA84, BM85a, 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 [GH87]. Automatic [RDW88]. automating [BBJ88]. automorphisms [ST88]. average [BkBT82]. avoiding [Mom81]. axial [ST82]. aza [BGT84]. azabicyclane [FSH°84]. azapurine [SOR87]. azines [SAV88]. azoxyalkanes [By83].

B [Cra85, DBVMB84, GDOS89, Kro88, PD83, CvrRS81, De 86b]. **B-DNA** [De 86b]. **Babu** [Li87]. bacterial [Tin81]. **Balaban** [Ano86b, Ano86b]. balance [MH83]. band [LS84]. bare [Mey88]. Bargon [Jor81]. barrelene [SAF88]. barrier [Ham87, Hin80]. **Barriers** [WM88, ADY89, AM88b, BMLR88, BW81, KJS2, PUC89]. base [Aud88, GT82, SRKT87, SK85]. based [BMB85a, BMB85b, Dyk88, MB84, 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, LM89, M89, MSC+88, AKRA84, ARS85, Bau84, BP81, CM89, CCSvRS83, Cre82a, Del84, DHK89, DH86, DH87a, DH87b, DH88, FA86, FV85, GT84, Gro87, HR87, MK85a, MFG89c, MFG89b, MTN87, MR80, MH83, NRS84, NRR82, OTW81, PH83, RAS85, RA87, ST89, SH83, SCCvRS82, SCvRSH87, SM87, SGW83, TKA+81, WP83, WM88, YNAK88, ZW83a, ZW84, AKRA84, Mag84, MFG89b]. basis-set [MH83, AKRA84].


binding [BP81, BC89, Cri87, GC85, Hil80a, Hil80b, KCF84, MK85b, De86a, De86b]. biochemical [Gol87, KB88, ZD87]. biological [JG89, SMORT5, SN83, TMOW85, WG89]. biologically [FK84, VV88]. biopolymers [AV84]. biphenyl [HR85, HR87]. Bis [BL81]. bit [HD88]. Bivariate [Si89]. BLMO [ZW84]. blocker [SHDP89]. blocks [NSKK87]. BNC [GT84]. body [BMLR88, BG82a]. Boltzmann [DM89]. Bond [Bai86, BE87, AG88a, BTG81a, BTG82, BG84, Del81b, Del81c, Del81d, Del81e, Del83, Del87, Gre84, HRKW89, Iku84, Jug84, KPE+84, LSROT80, LD87, MK85a, MFG89c, MFG89b, NSG+81, NR80, OLBM83, SAP88, Wil88]. bond-orbital [ZD87]. bond-polarization [MFG89]. bonded [Aid88, Dyk88, HPR80, KSL87, LSROT80, TMOW85]. bonding [AG88b, AK88, BTG81a, BG81b, BG82b, BG82c, DS80, Gol87, Gre84, Kin87, MK85b, NRM85]. bonds [Cl81, Cl82, Cl83, Fab88, LC82, PS87, SSSA82, WW81, WM88, ZD87].

Book [Boy86, Car85, Cra85, Gar82b, Gar82a, Gil87, Jor81, Jur88, Kro88, L87, Lip83b, Lip83a, Lip86, Ran86, Sch86, vRS86, Str85, Tri82, Wer82, Wil86].


C [FS82, Gar82a, DGO89, KPE+84, VM86, BL88, BTG82, BGT84, CvRSKJ81, CW80, Cz88, CvRS81, FWB85, FS82, FKS85, FKS86, GDO89, HHH+86, Kao88, LHOM84, MTN87, ST80, SN87, VM86]. C1 [SAP88]. C2 [SAP88]. Cahn [Mey80b]. calculate [BKL87]. calculated [BF82, BC83, BTG85, BTG86, FS82, GL88, GL89, HL83, LS89a, MSSS80, MSS82, MH83, OU84, TM85, WP82, ZW83a, ZW84]. Calculating [EM84, GSH88, Cri89, KCF84, Lin88, Mul88a, Mul88b]. Calculation [BkBT82, DFC+84, FWS89, IVRSS87, KI81, PV82a, RLR88, BR87, Bau84, Ber83, BN85, Bre81, BA82, Cha83, CW80, CP81, DS87, Dyk88, Fui87, Gal82, HW82, HG89, HL83, Lew89, MFG89e, MM87, MR80, NSGK+81, NN87, PLFL85, PR84, RLR89, ST81b, 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, CCSV83, Cre82a, Cre82b, CG86a, CT87, CL85, CE87, DGW+81, DTPR85, DM83, DR83, DH83, EWM85, Fab88, FKK85, FGR89, FWB85, FS83, GT84, GHT87, Gol87, GHHS85, GL87, HHK+86, HLG88, HW88, Hur88, Iku84, Ja88, JdKdWB87, Kar81, KHRvH87, Kro83, KKR+82, KSB85, LRP87, LCC87, LB89, LM85, Lew87, LGB+89, MK84a, Mag84, MK84a, Mey84, MH83, MSC+88, MM83, MM89, PW82, PW81, PL87, RAS85, RV85, SMKH87a, SMKH87b, SDKM87, SAV88, Sax85, SKJ88, SK89, Sch88, SL81]. calculations [ST87, SK85, SHK83, SB82, SCCV83, SCP82, SDB87, Str85, THW80, Van88, VDD86, Ver82, WP83, YNAK88, ZD87, AF83, DHS84, FA86, TMOW85, Lip86, Wer82]. calicene [HSEC83]. CAMSEQ [GCW88]. Canada [Ano86j]. Canadian [Ano86j]. cancer [BT80a, BT80b]. canonical [BMB85a, KDDHK89]. carbamate [KL87]. carbanions [BHR+86]. carbonic [BHR+86, GBT82]. carbonions [BP83]. carboxyl [ASS+85, BTG81a, MR83]. carbonyl [BT80a, BT80b]. carbonos [BG82a]. carborane [GDO89]. Carboranes [OG86]. carboxylate [BP81].

catacondensed [RHS89]. catalysis [FW89, Per84]. catalyzed [OLBM83].
[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**
[LD^+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, JBF86, MK85a, PUN86, Top87, ZW83a, ZW84,
BTG81b, CDL^+87, DM89, FGR89, Gla89, KPRT81, Kin87, KSS83, KPE^+84,
KSB84, PHG89, WBS80, GHT87]. **compatible** [CHS84]. **complex**
[CPTC84, DBVMB84, FM87, OTW81, SK86, TMOW85, YJ86].
**complexation** [DAU88]. **complexes** [BMLR88, Del81b, Del81c, Del81e,
Del83, Del87, Del89, Gen87, GRS88, HS82, JI81, KM85, Lin88, Ved88].
**compliance** [MR83]. **Component** [De 86a, SK85]. **Components** [SLR^+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, Ano86i, 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, Ball82b, Bal83, Bal84, BR85, Bal88, BL88, Cio87, CG86b,
DA83, KSJ83, KMS^+87, Lii87, LB89b, LB89a, OMK^+88, PLFL85, RB85,
TG86, BKK80, KB88, RKM^+85, RMB86, SAS87, TS83, Tri87, vBCG^+84,
Gil87, Boy86, Ran86]. **Computer-assisted** [DA83, Lii87].
**computer-oriented** [AS87]. **computerized** [Tin81]. **computers**
[BD82, CBR87, Gar82b]. **computing** [KNS85, SK84a, TTZWGKC81].
**concentration** [TTZWGKC81]. **concept** [JFG89]. **Condon** [DK85].
**Conference** [Ano86i]. **Configuration** [Wen82, Ada89].
**Configurational** [SRKT87, BMG84]. **Conformation**
[BP82, FSH^+84, HLPT82, HPW82, LS89b, SRPY88, Tai81, TMrGM88].
**Conformational**
[Ano88c, CwRS81, CP81, Cri82, Cri84, CL85, DPCS80, EIO85, FMT84,
FSH^+84, Fro86, GCW88, HW88, IL86, K884, OES89, PPT^+80, RMB86,
VM86, YJ86, ZPPC82, BSS88, BA82, CMR88, CP87b, DPSF^+88, Dod84,
FGR89, Ham87, LS89a, LDP80, LS88, MR80, NLB85, OTP87, Ös82,
RF86, SDKM87, SKV^+85, SKE^+84, VVVG81, VY88, VU83, WG87, Wer82,
Bur80b, KSS83, KVV^+84, KSB84, Mey81, SVS^+81, Sla83]. **conformations**
[BHW87, Che89, Cri89, Fab88, FSL84, G87a, HR87, JMB87, PR84, Sau89,
Sch88, ZPCR82]. **conformers**
[EIO85, KMS85]. cyclohexasulfur [LRP87]. cyclononane [FGR89].
cylooctane [IO84]. cyclooctasulfur [LRP87]. cyclopentadienes [Kel80b].
cylopentadienyl [Kel80b]. cyclopenteny1 [GHHS85]. cyclopropyl
[HML83, LH88]. cyclosporin [PHG89]. cytosine [Del83, PV82b].

d [Gil87, Kro88, Str85]. Damping [CU89]. Danuher [Aro88c]. data
[BF82, BC89, BBJ88, Cre82a, Cre82b, HD88, KSB84, KJ85, Mor85, PPT+80,
vRS86, Sch88, Si85, SS84]. databases [RDW88]. decane [Os82].
decanes [Bur80b]. decarboxylation [LCL84, Rue87]. decay [SS84, Sz87].
decomposition [FBD80, HB82, KHRvH87]. Dedication [Ano86a]. defects
[BG82a, SDL82]. defined [Gla89]. deformation [CE87, Kar87, LTLA87].
Degenerate [LvRS89]. degree [KR87]. dense [CM89]. densities [CE87].
density [AVF84, Bac89, BW83, Gh89, HAKW87, Jug84, K81, Mar87,
MSG80, OTW81, RB87]. Deorthogonalization [CP89a]. deoxyribose
[SPBO87]. dependence [Del84, HRKW89, Ehr84]. deprotonated
[ZPPC82, ZPCR82]. derivative [Bra89, MHA89, PHG89].
derivatives [BC83, FSST84, FS89, FK84, GHHS85, Kao88, WM89]. derived
[BR89, BG81b, CF87, KJ85, TMrGM88]. described [Bau84]. description
[BMB85a, BMB85b, LPB84, LWD82, MB84, MBB85, PAST87, P87,
RK85, ZD87]. design [Fuj87, HKB80, LDP+87, Cra85]. designs [Sil89].
detailed [CF87]. detection [BFF86]. determinants [SS84].
Determination [BFAG81, CRR85, CP87b, LCL84, OC88, SWM83,
TMrGM88, BHW87, D86a, MFG89b, SHDP89]. determined [BPP82].
determining [BBJ88, DE83]. deuterium [AF83, HLH83]. Development
[YNAK88, LPB84, Ran86, SHK83, CUCP89]. developments [DCG81].
development [ZW83b]. Dewar [Kel80b]. diabatic [BMR87].
diacetals [Bur80b]. diagnostic [Ran80]. diagonalization [BR87]. diagrams
[GDP+85]. dialkylcyclooctatetraenes [Tos84]. diamine [Ham87].
diaminomethylene [ASFW89]. diaminedichloroplatinum [KJ85].
diamions [WP89]. diatomic [BE87, DK84, DH89, 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 [CCvRS83, SCCvRS82, ScvRS87]. diffusion
[AS81, Gar89, Per84, RV87]. diffusion-limited [AS81]. Digital [TS83].
Dihetero [IL86]. dihydrofolate [Gre85]. dihydroxycarbene [FBD80].
dilute [GLLOB88]. Dimensional
[GC86, IL86, AM88b, GPC88, GDP+85, KSI88, SI88, SDL82, SK84b].
dimensions [LW88]. dimer [Has84]. dimerization [VU83]. dimers
[BG82b, VM86, ZP84]. dimethoxytetrahydrofuran [DPF8+88]. Dimethyl
[IL86, KMS85, OE89]. dimethyl- [OE89]. Dimethylcyclopentyl
[VMNGTV86]. dimethylpentane [CL85]. dimethylphosphate [MB87].
Diophantine [Bur82]. dipeptide [RMB86]. Diphenyl [TKK+81].

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].

dithiote [God87].

dithioglyoxal [God87].

divinylketone [Ska83].

dNA [Aid88, Dar89, De 86b, SRKT87].

docking [Kar86, PLFL85].


doubly-extended-guanidine [JG89]. Driver [Gil87]. driving [BA82].

Drug [Ano88c, BC89, Cra85, SDKM87]. during [CS82, SOR87].

dynamic [Mit88].

dynamical [Fn87].

dynamics [GM86, HB82, IL86, SL86, BBO +83, CU89, FM87, Fuy87, GHF87, GCW88, HLC88, NKC85, NK86, SHDP89, TJ86, YE89].

easily [KS83, KVV +84, KSB84, SSSA82, SVS +81, SKV +85, SKE +84, VSS82].

economical [NR82]. Ed [Jor81, Gar82b, Str85]. edge [Bal88, HB89, LB99a]. edge-weighted [Bal88, HB89]. Edited [Lil87]. editor [DMB88].

Effect [DPSF +88, HLH82, ASS +85, ASF89, BTG85, BTG86, BW89, FSH +84, G85, GT84, GL87, Kim85, NLA84, TS81a, TM84, WM88].

effective [KSS85].

effects [FSV86, RS85, AH84, AF83, AKRA84, BTS +83, BCT83, CS82, DVA83, Del81e, Del85, Del86, Del87, Ehr81, Ehr84, EH83, HPR80, HLH83, JI81, KPR81, KSL87, KSJ82, Mag84, MSC +88, MM89, PR80, Rit86, SSSA82, SMF89, SMG87, WB80, BTRT88].

Efficient [CCSV83, Dy88, KO86, CF88, FB86, Mas88, OTP87, PR87, SL81, Sens87].

eigenvalue [DK84, HT82, KDKC83, KKE88, Mas88]. eigenvalues [DK88, Gal82, NN87].

eigenvectors [G82, S87].

elastase [FM87, Fuy87].

elastin [C89].

elastic [WP83, ZM88].

electrically [Dy88].

electrochemiluminescence [AS81].

electrode [BFAG81].

Electron [AVF84, CPTC84, Cla82, GRS88, OT81, Bae89, BNR86, BW89, CHS84, CV88, Cla81, Cla83, CS80, DCG81, GDP +85, GT84, HLH82, KF88, KKR +82, LCC87, MM87, PW82, RLR88, RLR89, RB87, RDK83, WM88, ZW83a, ZW84, K87].

electrononegative [AS +85].

electrononegativity [LD89].

Electronic [KS83, KJ82, LY87, PPV83, SM80, ABE +85, AVBF84, BT80a, BS80b,
BE87, BKL87, Gor88, HAKW87, Lew87, NVGB81, PW82, RP80, SSSA82, SMG87, TM84, WD88]. electrophilic [FS89]. Electrostatic
[EHr86, HLG88, PASTB87, CF87, CW81, EM84, GSH88, LDP80, LZP84, MK4b, NSGK+81, PHG89, PR80, SK84a, Wi88, ZP85]. element
[KS88, MK85a, Si88]. elemental [WKP+80]. elements
[Bal83, CPTC84, CCSvRS83, DbCV+86, DH86, Gro87, KDEHK89, MHA89, PKD88, ScvRS87, SGW83]. Elizabeth [Ano88c]. ellipsoid
[ELB87]. Elsevier [Lip83b]. embedding [Cri82, Cri84, CP87b, Cri89]. emission [BCT83]. Empirical
[NK86, PW82, BG81b, BG81a, BG82b, CP87b, RPV87, SDB87, VDD86]. employing [WM89]. emulsion [TS83]. Enantioselectivity [LBZ89].
ended [BD82]. energetic [CPTC84, SPBO87]. Energetics
[GB83, SBLB83, HW88, KC87, OTPH87, VU83, VU84]. Energies
[EHr86, AYS80, Bys83, CvRS87, 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, BHH87, BSSW88, BBO+83, Car82, CDL89, CP81, Cri82, Cri84, CP87b, Del84, DPCS80, FWS89, FST81, FSPT82, FT89, FKS85, GB87, G88, Ham87, Has84, HHR87, I084, KSHD88, K82, LDM89, Lip86, LDL+88, Lop89, MHA89, MT82, NK86, Osa82, PLFL85, PR87, RDAS83, SDKM87, SOR86a, SOR86b, SORT86, SOR87, SPBO87, SO87, Sch88, ST87, SHK83, Tay84, TM85, TMrGM88, VK80, VSSS84, WG87, WM89, WMH88, WD88, WK81, WSP88, MK84a]. Energy-optimized [FA86]. enethiol [BSM83]. engineering [Gil87, Wen82]. England [Jur88]. enolic [LCL84]. enol [BT80b]. enthalpies
[Bys83, IvRS85, IFvRSS87, Wib84]. Enumeration
[BCC87, KHS86, KMST86, Cio87, Has87, K87, KMS+87, OTPH87, TK89]. environment [Run80]. enzyme [FM87, TTZGW8K81]. enzyme-ligand
[FM87]. EPEN [BG82b]. epicatechin [VM86]. equal [Dod84]. Equation
[EHr86, CPV84, DK84, DM80, GS85, GF87, K88, NS87, 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
[GS88, MFG89b, MH83, RP87]. errors
[MSSS80, OTW81, TM85, ZW83b]. essential [Fab88]. ester
[FG86, CF83, CDL+87, SBS82]. ethylenes
[FSST82]. ethylmethylamine [ABP80]. Ethylmethylsilane [PUNC86]. evaluating
[MBBA86, MR83, Sch89]. Evaluation
[FT89, MSSS80, MSS82, OUV84, BNR86, BCT83, JBFR86, Kar81, KR88, Ran82, Sch82a, ScvRS87, Szoo87, GR88, MK83, MK84b]. evaluations
[EM84]. Examination [ZP84]. example [RFLC89]. examples [Coo77].
exchange [KvRS89, SK86]. excitations [Wen82]. excited
[Cha83, Del81a, Del81c, DFC84, JH83, MM87, SM80]. excluded [HG89].
exclusion [SLB83]. expansion [CP89b, NF84, PKD88, SF86]. expansions
[LZP84, ZP85]. expectation [ZW83a, ZW84]. experiment
[KSS83, KVV84, SSB84, SSSA82, SVS81, SKV85, SKE84, VSS82].
Experimental [SK84b, BHW87, Sil89]. experimentally [ACvRS81].
Explorations [LDL88]. exponents [ZW84]. expressions [FVV85, Sch89].
Extended [DH88, WP83, BMB85a, BP81, GS85, JG89, Kin87, KSL87, Koz87, MBB84, MBB85, RKM85, WG89, DH86, DH87a, DH87b].
extended-guanidine [WG89]. extension [CU89]. external [Lin88].
Extrapolation [SK84b, BHW87, Sil89].

F [CvRS81, DD81, Del89, FKS85, FKS86, MFG89c, CCSvRS83, HPR80, JDS89, KT88]. Factors [KMST86, DK85]. family [Mil87]. Fast
[BC87, CBR87, Mat88, SCP82, Ber83, Kar86, LV88, TTZGWQKC81]. Faster
[MM83]. FCH [JDS89]. Fe [GLLOB88]. feasible [GC85]. features
[KSS83, KVV84, SSB84, SSSA82, SVS81, SKV85, SKE84, VSS82]. Feldmann [利87]. fenchylidene [FSST82]. Ference
[Boy86]. ferrous [HS82]. FH [Del87]. Fibonacci [EB87].
fields [BTG80, HP84a, MB85, 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-
[FBB86, PH83]. first-order [Ada89, GHF87, KBS88, SHK83]. first-row
[CCSvRS83, DHK89, DH87a, DH88, KTVRS86, SCCvRS82]. Fischer [CS82].
fitted [NR84]. fitting [Dar89, LMV86, LV88, SAS87]. five
[DA83, DVA83, DPSE88, Ham87, Hil80a, Hil80b]. five-membered
[DA83, DVA83, DPSE88, 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, ASS85, Rit86].
Fluorine-Substituted [FKS86]. fluorobenzene [BTG85]. fluorophenyl
[GG89]. fluorophosphine [SMG87]. fuctional [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,
CCV99, EIO85, GBT82, HP84a, HP84b, HH87, Hur88, LA85, MF85, MR83,
PV82a, RFP86, SK83, WM89, WP82, WKNC86, XB86, ZP89]. force-field
[HP84b, RFP86]. formaldehyde [HE85, HE88, SWM83]. formalism
[BMR87, NRM85, SL82]. formamidic [ZP84].

Graphite [SA80]. Graphs [Ano86b, BF85, Bal84, BR85, Bal88, BL88, DE83, EB87, HO83, HB89, LB89a, MBB84, Mi87, RB85, Ran83, ROK86, Sim87, STZ88]. Green [SDL82]. Ground [DM83, DR83, DH83, DHS84, BG80, Del81a, DTPR85, Has84, LR87, Ska83, WSP88, Del81b]. ground-state [WSP88, Del81b].

Groups [Di86, 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].

hydrogen-bonded [Aid88, LSROT80]. hydrogen-hydrogen [WM87]. hydrogenation [IFvRSS87, SAF88]. hydrolysis [KJ85, LKL87]. hydrophobic [GPC88, Lew89, KS82]. Hydrophobicity [GC86]. hydroxyacrolein [BTG81b, GBT80]. hydroxy [EWM85]. 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, Di87, FB89, FSST82, HB82, Hils80a, Ja88, Kels80b, KM85, Koz87, LS89b, LSROT80, LD87, MFG89b, MK85b, MSS890, MB85, MH83, RAS85, RPAF83, SMKH87b, Ste89b, VU84]. iii [BHR+86, AH85, BMBB85b, 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, Jun88, RRG+84]. infrared [WW81]. Ingold [Mey80b]. inhibitor [Fu87]. inhibitors [Gre85]. inhomogeneous [ZR81]. Initial [FSL84]. Initio [OG86, PUNC86, Wib86, Aid88, ADY89, ABP80, ASS+85, AFSK82, AVBF84, BT81, BMLR88, BR89, BP81, BG86, BTG80, BTG81b, BTG81a, BTG82, BTS+83, BPP82, BN85, BCT83, BTRT88, Bre81, BSM83, Bur80a, Cao89, CrvRSS81, Cre82a, Cre82b, CE87, DM86a, Del81a, Del89, DTPR85, EWM85, FKS85, GBT80, GBT82, GDO89, GT82, GT83, GT84, GHT87, GL87, GL88, GL89, HW82, HR85, HR87, HRRW89, HRS83, HSEQ83, HT88, HE88, IvRS85, Iku84, JI81, JFG89, KS84, Kar81, KB84a, KB84b, KHRvH87, Kvr88, KSS83, KPE+84, KV+84, KS84, KSL87, Koz87, LSROT80, LCY82, LHS87, MCF88, MFG89c, MFG89a, MV87, MTN87, MH83, MSC+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 [Ano86]. instruction [Tri84]. Integral
Integrals [KO86, DS87, FVV85, KF88, LCC87, PWS82, 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, BTT+83, Bre81, CF83, EWS87, Gre83, KTVRS86, KPR87, LV82, LD87, MV87, PASTB87, SHK83, Wen82].

Interactions [MKSW83, MK84b, BT80a, BT80b, Fra82, GPC88, GRS88, HLG88, KMS85, LS87a, LS87b, LCY82, PL87, PR80, SRKT87, SK85, WK81, WM87, HPR80].

Interactive [De 86a, De 86b, SOR86a, SOR86b, SORT86, SOR87, SLR+86, Ada89, BT80b, BTT+83, Bre81, CF83, EWS87, Gre83, KTVRS86, KPR87, LV82, LD87, MV87, PASTB87, SHK83, Wen82].

Interactions [MKSW83, MK84b, BT80a, BT80b, Fra82, GPC88, GRS88, HLG88, KMS85, LS87a, LS87b, LCY82, PL87, PR80, SRKT87, SK85, WK81, WM87, HPR80].
Knop [Ran86]. knowledge [Wen82]. Koopmans [BG82a, GT83]. Kowalski [Kro88].

L [Kro88, Lip83b, Lip83a, Str85, Wib86]. laboratory [Coo77, Car85].


M [Kro88, Wer82]. machine [BFF86]. macrocyclic [FSL84]. macromolecular [BB0+83, LV88, PV82a, vGBC+84, Lil87]. Macromolecules [De 86a, De 86b, GM86, BK86, Kar86, Kar87, VK80]. Madelung [Tay87]. magnesium [JII88]. Main [SLR86, BE87, DH86, SGW83]. main-group [DH86]. major [BF86, TMrGM88]. maleic [HH80]. malformin [HLPT82]. maneuver [Kar86]. manipulating [vGB84]. manipulation [FE87]. many [BG82a, BMLR88]. many-body [BG82a, BMLR88]. Mapping [ANO88c, Ke80a, Ke80b, Ke82, SJKM87]. maps [NSGK+81]. March [ANO88a]. Martin [ANO88c]. master [GF87]. Masthead [ANO88a, ANO88b, ANO88c, ANO88d, ANO81a, ANO81b, ANO81c, ANO81d, ANO82b, ANO82c, ANO82d, ANO82e, ANO83b, ANO83c, ANO83d, ANO83e, ANO84b, ANO84c, ANO84d, ANO84f, ANO84g, ANO85c, ANO85d, ANO85e, ANO85f, ANO85g, ANO85h, ANO86c, ANO86d, ANO86e, ANO86f, ANO86g,
Ano86h, Ano87e, Ano87f, Ano87g, Ano87h, Ano87i, Ano87j, Ano88k, Ano89d, Ano88e, Ano88f, Ano88g, Ano88h, Ano88i, Ano88j, Ano88k, Ano89k, Ano89d, Ano89e, Ano89f, Ano89g, Ano89h, Ano89i, Ano89j], matching.

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].


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, IO84, JT80, Kar87, LG8+89, LA85, LTLA87, MK84a, MK85b, Mey80a, Mey81, Mey86, Mey88, MM89, NLA84, OE89, PL87, PR87, SHDP89, SRPY88, SA80, TLA89, TmRM88, Tri88, VDD86, Ved88, VCB89, vdGB84, Lip83a].


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, JJ81]. Method [ KHS86, KO86, SJ86, AS88, Ada89, BD82, BFF86, BHW87, BC83, BA82, CP87a, CG86a, Dar89, Dil87, DCG81, FGR89, FBBA86, HA89, HL83, JBF86, Kal87, KT88, KSI88, KI81, KN85, KDEHK89, LCC87, Lew89, LW82, Mit88, MS88, Mul88a, Mul88b, OMK+88, PW81, PR87, RDK83, SI88, Sch82a, SO87, SAS87, Sil85, SK86, SMF89, STY87, SS84, Sz87, TDK83, TITZ8GWQC81, VK80, VVV81, WMMH88, vdGB84, AR85, 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, EG+89, FS83, Gil84, GT82, GT83, Has84, Iro80, KSS83, KPE+84, LK87, LA85, OE89, SVS+81, SCCRS82, MAR+84]. methyl- [ OE89].

methyl-and [ FS83]. methyl-CH [ KPE+84]. methylamine [ BG82b].

methylbutanoate [ SK8+85]. Methylcyclohexyl [ VMNGTV86].
Methylene [FOSV86, BW81]. methylhistamine [Top87]. methyloxiranes [DPCS80]. methylphenylalaninamide [KYJ88]. methylpropanoic [SKE+84]. methylpyrazole [CSCD+89]. metric [Cri89]. Metropolis [KS82]. Microcomputer [Tri84, Sch86]. Microcomputer-aided [Tri84]. Microscopic [Kim85]. MIDI [STH82, TSH81]. MIDI-1 [STH82]. MIDI-3 [TSH81b]. MIDI-4 [TSH81b]. mimic [VCZB89]. MINDO [BSSW88, CZ88, DH83, JdKdWB87, Top87, VFM+89]. MINDO/3 [BSSW88, CZ88, DH83, Top87, VFM+89]. MINI [STH82, TSH81b]. MINI-1 [STH82]. MINI-3 [TSH81b]. MINI-4 [TSH81b]. minicomputer [Coo77, Car85]. minicomputers [See81]. Minimal [TTK+81, RP+86]. minimization [BHW87, BBO+83, BS87, GS87a, Ham87, LS89c, MK84a, NK86, PL87, PR87, RDA83, RPA83, SO87, TMG88, VK80, WM88]. minimum [LS88, ZW84]. mixed [BG82b]. MM [AF83, WP82]. MM2 [HLG88, LGB+89, TLA89, AP87, AK88, CUCP89, GCW88, PL87, PUNC86, PUC89]. MM2/MMP2 [PL87]. MMP2 [OE89, PL87, STY87]. MND [Bai84, BF82, BSSW88, DGW+81, DM83, DR83, DS83, DFC+84, DHS84, DR86, FS83, FS89, GP85, GR88, HGT87, GOL87, HHH+86, JDWB87, OUV84, Top87, Ver82, VSS84, VFM+89]. MNDOC [CT87]. MO [AFK82, BT81, EWM85, GDO89, HTT88, Is84, Ja88, LS87, RBEV80, Gro87, NR80]. Mo-Cd [Gro87]. mode [HL83]. Model [AS81, De86b, KW86, SMKH87a, SMKH87b, AM88a, CW81, FT89, HHR87, Ke88a, KLo83, LP88, LR87, MS88, OLM83, PR80, SLB83, WK81]. modeling [EW87, Li87, LS88, LY87, OTP87, Rou87, TMOW85, WK81, GPC88]. models [BR89, BC89, Boy86, Cri87, EM84, Ehr84, Fra87, KvRS89, PH89, STZ88, Wil88, Rue87]. modes [BC89, GC85, Gor88, WM89]. modification [Si81]. Modifications [ST89]. Modified [CZ88, CP80, FBBK85, LWD82]. modular [Sch88]. MOL [Lew87]. molar [Lew89]. Molecular [BMG84, BW83, BP81, By83, CAO89, CMR88, CM89, Del81b, Del81c, Del81d, Del81e, Di86, DH86, DH87a, DH87b, Ehr86, FGR89, FM87, GS87b, GHHS85, GL88, HI80b, HP84b, IL86, KAR87, KMS85, KO86, LRP87, Lew87, LG89, MAR+84, Mey80a, Mey81, Mey86, Mey88, NF84, OTP87, PH83, SJ86, Sim87, SLC86, SFO6, TK83, Wil86, AGL82, AH84, AG88, AS88, AG88a, Aid88, AD89, AF83, AL87, AKRA84, ASFW89, AM88a, AJHM88, BNR86, BMB85b, BG87, BR87, BD82, BGT84, BCT83, BSS88, Bur80b, CRR85, CHS84, CW81, Cri89, DAI88, DE83, DHP83, De89, Di87, EM84, Ess83, FSL84, FS89, Fra82, FBB86, Fuj87, GTB81, Gor88, GCW88, HR85, HK87, HK89, HI80, HS82, HP84a, HL88, HLC88, HB87, HHL80a]. molecular [IO84, Jaf88, JT80, JBF86, KS84, KM85, KV8+84, KSB84, LCC87, LS87a, LS87b, LM86, LA85, LTL8a, L89, LB89, LS88, MK84a, MK85b, ME84, MF85, MH83, Me87b, 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, TK89, TJ86, TM85, TMrGM88, TW82, VSS82, VVVG81, VDO86, Ved88, VZB89, WP83, Wi88, ZM88, ZW83a, ZW84, vdGB84, DH88, FW85, GL89, KKR, KRR82, LCL84, SKV85, 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, Bait84, Bal83, BFAG81, BF82, BkBT82, BG86, BGT82, BW89, Bre81, BG82c, CvRS81, CS80, CG86a, DM86a, DM83, DR83, DH83, DHS84, DHK89, Dod84, Fab88, GSH88, Gla89, GSB85, HG89, JB85, KT88, Kar81, Kei80b, Kei82, 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]. Müller [WD88].

MOM [ZW83a, ZW84]. moments [Bau84, GF87, HE88]. MOMM [BKL87].

moments [Bau84, GF87, HE88].

MOMM [BKL87].

mono [PR80].

mono- [PR80].

monocenter [FVV85].

monohydrate [OC88].

monomethylammonium [Gre83].

monopole [LZP84, ZP85].

monopole [LZP84, ZP85].

monosubstituted [EWM85].

multiconfigurational [RPD86].

multidimensional [LDL88].

multiexponential [SS84].

multiphoton [BG87].

Multiple [RFLC89, LS88, MSG80].

multiplication [BC87, LM89].

multiplier [Van88].

multiply [CBR87].

multiplier [Van88].

multiply [CBR87].

multiply [CBR87].

multiply [CBR87].

multipolar [PHG89, Wil88].

multireference [Ada89, CP87a, FBKK85].

MuMATH [Tri87, Tri88].

mutagenesis [Tin81].

mutagenicity [KR88].

myelin [GS87b].

N [Del89, GHT87, LB87, Ran86, TKK+81, TG83, BTG82, B+83, BGT84, CvR81, HHK+86, Iku85, KT88, Kao88, KYJ88, TW81], Na-CI [SCvRSH87].

NaBH [BMLR88].

naming [Cio87].

naphthalene [DHP83, HW82].

nature [OTW81, WW81].

NCN [ASFW89].

NCN-containing [ASFW89].

NCOCH [FS82].

NDDO [ZW83a, ZW84].

near [BFF86].

Nel [DBVMB84].

neighbor [SLB83].

neighbors [YE89, vGBC+84].

net [CW81].

networks [HAKV87].

neuromuscular [SHDP89].

neurotensin [CP81].

neutral [BFAG81, DAU88, DM86a, Del89, FS83, SK85, ZPPC82, ZPCR82].

neutrals [HPR80].

Newton [Di87, PR87, SO87].

Newton-like [PR87].

NG [ZW83a].

NH [Del87, HPR80, LS87b, PMZ86, TMOW85, Ada89, BHR+86, Del89, KVR89, KPR81, NRS84].

NHF [LS87b].

NHOH [LS87b].

Ni [RAS85].

nitric [LSROT80, Sie85].

nitrobenzene [KHRvH87].

Nitrogen [ADY89, Del85, Del86, FS83, JH83, LB87, MSH82, RS85].

nitrophenols
orbits [BMB85a]. order [Ada89, CP87a, FBBA86, FC88, GHF87, Gre84, Jug84, KSI88, KBS88, Per84, SHK83, Tri87, WD88]. ordered [BMB85a, BMB85b, MB84, 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].


P [Ano86b, Del89, DCNG85, Wib86, DCNG85, ROK86, TKK+81].


Parametrization [CMR88]. parent [MFG89b]. Part [ARS85, RAS85].


penetration [PW82]. pentapeptide [CP81, YJ86]. pentenone [ST80]. PEOE [HLG88]. peptide [OLBM83]. peptides [AH85, LBI+89].


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, CHS84, ČFHS85, FE87, Koz87, LS84,
PR84, TKI89, TJS86, Tin81, Ved88, WK81, YNAK88, DA83]. programs
[Boy86]. Progress [Lip83b]. projection [Gla89, Ja88]. 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,
BK87, DE83, DH86, DH87a, DH87b, DH88, EIO85, FSH+84, GTS82, JSKI88,
LZP84, Lew87, MH83, MM83, PH83, Ran83, ROK86, SPBS87, 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]. pyrolopyrimidine [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,
NSK89, NRM85, Rap84, SHDP89, vRS86, See81, SK86, Tos84].
quanti-mechanical [FG89]. Quasi [SDL82]. Quasi-one-dimensional
[SDL82]. quasiclassical [DBVM84]. Quasiperiodization [RH87].
quasirelativistic [Klo83].

R [Gil87, KT88, Kro88, Ran86, Wib86, Del81e]. racemization [FWB85].
radiation [Ehr89, LPPB84]. 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, KB888, SF85]. rates [MM89]. rationalized [MM89]. Reaction
[CF83, AM88b, BG88, DLM885, GT882, Gil84, HB82, HMA82, HBK80,
LHC84, LLC85, LSLC85, MM89, Per84, SK86, TTZWGQKC81, VSS884,
ZR81]. Reactions [BHR+86, AJMM88, BW81, BTR88, BK882, EWM85,
FS89, GHF87, GT84, KvRS89, Kel80a, OLB83, VSS884, ST80]. reactivity
[JB85, LCL84, NVGB81]. real [FV85, Gal82, PLFL85]. real-time
[PLFL85]. Rearrangement [VMNGTVM86, FBD80]. reassessment
[GT81]. Rebek [LZ89]. Receptor [Ano88c, GC85, SK86]. recipes
[Sch89]. recognition
[LS89a, LS89b, LS89c, LZ89, LBZ89, MBB84, OMK+88, VCZ89].
recurrance [RLR88], recurrence-based [RLR88]. Recursion
[DS87, HO83]. redistibution [OTW81]. reduced [HD88, ZW83b].
reductase [Gre85]. reduction [Gre85]. reequilibration [Mor85]. reference
[MSC+88]. Refined [HR87]. Refinement [Dil86, WK81]. Regional
[YF86]. regions [KK80, KSJT83]. regioselectivity [AJMM88, FS89]. regular
[KB84a]. Reinforcement [WB80]. related [AV84, Koz87, TLA89].
relating [Ir88, Sin81]. relation [BT80a, BT80b]. relationship
[BT82, Gre84, KR88, WW81]. Relationships [GC86, GPC88]. Relative
[OG86, CPTC84, GHT87, Iku85, JI81, MR80, SAV88, TG83, WM88, ZW83b].
Relativistic [KB85, LB89]. relaxation [AP85, Cha83, CPH85, DM89].
relevant [BTR88]. Reliable [RA87, Mul88b]. Remarkable [vRSS866].
remarkably [KTvRS86]. Remarks [IO84, Mey84, HAK88]. removal
[MK84b]. renormalized [Bra89]. Representation [CW81, Wil88, Ehr84,
GDP+85, HP84a, KE89, LDM89, LzP84, LTLA87, ZP85]. representations
[MR80, ZP89]. repulsion [FV85, PW82, RDK83]. Research
[JR88, RN86, WER82, TR84]. resonance
[BR87, Bro83, JS89, MT82, WG89, AH84]. Resort [Ano83a]. Restricted
[RDA883, RPA83, GT89]. resulting [FS82]. Results
[PUNC86, DK84, GD89, HE85, SDL82]. Review
[Boy86, Car85, Cra85, Gar82b, Gar82a, Gil87, Jor81, Jur88, Krok88, Lii87,
Lip83b, Lip83a, Lip86, Rau86, Sch86, vRS86, Str85, Tri82, Wen82, Wib86].
Revised [G8587a]. revisited [CP87a, Zie83]. RHF [ZW83a, ZW84]. ribbon
[Dar89]. Richard [Lil87]. Richards [Str85]. rigid [Lin88, Di86]. rigorous
[ZM88]. ring [AYS80, Kel82, KR88, LB87, Mat88, RFP86, Tri88]. rings
[ADY89, AL87, DVA83, DVSF++88, Ham87, JHS83, LTLA87]. RIPS
[GFR89]. RN [Gro87]. RO [JI81]. role [CE87, Gor88, YJ86]. Rosenblit
[Cra85]. rotamers [PK88]. Rotation [BGT84, SAP88, DK84, DK85,
Fab88, Hin80, KJ82, L84, PUC89, Rau83, WM88, KD83]. Rotational
[PUNC86, SLC86, ABP80, Bur80a, FSL84, FW85, HE85, HT87, ST87].
rotor [SN87]. row
[CCSvRS83, DH86, DH87a, DH87b, DH88, FB89, Gro87, KTVR86, MK85a,
Mag84, PH83, SCCvRS82, SCvRS87, SV83, TH80]. rules
GLLOB88, MC88, OC88, RMB86, TJ86, ZR81]. simulations
[Che89, HLC88, KS82, RPV87, SK86, WKNC86, YE89, vGBC84]. SINDO1
[JS87, IJ87, JS88, IJ88]. 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
Strategies [BP87b, CG89]. Strategy [YF86, NKC85, Sch88]. stretching [BTG81a, BTG82, MHA89, RK81]. strictly [PS87]. strong [LSROT80].

Structural [LUNV85, LB86, BFS82, KSS83, KVV+84, KSB84, SSSA82, SVS+81, SKV+85, SPBO87, SKE+84, VSS82, PR80, SSSA82, SKE+84].

Structure [GC86, JSK88, rVSSRH86, ABE+85, AYS80, AVBF84, BMB85b, BMR87, BTS+83, BB83, DS80, GPC88, GT82, GB83, HW80, HAKW87, KK85, KR88, KS83, LS89a, LS89b, LS89c, Li87, Lip86, LYH87, NVGB81, OMK+88, PW82, PSS80, PFR82, RDW88, RP80, RRI88, SVS+81, SWM83, SM80, Tim81]. Structure-Activity [GC86, GPC88]. Structure-Directed [GC86].

Structures [BPP82, OG86, ASS+85, BMB85a, BMB85b, Ba85, BE87, Bro83, CvRSK81, CG89, Del89, FS82, HR85, HR87, HRKW89, JT80, KvRS80, KC87, KYJ88, KVV+84, KSS84, KMS85, LV88, MESS80, MESS82, MB84, MB85, PPT+80, PUC89, RKM+85, RRG+84, Sch82b, Sch88, SMG87, VSS82, VVVG81, WKP+80, WM88]. studied [Osa82]. Structures [BG81b, BG81a, BG82b, BG82c, DLM85, Jur88, Wer82, AJMM88, BP81, BG86, Bys83, CDL89, CMRW86, FMT84, God87, Gre85, HMA82, HSS83, HSEC83, J81, J85, Kao88, KB84a, KB84b, KM85, KSS83, KVV+84, KSB84, KK85, KR88, KSL87, LCY82, LLCS85, LKL87, LDP+87, LZ89, LBZ89, Lip87, MK85b, MT87, OMK+88, PUC89, RMB86, SHDP89, SOR86a, SOR86b, SORT86, SOR87, SSSA82, SVS+81, SKV+85, SKE+84, VSS82, VVVG81, WSP88].

Study [SMOT85, VMNGT86, AG88a, Aid88, ADY89, Bai84, BMLR88, BTG80, BTG81a, BTG82, BTS+83, BGT84, BS83, Che89, CF87, CDL+87, DAA88, DSS80, DHP83, Del81a, Del89, EIO85, FBD80, FS89, Fra82, FK84, Gen87, GBT80, GBT82, GI84, GS87b, GT82, GT83, Gre83, GCW88, Ham87, HT88, HML83, Iko85, JDS89, JMB87, KS84, KvRS80, Kin87, LV82, LSROT80, LCL84, LHC84, LHM84, LLCS85, LHL87, LDP+87, LZ89, LBZ89, Lip87, MK85b, MT87, NRM84, OM88, PUC89, RBEV80, RP87, Rue87, SS81, SSSA82, SAP88, SAF88, SM80, SMG87, SK84b, TLA89, TKK+81, TG83, Top87, Tos84, VV88, VVSS84, VFMT89, YJ86, ZPP82, ZPCR82, ZPBCS82, ZRG80, CvR88].

Subgraph [KHS86, TK89]. subject [Cri89]. submatrix [LM89].

subroutines [CBR87]. Substituent [EH83, FO86, Mag84, Ehr84, HPR80, KPRT81, PR80, SMF89, Del81e].

substituents [BTG81a, DPF+88, KPRT81, SCC8R82]. Substituted [FK86, HML83, Ke80b, Ke82, LH85, MFG89a]. substitution [Rit86].

substrate [TTZ89QK89]. substrates [Gre85, MM89]. substrutuctures [BFF86]. sulfamates [OMK+88]. sulfide [SB82]. Sulfilimine [TTK+81].

sulfides [Tai81]. sulfur [Bai84, DM83, DR86, LB87, Mag84, MSS82, ST89, TSS81].

sulfur-nitrogen [LB87]. sulphur [JI87]. supercomputer [WG87].

superiority [SCC8R82]. supermatrix [Cao89]. supermolecular [KE89].

superposition [AK84A, MFG89b, OTW81]. Surface [LP88, BMR87, Car82, CDL89, Has84, LDL+88, Lop89, Mey88, MK84b,
PASTB87, ST80, WSP88, Mey86. Surfaces [YF86, AM88a, DPCS80, FKS85, IO84, KE89, KJ87, Ōsa82, VSSS84]. survey [Kel80b, Kel82]. susceptibilities [WP83]. SW [TW81]. symbolic [KBS88, Tri88]. symmetric [FWB85, LB89b, ST82, ZP89]. symmetrical [ZP89]. Symmetry [KO86, Ran83, ROK86, Bal83, BW81, Cao89, CHS84, DE83, FSL84, HLH83, Jaf88, KJL84, 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]. Systematic [HBK80, SDKM87, TM85, CP80, ST81a, ST81b, ST82, 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, TTZWGQCS81, vGBC84, Jur88]. Szymnsky [Ran86].

T [Ano86b, LR87]. T.-S [Ano86b]. tables [LB89b, SN87]. taste [OMK88]. tautomer [Gre85]. tautomerism [BSM83, CSCD89, ROK86, Top87, Zie83, ZPPC83]. tautomers [BT80b]. Te [RBEV80]. technique [BD82, DE83, Gar89, HO83, Kel80a, LMV86, Per84, RPD86]. techniques [SL81, TS83, RDAF83]. technologists [Ran86]. Teller [LR87]. tempered [DHK89]. ten [KKR82]. ten-electron [KKR82]. 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, CSCD89, CE87, FK84, GTB81, HUr88, Iku85, Kao88, KPR81, KSS83, LDP80, PUC89, Ran80, VSS82, WK81]. theorem [GT83]. theoretical [RRG84]. Theoretical [Ano86k, CDL87, CMRW86, FKS86, Gen87, Gre85, HMA82, Iku85, Kao88, LLC85, LSRC85, LKL87, LPB84, LZ89, LBZ89, Rue87, SAV88, VU83, VU84, VFMI89, BKKB80, BKT82, Cre82b, FBD80, Gre83, HT88, HPR80, HML83, HLH82, JDS89, KvRS80, KPR81, Kin87, LHOM84, LH85, Lip83b, LUNV85, OMK88, PR80, TW81, WB80, LDP87, RRH86]. Theoretically [KJ85]. Theory [CG86b, KKR82, PD83, BT80a, BT80b, Boy86, Del81b, Del81c, Del81d, Del81e, Del83, DH86, DHI87a, DH87b, DH88, Ehr81, FE87, FC88, GlS89, Kin87, KR88, LCL84, Mez87b, NM85, 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 [LCV82]. Through-Space [DVA83, CGN87, DCNG85].
Tim [Lip86]. Time [RPV87, FBB86, Gar89, PLFL85]. time-independent [FBB86].
time-step [Gar89]. Toluene [XB86]. Tool [CG86b, GRS88, HK88, See81]. Topological [Bac89, IL86, BM81, 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, IO84, LA85, MHA89, Osa82, 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, BL80b, CDL89, LLSC85, ST87, TMOW85, ZP84]. Transfer-Matrix [KHS86]. transferability [SSA82]. transferable [NSKNK87]. transform [SF85]. Transformation [TG86, CHS84, 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, VV84]. transmission [CG87, DCNG85].
Triplet [FO86, CF83, DPC80, HW82]. triplet-state [DC80]. Tripos [CCV89]. tRNA [LDP80]. Tropsch [CS82]. truncated [SO87]. Tubercidin [SOR86b]. twisted [HR85, HR87]. Two [BR87, CF88, LE88, MM87, Osa82, PW82, RL88, RLR89, S88, SN87, SK84b, LCC87]. two-center [PW82, RLR88, RLR89]. two-dimensional [S88, SK84b]. two-electron [CHS84, MM87, LCC87]. two-parametric [Osa82]. Type [JG89, WG89, Aid88, AK84, Bre81, Mas88, ST89, STH81a, STH81b, STH82, TH80, TSH81a, TSH81b, Tat85, BG80]. Tyr [CP81]. tyrocidine [TMRGM88].

UMP2 [CFHS85]. unbranched [RHP89]. uncatalyzed [OLBM83].
uncomplexed [MK84a]. unconventional [CG86a]. Undecanes [IL86].
undecapeptide [PHG89]. unified [Jug84]. unimolecular.
[FS82, HB82, SF85]. Unique
[BMB85a, BMB85b, MBB84, MBB85, RKM+] Units [De 86a].
unrestricted [MSG80, RFLC89]. unsaturated [AYS80]. unsymmetrical
[Kel80b, Kel82]. unweighted [ZW83a]. upon [HT82, RS85]. Uracil
[Zie83, Del81b, Del81d, Del81c]. urea [BHR+] Use [CHS84, Dil86, BA82,
Dil87, GS85, Hur88, Kar87, KR88, MR83, RV85, TSH81a, Top87]. used
[LD8+] Useful [CG86b]. Usefulness [FBKK85].
valence [Bai86, CvRS81, HR87, Jug84, JFG89, HLH83, LDM89,
LRP87, MR80, NRM85, ROK86, ZD87]. valence-orbital [ZD87].
valence-orbital/bond-orbital [ZD87]. valences [JB85]. valency [Mag84].
Validity [CCV89]. Validity [AM88b]. valinomycin [MK84a, MK85b].
value [Gre84, Ran80]. values [GBP85, ZW83a, ZW84]. vapor
[VVV81]. various [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 [BK87]. velocity [HLC88]. Venkatagahavan
[Li87]. Versus [ST89, Ada89, FB89]. very [Kar87, LM89].
[BT81, KB84a, STH81b]. via [DVA83, HLG88]. viable [ACvRS81].
bond [DK84, DK85, KDC83]. Vibrational
[DK88, DBVMB84, BTG80, Gor88, HE85, HLH82, HLH83, HE88, Lin88,
MAR84, MSA88, PKB88, Ska83, SBS82, VVV81, X86]. vibrations
[LPB84, PV82b]. vibronic [LS84]. vicinal [DVA83]. view [GBP85]. VII
[KB84b, MKSW83, TSH81b]. VIII [BG82a, BTRT88, RKM+] well.
vinylic [Rit86]. violuric [OC88]. virtual [CP80, FBKK85]. voltage [Kim85].
Volume [Ano86b, HG89, Lip83b]. volumes [KE89]. Voronoi
[BC89, Cri87].

V [Cra85, Ran86, Wib86, AG88b, MBB84, Mey81, Mey88, Run83, STH81a].
vacuo [SHDP89]. Valence [Bai86, CvRS81, HR87, Jug84, JFG89, HLH83,
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]. vapor
[VVV81]. various [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 [BK87]. velocity [HLC88]. Venkatagahavan
[Li87]. Versus [ST89, Ada89, FB89]. very [Kar87, LM89].
[BT81, KB84a, STH81b]. via [DVA83, HLG88]. viable [ACvRS81].
bond [DK84, DK85, KDC83]. Vibrational
[DK88, DBVMB84, BTG80, Gor88, HE85, HLH82, HLH83, HE88, Lin88,
MAR84, MSA88, PKB88, Ska83, SBS82, VVV81, X86]. vibrations
[LPB84, PV82b]. vibronic [LS84]. vicinal [DVA83]. view [GBP85]. VII
[KB84b, MKSW83, TSH81b]. VIII [BG82a, BTRT88, RKM+] well.
vinylic [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 [Run80]. Water
[De 86a, De 86b, BG82b, BG82c, CDL89, Del81b, Del81c, Gen87, GLLOB88,
Iku84, JI81, KTVRS86, KYJ88, KSL87, LV82, LCC85, Lin88, MCC88, 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].
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