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Title word cross-reference

\[ 0.0 \leq x \leq 0.3 \] [WZ99]. (110) [Bre99]. (4s) [KSW98]. (5s) [KSW98]. \((C_{2v})\) [AFM99]. \((d + s)^3\) [Bec97a]. \((\Gamma)\) [LMAK93]. \((J = 0)\) [CB93b, CB94a].
\((n = 0, 1, 2)\) [WMZ98]. \((n = 1, 2, 3, 4)\) [HL93b]. \((n = 1, 2, 4)\) [XKKB+99].
\((n = 1, 2, 3)\) [IBS95]. \((n = 1, 2)\) [ST97, WMD95]. \((n = 1, 2, 6)\) [GFY+99].
\((n = 2, 3)\) [XSG97]. \((n = 2, 3, 4, 14)\) [Bou94]. \((n = 2, 2, 4)\) [CCS99, SPR94].
\((n = 4, 5, 6)\) [RT98]. \((x = 2, 3, 16)\) [LXWZ99]. +
[BAA91, BYGA99, CR96b, CB93b, CB94a, DV91, HZ91b, MSM96, MLK94, Oku98, PGM95, RNS93, Sha92, SC95, XY95]. 0s [RLR90]. 1 [SWD+99]. 1 \(^1\) [BP93b]. 1 \(^1\) \(B^+_2\) [NNH98]. 1 \(^2\) [BP93b]. 1 \(x\) [GFRR94]. 1/2 [BHX96]. 1 \(r_{ij}\) [PCO+94]. 1/2 [GLMP98]. 10\(D_q\) [MBA94]. \$187.00 [Kar96]. 1s [FAV92]. 2 [HGL99, LU90, LCP+91, LSGS91, SSM+99]. 2 \(^2\) \(A^+_g\) [NNH98]. 2 \(^3\) [BP93b]. 20 [LS99]. \$208 [Ber96b]. 3 [Boe91, CB93b, CB94a, RT99]. 3n [Roo93b, RL97]. 4 [BT95, RT99]. 4n + 2 [OS95]. 5 [MMCC99]. 540 [MUL99].
6 [SSM⁺99]. $60.00 [Mon93]. 7 [SSM⁺99]. $79.00 [Str91]. = [ANB94, Al99, BCY95, BZQ95, GAR97, Kor90, NBS95, NG95, NL96a, PZTPMC99, STM97, SG96b, SL97, SNH99, YZX96]. [2 + 2] [Fir94]. * [BB94, JKK⁺92, LJ95]. + [ANB94, BCMÖ97, BB95, Bou94, Bro95a, CWZ98b, CLOFR98, CD90, Cs96, DS90, DSS90, FV96, Gao93, GS94, GPS90, JM93a, KSF91, KKWT99, KG93, KA95a, LHL91, MO94, MMR92, NBS95, Pal94, PS93, PH94, Pro95, RNS93, SPS96b, SZ97b, SC95, STC96, TFS95, UJS90, WY99, WMD95, YD96, YSHD97]. +{(−)} [BCY95]. + [BK49b, ELM96, UJS90, ZTC97]. − [CLOFR98, CD90, Cs96, HZ91b, KKWT99, KK93, KG93, MTNF99, Oku98, Ort98a, PG95, SKE92, SEKE98, WYZ⁺92]. 0 [ZTC97]. 3 [Kal90]. 7 [DM97b]. 0 [CBAM97]. 1 [BC95, BYGA99, CB93a, CRsP93, GAR97, HMK96, LP99, LU92b, NÁJ91, NÁJ92, RNS93]. 11 [GAR97]. 13 [BZ92, GS97b, GAR97, KH96a, RN96]. 13 [SCL96]. 17 [KH96a]. 19 [GAR97]. 1A [CC98]. 1A [KA96]. 1Δg [FSW⁺91, MLK94]. Φg [Pet92]. Πu [Pet92]. Σ [CWJ⁺99, FSW⁺91, SES93]. Σ⁺ [BFV⁺93, PVC⁺90, TGS99]. Σ⁺ [RA96]. 1Σ⁺ [BP93b, MLK94]. 2 [BRL92, BLK97, EL96, KA95b, LU92b, LK94, Man99, PS93, Sz97b, UJS90, WY99]. 2+ [BL99, BB95, BDH⁺97, CA95, CG97b, EJ93, FLL91, GS94, JM93a, KG93, MMR92, Pro94, Pro95, T97, W90]. 2+/3+ [ZBL99]. 2.6 [XSA⁺92]. 2− [BGM95]. 2− [BADM97]. 2− [DM97b]. 207 [GAR97]. 20 [GAR97]. 2A [Pet92]. 2− [LM93]. 2Πu [MM94]. 2Σ⁺ [LB97, Man95a, Man95b, RNS93]. 3 [BP93b, CB93a, CRsP93, LU92b, NÁJ91, NÁJ92]. 3+ [BGM95, BDH⁺97, DND95, MN95]. 3− [CIX⁺92, NG95]. 35 [GAR97]. 37 [TWK⁺92]. 3Πg [TGS99]. 3Σ⁺ [FV96]. 4 [HML98, LU92b, SES93]. 4+ [ABC93, SK99a]. 4− [NM92]. 5 [LU92b]. 5+ [BMA90, Cze99, SK99a]. 6 [Tew94, Tew97]. 6+ [BMA90, SK99a]. 6− [REU⁺91, XCY98]. 7+ [SK99a]. 9 [KP97]. e [BLK97], ∞ [KP97]. M [PAT93]. N [PAT93]. n+ [WMZ98]. o [L97]. 0 [AS93, KJL96, LK90, UJS90, YZX96]. 0 [GS90b]. 0.4 [L97]. 0.6 [L97]. 0.8 [M96]. 1 [DM98, ELM96, GJOV97, GS90b, MW92, NÁJ91, NÁJ92, WP90]. 1− [SPF93, WZ99]. 1.2 [Min96]. 10 [BKM90, REU⁺91, VR92]. 105 [RKPE95]. 111 [RKPE95]. 12 [CIX⁺92, Cs96, Eva97, TST⁺99]. 123 [RKPE95]. 13 [L97]. 14 [LGT94]. 7 [DM99]. 1A [PW97]. 2 [AS93, ARBB95, ANB94, ACHT95, Ali99, ABC93, ABDM94, AD98, BA91, BZMR92, BIL95, BU94, BD97, BBC92, B94, BFR90, BYE⁺97, BCY95, BDH⁺97, CW93, Cai93, Cai94, CPBC95, CR96b, CG96b, CB93b, CB94a, CRK⁺91, CF93, CL95, CPD⁺98, CPD⁺99, Cun92, D90, D91, DND95, D97, D97, EB95, FDC92, FS95, FC199, FSW⁺91, FB90, MFD⁺96, GKKM96, GJP97, GPS90, Gin97, GV93, GJOV97, GZ97, GL96, GS90b, HMG93, HS92, HBL99,
HP98, Hir92, HHPT91, IBS95, JMP99, JKK+92, Jen94, JMD95, JJ97, Jur97e, KJ95, KA96, KP97, Kor90, LW92, Li93, LF95, LV97, Loh91, MSD95, MALT96, MLT98, MTP+98, MMH95a, MECE97, MHY98, MK90, MLL99, MM94, MGNK95, MCA95a, MTD93, MTTS93, MLK94, MRST95. 2

[Min94a, MZ95, MDM94, MD91, NM95, NÅ 91, NÅ 92, NL96b, OLS+95, Oku98, Ort98b, PGM95, Pal94, PBS99, PSBL98, PPK96, PGS97, RN96, RA91, RD97, RA96, RCWN94, RKH+98, Roz97, RP98b, RS97b, RN93, SE93b, SM96a, SDP+95, SAB+97, SC99, SL93, SP92a, SRP+98, SX96, SBAD90, SP92b, SZC97, SST93, STMR97, SCS94, Sla92, SZCO99, Sme92, SGGMGFS96, SES93, SG97, SGB98, Sta98b, SC95, STC96, SC99, SNH99, TJ97, TGS99, TMA97, TPR96, TFSZ95, TZCT97, TS92, TMD96, VH96, VÅJ+92, VBN95a, VBN95b, VR92, VJ95, VJ97, WFS93, WY99, WI96, WDS97, WL99, WL92, WMD95, YNMT98, YNST99, YD96, YSHD97, YK97, ZC96, ZTC97, ZBL99, ZGSP97]. 20

[Min94a, MZ95, MDM94, MD91, NM95, NÅ 91, NÅ 92, NL96b, OLS+95, Oku98, Ort98b, PGM95, Pal94, PBS99, PSBL98, PPK96, PGS97, RN96, RA91, RD97, RA96, RCWN94, RKH+98, Roz97, RP98b, RS97b, RN93, SE93b, SM96a, SDP+95, SAB+97, SC99, SL93, SP92a, SRP+98, SX96, SBAD90, SP92b, SZC97, SST93, STMR97, SCS94, Sla92, SZCO99, Sme92, SGGMGFS96, SES93, SG97, SGB98, Sta98b, SC95, STC96, SC99, SNH99, TJ97, TGS99, TMA97, TPR96, TFSZ95, TZCT97, TS92, TMD96, VH96, VÅJ+92, VBN95a, VBN95b, VR92, VJ95, VJ97, WFS93, WY99, WI96, WDS97, WL99, WL92, WMD95, YNMT98, YNST99, YD96, YSHD97, YK97, ZC96, ZTC97, ZBL99, ZGSP97]. 20

[Min94a, MZ95, MDM94, MD91, NM95, NÅ 91, NÅ 92, NL96b, OLS+95, Oku98, Ort98b, PGM95, Pal94, PBS99, PSBL98, PPK96, PGS97, RN96, RA91, RD97, RA96, RCWN94, RKH+98, Roz97, RP98b, RS97b, RN93, SE93b, SM96a, SDP+95, SAB+97, SC99, SL93, SP92a, SRP+98, SX96, SBAD90, SP92b, SZC97, SST93, STMR97, SCS94, Sla92, SZCO99, Sme92, SGGMGFS96, SES93, SG97, SGB98, Sta98b, SC95, STC96, SC99, SNH99, TJ97, TGS99, TMA97, TPR96, TFSZ95, TZCT97, TS92, TMD96, VH96, VÅJ+92, VBN95a, VBN95b, VR92, VJ95, VJ97, WFS93, WY99, WI96, WDS97, WL99, WL92, WMD95, YNMT98, YNST99, YD96, YSHD97, YK97, ZC96, ZTC97, ZBL99, ZGSP97]. 20

[Min94a, MZ95, MDM94, MD91, NM95, NÅ 91, NÅ 92, NL96b, OLS+95, Oku98, Ort98b, PGM95, Pal94, PBS99, PSBL98, PPK96, PGS97, RN96, RA91, RD97, RA96, RCWN94, RKH+98, Roz97, RP98b, RS97b, RN93, SE93b, SM96a, SDP+95, SAB+97, SC99, SL93, SP92a, SRP+98, SX96, SBAD90, SP92b, SZC97, SST93, STMR97, SCS94, Sla92, SZCO99, Sme92, SGGMGFS96, SES93, SG97, SGB98, Sta98b, SC95, STC96, SC99, SNH99, TJ97, TGS99, TMA97, TPR96, TFSZ95, TZCT97, TS92, TMD96, VH96, VÅJ+92, VBN95a, VBN95b, VR92, VJ95, VJ97, WFS93, WY99, WI96, WDS97, WL99, WL92, WMD95, YNMT98, YNST99, YD96, YSHD97, YK97, ZC96, ZTC97, ZBL99, ZGSP97]. 20
$S = 0, 1/2$ [LP97d].

$S^+ \leftrightarrow S^-$ [Par99], $sp$ [Ell91]. $t$ [RW92]. $T_1$ [TWK98]. $T_0$ [DBM99]. $\rho$ [LKLBD98]. $U(2n)$ [BG98b, BG98c, BG98d]. $v$ [BYGA99, KL91]. $v'$ [BYGA99]. $Y'' = F(X, Y)$ [Sim95]. $Z$ [KSH94, Rey90]. $Z = 1 - 24$ [PZ91].

$*$ [FL95, NNH98].


-2 [CAM+97]. -acetylpropanamide [ZH99a].

-2 [CAM+97]. -acetylpropanamide [ZH99a].

-2 [CAM+97]. -acetylpropanamide [ZH99a].

-2 [CAM+97]. -acetylpropanamide [ZH99a].
-poly [GT97]. -polyazamacrocyclic [HBGR99]. -propiolactone [BH92].
- protonation [SSM+99]. -Pyridylacetic [NSS+95]. -quinonenediimine
[Mor93b, Sam97, Har90]. -representable [KLM91, KL92a, SFM94]. -residue
[LS99]. -S [BUZ94]. -separation [MHS95].
- Pyridylacetic [NSS+95]. -quinonenediimine [SWD+99]. -reduced [KG98].
- related [Nal92a]. -Representability [Mor93b, Sam97, Har90]. -representable
- subunit [SCMF93]. -Tetrasilane [Yam97]. -tetrazine [Ort97]. -Type
[BFD98, Wil96, Boe96, Ell91, SMM+90]. - wave [DBM99].

/M [BDH+97]. /Molecular [BLBP97]. / [Pet92]. /1 [Boč90]. /6
/Cu [Eng92]. /INDO [KSIH92]. /MC [FZZ92]. /MCLR [NÅJ91]. ?
NSaha:1999:LES. /Q [RSCP91].

0 [Ber96b, Brá95, Car96, Deu96, Kar96, Lin96a, Sjö96, Tri96].
0-19-509775-0 [Mic96a]. 0-19-855573-3 [Str93]. 0-387-57874-9 [Brá95].
0-387-94376-5 [Sjö96]. 0-387-94380-3 [Car96]. 0-444-82171-6 [Tri96].
0-7923-3264-4 [Ber96b]. 0-7923-3664-X [Kar96].

1 [ARB95, BRA+99, Brá96c, HRH99, JZ95b, KJ95, MAL93, Mav98,
MCM98, DZB92h, RA91, SB98, SAL+94]. 1-Bisnitroxyphenylethylene
[TD96b]. 1-D [MCM98, SB98]. 1-dimethyl [MSRP90]. 1000-Tesla
13-Molecule [PVLG93]. 13C [Mon98, PRC98]. 155.00 [Ano92].
1987 [Cal90d, Cal90c, Cal90a, JPP87]. 1988 [ Ağr90, Cal90g, Lun91]. 1989
[Cal90e, Cal90b, Lun91, Tay91]. 1990 [Ano90a, Ano90b, Ano92k]. 1991
[Ano91a, Ano91b, Ano93b, Bir94, Eri92, Lun92, Kar93]. 1992
[Ano92a, Ano92b, Ano93g, FMT93, Jør92, Kar93, Lun93]. 1993
1996 [Ano96a, Ano96b]. 1b [FMS+99]. 1b-adrenergic [FMS+99]. 1D
[LO93, TDK+94]. 1S [JM95].

2 [BP93b, JZ95b, Jur98b, Lin96a, MTD93, MCM98, OSA+97, PVLG93,
RK95, SB98, SP92b, Sta98b]. 2- [AEHM91, MH98]. 2-alkenylfurans
[EVSN92]. 2-Aminoethanethiol [Bue96]. 2-Aminoethanol [Bue96]. 2-D
[MCM98, SB98]. 2-diazaacyclobutadienes [JZ95b]. 2-Dihydro-1
[JZ95b]. 2-dimethylcyclopropanone [CAM+97]. 2-Dithietes [MF96].
2-electron [DWB98]. 2-Hydroxypropanal [OSA+97]. 2-Hydroxypyridine
[MTD93]. 2-isomer [MZ91]. 2-Nitrophenylcyanate [Mor96c].
2-Nitrophenylthiocyanate [Mor96c]. 2-Pyridone [Al95, MTD93].
2-substituted-1 [SLG+96]. 2-Trifluoromethylvinyl [KH97]. 2/6


4 [AAS93, Ber96b, TD96b]. 4- [BBB+95]. 4-31G [AKCS91]. 4-aminobutanol [KR93]. 4-chloro-indole-3-acetic [RTKP96]. 4-Currents [AA93]. 4-dihydropyridines [PHBB94]. 4-Diphenylpentane [LV93]. 4-Nitro-1 [PGS97]. 4-phenylene [Lah92]. 4-trioxane [BJM+94]. 4.2 [RBB+94]. 45.00 [Cal93]. 48 [CAK+96]. 4CuCl [BBC92]. 4d [MS93b]. 4th [Br¨a95, Str92].


7-cyclooctatetraene [PMS94].

8-tetrachlorodibenzo-p-dioxin [MEP90].

9 [Br¨a95, Dun96b]. 9-dimethylguanine [YJL92]. 9-j [Lai94].

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

A/T [LSGS91]. AA [SST93]. Ab-initio [FR92, FR93a, RK91, SKRK90]. Abacus [Mon93, Sri97]. able [GV92]. above [CB96a]. above-threshold
alkaloids [Bha99]. Alkane [CD90, WGR+94]. Alkanes
[Gin95, Gin96b, MK98b, BKM90]. Alkenes [ET99a]. alkylfurans
[LF96]. alkylation [BvV91, BHv96]. Alkylation [Cha95]. Alkylidenes
[Bc97a]. Alkylperoxyl [ET99]. Alkynes [Jay92]. All-
[MI93]. All-Electron [SSO+97, SG93, BK97, MKRW99, SG92]. All-trans
[KB94, YAD92, CPA98]. All-Valence [RL92, MAAP90]. Allene [FF94].
Allinger [An96-58]. allotropic [WTSN94]. Allowed [Pon97]. alloys
[JL98, FD96a, MLR+98]. Allyl
[RL97, BT96, FS99]. allyl-nickel [BT96]. Allylic [PRB96, PBHB95].
amost [EMS92]. AlO [MCOS94]. Along
[Pon97, AM90a, Art93, LV97, LAM91, LAM92, Pal92b]. alpha
[AP93, Jn96, KSW98, HFTP91]. alpha-Aminoisobutyric [AP93].
alphafunction [Jj96]. alpha-particles [KSW98]. Alternant [BE95, BE98,
HA93, KBG97, TDK+94, TDO97, ZSK97, AH92a, Dia99, Hal93].
Alternating [Kup94]. Alternation [LP96, LN96, MD93c, TAY+97, CP99a].
Alternative [GR95b, GR96b, Gin96a, Hkc96, JK95, MAPLB92, SB92b,
ZY90, BT96, LU92a]. Altmann [Lin93]. Alumina [NMvB+98].
Aluminum
[BpL97, BpL94, BBRT94, Kie97, LB94, VG90, BHL+99, GL92]. AM
[MAL93, ARBB95, BH92]. AM1 [PHM+91, PBHB95, BHPB93, BHPB95,
BPHB96, GARC97, KK99b, KGM97, MK96, MAL96, Ml98, PIC94,
PBB92, SM97, SSM93, BP92b, DE92, SBD+92]. AM1-based [BPHB96].
am7 [HS92]. America [Bir94]. American [Bir94]. Amides
[BK94c, Mar97c, RB97]. Amino [Sen96]. Amino [BDG96, DB94a, Jur98a,
Sm96, BOL+90, GL97, HGL99, Kkm99, Les92, Tew92, TBP99].
Amino-Nitro [DB94a]. Aminoalkylation [MK98]. aminobutanol
[K93]. aminobutyric [Ram90]. Aminoethanethiol [Bue96].
Aminoethanol [Bue96]. aminohexanoic [Ram94]. aminomimidazole
[HGL99]. Aminoisobutyric [AP93]. aminopentane [Ram90].
aminophenyl [SWD+99]. Aminopropionamide [CFR96]. Ammonia
[MSCS95, CBL95, HW91, WG99, ZY94]. AMO [PˇCe90]. Among
[AMKS93, ZC95, Csa93, DM92]. Amorphous [TNM98, B92, Tos95].
Amphipathic [NAK95]. Amplitude [Day96, MSRFP93]. Amplitudes
[Day95, MMD96, MPP95]. Amsterdam [Tay91, Tr96]. Analogic
[Reg92, RFF89]. analog [LU90]. analogous [Tri98c]. Analogs
[KG93, LS92a, LBBE98, MvC94, SA98, SM98, WY96, BBSS96, Les91,
LU92b, RA91]. analogues [Mep90, WSTB90]. Analyses
[CDDV93, CD+94, NYK98]. Analysis
[AZAC97, AFTM5a, AFTM95b, AFO+97, AFTM98, AM90a, Art98,
AM98, BW99, Bue96, BP95, CB94a, CV99, Dia99, FS94, FS95b, Gho95,
GARC97, Hc91, Ik94, Ja97, Jck92, Jbt+95, KT96, Kj93, LP97b, LL97,
MI93, Mor96c, MT96, MSP92, NK96a, Na94, Na95a, NM95, N93b, NB97,
OSA+97, PP95, PO97, PKM94, Par97, PV94, PG97, PS94a, PB95c, PJ96,
Pon97, RKN97, RT98, SLtM+94, SB95a, SM96b, Sch95b, SS91, SLDB91, TMD96, VB94, WHF92, ZM96, Ali99, AYA95, AFZ+99, BE93, Bha99, BRV99, CB93b, CC91b, CDG04, FLHT90, GVV+90, HSES94, ITT+94, ISOA99, Jac98, Kin93, KRRB99, KC97, LLL91, LAM91, LM92, MESH93, Min90a, MEP90, MSRP90, Na92d, Na92h, NM92, PL91, PLBB99, PB99, RTKP95, RT99, RAM91, SCA93, Sch95a, SC96, Tac92, [Tac94, TYTY91, TWWC91, VX99, VES+99, ZPBC97, Ish92, YITY93]. Analysis [Tac94, TYTY91, TWWC91, VX99, VES+99, ZPBC97, Ish92, YITY93]. Analytic [GKK97, GC91, Loh96, MZM94, Sza95, TK92, CJM+91, DS92]. Analytical [BPL97b, CTC95, DDG93, DW90, GRK96, Gus98, HO94, IHG95, KKK97, Mor96a, QS98, RDK97, SZL95, Tac96, BMA99, Hos97, WB93, RDK02]. Analyticity [RH96b]. Ananalysis [P˚AS+97, SMO+96, BBSS96, LV97]. Analyzing [KC98a, KLC98a, KC98b, KLC98b]. Ancillary [CAK+96]. and/or [NMN+97]. Andreas [FMT93]. androstane [PTKS+92]. androstanediones [KPTVT+97]. anesthetics [DB97]. angle [STKK92]. angles [FCMB99, MEB91]. Angular [Can97, Obs96, Pal93b, TN96, YPC97]. angularly [DSW93]. Anharmonic [CB93a, MS97b, RDF98, Sch95b, BFV92, LC90, LF99, Réa90, Sch95a, WN90]. Anharmonicity [SB95a, Tes96b]. anhydrase [GK92]. anhydride [HM99]. Anion [BSP97, CFDS90, ESP98, Jur99a, RML97, Yan97, CJX+92, Jur99c, Pro95, XYC98]. Anionic [FLRV97, GSJS97, KSN95, D90, KSN93, KJL96]. Anions [RMP93, Can97, DBG92, DZ097, MKM93b, PZ95, YMNT98, Can94, KSSG95, MW90b, MRST95, MCB99, Pro94]. Anisole [DZOR98]. Anisotropic [BH96, Bra97a, WG95, BMFP92, DOPS91, MK90]. Anisotropies [Can97, RGT95]. Anisotropy [GARC97]. Annealing [BLRD92, MT96, BV93, IBS95, JH90, K194, LS99]. Annihilation [LZ96]. Announcement [Ano90g, Ano90c, Ano90d, Ano90e, Ano90f, Ano91c, Ano91d, Ano91e, Ano92h, Ano92c, Ano92d, Ano92e, Ano92f, Ano92g, Ano93c, Ano93d, Ano93e, Ano93f, Ano94d, Ano94e, Ano94f, Ano94g, Ano94h, Ano95c, Ano95d, Ano95e, Ano96c, Ano96d, Ano96e, Ano96f, Ano96g, Löw94a, Par95a, Par95b, Par95c]. Anomalous [SWD+99, NMN+99]. anomeric [MT91]. Ansatz [GR95b, GR96b]. ansätze [SB92b]. Antagonist [MTP+98, WD91]. Antagonists [DBF+96, MTD93, ARBB95, WL9+94]. Antalya [Yur95]. Antarafacial [RW92]. anthracene [KL93a]. anthraquinone [HGP91]. anti [BD95b, TCZ91]. anti-malarial [TCZ91]. Antiaromaticity [MP94, PMS94, ZH99b]. antibiotic [NSS92]. antibiotics [BS95]. Antibound [BR97]. anticancer [BS95, SC96]. Anticonvulsant [MAAP+98, TBB98]. Anticonvulsivant [BB95]. antidepressant [CMA+99]. Antiferromagnetic [SB95b, YITY93]. antihydrogen [AZ99], antileishmanial [Bha99]. antimalarial [BJM+94, DBR+96]. antioxidant [BP90]. antiparallel [Xu99, Per93]. Antiparallel-spin [Per93]. antisite [CFDS90]. Antisymmetry [Pal95, VA90]. Antitumor [FT95, FT96, FT97a]. Antiviral [DZB92a]. Any [AB97, KJ95]. Aperiodic
Apoenzyme [FVN98]. Apomorphines [GJOV97]. appearing [PCO+94]. Applicability [Lef99, MMH95a, MUMH97, MMH95b, PS94b, SMPJ94, Sch93, ZP90, PL93, TNS96].

Application [ASP97, ABR95, AT97, Bat92, BCM97, BD94a, BG98a, BKL94, CCM+96, CT96, CFMA93, CGMG92, CB94b, DA92, DRBE96, DA91, Dum99, EBG95, FSVZ97, FFD98, GDY97, GW98a, IKC96, Her98, IK94, JM95, JM96a, KFS98, KT94, KKE+96, KL97b, KL97a, LT90, MR92b, MD93c, Nic99, NV94b, NS93b, PM93, SCL96, SDW+98, SZL95, SZ97a, SP90, SS99b, STY+98, SGGMGFS96, Ste96, SATP94, TNS999, TMS98, TC98b, VH96, BZMR92, CT95, Che92, CM99, DWM90, HC96b, HDB+95, LC90, MRC99, MK94, Or97, Rom92, SN99, SG99a, SOK+98, Sim95, TG999, WP91, WA94, Wi99b, BTKVG99, BD95a, Boe93, CCWF96, CA92b, CTC95, GRB+93, Har94, LCL98b, KZ91, KCL95, LKM99, LV97, Lin91, LJS94, MFH91, Nag96, NYNY99, NV97a, PS92c, RVP92, SS90].

Applications [ADB96, Cal90b, CWZ98a, DQB97, Enk97, GP95, GG97b, GLBM96, Hom93, KBB+90, Kup98, LLC+94, LDJH92, MP97, NS93a, O'C96, PEBS97, PG95, SM96b, SB96, T97a, Wi96, ZLHZ94, Ada94, Ave89, Bal90, CC92b, Ced90, Del92, Har91, Kha91, L92b, Na95b, Sem96a, ZM95, CV91, CB95, Csi77, KS90, LBL98, Or98a, PK92b]. Applied [BLE96, BC96b, CJH98, CB96b, Da94, KD98, KPT97, K96, LCL95, Muk92, PDT97, RDK97, Rox97, V95, V97, AZ99, CFMA95, Cze99, Ell91, FH90, FR98, HMK99, NPL90, RD92, Ana93g, Sta93]. Approach [AC94, ATI97, AO93, ABL97, BM96, CL95, CLSI94, CG96, DI99, DFDK99, DC95, Del98, Dew92, FK94, Fer96, FFD98, FB97a, FB97b, FB97c, Fl97a, Fr93a, Fr93b, GJ95, GD94, GSD97, GSGA98, GGY97, Har97b, Hu96, JP95, JZ95a, JZ95b, Jur96a, KSR95, KNA94, KPT94, Kry98, Kup98, LY98, LP96, LD95, LBEB98, MK93a, May98, MK96, MP97, MP98, MSCP92, NY98, Nic96, NS93b, Pa97b, PPP97, PC95, RP96, SA96, SAR96, SM96c, SG94, SGGMGFS96, SL95, SP94, XY95, Ada94, AM90b, BA91, Br96b, V90, CPA98, Csa90b, CK91, DM92, DB94b, EM92, FMR91, Fl97b, FJR96, FDD95, GDYY97, GDB98, JK90, KSS92, KK99, Kn99, KFK91, KPM+90, KLM91, KSW98, LF94, LLL91, LF99, LP92, MM99a, Ma99b, Min90b, MAPLB92, MSF91].

Approach [MV92, MSC92, NYNY99, NM96, NS92, NMC92, OKY+99, PBN90, PA92, PY92, Pic92, PB95b, PS92b, PFK99, RTS91, RSCP92, Roe91, RK91, RMF90, SK99a, SGK99, SCP91, TD03, WL94, WG99, Wil99a, WP95, Yu95, YUSM99, ZY90, ZM90]. Approaches [BA97a, BB96a, BAK96a, Chr97, FGR98, FWC+93, JOC97, NB97, PTP95, RZ96, RWT92, CG96, Chr92, He95, HBGR99, Mat97, PP92, PČe90, RWT91, Sch92a]. Appropriate [Gi95, MYN+96]. Approximants [CG95, CB93a, LB97]. Approximate [AG91, BMA99, CV94, Fer95, HHKM95, KS98, Mez97b, MYPL90, MP91, NP96a, Nuni95b, Or98a, Or99, OYL91, PTP95, SDW+98, CD92, CP90,
JGP91, Rin96, RSCP92. Approximately [SFM94]. Approximating [BMDM90, TN96]. Approximation
Atom-Symmetric [YLD97]. Atom-Vacancy [FD93b]. Atomic [AC97, ABR95, AYDR96, AR99b, AC94, BP93a, BK96, BGS98, Can97, CC97b, CA97, CDDV93, DDD93, DZF93, ETV94, Fan97, FD93, GP95, GD94, GZ97b, HW84, HW87a, HSS+95, Ish90, KSH94, KS95b, KBL95, KS96, KN99b, KY93, LKBJ97, Lin97, Lin96b, LBKLC98, LK93, Mar97a, Mic94, MM98, Mon98, NK98, Pah98, Pen93, Pen96, RH95b, Roz97, SKN95a, SKN95b, TSP93, VBD+98, YD97, Zha96, ACAT92, AYA95, AR99a, Can94, Csa90a, Csa91, DM94a, Dav90, GL92, Har94, HFM91, Hos97, KKNY99, KE90, KN99b, KY92, LMV92, LM93, LO90, MFR91, Mon94, NWT92, PBPN90, Par99, PZ91, Rau02, RR95, SW92, SKK90, TN96, TBW90, UBA92, VA90, WSTB90, Yu95, ZYZ90, WS92].

atomic-electron [TNI96]. Atomic-Molecular [Fan97]. Atomistic [KJD+93]. Atomization [EPB97]. Atoms [ABR95, AM98a, AH97, Bad94, BOX94, BKM93, CBAM97, CC95, CV99, CGR+94, Dat95, DPP+94, GSD97, Gin96b, GLMP98, HWB95, HC96e, JOC97, JM99, KWT95, Koh95, LV98, Mar91, Mar97a, Mar98b, McD97, MA99b, MTL97, PCC93, Pie93, PDT97, PB97a, QS98, RPJZW96, Rae91, SMP94, Sch98, SD96a, SGK+95, SKZ96, SHE97, SS97b, SFGW96, ZwJP95, ASM91, BK95, BKL91, Boe97, Bra95, Bra98b, BGS97, Cal93, CCWCF96, Csa94, DDS9, FR98, GL99, GW91, HW92, HW96, HW90, HBJ+92, HFM91, KM99b, LaF90, LBL98, MFH91, NM91, PS99, PZA92, PG95, PA99, SAB+97, Sco90, SB90, Sem94, SK99b, SKC99, TK92, Tit96, TC98c, VG90, ZP92b, ZB92, ZPBC97, Cal90e, Bra98a].


Auxin [RT98, RTK95, RT99]. auxins [RTK96]. Average [JM93b, KPR97, MR92b, MSP90, PAAM98, SGK+95, MR92]. Averaged [CAJ94, CJH98, KS95b, BBS91, SA97, ZS97b]. Averages [Pop98, Val96, Ort93]. Avery [Cal90b]. Avian [NK96a]. avoid [TS92].


Azabutadienes [Mor96b]. Azasilatranes [DS96]. Azide [YK97, SK91]. Azido [DZB92a]. Azines [DT96]. aziridines [PW95]. Azo [Shu96].

Azotobacter [SZ98]. azulene [GS90a, GS90b].

B [Cal90d, Cal90c, KJ95, Kor90, NÅJ91, NÄJ92, RA91, Sta90, FSW+91, BS91b, Bou98, Bou94, DBLV94, GK90a, JM93a, LBT94, LP99, Mar97b, SST94, WP90, MLK94]. B-DNA [BS91b]. B-spline [DNLV94]. B.C.C [PTL90]. B.V [Ag90]. B3 [Csa96]. B3LYP [Bau98]. Ba [BSS+97b, DDN95, L97]. Bacillus [HB94]. Back [Hos97].

Back-of-envelope [Hos97]. Backbone [FWT+96, LV93, PFMC97].

Band [AGL97, Ara94, CL97, CCC+95a, CM94, FFD98, GSSD+96, Gin95, Lad97b, Min94a, Min98, MAD98, NC95, SK91, Spr96, TDK+94, And90, BBS90, Boe93, EC96, Fau92, FFD96, For92b, KPM+90, LO93, MW92, SBAD90, SS92g, TWWC91, VCMML90, Yam90, YYL90, BRS96]. Band-Structure [CM94]. Bands [DFD97, Gin97, SMB97, BAD97, Loh91].


Barry [Bra96b]. Base [Bra93b, CD93, FW92b, SPG97, SH96, Tew94, ZL98, BH96, FL95, LJS94, PS99, TCB99, Tew97, YNO92, FW92c]. Base-Pair [FW92b, FW92c]. Based [BDG96, BPL94, CDDM96, DMFR93, GLBM96, Gsm98, J95, JBT+95, KS97, Kon94, MS97, Mos98, MV99, RB95, RABZ94, RWT92, SZ95, S97a, S97e, SDE94, SL98, Wen98, ZL9794, BJM+94, BBLK94, BFRN90, BPHB96, CKB91, CB99, EKI94, FKR92, FF90, GSC99, Jac92, JM96a, KRZ91, KSIH92, LP98, MM99a, Min90a, PLBB99, RWT91, SGCC99, SSC92, Suh93, TYY91, TGS99, TD03, DGM90].

Bases [AP96, BNL96, JBS97, SM98, CXFP99, DLR+90, DS90, FHHE90, GT97, Les92, MB91, SSM+99, WS92, YJL92]. Basic [BKR97, Chr99, Tay91, D96b, Jac92, LM95, Bud92, HC96a, NM92, Str91].

Basicity [BK94c, PZTPMC99]. Basis [AH96, AM95, AWA96, BC96a, BR94, BEJ98, Bro96, BDH+97, CM96a, CHM95a, CHM95b, CHMA95, CSS93, Dat95, DLV95, Fer96, FFD98, FR93a, Flo97a, Gin95, GT93, H97, Hi98, HS91, HS92f, HS92e, J99, Jur98a, Jur98b, KSR95, KKT97, KL97a, Kru92, Kut94, L95, LTP96, MSD95, NNM96, PG94, Pah98, PVLO93, PH94, Pen93, Pen96, PMN+92, PDT97, RPJZ96, S97, SPOAS97, SA96, Sur94, T97, T99, T99, US97, UBA92, WI96, AM92, AH92b, Bla99, BC97b, Boe96, BSP98, BGS97, BG98b, BG98c, BG98d, C91, CB91, DLV94, DWM90, DBF+92, Flo97b, FR98, G91b, HBJ+92, ISOA99, Ish91, Ish92, JRS+99, JEB92, J96b, KH96a, KH95, KYW95, Les91, LP92, LO90, L99, MHS95, MFH91, MS92, NE95, PC0+94, PK99, PB99].

basis [Qui02, RA99, RLR90, REU+91, Sam92, SS92f, Sta98d, SBZ92b, Tal93, TKSH93, Tit92, VCCM92, VAVN91, WBP91, WS96, Wil99a, YNO94, vMVvLvD97, HBJ+92]. Basis-Set [CHMA95, PH94, AM92, MFH91, PB99, WS96]. BaTiO [AMC97]. bay [KL93a, VS95]. bay- [KL93a]. bce [MESH93]. BCS [Aon98, PC95]. Be [JM95, TST+99, CL94, CDDV93, L994c, Sta98c, BSHP97, BKL98, JM93a, JM96a, KP97, LBC97, RA96, REL+90, RKPE95, FMD+96]. BeC [DTA+96].


Brä96c, Brä98b, Brä98a, Brä98c, Cal90g, Cal90d, Cal90f, Cal90c, Cal90e, Cal90b, Cal90a, Cal93, Car96, Deu96, Deu98a, Deu98b, Deu99, Dun96b, Eri92, Gre98, Jen99, Jor92, Kar93, Kar96, Kla93, Kra96, Kum93b, Kum93a, Lin93, Lin96a, Lun91, Lun92, Mat97, Mic96a, Mic99, Mic97, Mon93, Mon94, Mon99a, Mon99b, Pan99, Deu97, RKS99, Sjö96, Sta90, Sta93, Str91, Str92, Str93, Tay91, Tri96, Tri99, Wha96, Zer99b, Zer99a, BD95c.

Books
[Ano98a, Zer98a].

Boolean
[Löw92g].

Borabenzene
[KEG+97].

Borane
[BP92b].

boranes
[MAC96].

borazine
[MZ91].

borealis
[SKC99].

Born
[AZ99, CW97, CFB97, KLM91, RL98, STY+98, SNNY99, Suk95, Sut99a, TN96].

Born-von
[CW97].

Boron
[BF96, Bou94, WYW96, BFV+93, LMV92, LFD99, VCMLL90, ZSK97].

boron-like
[LMV92].

Boron-Nitrogen
[WYW96].

Boronlike
[VIK98].

borrowing
[McH91].

Bose
[MVL98].

Boson
[MS97b].

Bosonic
[Oht98].

Boston
[Cal90e, Cal90b].

Both
[Gin95, RP98a, BA90, DO90].

bottlenecks
[Ran93].

Bound
[BGS98, CB99, Csa96, FKK99, FS95c, GSJS97, HMLK98, VJ95, VJ97, EE91, KD92, LS99, Ni94, Roc99, WTD+94].

Boundaries
[CLKMTA95, TSPK97].

Boundary
[AM97, BE95, LKMC93, LCLO95, PTH+97, LV97, YNNR97].

Bound ed
[Núñ94b].

Bounds
[AR99b, Fer91, TVP93, Taš96a, Žit94, AR99a, Csa94, Csa95, Fer90, LK94, PG95, PFK99, TP90].

Box
[LLL97, LKMCVT95, LKMCVT96, OKI98, Whi99].

Boxes
[Aqu95, LKFF98, A95].

Boys
[PK99].

BPb
[BUN94].

Br
[DKM97].

Bragg
[Jac92].

brain
[BPHB96].

Branch
[RG96].

branched
[Art94b].

branching
[CDG04].

Brandt
[Car96].

Breach
[Mon93].

Breaking
[DDH+96, GS94, NFVM94, OOD96, SW97, CGG96, CRK+91].

breaks
[CH91].

breakthrough
[BBCL92].

Breathing
[AMD+97].

Breit
[EK94, FM92b, Ish90, Ish91, Moh92].

Brewer
[Br95].

bridge
[AB99].

Bridged
[BAD99, CdbKZ99, DBG92, FWS97, Gal98].

Bridges
[Shu96].

Brillouin
[DMFR93, GLM91, KS90, LVW97, Wel98].

Britain
[Kra96].

Broken
[CC98, Coo92, Nob99, Oz92, YO92, RVP92, Ran93].

Broken-symmetry
[Nob99].

bromide
[TBP99].

bromine
[CB91].

Brownian
[NH90].

Brueckner
[AS94a, KKJ94, MHN98, Ort98a, Ort99, Scn95, WB94].

Brueckner-Coupled-Cluster
[Scn95].

BSSE
[FGRS98, GRT96, HVS98, MV91, MVHV96, May98, VM92].

BSSE-Free
[FGRS98, HVS98, MV91, MVHV96, VM92].

buckminsterfullerene
[FLLZ91, TMH94, FLWZ90].

Building
[Emc97, Mar94b, PFMC97, PŠ97].

Built
[GVC96, LDJH92, LDJH92].

Bulk
[OLC+96, RHC96, Tri97, LXWZ99].

bupivacaine
[DB97].

Butadiene
[DC97, BT96, PC90].

Butane
[SM96].

Butenolide
[MM95].

Butyl
[RW92].

Butyldene
[PK99].

butylcyclopropanone
[CAM+97].

butyrolactone
[BH92].

C
[Ågr90, Ano92j, Ano93h, BL99, BSS+97b, Brä95, Brä98b, Cal90f, CCC+95a, CMF+98, Eva97, GFY+99, GAR97, JKK+92, Jen99, KJ95,
Kor90, MCCF95, RA91, SC98b, SC99, Wha96, XY95, YZX96, AS99, BZ92,
BB91, BSS+97b, BKM90, CCC+95a, CD93, CXPFP99, CL92, CC92c, DR92,
DM98, DM99, EDF+98, FLWZ90, FLZ91, GV93, GS97b, HMG+92,
HRRBL97, HZ94, HOE+97, HL93b, JM93a, KP96, KH96a, LMR93, LU92a,
LFS94, LL99, LSC98, LSC99, MR99, RN96, RRC94, RA91, RK92,
SK99a, SCA93, SDO91, Sc93, SK92, SL97, SZCO99, TST+99, TPR96,
TFSZ95, TZCT97, TMD96, WYW96, XY95, YZX96, JTZ+96, MPSF97]. C-
[SAC93]. c-BN [MPSF97]. C-H [HZ94]. c-Myb [JTZ+96]. C-NMR [BZ92].
CA [SST94, BC97b, FLZ91, CCC+95a, HBJ+92, Pro95, YDDP92, W99].
CaC [DTA+96]. cadmium [LMMK93]. CaF [LW92]. cage [BBZ91]. cages
[FLWZ90, FLZ91, ZSK97]. Calais [Löw96d, Pau97]. Calcium
[BPL97b, WLB+94]. Calculate [ZLHZ94, CE90, MIA+92, MIW91, RSCP92]. Calculated
[CHAR95, Cfrau+94, DE92, Dat95, HS95, KD95, LV98, YLLJ96, BHKK93,
FR93a, GFS92, LH94, RRC94, SN99]. Calculating [ˇCHMA95, CG94, Coh97, DZO97, HZ99, JM96b, RSCP91, SF94, Val96,
CB96a, Har94, NZ92, Roof93b]. Calculation [ASP97, AL98, ALRP96, BZ92, BLB95, BB97b, BL92b, CJA94, CÁ92a,
CC97, Csa91, DDDG93, DZ98, DZ96b, ET94, FCSV98, GSD97, GMI95,
Har97b, HU94, Iga95, Jas94, JR96, Jon97, JM96c, KMR92, KKK97, KSY97,
KPT94, KL97, Lev94, LTP96, LD94, LR94, LS92b, MA98, MHS95,
MA97, Mez94a, MV97, MAD98, M96b, PSAUS90, PVGL93, Pen93,
Pen96, PMN+92, RN96, RP97, RLR90, RL97, SM96b, SB97, SSO+97,
SZ96, SZ97a, SCP91, Sen96b, SSM93, Sme92, SATP94, VDCK97, WD97,
WR96, WZ99, YLYB90, YLD97, ZW96b, BDK90, BP90, BL98, CM92,
CS96a, Csa90a, CB91, DDD99, DD97b, DD92, DOP91, DT94, DB94b,
EMP92, FGM90, HZF+91, KPV+95, KNN96b, KE90, KD92, KCL95,
KKS91, KSI92, Kur90, LRR92, LL99, MRC99, MLBP95, MPP92].
calculation [MD93b, MD92c, OS91, Rey95, RH92, REU+91, SAW97, SS92a,
SN99, Sch92a, SP90, SSC92, TTM99, Tit96, TŠPK94, VZ92, Wen93,
WL92, WK9+95, YB92, ZZ94, Kov90b, Mun92]. Calculations
[AHI96, AH97, BB97, Bér97, BNL96, Boe92, BEJ98, BPL94, BS94,
BJL98, BL98, CM96a, CM98, CH95a, CH95b, CHMA95, CCC93,
CF97, CM94, CLKM9A95, Cul95, DHL+94, DREW98, DRB96, Dun96a,
Dun97, EP98, EMMS94, Fer96, GKKM96, GD98, GMS97, GTR96, GT93,
GP94, Gre94, GP97, HMGPP93, HLS94, HBL99, HNB92, HMLK98, HC96e,
HZ94, IAN+94, IK97, Jac97, JCÁ96, Jen94, JL91, JAG95, JSG97, Jura96a,
KL98, Kar98, KS98, KBL95, Kol97, KA95a, KL97b, K97a, LMC97a,
LPM97a, LMR96, LBM94, LY98, LFS94, Lind96b, LCO95, LL92, MMY+96,
MS95, MF96, Mar95c, MA95, MSC95, Mor93a, Mor97b, MRD92, NV94a,
NV94b, Núñ97, NV97b, Oka98, Or98, PCE95, Pah98, Pra97, RML97,
RSD97, Ry94, SB95a, SO94, SNMB97, SPF96, SRS92, SG93, SST93].
Calculations [SR96, SBIP97b, SLA97, SBD+92, SAL+94, SH96, Sta96a,
SL97, SDG97, TJ95, Tri97, VV95, VK98, WD95, WZW96, W96, YNY99,
[BA91, BBMM99, CT95, For92b, Geg91b, LB96b, LAM92, MVS97, Pal91, PDo92, PCD99, RRC94, SC99, TMA97, Whi99, CLGW95]. cases [hJH97, Löw92h].

[BB96a, BBOR96, BCD99, GMM97, JK90, KP92, LH99, MCOS94, Pr97, SG93, XLW+99, YTYS97]. CASV

[GZ97, GZ06, Deu98b]. **Challenges** [KPD93]. **Challenging** [BA97a]. **Chalmers** [Gre98]. **Change** [KS98, RD90, TTOY93]. **Changes** [FW92b, FW92c, AM90a, FL95, Hag96, Pal93a]. **Changing** [SB97a]. **channel** [FKK99, KO91]. **channeling** [NST94]. **Chaos** [GBMA94, CPW92, Kar93]. **Character** [Bor94, CLSI94, Her97, KM92, PB97b, PGGH95, FJIR96, NNH98, TG96]. **Characteristic** [PM95, YD97, ZW96b, DM97a]. **Characteristics** [KZ99, RW92, SN99, VH96, Voj96, EZ93, GS91, TP94]. **Characterization** [DTA+96, HS99, JI95, KC98b, PV94, RK97, CPD+98, KJL96, KLC98b, LM92, Ran95, RK99, WM92, AKCS91, SCMF93]. **Characterizations** [BPL94]. **Characters** [WFK97]. **Charge** [AYDR96, AC94, ATI97, BK96, BLBP97, BK95, BAD99, CLSI94, CM94, Del96, HP98, HSS+95, KO95, KMM95, Kup94, KKM99, LK90, Lon99, MK99, MKM96, MKM97, MM98, Mon98, MM95, MNM+97, NNM+98, Nal94, Nal95a, NM95, Na97, PC91, SBM97, SBAD90, SG94, SR96, SMO+96, SHC+98, Sta98a, Sur95, Sur97, WPB98, YDFS98, AS91, BADM97, CB95, Cu91, DM94a, GZSV99, GB599, HE90, HSES94, LK99, MES93, MCA95a, Nal92d, Nal92b, NM92, Nal98, Sta98a, SN90b, HE90]. **Charge-** [NMN+97]. **Charge-Conjugation** [Kup94]. **Charge-dependent** [Lon99]. **Charge-Exchange** [KO95]. **Charge-Mediated** [NMN+98]. **Charge-Transfer** [AT97, CLSI94, SBM97, Sta98a, WPB98, PC91, GZSV99, LK99, Sta98b]. **Charged** [Brä98c, GH96a, HL93b, NBS95, PCC93, VBF95, WA94, Woo99, BKS97, GW91, HFM91, MF91, NYK98, TIA+92, VF99]. **Charges** [AC94, BKM93, CV99, CDDV93, LV98, Mon98, Roz97, SK99b]. **CHD** [RT96]. **Chebyshev** [NS95b]. **chelates** [HBGR99]. **Chemical** [ADB96, AR96, AFTM95a, AFTM95b, AFO+97, AFTM98, AK97, AH96, Bir94, BSHP97, BPL97b, BK98, CN94, CXL97, CCE+93, CL95, CCG+96, DP94, Dun98, ESP98, ETV94, FSSF96, Gho94, Gin95, Gin96b, GJPMML91, GJLA99, Gre94, GWCT97, GKS99, IK94, KSKJ94, KZ94, LP97b, LL94b, LÖW94c, MB97a, May98, Mon98, MTD96, MM95, NOYY94, NN94, Nal92a, Nal95a, Na97, NS95a, NS95b, Nef95a, Nef95b, NV94a, NV94b, PRC98, PZ95, PS94a, Pon97, Pon98, PCD99, Ryd94, RKG96, SKJ98, Sch93, SR96, SDE94, Sur94, Sur95, Sue96, SFGW96, TKNI96, Vd96, VB94, VBF92, WS94a, Wen96a, YDFS98, ZCT98, ZZZY96, Aks+90, ABSW95, Ano92k, AFZ+99, BZ92, BA91, Ber96b, Bhaa9, BS98c, VD90, CM92, CRK+91, DVJ93, Deu98a, DO90, ESV92, FLW92, FLZ92, FL95]. **chemical** [FS99, GKM90, GS97b, GB90, HZ91b, Kar96, Kha91, Kry96, Lad94, Lan95, MUL99, MD94, MD95, MCA92, MCT99, ML99, MV92, NOY92, Nag96, NOY98, NM96, NE95, NV97a, OYNY98, PTL90, RT99, RD90, ST98, SG92, TIA+92, TP92, TNSM99, TTL92, TMA97, TŠPK94, TCM99, TMD96, WJC+98, Wen96b, WZ96, WZ96, YOT93, Yur95, Mon93]. **Chemical/Molecular** [VBV92]. **chemically** [SES93]. **Chemisorbed** [BDD93]. **Chemisorption**
[FWBT94, NM95, SFGW96, FL91, LaF90, MtPC+96, NF92, SW92].

**Chemistry**

[All94, AAS93, Bad95, BG98a, BR94, BPL97b, Cal96b, CCC93, CC98, Cle92a, DN96, Dew92, Enk97, GZ98, HPSC97, JPP87, KPD93, Kir95, Kor95, Löw90c, LZ92, LZ94, Löw95f, MDS08, Mos98, Nic99, Ryd94, SS97a, WSM+94, Ano90g, Ano91g, Ano92j, Ano96-58, BAF95, Brä98b, BBE95, Cal90c, CDB99, ˇCVW91, Coo05, Csi77, CD81, DS99, ESTM95, FS99, Gur99, HW04, Hei95, Hei90, Hin88, Kel97, Ken93, KWZ98, KH95, KH96c, Kra96, LGT94, LZ91, Löw91a, Löw91b, Löw91c, Löw91d, Löw91e, Löw92a, Löw92c, Löw92d, Löw92a, Löw93a, Löw93b, Löw94b, Löw95c, Löw95d, Löw95b, Löw96a, Löw96b, Mat96, Mat97, NSAS+90, Pär98, Pan95, Qui02, RS00, SR93, SR02, SP95, SN97, Smi96, Str92, Tay91, Tet93, Tri96, UBA92, WA94].

[GARC97]. Close [Hed95]. Closed [AM98a, BMA93, BEG94, HT97, Pal97a, PKM93, MC91a, MC91b, Moh92, MCB99, VDL95]. Closed- [BMA93].

Closed-Shell
[AM98a, BEG94, PKM93, MC91a, MC91b, Moh92, MCB99, VDL95].

Closure [BO93], Clothing [DM96], cloud [VDBPR97b].

Cluster-Series [MI93]. Cluster-Size [BDD93]. cluster-type [CS99].

Clustering [Mar95c, Ike99]. Clusters [AML+95, AMD+97, ABR95, Boc96, Bou94, BDD93, DDH+96, DRBE96, GD96, HLS94, HU94, Jur98b, KSN95, Loh96, MMP+94, MDJ98, MLR+98, NM95, NG97, NC95, NS97a, NS97b, PTP95, Ros96, RKPE95, SPF96, VDCK97, VBF95, ARDP92, ACB+99, AGNS92, AD92, BGS99, BUZ94, BMDM90, BAL95, BFP93, BYE+97, Cas91, Cas97, CS96a, CBL95, CCS99, ČPV90, CPD+98, ČZ92, FLWZ90, FG90, GKM90, GFY+99, GW979, GRB+93, Gur99, HCR94, HSL92, IBS95, KSN93, Kap99, Kar90, Ki94, KS94c, KF96, KBBK90, KJ97, LP98, LXW99, MD92a, MRR99, MA95, MNC95, Mur90, RRC94, REL+90, SCP93, SKE92, VG90, VFBP96, W96, WMZ98, XSG97, YNNR97].

CN [JMP99, NG95, NG96, Bau97, Del92, JMP99].

CND0 [Boc90, DDP93, KSH92].

CO [Bou96, BL98, SC98b, SC99, VR92, Ano93g, NG95, Cas92, CLGW95, EZ92, hJH97, LD95, MLT98, NL96b, PBP92, RKH+98, SM96a, SDP+95, SCS94, SG96b, SG97, YBM97, Jur99c].

CoAl [DDC97].

CoBalt [GK92, SFGW96, WWFR99].

Cocatalysis [Sak97].

CoCl [CCWC96].

coefficients [Kin94, Xu99].

Coefficients [BK94a, BP93c, De 97, GL96, MK98a, PAT93, RWT92, ZW96b, BP93b, CBT93b, Kat91, Kat98a, Luk92, PC99, PZA92, RWT91, SDO91, SMH92, Wen93].

Coenzymc [FVN98].

Cofactors [DV98].

color [KŽ90].

color-pairing [KŽ90].

COLUMBUS
Combination [AS96, KEG+97, PMN+92, BJA99, TNI96].
Common [HH97, LSS96, Van96]. Commator [MV98b]. Como [FR94].
Companions [Par94b]. Comparability [BKM90]. Comparative [ADPS98, BLE96, GJ96, VBV92, Ano96-31, DV96]. comparing [OS92, GS97b].
Comparison [AOH96, BBTU97, BBC+96a, CLGW95, CL92, Csa95, DS90, DZO97, GL92, JMS95, Jur96b, KLC98a, LJ95, LP94, LS93b, MPJ98, MR94, PC90, PB96, PAAM98, Pra97, RL94, RRS97, STZ96, Sza95, Tri97, ZON+96, ZC95, CGG96, KF96, LG96, Ort93, Par92b, Sch92b, Suh93, CZ94a, PČP92, RTKP95, SB92b].
Comparisons [CS96a, MM99a, Sem94, TFSZ95, DBF+92]. Compensation [ST96b]. Competition [KM92]. Complementarities [NK96a].
Completeness [Hi98, JB97]. Complex [AMRT94, BPL94, Cio94, CCE+93, DP94, GS92a, GS92b, HPSC97, KW98, KB93, KE93, KK93, MA93, PM93, PV94, PV98, SWF93, SL93, SDW+98, SSD96, VH96, Ano93a, BS91b, CPN91, GZD99, GZDZ97, MLL99, MLK94, NL96b, Sch92e, SC99, WM92, WFS93, ZBL99].
Complexation [XY95]. Complexes [ATP97, BKWL97, Bér97, BCRL94, Cl9799, CC96, DL92, LL97, JKK+92, KS94b, MCM95, MBA94, MBP97, NG95, RK96, SM97, SB97a, SBIP97a, STM96a, Sta98a, TMS98, TSS97, XY98, BCLS94, BDPS97, Bro96, CC92c, Cun92, DSS90, Del92, EE91, FZZ92, FWS97, FS99, HRR97, HB97b, HWB97a, ITT+94, Kar90, MAC96, NL96a, OSS95, PC91, ROL+90, RCW94, SC96, STM96b, VAB94, VM92, WG99, WMD95, WWFR99, YZX96].
Complexity [Art94b]. Component [CJH98, HBL99, LX95, LKL99, MBV+98, SS97b, vvBS96, BOL+90, BSS97a, KBKT93, Zho93].
Components [GB97, Q98, Luk92]. composite [BG98b]. Compound [DL92, LEG+94, GC91]. Compounds [BLE96, BHP95, CF96, DBZ92a, Dau94, DD93, ET97, EMMS97, FT95, GKK96, GARC97, J93, LL92, NN94, PD93, RGH94, SR96, SBIP97b, Sta98a, TB95, VV95, VDD96, BJM+94, BH92, CMA+99, FT96, FT97a, FEE+98, JF92, Kh92, Kin94, LRM93, LRR92, LC93, Loh91, Lun91, MUL99, MKK96, RC92b, SJ97].
Computational


[BJM+94, BPL97b, GBL97, HPSC97, HBGR99, Hin88, Jay92, Jur98b, Jur99b, Jur99a, KPD93, KÅ99, KRRB99, Kry93, LSS96, MZ93, MPOG99, Mos98, NSAS+90, NGM+95, PMO90, PW97, PM95, PTM92, Qui92, RC92b, Sza95, TNS92, VRR92, Wen96a, An90i, An90j, An90k, BAF+95, CL92, Coof95, CF99, FCA91, FADC91, KK92b, MSRP90, PAC90, PACO90, Pos91, SCP93, Tri96, Wen96b, CD81, An92k, An92j, Cal90g].

**computationally** [BS95, TSS95]. **Computations** [FGRS98, Löw90c, Ryc94, Sim98, LS99, Löw91a, Löw91b, Löw91c, Löw91d, Löw92b, Löw92c, Löw92d, Löw92a, Löw93a, Löw93b, Löw94b, Löw95c, Löw95f, Löw95d, Löw95b, Löw96a, Löw96b, MRST95, MSC92, Sin92, SZCO99].

**Compute** [BR94, MKM96, RL94]. **Computed** [HH92, Jur97g, SBD+92, KSF91, MR97, MSPS90, Nes94]. **Computer** [BPL97a, BRA+99, GMI95, Har99, SKZ96, ACB+99, Jon92a, Löw92g].

**computers** [Cle92a, FKHD97, Har91, Ken93]. **Computing** [DB99, RWT92, ST96a, Sim97, TNM97, WPB98, BDPS97, Con92, Jur99d, Ken93, LGBL94, OS90, PS92c, RWT91]. **Concentration** [SR96, BPHB96].

**concept** [VD90, KLC98b]. **Concepts** [Na195a, Na195b, Atk91, LM95, Na192d, NM92, TD03, Dun96b, Str93].

**Concerning** [GL94, HM95, Ney95b]. **Concerted** [Pon97]. **Concluding** [Löw90d]. **condensate** [DBM99]. **Condensation** [TM97, MVL98, PL93]. **Condensed** [ACPR98, Cab96, Chr94, CCZ97, Her98, Löw90c, Mar94b, Mar97a, Mar97b, BCD91, CDB90, Chr92, Lei99, Löw91a, Löw91b, Löw91c, Löw91d, Löw92a, Löw92c, Löw92d, Löw92a, Löw93a, Löw93b, Löw94b, Löw95c, Löw95f, Löw95d, Löw95b, Löw96a, Löw96b, Lun92].

**Condensed-Phase** [Her98, Mar97b, Cab96]. **Condition** [BA93, Pon98, PCD99]. **conditioned** [JK92b, SBZ92c]. **Conditions** [AM97, BE95, LP94, YO92, HYS91, NST94, YNNR97, ZP92b]. **Condon** [AD97, LKMCVT95, LKMCVT96, PRSD92, PSM94, Pa197a, PL99, RSCP92, VV91]. **conductance** [CDB90]. **conducting** [AM93, Sta98e]. **conduction** [EC96]. **conductive** [TYY91, TYTY91]. **Conductivity** [BMK96, LRM96, LRM97, RML97, yYL94]. **conductor** [TN96]. **conductor-like** [TN96]. **conductors** [Sta98b, Yam90]. **conduisant** [GK90b]. **cone** [BR92, KH95]. **conference** [An91g, Fuk90, Löw90d].

**Configuration** [BEC94, BLM95, BL98, DM94b, EBG95, Huz96, JCM+92, KSR95, MHG95, MR92b, PS96, Pen96, PAT93, SWF93, YJL92, BE93, CC91a, CGG96, DM92, Duc90, HC91, IHG95, MM93, RTS91, SWD+99, SG90, SBZ92d].

**configuration-interaction** [CC91a].

**Configuration-Interaction-Oriented** [SWF93]. **Configurations** [CC97a, CDC98, HM97a, FW92a, WM92]. **Confined** [CLKMTA95, PZWJC96, WGR+94, ZWPJ94, SR99]. **Confinement** [RM99, ZWP95, Art96]. **confinements** [PKJ99]. **Confirmation** [Tri98c]. **conformal** [CSH99].

**Conform** [MV+97, SKJ98, SRS92, Csi82, FT97a, WTD+94, Luo95].
Conformation-Transitional [Luo95]. Conformational [Bue96, CDDV93, CDM+94, DZOR98, GSSD+96, HS92b, Jac97, LS99, LVCP91, MSM96, MT96, MIP99, NSS92, NAK95, NMS99, NP96b, PL92, RL95, RKN97, RT98, RGH94, RK95, Tew92, Tew94, VDD96, WHF92, Cab96, ITT+94, JGCJ96, MG90, MT91, RTKP95, RTK96, RT99, SDP+95, SSM+99, Jac98].

Conformationally [AV92]. Conformations [BRA+99, FT95, SST93, FT96, LCP+91, LU92b, LE92, Pal94, Ran95, SST94]. Conformers [PK99, AGAP98, HRH99].

Conjecture [Csa96]. conjectured [TP90]. Conjoint [GR96a].

Conjugacy [Pal95]. conjugate [MBP91]. Conjugated [JCA97, Kan93, KBT94, GFS92, GX98, HZ91a, Kir92, KRBT94, LB94, MB92, PVN90, SP90, YB99, YAD92, GRK96]. Conjugation [DB94a, Kup94, OKI98, PB97a, Kor90, LL99]. Connect [VdV96].

Connected [JM93b, MZ94, LP98]. Connecting [Pal97a].


Consequences [Suk95, BSS+97]. Conservation [FSAV97]. Consideration [Zap95]. Considerations [ECBH96, BSP98, MKR99].


Constant [EPB97, FGRS98, FF94a, LC90, Sta91, TFF+91]. Constants [EPB97, FGRS98, FF94a, LC90, Sta91, TFF+91].

 Constraints [IK94, Sad97, TKMA92, Val94, Cui91, KDB90, MK90, WW97, ZP92b]. Constrants [BDT96, GGHP94, KKW99, MYPL90, MP91]. constructed [EIl92]. Construction [Ban91, Bro93, CW98a, CH95a, Her97, MD93a, Mey94, Mey97, DMT97, ZW98a]. Contact [HNB92, PV91].


Continu [AB97, Nic99, BRV90, Rod91, Sme92, Tom91]. Continuum [DBLV94, PTH+97, WR96, CT95, DV93, FM92a, GJMML91, MCT99, RV92, TCM99, BF93]. Contour [Ort95]. Contracted [CV94, PDT97, CB91, SS92d, TK93, VAV91, MAZ98]. Contracting [Val96]. contraction [ISH1, SS92].

Contributions [LZ96, WL99, GS90b, VAJ+92]. Contributions [LZ96, WL99, GS90b, VAJ+92].
[Ano98a, Ano98b, Ano98c, Ano98d, Ano98e, Ano98f, Ano98g, Ano98h, Ano98i, Ano98j, Ano98k, Ano98l, Ano98m, BK96, Ano90g, Ano90i, BPVP92, CDB99, Cim96, GSKC99, KK92b, LZ91, PBPN90, Per93]. Control
[DDH+96, Jos97, MY99, TC98c]. Controlling [BRZY97]. Conventional
[FGRS98, Nic99]. converged [FADC91]. Convergence
[BF94, BDD93, Csa94, DP96, Hom93, KZ99, Kin99, Kol97, LXWZ99, N´u˜n97, Sel93, WBD97, CFMA95, GR95a]. Convergent [TM93]. Conversion
[ML99, GS90a]. Converters [KB93]. convolution [PLS99]. Cooper
[AS95, Tac94]. Cooperative [DD99]. Cooperation [SS92c, Suh94].

Coordinate
[KZ99, MD93a, Nag95a, NM95, PM93, PDT97, SWF93, BA92, W98]. coordinated [ASM91]. Coordinates [CN99, DZF93, DZ94, LB97, LKB97, MBA97, Zha96, BRV90, CTF92, GS92b, Sch92b, ST91, TFYY91].

Coordination [Dan94, Ryd94, TD03], copacking [WP91]. Copenhagen
[Kar93]. coplanar [Les92]. copolymers [BL92a]. Cooper
[B´er97, ETV94, Fot94, LB94, PM93, KCP90, Yam90]. Core
[EMMS97, Lad97b, PB96, RRS97, BDPS97, CLGW95, LO93, Per93, SS98].

Correction [CSS93, CS98, DD93, GR96a, Kry95, IHG95, KF96, MRD92, P091, Sut99a, TC98c]. Corrections [AZ99, Del98, EMMS94, KS94a, Lev97, LTP96, PPP97, PP98b, See93, BLG95, LP98, WS92]. Correctly [Bau98].

corrector [Sim95]. Correlated [CZ94b, CSS93, GKA97, Hoo94, JBS97, Kin96, KP97, KLT97, Kup94, Mar95c, NG+99, PP94, PK96, Ryc94, SE92, SO94, SN98, BBM99, Che92, FW92a, KM99b, CA95b, Lev99, Mar94c, MB93, PP91, PˇCP92, PA99, ZA95, PC99]. Correlation
[AL98, ABR95, BP93e, BP95, BCL98, CBT93a, Can97, CGLP96, CC97b, CGR+94, CA97, DW97, DC97, FT97b, FR93b, FS93a, FS94, FS95b, Fue94, FS92, GS94, GJGPZ97, GS97, GSA98, GLMP98, GBV97, GSKC99, Hed95, HP97, HM97b, JCA97, JMD95, JI97, KNA94, Kin94, KM97, KBL95, KH96b, LO93, Lad97b, LRM93, LMR94, LP94, LG95a, Lev97, Lin94, KLBD98, LBLK98, Löw95a, Luk92, MSD95, Mar95b, MK96, MK97b, MK98a, MPJ97, MPJ98, Muk96, NK97, NKB97, PKM93, PC95, PP98b, PR97, PSS97, QS98, RS98, Ros96, SMPJ94, SBM97, SA96, SF+98, SW97, SS97b, SM95, SU94, SK98, WS98, Xu96, YNNY99, YDFS98, Zie95, Ada91a, ADB95, AC95, Bec94, BMDM90, BKL91, Bro96, Bud92, BFW92, CBT93b, Can94, CGG96, CLGW95, Csa91, Dav90]. Correlation
[DSS90, DDN95, EKI94, FG90, För92a, GN90, GL95, GVB96, HC96d, Ish92, Iva96, Iva97, KBB93, KKK90, KL93b, KKL90, KCL95, LCB98, LS92b, MHN98, MK95, MSF91, MD92c, NOS94, PGM95, PP92, Per93.
[BKLV94, BKLv95, KMV˚A95, BL91, BFL91, Rin96, TGS99]. crown [Tho96].

Cryolite [BPL97]. Crystal [AOH96, DM96, DTM96, KD98, KPTS94, MSS99a, Pan93, PVLG93, RK95, STM96a, Sta96a, Sta97, Sta98a, TSPK97, AS93, BLA95, CRK+91, DO90, GGHP94, PS99, PS92c, RK91, SKRK90, SJ97, Sta95, Sta96b, Sta98b, Sta98d, Sta98e, WL90]. Crystal-Field [STM96a]. crystal-orbital [Sta98d, Sta98e, WL90]. Crystallography [HMK99, MHK95].

crystallization [IPA94]. crystalline [CCC+95a, ETV94, GT97, Sta97, AST95, Boe96, BJA99, CRK+91, HMK99, NWT92, PAC90, PACO90, PD92, TNS92, WSTB90, ZWD98a, ZWD98b].

crystallization [IP94]. crystallography [HMK99, MHK5].


cu-o [AS93, VBN95a, VBN95b, Min96]. Cuprate [DMB97, DBM99, Mat96].


Cyanoketine [RW92]. Cycle [KP93, PK92a]. Cyclic [BEG94, BE95, BE98, BČ96, KBGE97, LP96, TBČ95, Che92, ITK91, Kar90, LR98, MB91, PP92, PP91, PČ92]. cyclicity [BBKL94, BBLK94].


Cyclopetadiene [Bra97b, SL98]. Cyclopentadiene-Based [SL98]. cyclopentadienyli [BB94]. cyclopropabenzene [EMMPHP92].


Cytosine [GL98, PCE95, ZL98, BHV96, FL95, PWL98, TG96].
D [Ano93g, BBC92, Bra95, BYGA99, Cal90c, Cal90a, Dun96b, Lin96a, LU90, LCP+91, LSGS91, Mat97, Mon93, Mon94, Sta93, PAT93, SST93, ST94, CBT93a, CB93b, CB94a, GJOV97, HP98, IHC95, MCM98, SPH98, SB98, SNT93]. d’activation [GK90b]. Dahmen [Car96]. DAN [Mun92].

Dancoff [DP97, VZ93]. dans [GK90b]. Dahmen [Car96]. DAN [Mun92].

d’activation [GK90b].

Dahmen [Car96].

DAN [Mun92].

dans [GK90b].

Data [BMG+98, HL93a, HPSC97, Jur96a]. Dative [SL93].

David [Gre98, Jør92].

Davidson [JGP91].

Davydov [För97].

Day [Dav98].

dC [GT97].

DCI [RN96].

DCNQI [Sta98b].


deaminations [HDB+95].

deaminoarginine [SS90].

Debye [ZW96a].

decane [Lu99].

Decarboxylation [FB96, NSS+95].

Decay [ABB93, VBF95, Ale95, GZD97, SLS91]. Decomplexation [XY95].

Decomposition [BAK96a, BAK96b, Jur99a, Pás97, PGS97, PSC97, YPC97, AKCS91, CRK+91, RK92]. Decompositions [AT93, MR94].

decoupled [Nal91, Nal92c]. Decoupling [BJLK98].

decsilane [Lu99].

Dedication [Ano92m].

Deduced [MPJ97, MSF91, Sin92].

Defect [LBM94, LMMK93, MKDL93, Mar99b].

Defects [Kry98, MI93, MPSF97, CFDS90, GKM90, Kun90, LW92, MG99, SX96].

Deficiency [Mez97a]. Define [Bad94]. Defined [Mor96a]. defining [BP93d].

Define [KS95a, Ols96].

Deformation [Ad99, BKLv95, ČHM95a, GR94, Mon98].

Deformations [B98a]. deformed [DSW93].

Defranceschi [Cal90c, Eih97]. Degeneracy [B96a]. Degenerate [CJA94, JG95, LD94, Pa98, RDF98, AI99, KSF91, MHP95a, MHP95b, MRD92, YG90].

degenerated [HOF+97].

degree [Art94b]. Degrees [NP96b].

Dehydration [BAK97].

dehydroalanine [NMS99].

Dehydrogenase [CAK+96, Ryd94, GVK99, RAM91]. del [BG98b].

del-operator [BG98b].

Delayed [MBV+98].

Delhalle [Cal90c].

Delocalization [CD93, KM92].

Delocalized [SBL+94].

delta [SBL+94].

Deltafunction [LB95].

Deltafunction [LB95]. Denmark [Kar93].

Dennis [Ano92k].

denominator [LC90].

dense [KH96a, Mar90, MA9+91].

Densities [AZAC97, CC95, CM94, DBB94, DMFR93, FUI97, HSS+95, KKT93, Kup94, Mar96, Mic94, Núñ95b, Núñ96, OH97, PV97, PS94a, PB95c, PJ96, SRM98, SP94, CCWF96, CMB95, KM99b, MS91, MAC96, PA99, VES+99, YKN+99].

Density [AMRT94, ART94a, AL95, ASP97, ABR95, AM98a, And94, AYDR96, À94, AS94b, ADM98, Bad95, BDBG96, BAR94, BIM97, Bé97, BM96, BDK90, BCR94, BG98a, BAL95, Bra97b, BS94, BYE+97, BCL98, CDBK99, CG97a, CZ94a, Cha98, CGLP96, CSP98, Cio94, Coh97, CPA95, CA97, CB94b, Dau94, DPP+94, DZ94, DDD98b, DZ96a, DI95, Dob98, DKKB97, Dun96a, Dun97, Eng95, EMMS94, EMM97, FEE+98, FP94, FT97b, FWC+93, GMS97, GR94, GR96a, GG97a, Gho94, GD94, GSD97, GD96, GWB97, GBRA94, Gör98, GPD94, GG97b, Gre94, GWCT97, GLBM96, GK91, GDF92, HMG93, Hag97, HHKM95, HM95, HM97b, HBH98, Jac97, JBT+95, JBT+95, JBT+95, JBT+95, JBT+95].
Density [KVB97, KS94a, KSSG95, KBA96, KD98, KS94b, KVS98, Koh95, KMM96, KL97c, LZ96, LY98, LP94, Lev97, LLZ98, LKLB98, Lu99, LLBM+95, LAS+95, MG97, Mar94b, Mar94d, Mar95a, Mar95b, Mar98b, Mar98a, MRT97, MFP96, MSMR99, Maz98, MB98, Mez97b, Mic96b, MDJ98, Mor93b, MCA95b, MNC95, MSCP92, Nag94, Nag98a, NV97b, OHS97, PCE95, PY99, PP98a, PMDM97, PZDM97, Per98, PB96, PEB97, PRTV97, PAC90, POC90, PG99, PAM98, PK96, PS94b, RL95, RP98a, RSD97, RRS97, SP98, Sam97, SPOAS97, SDW+98, SS90a, SD97, SPC96, SZ96, SZ97a, Scu95, SCP93, Sha95, STY+98, SNY99, STMR97, SR96, SPM94, SMO+96, SAL+94, SC97, SH96, SL95, SD97, SC99, SAT94, Suk94, Suk95, Sur97].

Density [TKNI96, Tac96, TC98a, Tet93, TG95, The97, TSP96, TSP97, TB95, TCM95, Tri97, Val94, VB94, Wk95, WR96, YNY99, YNN97, ZC96, Zat95, ZC95, ZF99, ZL99, Ali99, AC95, ABSW95, An92, BOL+90, BOA95, BMDM90, BCD91, BDPS97, BS92, Ca90a, CCA98, Cha92, CLG95, CP99b, CMA+99, CES97, CA91, CEM+96, Ca90a, Ca90b, CK91, Cae92, Cee99, DA91, DDC97, EDH+92, GP92, GRBB92, GNF90, GW91, GSKC99, HCR99, HMG+92, HAR94, HK95a, HJ96, Hol98, Huf99, Jac98, JWG95, Jur99d, Jur99c, KK99a, KC97, KL90, KLM91, KL92a, KL92b, KB90, LC98, LBL98, Mar92b, MHN98, Mar99a, MV96, MCE97, MLL99, MH93, MRT95, MRST95, MR97, Min90b, MYP90, MP91, MSF91, NNY99, NM94, Na95b, OGG90, PA99, PSM98, PP90, Per93].

density [PG96, PNB94, PG95, RVP92, RD90, REK92, SH90a, SN99, SG96a, SCP91, SP92b, SP95, Sem96a, SPM+96, SSC97, SCS94, S99, SG96b, Spr93, SD91, SH99, TNS99, TP90, The94, TC98c, TGD97, Tri96, V96, VV98, WW97, WS92, WGP99, WM98, YB99, Yor95, ZTC97, ZY94, Zie96, CES97, Mar99a, PM98, PD97, CA90a, Ca93].

Density-Dependent [KLLB98, Scu95].

Density-Functional [Dun97, G98, H97, P97, Scu95, The94, TC98a, TCM98, Tri97, Bec94, BF91, BFL91, BMA99, CT95, CCS98, C99, D97, FMR91, GBS99, KCI95, Lon99, PG96, RH92, Rod91, RM90, TC98c, YB99, SB92].

Density-Matrix-Response [TC98a, deoxyadenosine [KJ96].

Deoxynucleobase [GSD+96].

deoxynucleobase [KJ96].

Deoxyxynucleotides [GD92].

Dependence [CR93, EPB97, FP96, FMD+94, FDAC90, GLY94, KSH94, MPV94, MBA94, SC98a, SG90, AM92, FV96, FR93a, HSWS95, LP99, MJL99, MPH99, PP99, SLS91].

Dependences [AN99, AV92, AM97, CT96, C98, DFD99, DD98b, FB97, G98, JR96, KLLB98, KSY97, LG95b, Mor96b, RB95, RW98, SB95a, Scu95, ST93, TC98a, TCM98, Tri97, Bec94, BDP+92, BFL91, BMA99, CT95, CCS98, D95, FMR91, GBS99, KCI95, Lon99, PG96, RH92, Rod91, RM90, TC98c, YB99, SB92a].

Depleting
[Sen96, Jur99c, MSRP90]. **Dimethyl-Amine** [Sen96].
dimethylcyclopropanone [CAM+97]. dimethylguanine [YJJ92].
dimethylimidazol [Cio93]. dimethylnitramine [CRK+91].
**Dimethyluracil** [PIG94]. dinaphthonorbornadiene [SCC91]. Dinuclear
[Bér97]. diol [Enc96, KM90c, WP92]. **Dioxide**
[AMRT94, AMKS93, SLG+96, TFT+91]. dioxin [MEP90].
dioxodihalides [TGDS97]. Dioxogen [Bér97, BB9+96a].
Diphenylacetylenes [DB94a]. Diphenylpentane [LV93].
diphenylpolyenes [LB94]. Diphosphate [FVN98]. dipolar
[MK90, SAL+94]. Dipole [BP93c, BP93b, Can97, CJA94, GSJS97, KSF91,
MS98, Mon98, SPS96b, SC98a, Sut99b, DOPS91, KY91a, KY91b, KM90c,
MK90, Par92b, SDO91, SSC92]. Dipole-Bound [GSJS97]. Dipole-Moment
[MS98]. Dipole-Octupole [BP93c]. Dipositronium [PK96]. Diprotonated
[Sta95]. dipyrtylid [AEHM91]. Dirac [DJ12, Csa92, DJ95, Dat95, DN96,
EKI94, GC91, Ish90, MHN98, MC91a, MC91b, Moh92, VIK98, ZP92b].
**Direct** [AL98, BTTS97, BD94a, BD94b, BD95a, CMB95, DRBE96, FGRS98,
FP94, GVB97, KBGE97, VdV96, VHFL93, ZDO96, SO97, VR90].
directional [BMP92]. Directly [BDNT97, Sin92]. Dirichlet
[Núñ95a, Núñ97]. discovery [Kha91]. Discrete
[HR95, OLC+96, VJ95, VJ97, Ale95, Geg91b, Ish92]. discretized [CGMG92].
**Discrimination** [Reg92]. disk [Brä96b]. Diskette
[Ano95f, Ano95f, Ano95h, Ano95i, Ano95j, Ano95k, Ano95m,
Ano95n, Ano95o, Ano95p, Ano95q, Ano96h, Ano96i, Ano96j, Ano96k, Ano96l,
Ano96m, Ano96n, Ano96o, Ano96p, Ano96q, Ano96r, Ano96s, Ano96t,
Ano96u, Ano96v, Ano96w, Ano96x, Ano96y, Ano96z, Ano96-27, Ano96-28,
Ano97a, Ano97b, Ano97c, Mic96a]. disorder [Lás93]. **Disordered**
[DFL98, LRM96, SLtM+94, BCD91, CDB90, LO93, PK90]. dispersed
[EZ93]. **Dispersion** [BP93c, HP98, MJ9393, ADB95, BP92a, CPA98, MK90, BP93b].
**Dispersion-Energy** [BP93c, BP93b]. Displaced [Coo94]. Displacement
[KMM95, MK99, MKM96, MM98, KKM99]. displacements
[MNTF99]. Dissimilarity [Mez97a]. Dissipationless [ML96]. Dissipative
[AT9+96, BS93, KMM96, O’C96, Sch99b, BCD91, Sch90, Sch94].
Dissociation
[Ata97b, DM95, Jos97, JM96c, Jur97b, LTP96, Mar95b, Rot96, Ata97a,
CLOFR98, CKB91, HMG+92, JY94, Jur99c, Rot97, SP92b, VES+99, ZGPS97].
Dissociative [CFB97, MD91]. Dissociative-ionization [CFB97]. Distance
[GM93, HSS+95, LNT99, MC94, MBA94, HSWS95]. Distances
[GR95b, GR96b, HP97, BBLK94, BDPS97]. Distortion
[Kup94, WTD+94, WG95]. distortions [Cas97]. Distributed
[AC94, FFD98, Wil96, Wil99a, LGBL94]. Distribution [And94, KBWJ96,
ML97, MK98a, MV99, Ols96, RPKMK95, SHC+98, TSPK96, ASM91, DOPS91,
GSM+92, HE90, MYPL90, MIW91, NA92d, SAD90, WN90]. Distributions
[BK96, CYY95, HA93, LP97a, MFAT98, PV94, PV98, SPC96, SMO+96,


DM [Br¨a95, Br¨a96b, Br¨a96c, Car96]. DNA [BS91b, BDP92, Bor94, BPL97a, Brom91, CD93, GBS99, JTZ96, JDB99, KL93a, LP97a, LF90, LSG98, PWL98, PBR96, RBB94, SM98, SSt93, SSt94, SH96, Toh99, TG96, WP90, YDP92]. Do [ATP96, JCM92, DLF99]. Doctoral [Ano99n].


donor-DNA-acceptor [GBS99]. donor-pair [GDF92]. Dopamine [GJO97]. Doped [DD97a, DP93, DM96, DTM96, Dun99, LRM97, LF95, Yam97, AM97, BRS95, DDU96, DS99, DD90a, FS95a, LTI96, Min94a, SMM+90, SBL+94, TTO93, YZX96, YIL90]. doping [AKS+90, ABCM93, CEZ99, MS94, SAB+97]. Dordrecht [Ano92n, ABCM93, CEZ99, MS94, SAB+97]. Dordrecht [Ano92n]. Dressed [PLA98, xLT92]. DRF [DV91]. Driven [GW98a, MT91, RD90, XSA+92]. d’unification [AKS90a, GRS+90b]. duplex [YDP92]. duration [Hag94]. During [YBM97, Dun96b, LM95].

Double [BL92b, CDD96, Gra97a, KBL95, Kor90, Mey94, Mey97, Par97, PB95a, TKSH93, Ert90, FCMM99, MTL99, NL96a, PBR96, Sta98b, BK98].

double-helix-mediated [PBR96]. Double-Ionization [Par97].

double-Linked [KBL95, BKO98]. Double-Point [Mey94, Mey97].


Duschinsky [PSD97]. dushinsky [GS90b]. DV [LH94, SST93, SST94].

DV-X [LH94, SST93]. DVR [BZ98]. Dy [Li93]. Dye [Shu96, BDZ94]. Dyes [Che96, BBS90]. Dykstra [Agr90]. Dynamic [ALR96, BAN97, CA96, GS93b, MFP96, PP95, SASS99, TFOY92, WSW98, Art93, BCX92, BP92a, Chr92, LOC93, LTY92, SDO91].

Dynamical [AT93, FWBT94, Her98, SSM90, FLHT90, KPW+95, TD03]. Dynamics [ABB93, ADB96, At97b, BS93, BTS97, BM96, BCM97, BSH97, Br93b, CN94, CD93, CFB97, CCT98, DHL+94, DD98a, DD98b, DKBB97, Dun98, FWT+96, GBS+93a, GH99, GLBM96, GW98a, HGC93, HL93a, Hop90, KMM96, LLC+94, LM95, MHA98, MY99, MK98b, Mon94, NY98, Nie96, OMT97, ODD96, OK98, PTC94, PPS96, PPK97, PP98b, RB95, SB95a, SB97a, SB97b, SMNB97, SD96b, SM92b, The94, TBW90, WGR+94, WZ96].
ZZCSE94, AEJ91, Ata94, Ata97a, BZ90, BA91, BJ92, BFL91, BFV+93, BMFPV92, Cor92, DD95, DÖ94, ESHP99, EE91, GVK99, GGHP94, HM99, Hag99a, JO94, KDH90, KY95, KJ97, Kry96, LADV92, LU90, MD92a, MCB99, MJLL99, Nag96, PY92, RC99, SHF94, Sch92c, SCP95, SKC99, TW90, TW92, TCB99, Tho96, TMR99, TD03]. **dynamics** [Tu91, WLB+94, WGP99, Yur95, Kar96, Deu98a, Dun96b]. **Dyson** [SS98, TMD96]. **Dyson-corrected** [SS98]. **DZP** [JG95].

**EA** [Bau98]. **Early** [SL93, Cle92a]. **Earth** [DTA+96, Sta98c, CM95, CSa94, LRM93]. **easier** [BAF95]. **Eckart** [Ell92]. **Eclipsed** [Pal94]. **ed** [Car96, Sta90, Str92]. **Ed.** [Mic97]. **EDA** [SBM97]. **Edge** [BSS96, CF96, ML99]. **Edge-** [CF96]. **edge-to-loop** [ML99]. **Edited** [Año92k, Año93g, Año93h, Cal90c, Cal90e, Enk97, Eri92, Kar93, Lun91, Lun92, Mon93, Stan93, Tay91, Ber96b, Kar96, Mon94, Tri96]. **edition** [Brä95, Str93]. **Editions** [Str92]. **Editor** [Cal90d, Mat97]. **Editorial** [Löw90b, Löw90c, Löw91c, Löw91e, Löw19b, Löw92b, Löw92c, Löw92d, Löw93a, Löw93b, Löw94b, Löw95c, Löw95f, Löw95d, Löw96b]. **Editors** [Dun96b]. **Eds** [Kra96]. **Effect** [AMK93, ABDM94, BSS96, Bau97, Bre99, ČHMA95, CEZ+99, CL90, DB94a, DZ96b, FLF96, GFS92, GMS97, GH99, HGP91, KUN+98, KEM93, MV98a, NK96a, PBD97, PR98, P99, SY91, SIM93a, SS92c, S93, ST96b, TG96, Van94, WBD97, Xu96, ZLW99, Aon99, BLG95, EMM99, EC96, EMS90, EBMS92, Gao93, GSP93, GS90b, HZ91a, ISO99, KA96, LF90, MT91, Pet92, SG96a, SLG+96, V95, WW97]. **Effective** [Ara94, BCLS94, Coo95, CPT96, CL94, CL95, FD96a, Gln97, GG97b, GvL96, KFS92, KPT94, KA95a, MTL97, PG94, P97, P98, P99, Sch99b, SR96, STM96a, SJ97, BAR94, BC97b, CB99, DP96, Ell91, ERC91, FDD95, H93, KDB90, KLO+98, PO91, RCB+99, STM96b, SBZ92d, TM99, Tom91, TC98c, Van96, WBP91, YZ92]. **effectiveness** [WK90]. **Effects** [AL95, Ata97, Bow98, BKLV95, CBT93a, Can97, C94, CV99, CPA95, CC97, CDC98, CC96, DLG95, DP94, DC97, DZ98, E92, EM92, EMM94, FT95, FDF97, GJ97, Gra97b, Hag94, HBL99, Ish91, JCA97, Jay92, KM92, Kar98, Ken97, Ken98, KZ94, KY93, KN92, KMM95, LDF94, MSD95, MB97a, MK96, NONY97, NK97, NG96, N97, Oku98, PCE95, PK93, PVL93, RP9+97, SB95a, SR96, See97, SAFK97, SFG+98, SM92b, SM95, SU94, SKS98, WSW98, ZWP95, ADB95, BDZ94, Ata94, BMDM90, Bo90, BB94, BF93, Bro96, Cab96, Can94, Cas91, CP99a, CA90b, Cul91, Dia99, DN95, FT96, FT97a, FKB92, GPML91, Gur99, Jug90a, KTK+90, KL93a, KKL90, LM91, L99, LF90, xLYT92, LE92, MG90, MRB+96, MAK+91, MCA92, MCT99]. **effects** [MRT95, MR97, PGM95, PZ99, PHBB94, PK94, RCB+99, RH92, SCA93, SLD91, Suh92, TL9L92, TMR99, TUK90, TCM99, VX99, WGP99, XKB+99, YJL92, ST9K, TB99, T95]. **Efficiency** [KKT97]. **Efficient** [CZ94b, Hag95, Hag96, Hag98, LP97d, MFCA93, PH98,
WWM+98, BS95, Sim99c, TSS95. Efforts [Sha95]. Eigenfunctions [Fan97].
Eigenproblems [Ada99]. Eigenspectra [SB98]. Eigenstates
[PB95a, XY98]. Eigenvalue [HA93, Sad97, FKK99, JK92b]. Eigenvalues
[Aqu95, FK94, GW98b, KBW196, KP93, MS97a, Mor96a, PK92a, Sie93,
ST96a, Sim97, TE96, A.95, Egu96, Fer90, LLL91, LLSY92, She90b].
Eigenvector [LLSY92]. Eigenvectors [Wu1994, NZ92]. eight [YAD92].
Eighth [Sim98]. Eighth-Order [Sim98]. eikonal [CF93]. Einführung
[HW87a]. Einstein [MVL98]. Einstein-like [MVL98]. ejection [BJ92].
El-Sayed [Kra96]. Elastic [Sim98, KFK91]. elastin [LUU90]. elastomeric
[LCP+91, LU92b]. Electric
[ABB93, ABDM94, Bau97, CJA94, Gus98, HC96e, Kar98, KBM92, MKM93b,
NY98, NG95, OK96, SKZ96, ZZ93, ASM91, CT95, Can94, DB94b, Fer92,
KA96, Kic97, KY91a, KY91b, Mar91, PNB94, SM94, SBAD90, LF90, MCT90].
Electric-Field [HC96e, MKM93b, NG95, KBM92]. electroactive [GJD97].
Electrochemical [CGS+94, YUSM99]. Electrode
[WR96, LRR92, Rey95]. Electrodeposition [SLtM+94]. Electrodes
[LLZ98, KPM+90]. electrodynamics [KH95, RW99, Woo99]. Electroluminescent
[PB97a]. Electromagnetic [CV98, OS95]. Electron
[AM98a, And94, Ara94, BMA93, BF96, Bad95, BK96, BS93, BCMO97, BGS98, CBT93a, Can97, CHM95a, ČHM95b, ČHMA95, Che93, CA97, CL94, Day95, Day96, De 97, Del96, DP97,
DDN95, DO94, DZO97, DZOR98, Flo97a, FS93b, Fr93a, Fue98, FU97,
Hag99a, Hed95, Ish96, IP94, JCA97, JMD95, JJ97, Jur97g, KM92, KPR97,
KNN96a, KBA96, KS96, KD95, KV96, LO90, LBLKC98, Löw95a, LBG97,
MM91, MS97b, Mar92B, Mar94b, Mar94d, Mar96, Mar98b, MB98, MB93,
MBA97, MRL99, MCM98, Mik94, MK99, MP93, Muc96, NMM97, NKUS97,
Nes94, NMPK94, Nū96, Oht98, Ols96, OHSF97, Ort98b, Paj91, PGM95,
PP92, PV97, PV98, PZWC96, PTC94, PS92b, Pon97, Pon98, RPK95,
RML97, Roe90, RDK97, Ros96, SS99a, SA96, SAR96, SSO+97]. Electron
[SF95a, SD96a, SN98, SG93, STMR97, SR96, SW97, SM95, Suh94, Suk95,
TN96, TC98a, TM93, TSPK96, TSPK97, TDK+94, US97, Ukar94, Val96,
WS94b, WS94a, WZW96, Wi96, Xu96, YNN99, YAD95, ZO95, ZON+96,
ZH99b, Agr91, AC92, ACHT95, An921, AMH+92, AH92a, BMA90, BBCL92,
BK97, BKYY99, BMDM90, BSP98, BCY95, Bud92, BFW92, Can92, CBT93b,
Can94, CG96, CB99, CB99a, Che92, Cio90b, Csa92, DM97b, Da90,
DBW98, DW90, FMR91, Flo97b, FR98, GP91a, GP91, GBV96, GW91,
GSK999, GH2, HSES94, JM94, KMR92, KG2, Kin99, KKL90, KM99b,
KTCN93, KCP90, KCLI95, KL90, Kry96, KSK91, KSW98, LBBK91, LB93,
LM91, LDJH92, LDHI92, LS92b, MAA+92, MG91, Mar94c, Mar99a,
MKRW99, MBG90, MKDL93, MHS95, MHY98, MAC96]. electron
[MM94, MAAP90, MFCA93, NNY+96, NM96, Ort91, Ort92, Ort93, Ort95,
Ort98a, Ort99, Pic92, PV90, PK99, PA99, Pos91, PK92b, PBR96, Rep96,
RH92, RB93, Roe91, RD92, RMR90, Sarb90, Sae92, SK99a, SP92a,
STKK92, SG96a, SB95b, SP90, SK99b, SG92, SH90b, Suh91, Suh92, Suh93,
SD91, SS98, SBZ92b, SBZ92d, SB92b, TST+99, TNI96, VES+99, WDS97, WW97, XSA+92, Xu99, YKN+99, YJL92, ZM95, ZO94, ZDO99, ZP92a, ZBL99, AD95, LRR92, RB93. **Electron-Electron** [SF95a, GVB96]. **Electron-Hole** [KM92]. **Electron-Pair** [KM92, WS94a, ZH99b, Rre91]. **Electron-Phonon** [BS93]. **Electron-Repulsion** [Ish96, MFCA93]. **Electron-Rich** [WZW96]. **Electron-spin** [LBG97]. **electron-transfer** [BCY95, ZBL99]. **Electron-withdrawing** [LRR92]. **electronegativities** [GW91]. **Electronegativity** [All94, CN94, DLG95, GJ95, Gho94, KN92, NaI91, NaI92a, NaI92c, Yor95]. **Electronic** [AEAO99, AHM97, ARDP92, AH97, AMKS93, Ano93i, Ano93j, Ano97d, Ano97e, Ano97f, Ano97g, Ano97h, Ano97i, Ano97j, Ano97k, Ano97l, BL92a, BUZ94, BBS+97, BXZ95, BKM93, BFH96, BS94, BJL98, CWX93, Cai93, Cai94, CMCR96, CSL94, CR96a, Cha97, CXL97, CA95, CCT98, Cio94, CSZ97, CF96, DJF98, DB94a, DZ96a, DL92, EZ93, FDC92, SF95a, GBRA94, HAEMA92, IAN+94, Ino96, JC96, JBT+95, Kan93, KGC+96, KEH+97, KPD93, KT95, Kru92, KGVM97, KG97, KG99, LMC97a, LBB91, L92, L98, L99, L93, LF95, LEG+94, Löw99, M93, MCL95, MHM95b, MRL99, MB92, MV+97, Mic94, MTD93, Mik94, MA95, MH98, MK97b, MC95, Mor96c, Mor97b, Mor98a, MPSF97, NP96a, NMvB+98, Nic96, NG96, PM97, PS93, P97, Pen93, Pen96, PAT93, Rat92]. **Electronic** [RHC96, RW98, RKPE95, RAA94, RS97, Sah95b, SD96a, SPFL93, SBL+94, SAFK97, SG92, SG93, SST93, ST94, SR96, SRF98, S97a, SB97b, SME96, SAL+94, SG96b, SG97, SGB97, SGB98, Sta93, SL98, T96, TKO+92, TTOY93, TH97, TCA+91, TPR96, T3CT97, TIP96, TCM98, VR95, W190, Wil96, WDC97, WTS93, YC98, Y97, AEMH91, AKS+90, BDZ94, Ano92o, Ano93g, BGS99, BOL+90, BBZ91, Ber96b, BAL95, BS92, Bro95a, Ca90e, C90, CPA98, CP99a, C92, Cio90b, CC91b, Cio91, Cio93, CCS99, CML92, Coo92, DFG99, DD98, Dia99, FLWZ90, LLL91, FMD+94, FMD+96, FKR92, FJR96, G95, GS91, GRB92, Gur99, IH90, JH90, J95, KTK+90, Khe92, KH90, KJL96, KPT97, K90a, K90b, KG98, LMC97b, Lan95, Li92a, Lás93, Li97, LVCP91, xLY92, LG96]. **electronic** [Mar94c, MCOS94, MW92, MB90, MEC97, MLL99, MS93a, Mez90, METH94, Mük92, Nah99, Nor91, NC92, PK90, Por92, PCF94, RRC94, RD90, Res99, REKP92, RK91, SP92a, SX96, SGG99, SK91, SP91, SWD+99, SS90, SLDB91, Spr93, Suh91, Suh92, TJ97, TMA97, TS95, Tit96, TSP94, VX99, WL92, XKB+99, XSG97, YG90, YBZ92, BSS+97b, FS99, LF99]. **Electronic-phase** [TKO+92, TTOY93]. **electronically** [PY92]. **electronics** [Avi92, Bir94, Sla92, Mic97]. **Electrons** [BRZY97, BW97, BL92b, B93, GFRR94, Hag98, OKI98, TAY+97, Bar90, Hag99b, Har90, LB93, LG92, SMH92, TP92]. **Electron-in-a-Box** [OKI98]. **Electrophilic** [MKM97, PHM+91, AFM99, DGMW90, TFR99, Yu95]. **electropolymerization** [HDY+91]. **Electrostatic** [BMP93, BMV93, DDG93, DD93, FT95, FP96, GJ97, HS92a, JSG97, K90c, KMM95, MK99, MM96, MM97, MM98, MM95, MSCP92, ...
MAAP, NK96a, PRC98, SKTN97, SM94, SGK+95, SG94, BMP92, CMSF93, CA90b, FT96, FT97a, KY92, KKM99, LLL92, MEP90, MSRP90, MBP91, MIP99, RAM91, SCMF93, SHF94, SLL+91, WGP99.

Electrostatics [Bec97b].

Element [Eid99, LVL+93, SGB97, SGB98, MSC92, NPL90].

Elemental [KL94, Mur90].

Elementary [ˇCHM95b, DKM97, DV98, FBKD97c, GMI95, GKS99, Iga95, Jur97d, KJ93, LBMR95, Mar97b, Mik94, Pa93b, Sum97, Sch95b, ZWZ96b, ZARB96, BCLS94, Braf98b, BG98c, BG98d, CC92c, DW90, For92b, FJR96, GVv+90, HW04, JRS+99, JF92, Kov90b, KA95b, Lin92, Lon99, MD99, PZ91, SP90, Sch95a, Tit92, WDS97, ZFZ92]. ELF [Fue98].

Elimination [CC96, FLF96, Kat97, MR94, Cun92].

Ellinger [Enk97].

Ellipsoidal [KL94, Mur90].

Ellipsoidal-Coordinate [KL99].

Ellis [Cal90d].

Elongation [ASI94b, IAN+94, MA195, MA197, RA199].

Ellipsoid [Agr90, Tay91, Tri96].

Embedded [EDF+98, PB95b, RS94, T95, VR95, SRP+98]. Embedded-cluster [PB95b]. Embedding [Zou92, Bre99, TS92].

Emitted [DMR96].

Empirical [L¨ow99, MS98, RWT91, RWT92, Ros96, GBVM93, LK90, LZ91, TD03].

Employing [JKK+92, KCI98, PPP97].

Enantioselective [SWM94].

Encapsulated [LEG+94]. Enclosed [Aq95, A.95]. End [Dia99, PTC94].

end-group [Dia99].

Endo [MV98a].

Endo-Lone-Pair [MV98a].

endo-hedral [HRRBL97].

Ene [Pra97].

enediyne [BS95].

Energetic [VDD96, KSN93].

Energetics [AL95, BF93, WR96, Fra99, SPM+96, SZCO99, WTD+94].

Energies [AR93, ADS98, BT95, BF95, BKL97, BLK97, BMP93, BZQ95, BDH+97, CV99, CM94, CS98, De97, DMFR93, DZO97, EPB97, FR93b, GSD97, GSJS97, JKR98, JGR88, JMR98, Jos97, JM96c, KSH94, KG93, KKE+96, LP97c, LS92a, LP94, LTP96, Loh96, Mar95b, MHA98, Maz98, MV99, NBS95, Pa97, PL98, Pec93, PAAM98, RS98, Ros96, ST93, SDG97, TJP93, Wen98, Ada91b, Ada96a, AMH+92, BHGC99, BCY95, BKL98, CA91, CB91, DKTZ94, EKI94, HC96c, HZF+91, Ish91, Ish92, Jur99d, Jur99e, KSS95, L92a, MK90, MS90, MBP91, NL96b, Ort92, Pa99, PG96, RR95, SF94, SCP91, SS98, SJR91, VES+99, VA90, VZ92, YAD92, WB93].

Energy [AR92, ART94a, ASP97, AP93, AM98a, AMKS93, Aqu95, BBOR96, BE98, BP93c, BG95, BRA+99, Bra97a, BILK98, BP95, BCL98, CCM+96, CM96b, CH91, CC97, Csa96, DP93, DM96, DTM96, DDG93, DPP+94, FP94, Fer95, FT97b, FDF97, FS93a, FS94, FS95b, Fue94, GS94, GR96a, GG97a, GB93a, GB93b, Gin97, GBRA94, GLMP98, GP97, HMP93, HLS94, HA93, HM95, IK94, IY99, JKK+92, Jas94, Jur97b, Jur97c, Jur98a, KPR97, KNA94, KS95b, KSY97, KT96, KPT94, KH96b, KCI98, KL90, Lad97b, LRM96, LKL97b, LBKLC98, MMP+94, MK97a, SM96, MD93a, Me94a, Min94b, MP97, MP98, MJS93, MV99, NM95, NS97b, Pa92b, PM97, PLA98, PV98, PPS96, PP97, PR97, Rot96, RK95, RRS97, SMP94, Sch97, SZL95,
SIM93a]. **Energy**
[SZC97, STM97, SATP94, Suz99, SV95, Sza95, Tac96, TBAP95, Taš93, Taš96a, TDO97, Val94, VV95, WS94b, WTSN94, Xr94, Žit94, A.95, AS99, AČHT95, AGNS92, And93a, AKCS91, AH92a, Bec94, BDK90, BP93b, BML98, BRV99, BV93, BF92, ČDM91, CCS98, Cin96, Cim91, CA90b, CEM+96, CTC95, Csa90a, Csa91, Csa92, DS99, DI95, DLF99, DS93, EC96, EMP92, Fer91, FGM90, FF90, FS92, GRBA92, GRBA+93, GL92, GV96, GZsv999, GSKC99, GH92, Gut99b, HFM91, HC96a, HC96d, Hr92, Jac92, JK90, JM94, KBBK93, KR93, KMP+90, KCI95, KK92b, LCB98, Lás93, Le99, LH94, LP99, LV97, LFD99, Löw90d, LLB99, LM92, MD92a, MS91, MNT96, MKKW99, MCOS94, MG93a, Mez90, MT91, MYPL90, MSF91, MD92c, Mur90, NN98, NIST94, NAI91, NAI92, NOS94]. **energy**
[OSS95, OYNY98, Ort92, OYL91, PGM95, PK90, PMDM97, PMDM98, PP90, PC99, PFK99, RG99, RSCP91, RK92, Rot97, RBB+94, RNS93, SK99a, ST97, SKE92, SEKE98, STS95, SN90a, Sin92, SS91, SLS91, SES93, TCS+90, TMA97, VÁJ+92, WP91, WDS97, WW97, W98, Yu95, ZP90, ZBL99, ZGPS97, Zho93, AST95, Loh91, NOY98, An92]. **energy-based**
[FF90]. **Energy-Evaluating** [Fer95]. **Energy-Partitioning** [JKK+92]. **Engineering** [Enk97, Lun92]. **Englewood** [Str92, Wha96]. **enhanced** [ML98]. **Enkephalin** [PLY92, LS99, LVCP91, PVU+93]. **Enolate** [PBB92]. **enolates** [SCA93]. **Enrico** [And93b, An92c-46, KK92b]. **Ensemble** [CC95, CCWCF96, HLJ96, OGK90, WT98, Nag95b]. **Ensemble-density** [OGK90]. **Ensemble-representable** [CCWCF96]. **Ensembles** [BRA+99, Nag95a, Nag98b]. **entanglements** [Art94b]. **Enthalpic** [BPVP92]. **Entities** [BPL94]. **entropic** [BPVP92]. **Ensembles** [BPL94]. **Entropy** [AZAC97, GH96a, GLMP98, NP96a, Wal94, Zie95, AYAZ95, GJPZ97, MP91]. **envelope** [Hos97]. **Environment** [DB99, FVN98, JCA96, Löw97b, Sch99b, CRK+91, NGM+95, RK91]. **environmental** [LF90, SLD99]. **Environments** [ZLWES99, Mar92b]. **Enzymatic** [GLBM96, SHB+96, BBSS96]. **enzymatically** [HDB+95]. **Enzyme** [ECBH96, HM99, KK92a, Kov98b, RMH+99]. **enzyme-inhibitor** [RMIH+99]. **epitaxial** [Mii97]. **epoxides** [KM90c, WP92]. **EPR** [Kr97, MA99a, PLB999, VABM94]. **Epstein** [Cim96]. **EPV** [SB92b]. **Equalization** [GJ95, Nal91, Nal92c, Yor95]. **equally** [AEJ91]. **Equation** [Aon98, BD94a, BD94b, Boe95, CV94, DF93, Eid99, Hag98, IK94, LVL+93, Maz98, MS97a, MS97b, NOYY94, PTH+97, RW98, Sch93, ST96a, Sim97, Taš96b, TE96, TZ97b, Zha96, AGH91, AA92, BS91a, BD95a, CC91a, CP92, FKK99, Fer90, Geg91a, Geg91b, Hag95, KH96c, PZDM97, PZDM98, Rod91, SN99, Sim95, Sim99c]. **Equations** [Áng93, Bec97b, BG95, Chr94, FK94, GRT96, Gin96a, HM97c, JM93a, JK94, JK95, Mar93a, Mar98b, NS93a, SE97, Ste96, Ter97, BBS91, CTF92, ČP90, CMG92, Har99, JKG99, Kry96, Nal91, Nal92c, New97, PP91, Roc99, Sch92c, SE95b, Vin92, WW97, ZZ94]. **equilibria** [Nal98].
Equilibrium [Gui98, KH90, MTD93, METHH94, Cab96, EMS92, NWT92, PSAUS90, Slag92, Zha92b, Boc95]. Equivalence [HM97a, NY996].
equivalent [PC91]. Erdahl [Cal90a]. ergodography [OYNY98].
Ergotamine [MM95]. Ermer [Tri98c]. Erratum [AR99a, CB94a, DJ12, FS95b, FS09, Her93a, Iva97, Jac98, KN99a, MD95, MT90a, MC91b, PMDM98, PZDM98, RDK02, Rot97, SKN95a, Sim99b, Vol90, Wen96a].
Error [CSS93, Ney95b]. errors [SEKE98]. ESR [HZ99]. essay [HZ92].
essential [DBM99]. Ester [HBH98].
esters [FRV97, KE91, MKBP97, PHBB92, PBHB95, PRB96, TSS95]. estimate [JS91]. Estimates [GP97]. estimating [SN90b]. estimation [BPH96].
Even [RR94]. evenly [JL91]. Event [Vo96]. events [Lev99]. Evidence [GHB99, KCP90, RW92, YJL92]. Evolution [AD92, BSB94, BM96, CG95, Fan97, KEP93, Mic96b, PGS97, R97, SB98, YBM97, Kha91]. evolutionary [GHB99]. Ewald [Har98a, LS93a, TW90, TW92].
Exact [AM97, BBC96, CD92, CR96a, CFB97, FS97, Gör98, HM95, HM97b, Hol98, JGP91, KCI98, LP94, LG95a, MAD98, Nag95b, SM92, Tas96b, vDL99, DB94b, Iva96, Iva97, NM91, OM91, PC92, TD99, FS90].
Exact-Exchange-Mixing [KC98]. Examination [CSZ97, DE92, MDM94, Ney95a, PKM93, Cul91, Jac92, JGC96]. Example [BRV90, KBBK90]. Examples [UW94, Fuk94, ZWD98b, And90]. excess [SLS91]. excess-energy [SLS91]. Exchange [AC95, ABR95, BZQ95, BP95, BCL98, CGL96, C94, CA97, DFD97, GR96a, GBGA94, GNN90, GSA98, Gör98, GvLB96, GvNBV97, GY95, HH97, HM97b, KLL98, KCI98, KO97, Lah92, LP94, LG95a, LBKL98, LR94, MS93b, PP98b, PS94b, QS98, SKN95a, SKN95b, Sim97, SS95, SS97b, SV95, AM93, Bec94, BCY95, CFMA95, CLGW95, Csa90a, Csa91, Csa92, EMS92, FWS97, FDAC90, FADC91, GRBA92, GRB93, GL95, GV96, KLI92, KCL95, LCB98, MS91, MS92, Nag95b, PRVS95, S99a, SS91, SS92e, TUK90, VBN95a, VBN95b, YOT93, KL92a]. exchange- [Csa91].
Exchange-Correlation [BP95, CGL96, GSA98, GBB97, HM97b, PP98b, Bec94, GV96, KCL95, LCB98, SS91]. exchange-coupled [YOT93].

Excitation [CS98, DI09, DP93, DM96, DTM96, DMFR93, LD94, LD95, Oht98, ST93, SDG97, Wen98, YLD97, DS99, IHG95, JY94, KSH92, LHNK99, LP99, PK90, SF94]. Excitations [GS97a, MVL96, Ada91a, BAL95, Cio91, GZDZ97, Sas90, WB93, ZM95].

Excited [BLB95, BC96b, CLE94, CCS98, CG976, DD97a, Dau94, FSBS95, Kani93, MB98, Nga95a, Nga98a, Nga98b, NS91, Nic96, PCC93, PTP95, RSD97, SE95a, SC98a, SE95b, SG98, Sza95, TG95, The97, TC98b, TCM98, VZ93, WS95, WD97, BG99, BJ92, BRL92, CC91b, Cio91, DDC97, IHG95, KP92, ML92, Mhg95, MLL90, MAAP90, MPP92, MDM94, MS99b, NHH98, OIK90, SE93a, SK99, SKR90, TGS99, VX99].

Excited-State [CG976, CCS98, SE95b, DDC97, MLB92, SK99]. Exciton [˚AGL97, DP93, DM96, RM99, SSC91, C˚A92a].

Exciton-Depleting [DP93]. Exclude [GRT96]. excluded [Art94b].

EXGEM [Roe90]. Existence [AFTM95a, AFTM95b, AF997, AFTM98, AFZ99]. exo [SLG96].

Expanded [GM94, PF98b, CA92a]. expanding [PC994]. Expansion [BF94, DL95, GLM98, JM93b, Ku94, MJ93, NS95b, Pan95, PB95c, SP94, SV95, TB95, TZ97b, TM93, WBD97, Hol98, Ish92, Le97, LP97d, LK92, Mar92a, MF91, Mur90, Pri98, RLR90, SPS96a, SKE92, SS91, SS92e, TH90, VFB96].

Expansions [BK94b, BC93a, GM93, HM95, Jon94, KZ99, KMP94, KMP97, KF98, MZM94, Mc97, MS93b, MTL97, P97, Sch95b, BMM99, Ell91, JTF90, MS92, Sch95a].

Expectation [KS98, NS95b, NJud95a, EMP92]. Experiment [BM979, Kar93, SSK97, SB97b, Ågr91, GS97b, HW84, HW87b, MA99a, RT95, Sen94, TGD99]. Experimental [BKWL97, HH92, Jur96b, SBM97, SS97a, BB95, HW87a, LHL91].

experimentellen [HW87a]. Experiments [HZ93, HW05, Mar98a, Bra95, Bra98b, HW92, HW94, HW96, HW98, HS93, LM93, OS92, TD99].

explain [Bha99]. Explanation [VS95]. Explicit [CP90, LBPL97, LBL99c, Kn99, Sim99c, KK92b]. Explicitly [GK979, JM93b, JBS97, KM99b, Ryc94, KA95b, ZA95].

Exploiting [RH96b, LP92]. Exploration [Jur98b, MB97a]. Explorations [Sj96, Sil95].

exploratory [FMD94]. Exploring [Sch97, TCS90, MD92a]. explosion [BCC99]. Exponent [GM94]. Exponential [G95, Gra97a, HS92a, HS92c]. Exponential-Type [HS91, HS92e, HS92f]. exponents [ISOA99, TTM99].

Expressions [GR96, IP93, LBPL97, Pal93b, Pan95, WW98, CXFP99, CTC95, DW90].

EXRHF [Roe90]. Extended [Cal96a, Day96, DP97, DMB97, HBJ92, Kov98a, KL97b, LLL97, MA195, Mor97b, Mor94, PV94, SSGMGFS96, YO92, AMC97, AM92, AM93, BA90, BHI92, BC93, CD92, DGM90, HK95a, HS92c, Loh91, MHN98, MD92b,
extending [PRVS95].

Extension [DHPC95, DNM97,jug96, Pop98, PSS97, TV92, XSA+92, Zho94]. extensive [HC96c, LSW99].

External [JOC97, Mar98b, NONY97, OK96, CA90b, KS95a, KA96, Mar92d, MCA92, NMN99]. extracule [KM99b].

Extrapolation [NV94a, NV94b, NV97a, WL90]. Extremal [KV96, TSPK97]. Extreme [Can94, Eng92, Mar92b].

Factors [AD97, ALRP96, BDNT97, LKMCVT95, LKMCVT96, Pal97a, PM95, Bud92, BFW92, Kin99, PRSD92, PSM94, PSCP92]. failure [SWD99]. famous [Klo90].


Few-Body [FS97, FS09]. few-electron [PA99]. Feynman [CBG94, Kry95, Pop98, VCCM92]. FF [Boe93, Boe95]. FFT [RW98]. FF [TG99]. fibered [MV92]. Fibonacci [SBM97]. Field [ABB93, ADB96, AM98a, AGNS92, Baut97, CPA95, DD98a, DOn99, Eng95, Hag97, HC96e, Hu96, JDJP99, Jos97, Kar98, KBA96, KPT99, Kol97, Le97, MB97a, MB98, MKM93b, MLT96, NONY97, NG95, Ols96, OK96, Pan93, PVL93, RB95, SKT97, Sch97, SB96, SG98, SKZ96, STM96a, Ste96, TMP97, TKMA92, TSS97, VdV96, WHF92, AS93, ACC92, AS91, BBS91, BZMR92, Cha92, DD95, DB94b, FNSV99, GRTR96, Hag99b, Ish90, KTK90, KA96, Kie97, KKNY99, Kla93, KKL90, KY91a, KY91b, KL92a, KBM92, Kum93a, LK90, LK95, LM91, LF90, MCA92, MRT95, M91a, MC91b, Moh92, NSTFC94, NMN99, ROE90, SM94, SBD90, SES93, SJ97, VR90, VES99, ZWD98b, ZJ90, ZJ93, ZJ96, ZJ02]. Field-Theoretic [Dun99].

Fields [BRZ97, BG95, CF97, DID99, HHHP99, JOC97, Ken97, Ken98, KL97a, KMM95, Mar98b, MS98, M97, NY98, RS94, RS97b, RS97a, SC97, Sch98, SS97a, Sul97, TC98a, YXX99, Adl95, Fer92, Hua92, LTS96, Mar91, Mar92b, RR95, SC91, Sen96b, TC98c, Den96]. figures [Brä95, Brä96c, Dun96b]. File [She91]. Film [MPV94, Boe91]. Films
Freedom [NP96b]. Freeman [Jør92]. Freeon [Cam92, MC97a, MC97b, Mat99]. Frequencies [AML+95, BP93c, GL97, Hea97, HZ94, JAG95, Jur97c, KLC98a, STMR97, BP93b, FB90, FR93a, Kal90, MHL94, MSS99b, NL96b, PSAUS90, TBP99, Zha92b, Pro95].

Frequencies [AML+95, BP93c, GL97, Hea97, HZ94, JAG95, Jur97c, KLC98a, STMR97, BP93b, FB90, FR93a, Kal90, MHL94, MSS99b, NL96b, PSAUS90, TBP99, Zha92b, Pro95].

Frequency [ASI94a, Bau97, BP96b, Far97, JR96, KSY97, Le99, LG95b, Mor96b, PLA98, SB95a, SB97a, CT95, CPA98, Fan90, RH92].

Frequency-Dependent [ASI94a, Bau97, BP96b, Far97, JR96, KSY97, Le99, LG95b, Mor96b, PLA98, SB95a, SB97a, CT95, CPA98, Fan90, RH92].

Frictional [NYY96].

Friedel [DMB97]. Friedrichs [RG96]. Friend [Par94a]. Frohlich [TMM97, MVL98].

Frontier [MCA92, RD90, SCA93].

Frontiers [Yur95, Yur95, Kar96]. Frost [Zho94]. Frozen [Fer96, LY98, SZ96, RK92].

Frozen-Core [Fer96, SZ96]. FSGO [KR91]. Fukui [KN92, NM95, Na97].


fullerene-related [LSS96]. Fullerenes [BT95, HT97, LT99, TH97, TL98, TLC98]. fullerides [BSS+97b, MCCF95].

Fullerites [Sta98c]. Fully [CTG97, FSVZ97, FAD91, PP91, TTM99].

Function [AC97, AB97, AYDR96, BSB94, BBC+96b, BK94b, BGS98, CZ94b, DLV95, Fer96, Fue98, GVC96, GBS+93a, Har97b, Har98b, KZ99, KN92, Kry95, LMR94, LDP93, LTP96, NP96a, NM95, NA97, NS93a, PO97, PMN+92, SD96a, SB96, SN98, BE93, Boc96, BC93, CT95, CC91a, CB96a, DDA92, HDHP92, DW90, FG99, FKK99, GC91, HS92d, Jak93, JDB99, Jor92a, Jor96, Lip91a, Lip91b, Mez90, MD93b, MIW91, Mur90, NOYF92, NS92, PS090, PTM92, Pri98, RLR90, SNYN99, Sir99, Sme92, TWK98, Urr94, WN90].

Functional [AMRT94, ART94a, AL95, ASP97, ABR95, ASI94b, BDG96, BIM97, Bér97, BCR94, BGG98, Bra97b, BS94, CM96b, CDB99, C97a, CJA94, Cha98, CB94a, CGP96, CSP98, Cio94, Coh97, CPA95, CGR+94, CA97, Dan94, DPP+94, DZ94, DD98b, DZ96a, Dob98, Dua96a, Dua97, Eng95, EMMS94, EMMS97, FP94, FT97b, FW+93, Fue94, GMS97, GR94, GG97a, Gho94, GD94, GSD97, GD96, Gör98, GPD94, GG97b, Gre94, GWC97, GLMB96, HMG93, Hag97, HHHK95, HM95, HHHK95, JB97, J97a, J97b, J97c, Jur97e, Jur97f, Jur97g, Jur98a, K98, KS94b, KYS98, Koh95, KH96b, KL97c, LLC+94, Lev97, LLZ98, LKBD98, LKLC98, Lu99, LLLM*95, LAS+95, Mar95b, MK97a, Mar98a, MRT97, MO98, MFP96, MFAT98, MD99, MSCP92, Nag94].

Functional [Nag98a, NV97b, OHSF97, PCE95, PP98a, Per98, PB96, PEBS97, PGS97, PSCZ97, PAAM98, PS94b, PSS97, RL95, RB95, RHC96, RP+97, RP98a, R1097, RRS97, RPH98, SPOAS97, Sun97, SSO*97, SD97, Sch95a, SZ95, SZ96, SZ97a, Scu95, SCP93, STY+98, STMR97, STH94, SAL+94, SC97, SH96, SDG97, SATP94, Suk94, Suk95, TKNI96, Tac96,
TC98a, TG95, The97, TŠPKM94, TB95, Wko95, WR96, YNY99, ZC95, Ali99, AC95, ABSW95, Ano92i, AH92a, BAR94, BOA95, BMDM90, BDK90, BAL95, BDPS97, BS92, BY+97, BPVP92, CCS98, CZ94a, CB93b, Cha92, CLGW95, CP99b, CH94, CMA+99, CA91, CEM+96, Cs90a, Cs90b, CK91, Ce99, DI95, DA91, DDC97, DM92, EDH+92, FEE+98, GW97, GP92, GN90, GK91, GW91, HCR94, HMG+92, Har94].

functional

[HK95a, HLJ96, Iva96, Iva97, JW95, JH90, Jur99d, Jur99c, KK99a, KSSG95, KMP+90, KZ98, KC97, KL90, KLM91, KL92a, KK92b, KPB99, LBL98, MG97, MM99a, Mar95a, Mar99a, MV97, MECE97, MSMR99, MLL99, MRT95, MRST95, MR97, Min90b, MS91, MCA95b, MNC95, Na95b, OGK90, PWL95, PY97, PM97, PM98, PM99, PP96, PA99, RVP92, Rey95, RY95, SH90a, SCP91, SP92b, SP95, Sem96a, SPM+96, SN99, SSC92, SCS94, SS91, SG96b, Spr93, SC99, SN99, TN99, Tet93, TP90, The94, TC98c, TGDS97, Tri96, Van96, VVO98, WW97, W98, WGP99, WMZ98, Yor95, YNNR97, ZC96, ZTC97, Z94, Zie96, ZPBC97, Cal93].

Functional-Based [JBT+95]. functional-group [MM99a]. Functionals

[ABR95, AD98, FS93a, FS94, FS95b, GR96a, GBRA94, LP94, LBKLC98, MP97, MP98, PV98, RRS97, SM94, SDW+98, SK95a, SK95b, SF95a, Val94, VB94, Ca90a, CLGW95, CES87, Csa90a, Csa91, Csa92, Fer91, GRBA92, GRB+93, GSK99, KCL95, MSMR99, OYL91, Per93, PG95, PR95, Sem94]. Functions

[AL98, And94, AM98b, BDT96, BR94, CM96a, CW98a, CC98, CJH98, CPT96, CT96, DTS97, DKWM97, DM97, FK94, Fer95, FDF98, Flo97a, FS93b, FS97, GM94, GT93, Gra97a, Gui98, GOAY98, HS91, HS92f, HS92e, Hoo94, IF93, KSG93, Kin96, KK94, Kut94, LB98, LD93, Maz98, Mic96b, MCM98, Mo97, MV99, Niu95a, Niu95b, Niu97, Oht98, OK96, PVL93, Pen93, Pen96, RH95a, RH96a, RP96, Ryc94, SP98, TKMA92, TM93, US97, US96, Wi96, AS93, AH92b, AA92, BBS91, BS91a, BCC99, BB99, BR90, BS97, Ced90, CA92a, CM99, DBL94, DM96, DBF+92, DW90, DS92, Flo97b, FS90, FM92b, G91b, GL99, GP91, Har90, Hos97, HYS91, IT91, J91, JEB92, K90, KPK91, KKW90, KT95, KR91, KA95]. functions

[LP97d, LV97, LDJ92, LDH92, M90b, MV96, MD99, MR92a, MPS91, MYL90, MP91, NE95, Par92b, PD92, PK92b, RC92a, Res99, SG90, SKR90, SH90b, VA90, Wil99b, YKN+99, YG90, ZP92a, ZA95]. fundamental [AH92a, Cha96, De90, Gre98, MM93]. Fundamentals

[BC95, Löw95e, HW84, HW87b, Cal90f]. funnel [MT93]. Furan

[LX95, MK98]. Furfuryl [MH98, Tew92]. Furfuryl- [MH98]. Further


G

[Ano90z, Ano92], Ano93h, Ano94-37, Ano99d, Brä96b, Cal90f, Cal93, Deu98b, Lun91, Wha96, DDC97, Ano94i, CD93, CP99, FMS+99, FL95, HBJ+92], G* [Les92]. G1 [Jur97a]. G2 [Jur97a]. GA
[SST94, BC97b, Bau98, DKM97, HBJ+92, MMRSN92, PCF94, SPF93].

GaAs
[BP96c, CFDS90, FS95a, LMAK93, Por98, SMM+90, SPFL93, SBL+94].


compounds [NTL96, KSK+99, MAK+91, MK90].

Gaussian [AM98b, BNLF96, BC97b, Boe96, BJA99, BB97b, BS92, CHM95a, CHM95b, CHMA95, CM99, DTS97, FFD98, FR98, FS93b, FM92b, GM93, GJP91, GKK97, HBJ+92, HH97, Hill96, JBS97, JM99, JZ95a, JZ95b, Jur96a, Jur97c, Kh95, KA95b, KL97a, Kut94, Le 97, M9D95, MRT95, MR97, MS92, MS93b, MTL97, PG94, P9T79, REU+91, SP92b, S9C92, TH90, TKSH93, US97, W9B91, W96, Wil99a, ZA95].

Gaussian-2 [Jur98b, SP92b]. Gaussian-based [SSC92].

Gaussian-Type [Jur96a].

Gaussian-Type-Orbital [Jur95b].

Gaussian [AM98b, BNLF96, BC97b, Boe96, BJA99, BB97b, BS92, CHM95a, CHM95b, CHMA95, CM99, DTS97, FFD98, FR98, FS93b, FM92b, GM93, GJP91, GKK97, HBJ+92, HH97, Hill96, JBS97, JM99, JZ95a, JZ95b, Jur96a, Jur97c, Kh95, KA95b, KL97a, Kut94, Le 97, M9D95, MRT95, MR97, MS92, MS93b, MTL97, PG94, P9T79, REU+91, SP92b, S9C92, TH90, TKSH93, US97, W9B91, W96, Wil99a, ZA95].

Gaussian-Type-Orbital [Jur95b].

Gaussians [ITK91, KP97, PK96, SF95b].

cO [RP98a].

GCA [BKL94]. GCOSMO [TNS96].

GdNbO [DDN95].

GdH [ML98].

Geg91a].

Generalization [MPP+97, Pen96, Val94, Csa90b, CK91, She90b, TR91, HSV98, MVHV96].

Generalized [ANB96, AH97, AT93, BPE97, CLZ99, Cul95, Day95, Day96, FR98, Gra97a, KMP94, KMP97, LDGA96, MS97a, MS97b, MPO99, MMD96, MTL97, MT96, NOYY94, PP98a, RG94, RG96, She90a, TC98a, TM99, TN96, Z95, Ave00, G9M91, JK92b, K9C93, KT95, KS90, KL92, LH90, Mar99a, PK92b, V9V91, Yor95]. Generalized-Gradient [PP98a].

Generalized-Overlap [Day95].

Generalizing [Kat93].

Generalized [RP96].

Generalization [BNLF96, CV98, LBLKC98, Mik94, SLTr+94, Har99, TC98c].

Generator [PDT97, BG98c].

Geometric [SL98, EZ93, KSN93, Sal92d, MM93, VX99]. Geometric-phase [VX99].

Geometrical
AKS$^+$90, BPL94, GMR$^+$93, RHC96, Zap95, Art96, BBS91, BR92.

**Geometrically** [KN99b, NK98, KN99a]. **Geometries** [AR93, AMKS93, Jur97c, RGHH94, STM97, LS93b, MIH94, PSAUS90, SCP91, Zha92b]. **Geometry** [GL97, Min90b, MAI97, MT96, TJ95, VFHL93, ZM97, Bro96, CTC95, FMD$^+$94, HSWS95, Kla90, KMR92, METHH94, SE92, Sch92b, SG90, WD91, XKB$^+$99]. **George** [Ano99d, Deu98b]. **German** [Br"a95, HW87a]. **Germanium** [NN94, VBD$^+$98]. **Germany** [Br"a95]. **germination** [HB94]. **Gerratt** [Ano99f, Ano99p, WRC99]. **GeSiH** [BML98]. **Get** [PZW93]. **GGAs** [KPB99]. **Giant** [KLT97, Nes94, RG99]. **Ginzburg** [Aon98]. **glass** [Tet93]. **GLF** [BD94a, BD94b, BD95a]. **Global** [L"ow97b, BA90, LM92]. **globular** [Kid99]. **Glutathione** [VC92, BMVV93]. **Gly** [GJLA99, LU92b]. **Glycine** [MTD93, Ram90, RC92a]. **glycol** [Cab96]. **glycolic** [FR92]. **glycylcarbonyl** [Tew94, Tew97]. **Glyoxalase** [VC92]. **glyoxylic** [BS91c]. **Go** [BPE97]. **gold** [Bo\v c96, HCR94]. **Golden** [Lef99]. **Goldstone** [PR97]. **Goldstone-Type** [PR97]. **Good** [Ros96, KTC93]. **Goodman** [Ano99c, Ano99g, Ano99h, Ano99n, Kas99]. **Gradient** [BPE97, EMMS94, EMMS97, FGRS98, GR96a, GvLB96, HC96e, HM95, KS94a, KP97, Min94b, PP98a, PB96, RRS97, SV95, Tri97, ZC95, ASM91, BDPS97, CLGW95, IH95, JH92, Per93, SS91, SS92e, ZPBC97]. **Gradient-Corrected** [EMMS97, PB96, RRS97, BDPS97, CLGW95, Per93]. **Gradient-Dependent** [Tri97]. **Gradient-Optimization** [FGRS98]. **Gradients** [NG95, SZL95, SE97, MHN98, Orf92, SBAD90, SE95b]. **Gradus** [And93b]. **grafted** [Art96]. **Graph** [JM96b, KP90, LL94b, MD93c, PM95, PM97, PV99, SY96, ZLHZ94, Ano92k, DM97a, Hal93, LTY90, Mon93, Rom92, She90b, She90c]. **Graph-Theoretic** [PMM97]. **graph-theoretical** [Rom92]. **Graphical** [KSS92, KZ90, RP96, SAR96, SGK99, RTS91, She90a]. **graphite** [GL99b, LaF90]. **Graphs** [Gin96b, GLFY94, LNT99, SM96b, SM97, BKM90, BBL94, LLS99, She90a, She90c, She90d]. **Gray** [Cal90f]. **Great** [Kra96]. **Green** [Ced90, DDA92, DDP92, EP98, FL91, HS92d, MM91, MD93b, NS92, NS93a, SNNY99]. **Green-matrix** [FL91]. **Greenstein** [Deu98b]. **Grid** [ADB96, CHM95a, CHM95b, CHMA95, SB98, DB94b, New97]. **Grids** [GPD94]. **Griffin** [CGMG92]. **GROMOS** [FVN98]. **GROMOS-MD** [FVN98]. **groove** [HGP91]. **groove-binding** [HGP91]. **Ground** [BEG94, BLB95, BK94b, Bra97a, CLSI94, CAJ95, DTA$^*$96, DD97a, DLV95, DMB97, FSBS$^+$95, Fri93b, GFR94, KA95a, Mar98b, MW90a, N93b, NOS94, PCC93, RR95, RS94, SE95a, Sch88, SIM93a, SGGM98, SG98, STM96b, SN99, TBCP95, Ccd94, CEZ$^+$99, DDC97, EJ93, KSW98, L93b, M99, M97, M99a, MLL99, MB93, NM91, New97, Orf93, PFK99, PZ91, RVP92, RK92, SE93a, SM92a, SW95, SSM90, Tri98c, UJS90, W96, WW97, ZA95]. **Ground-State** [Bra97a, DLV95, FSBS$^+$95, GFR94, Mar98b, N93b, SIM93a, TBCP95, MW90a, N94, RR95, STM96b, SN99, CEZ$^+$99, DDC97, M99, M97, Orf93, PFK99, RK92, SM92a, WW97].

H [Ano92k, BML98, Br995, Br995, BDH+97, Cal90a, CMF+98, CR96b, CB93b, CB94a, CF93, CXFP99, CEM+96, DZ97, Gac93, GP90, IB95, JKK+92, Jur97e, KP96, KJ95, KGV93, LCS98, MIL99, MW90b, MLK94, Mon93, Nag96, PZTPMC99, RG99, RA91, RCWN94, RNS93, RKG96, SDP+95, Ska92, SL97, SC98b, SC99, TJ97, WFS93, WI96, WMD95, ZBL99, GV93, ACHT95, Ata97a, ADM98, BA91, BZMR92, BDNT97, BBC+94, BP93c, BP93b, BP96b, BK94b, Br93b, BYGA99, CAK+96, CLOFR98, CB93b, CR96b, DB90, CD93, CPD+98, Csa96, Cun92, DE92, DSS90, FCVL98, GJP97, HMC+92, Hag99a, HB95, HZ94, JPM99, JKJ94, JG95, JEB92, JM99, Jur97e, KS95a, KKWT99, Kor90, LJ95, LA97, LG94, MCL95, MAL96, MTP+98, MMM95b, MK90, MTD93, MTS93, MD91, NY98]. H-Bond [OSS95, Ort98b, PBS99, PK97, RCWN94, RS97b, RNS93, Sch97, SP92b, Sem94, STC96, TMA97, TUK90, U692, UJS90, WYZ+92, WW99, WDS97, Y99, YSH97, HP98]. H-Bonding [CAK+96, DE92]. H.-J [Br98c]. Haken [Br98b]. Half [BP93d, FSBS+95, MS99b, OS90]. Half-Projected [FSBS+95, BP93d, MS99b, OS90]. halide [NMCK92]. halides [BR95]. Hall [Str92, Wha96, An99d, Gut99a, HL96, Sch99a, Sri97]. Halogen [Lu99, RL95]. Halogen- [RL95]. Halogenated [ET99, BMP92]. Halogenobenzoic [BKWL97]. halogenofuran [NVR+91]. Halogens [TV92]. Hamilton [Sch90]. Hamiltonian [AS96, Ano98, Bro95b, DB94b, EKI94, Ell91, Ell92, Gin96a, Jug90b, KBW96, KH95, KS90, Kru92, L690d, May98, Oku98, RPKM95, RABZ94, SB98, SZ97a, Sen96, SS99b, STM96a, STM96b, SJ97, SKS98, Trom91, VDBPR97a, VDBPR97b, ZM95]. Hamiltonian-crystal [SJ97]. Hamiltonians [BS97a, CT96, CB99, CY95,
Hyperpolarizabilities [ASI94a, BP96b, Cha97, LL92, Mor93a, NYKY98, SAS99, Shu96, YNY99, AD92, BP93b, KMR92, Kur90, LKM99, LYS95, MD92b, MPP92, Mun92, RH92].

Hyperpolarizability [JR96, KUN+98, Kan93, Mor96b, NONY97, SC98a, TSRP99, YNY99, BP92a, CPA98, CP99a, DBF+92, LL99, NYKY98, NYNY99]. Hyperradius [AGH91]. Hyperspheric [Ave89, AH92b, Ave00, BD94a, BD94b, CN99, DZF93, WBD97, Zha96, BZMR92, BD95a, NZ92, Cal90b]. Hyperspherical [Ave89, AH92b, Ave00, BD94a, BD94b, CN99, DZF93, WBD97, Zha96, BZMR92, BD95a, NZ92, Cal90b]. Hypersurface [RRS97, AKCS91, TCS90]. Hypersurfaces [BML98]. Hypervalence [JF92]. Hypervalent [Har96, DA91]. Hypervelocity [WSM+94]. Hypervirial [LBMR95]. Hypothesis [Jac92]. HZSM [MMCC99].

[AL95, LAS+95, Mey94, Mey97, TAY+97, FKR92, GJPMML91, KKL90, KRZ91, Mar94c, Moh92, RH92, SCA93, Suh91]. **Inclusion**
[Boˇc90, RL92, ČPV90, HWB97b, HWB97a, RWT92]. **Incomplete**
[LD93, KB92]. **Incorporating** [RPB+97]. **Increase** [KK97]. **Increased**
[Har96]. **Increased-Valence** [Har96]. **Indacene** [HHKM95]. **Indefinite**
[Löw96c]. **Independent**
[AV92, KPA95, GSPSM93, Kin93, Kin94, Luk92]. **Indicators**
[FJRS97]. **Indefinite**
[L¨ow96c]. **independence** [Lev99]. **Independent**
[AO93, SD98, TMDB98]. **INDO**
[DM95, FKR92, HZ99, JKK+92, KRZ91, PSBL98, RL92, SJ97]. **INDO/S**
[HZ99, KRZ91]. **indol** [RTKP95]. **indol-3-ylacetic** [RTKP95]. **Indole**
[WGP99]. **Induced**
[BS93, Gui98, MB98, MLK94, MSS99a, RM99, Tew94, Ata94, Ata97a, CA90b, FSW+91, NMM+97, NMM+99, Pal93a, SPFL93, SSM+99, TBW90]. **Induction** [Pie93]. **Industrial**
[RVL97]. **Inelastic**
[GYDY97, CF93]. **Inequalities**
[Csa93, Csa95]. **inequality** [TNSM99]. **Infinite**
[CW97, Del96, FUI97, LKMC93, NV94a, NV94b, Suh94, ALe95, CA90a, CMA93, FS92, LKVS97, MFC94, NV97a, Suh92, Suh93, TKO+92, TTOY93, YITY93]. **infinitely** [Dia99]. **inflammatory**
[BD95b]. **Influence**
[BKY99, BKF94, DWR99, GS94, JC96, Le99, MDD93, MKM97, PB97a, Tew97, BSS90, MT91, NGM+95, PACO90]. **Information**
[NP96a, YAD95, Zie95, Ano90h, Ano94i, HSWS95, Rg92]. **Infrared**
[GSSD+96, HJ94, MDD93, ZJS99, HS95, Lin91, TWWC91]. **Inhibition**
[Mav98, RAM91]. **Inhibitor** [BB97, RMM+99, SHB+96]. **Inhibitors**
[KKS99, MBV+98, ARB95]. **inhibitory** [HB94]. **Inhomogeneous**
[HM97c, Fer92, HLJ96]. **Initial** [GZDZ97, Hag96]. **Initiation** [Lad97a]. **Initio**
[AKD96, AST93, BTT97, BBC+96a, BLB95, BAK96a, BL92b, BCS96, BH+97, Bue96, BDD93, CWX93, Cai94, CMF+98, CLSI94, CMFA93, CA96, Cha97, CFR96, CPT96, DS96, DRBE96, DZ97, EMMK94, FF94a, FF94b, FT95, FLRV97, FWC+93, GDID98, GBS+93a, GL97, GL98, GW98b, GP97, HP97, HHHKM95, HHH98, Huz96, Jen94, JZ95a, JZ95b, JM96a, Jur96b, Jur97a, Jur97b, Jur97c, Jur97d, Jur97f, Jur97g, Jur98a, Jur98b, Jur99b, Jur99a, KUN+98, KKNS97, KL97a, Kry98, KG97, KG99, LV93, LJ95, LRM96, Löw99, LB95, MSD95, MCE+93, MF96, MDD93, MS98, MRL99, MTD93, MSC95, MR94, NNM96, NBS95, OSA+97, OHF97, Par97, PVLA93, Pen93, Pen96, PFMC97, RKN97, RM96, RML97, RKPE95, Ryd94, SE95a, Sak97, STK97, SNMB97, SPS96b, SG93, SLA97, SMO+96, SHC+98, SH96, Sta96a]. **Initio**
[STA97, Sta98a, TB95, VH96, YY96, Yam97, YD97, YK97, YW92, ZL98, Ágr90, ADB95, ACC92, ACB+99, AGAP98, AGM99, ANB94, AKCS91, ABC93, BL99, BMA90, BHL+99, BILA95, Bha99, Bha99, BB93, Bre99,
BHv96, BMG95, BCY95, Clofr98, CA92b, CMA93, CPA98, CRK+91, CK91, CP99b, CEM+96, DFG99, DV91, DLF99, DBF+92, DO90, ERC91, EMY96, Eva97, FA92, FF92, FT96, FF96, FT97a, FWS97, FFD96, FMD+96, FL91, FR92, FR93a, For94, Fra99, FADC91, GE92, GX98, HSES94, HGL99, ISO95, JMP99, Jur99c, K99a, KPW95, Kar90, KNN96b, KR93, KJL96, KH96a, Kir92, KKL90, KH96a, Kir92, KKL90, KK93, Kor90, KYW95, KG98, KL92b, LC92v, Les91, Les92, LW92, LWX99, LBG97, MD92a, Man95a, Man95b, Man99, MK96, MCOS94, MW92, McW99]. initio

[MLL99, MR92a, Mil97, MFCA93, MFCA94, MRBM91, Nov92, NL96a, OT91, OS92, PVC+90, Pa94, PAF91, PTS+92, Ram94, RTK95, RTK96, RD97, REU+91, REL+90, REKP92, RK91, RK92, RC99, SE92, SE93a, STKN90, SDP+95, SAB+97, SRP+98, SS90, SX96, SP91, SCP93, Sem94, SPM+96, Suh91, SPR94, TCB99, VR92, WFS93, WLB+94, WSB94, WL92, WKP+95, XSG97, XFF98, YNO92, YNO94, Y96, YSD97, YAD92, ZGPS97, LHL91]. innate

[Chu99]. Inner

[BZQ95, BDH+97, BCY95, ZBL99]. Inorganic

[KN92, Lun91, OCK99]. Insecticide [NAK95, KKS99]. insertion

[RD97, SM96a, WY99]. insights [BADM97, VABM94]. insights

[FMS+99, VR92, Woo98]. [Rau02]. Instability

[ATI97, CC97a, LN96, Sim93b, YOT93, Y92, RNS93, TKO+92]. Institute


[Dem99, Kov98a, MCCF95, NMN+98]. Integer

[Sri97]. Integrals

[AM98b, BR94, BB97b, DW97, FS93b, GY95, GIA96, Gus98, GOA98, HO94, HS91, HS92f, Jon94, Jon97, KZ99, Kin96, KBL95, LKB97, LDP93, LR94, MBA97, MS93b, MN+92, SP98, SBD+92, US97, US96, Bud92, BFW92, CM99, DD97b, FM92b, GP91a, GJP91, JE90, JEB92, Jon92b, Jon93, Kin99, L90, LK93, MRC99, MT90b, MHS95, MS92, MGLBP95, MFCA93, Ort95, POC+94, PW91, RLR90, REU+91, Sm99, SH90b, TIN91, Z93, ZF92, ZB92]. Integrals

[Integrals [FS94, FS95b]. Integrated

[CDDV93, KM97, MSM96, MK97b, KKK90, K91, MK5, MK6]. Integration [FS93a, IYF99, Csa92, JO94, Roc99]. integrations [JE90]. Intelligent

[AM98b, BR94, BB97b, DW97, FS93b, GY95, GIA96, Gus98, GOA98, HO94, HS91, HS92f, Jon94, Jon97, KZ99, Kin96, KBL95, LKB97, LDP93, LR94, MBA97, MS93b, MN+92, SP98, SBD+92, US97, US96, Bud92, BFW92, CM99, DD97b, FM92b, GP91a, GJP91, JE90, JEB92, Jon92b, Jon93, Kin99, LH90, LK93, MRC99, MT90b, MHS95, MS92, MGLBP95, MFCA93, Ort95, POC+94, PW91, RLR90, REU+91, Sm99, SH90b, TIN91, Z93, ZF92, ZB92]. Integrals

[Integrals [FS94, FS95b]. Integrated

[CDDV93, KM97, MSM96, MK97b, KKK90, K91, MK5, MK6]. Integration [FS93a, IYF99, Csa92, JO94, Roc99]. integrations [JE90]. Intelligent

[AM98b, BR94, BB97b, DW97, FS93b, GY95, GIA96, Gus98, GOA98, HO94, HS91, HS92f, Jon94, Jon97, KZ99, Kin96, KBL95, LKB97, LDP93, LR94, MBA97, MS93b, MN+92, SP98, SBD+92, US97, US96, Bud92, BFW92, CM99, DD97b, FM92b, GP91a, GJP91, JE90, JEB92, Jon92b, Jon93, Kin99, LH90, LK93, MRC99, MT90b, MHS95, MS92, MGLBP95, MFCA93, Ort95, POC+94, PW91, RLR90, REU+91, Sm99, SH90b, TIN91, Z93, ZF92, ZB92]. Integrals

[Integrals [FS94, FS95b]. Integrated
[CBG94, GJOV97, MR99, GT97, Mar93b, Nak92, OM91, SMH92].

**Interaction** [Agr91, BHL+99, BEG94, BP96c, BL98, CCB+96, MC97a, MR92b, NTL96, PS96, PRC98, PFM97, SWF93, SM96b, SF95a, Sch99b, Sur94, Sur95, TMDB98, VA90, Ada96a, Art94b, Bat92, BE93, BHV96, BLG95, CC91a, CPBC95, CCC+95b, CGG96, CLR+93, CDLP+99, DI95, DS93, Düc90, EVSN92, FM92b, GV96, HC91, ISOA99, Ish91, IHC95, KBKT93, KSS92, KRZ91, K90, LB94, LLB99, MRRSN92, MMCC99, MLT98, MH95, Men99, Moh92, NL96b, Ni94, Pai91, Pet92, Pro94, Pro95, RTS91, SWD+99, SBPP92, SEKEB98, SG90, SC93, SB92d, S91, Ta92, TSY99, TY99, TC98c, VAJ+92, WP90, WMW92, YZ96, YDPP92, YJL92, Yu95, PTL90].

**Interactions** [BP93c, DE92, GBVM93, Gin97, KSN95, Kar98, LV93, LS93a, May98, NNMH96, OLC+96, SE93b, SD98, SGB97, SH96, SPL97, TWK+92, ZRNZ97, Ada90, Ada91b, AGM99, And90, BP93b, BH92, BMP92, CG97b, CMSF93, CG99, GP98, GP99b, HVS98, HZ92, JMP99, KPTS+93, KPTVT+97, KY92, KH97, LaF90, Man95a, Man95b, Man99, MV91, May92, MVHV96, MK90, OB95, PL95a, PA92, RMH+99, SCC91, VR90, VM92].

**interactive** [Qui02].

**Interatomic** [RA96].

**Interband** [SMM+90].

**Interbasis** [KMP94, KMP97].

**Interbond** [Sur95].

**Interchain** [TIA+92].

**Interchange** [She91].

**Interconversion** [CBG94].

**Interconversions** [BHPB95, HRH99, Sla92].

**intercorrelation** [HG95].

**interdisciplinary** [LF94].

**Interelectronic** [GR95b, GR96b, Lah92].

**Interface** [CCT98, Kov98a, Sj98].

**interfaces** [WGP99].

**Interference** [May92, Si95].

**Interim** [Har97a].

**Interionic** [Mez94a].

**interlayer** [LaF90].

**Intermediate** [NMN+97, NMN+98, Pai97, PL98, S99b, ACZ91, BZ92, BHGC99, CP91, EZ92, FF96, Pai99, ZM95].

**Intermediates** [BP92b, EMMK94, HS95, HDB+95].

**intermetallic** [MECE97].

**Intermolecular** [Ada96a, Ada99, BH92, EE91, GBVM93, May98, McH91, Pie93, SPL97, TT98, V96, VR90, Ada90, Ada91b, BMP92, HV98, HZ92, JMP99, KBKT93, KY92, Löw90a, MV91, MVHV96, MR92a, MRBM91, Sco90, SJ91, VM92].

**Internal** [BW99, Che97, GWT97, KC98a, KLC98a, KLC98b, Na92b, Pa97b, ZZCSE94, CLZ99, CTF92, GX98, GS90a, MJLL99, Sch92b, WFS93].

**internally** [SS92d].

**International** [Deu96, Kra96, Löw91c, Löw91d, Löw92a, Löw95f, MDS98, Str92, An91, Lad94, Löw90c, Löw91a, Löw91b, Löw92b, Löw92c, Löw93a, Löw93b, Löw94b, Löw95c, Löw95d, Löw96a, Löw96b].

**Interpair** [JJ97].

**Interpolant** [CB96b].

**Interpolation** [DQB97, CLZ99].

**Interpretation** [BDG96, Gin95, Gin97, Pec93, PEBS97, Cio93, Kat98a, SH90a, SB92b, Tom91].

**Interpretations** [AGL97].

**Interreactant** [Na97].

**Intersecting** [BW97, Na94].

**intershell** [DI95].

**Interstellar** [AST93, PMM97].

**Interstitial** [EF+98, LFD99].

**Intersystem** [KVM95].
Intra [JJ97]. Intra- [JJ97]. Intracules [KKT93]. Intramolecular
[ADPS98, CDD+99, Flo95, GSPSM93, GL98, HP97, Ram90, SSP98, CSH99,
DS93, MKK96, NOYF92, Par92a, RC92a, Ram94, Sem96b].
intrasupermolecular [NOYF92]. Intrinsic [DZ94, MD93a, NSS+95, SX96].
intrinsically [AMH93]. Introduction
[ASH91, AVV93, Ano91h, Ano91i, Ano92p, Ano97m, Ano98n,
Ano98o, Ano99e, Brä93a, Brä95, Brä98b, Cal92, FR94, HWB05, Kas99,
KW998, Loe92, Löw99a, LZ92, Löw92c, Löw92f, LZ94, Löw97a, MCA92,
Mor98b, NOYY94, ÖSZ90a, ÖSZ90b, ÖSZ92, ÖSZ93, ÖSS293, ÖSZ94a,
ÖSZ94b, ÖSZ95a, ÖSZ95b, ÖSZ96a, ÖSZ96b, ÖSZ97a, ÖSZ97b, ÖSZ99a,
ÖSZ99b, ÖSZ99c, OAG99, RS97a, Smi96, Tri98a, UH95, HW85, HW87a,
HW87b, HW92, HW94, HW96, HW00, HW04, Kum93b, Rat92, RS00, Kla93].
Introductory [Kys90, Ber96a]. Invariance
[CAK+96, Jou97, JH92, Woo99]. invariant
[KKNY99, OS95]. Invariants [BDT96]. Inversion
[Sen96, ITK91, SP92b, WSB94].
Inversion-Bending [Sen96]. Inverted [TMA97]. Investigated
[KUN+98, ST93, Mar97c]. Investigating [KM92]. Investigation
[BBS90, BC95, Bra96a, Cha95, Cha97, CFR96, CS98, Csa90b, Csa96, DP93,
EK94, EMMS97, JTZ+96, Jay92, JZ95a, JZ95b, KBKT93, KY92, Lah92,
LLZ98, MCE+93, MV98a, MFF96, PKM93, PSCZ97, SWMB94, STS95,
STM97, YZX96, YK97, And93a, BBCL92, BB93, BS91c, BV93, CEM+96,
CK91, DM97b, DFG99, FLW920, FR92, GMB97, GJPF92, HSWS95, HB95,
JMP99, KR93, KS94c, KE91, MG91, MFA94, NGM+95, PTM92, Ram94,
RBB+94, SG96a, TFR99, WBH90, WMZ98]. Investigations
[BTN98, Bov94, KS94a, KVS98]. Involved [DTM96]. Involving
[BF96, GH96a, LX95, Nic96, PVLG93, WR96, Bud92, BFW92, HB95+92,
MG90, MK90]. Iodides [Sta97]. Iodine [DYD96, EMMS97, GZsv99].
Iodine-doped [DYD96]. Ion
[BCM97, BD94a, CA91, DD98b, GBS+93a, HNB92, PBB92, Ryd94, SD97,
Schr97, TK996, ABCM93, BLG95, BILA95, BJMK92, DMR96, DKT94,
EC96, FMR91, Klu92, KRZ91, MG97, NST94, RNF90, TM99]. Ion-atom
[DMP96]. Ion-Helium [DYD98b]. Ion-Molecule [TK919]. Ionic
[AMD+97, CBAM97, CLS94, GD96, KSKJ94, KM92, BR96, CLOFR98,
CDB90, GSP90, KTK90, Lum92, MAAP90, PBPN90, SP91, YNN97].
Ionization [AR99b, BMP93, CDDM96, CR+94, FLRV97, GW91, Jur97d,
KC98, LD95, MG93a, Moi97, Mor94, NKUS97, Par97, PAAM98, STM97,
Vo96, AR99a, CB96a, CF979, DDA92, GL95, KSS95, KTC93, KCL95,
MH98, MDD94, MSP99, MBP91, SP92a, SPB90, S92]. Ionization
[DMP96]. Ionized [IK97, NS97a, NS97b, RZ979, NS91, SB90].
ionizing [CH91, WK90]. ionone [TCB99]. Ions
[BF96, BPL94, CBT93a, GS94, GH96a, IK97, KKT93, KGv93, PAT93,
RDK97, VIK98, AMH+92, BUZ94, BKS97, BMG95, CBT93b, CF979, Dnv90,
FAV92, HAR94, II94, LRM93, LHL91, LBG97, Mar91, MLB92, MDM94, NM91,
NMCK92, Par99, PZA92, RDK02, SC91, SBPH92, YDD92, Brä98c].
IPGG, LCP+91, Ir

J [Ano92-45, Ano92-44, Ano93b, Brä98c, Cal90c, Cal90e, Cal90b, Dun96b, Eri92, GARC97, Gre98, Jer92, Kum93b, Kum93a, Lun91, Tri96, Lai94, WRC99, KA95b]. J, [Ano99f, Ano99p]. Jahn [Cas97, GMS97, RN93, Sim93b, Suk94, Suk95]. Janos [Brä96c]. Java [Mos98]. Java-Based [Mos98]. Jean [Löw96d, Pau97]. Jean-Louis [Löw96d, Pau97]. Jellium [VBF95, BFP93, JWG95, KF96, MD93b, VFBP96]. Jersey [Wha96]. Jerusalem [Cal90c, JPP87]. John [Call90g, Cal90a, Deu98a, Ano90j]. Johnson [DJ12, DJ95]. joint [FG96, Ano96-31]. Jortner [Cal90c]. Joseph [Tri95]. Journal [Löw90c, Löw91a, Löw91b, Löw92b, Löw92c, Löw92d, Löw93a, Löw93b, Löw94b, Löw95c, Löw95d, Löw95b, Löw96a, Löw96b, Löw91c, Löw91d, Löw92a, Löw95f, Löw91e]. Jr [Call90a]. Jr. [Ano91-27]. July [CD81]. jumps [Fan90]. junction [LSGS91]. June [CD81, Kar93, Na95b, Fuk90, Löw90d]. Justification [NS95a, Ney95a, Ney95b]. Justin [Kum93a].

[KSH94]. Large-Scale [BBS+97, HL93a, BMFPV92]. larger [OSS95, RA99].
Laser [Ata97a, BRZY97, CFB97, DiD99, DDH+96, DD98a, GW98a, Hag97, Hag98, MY99, TC98a, Ata94, BCC99, Cha92, DD95, Hag94, TC98c].
Limited [LL94a, LKMC93, WZW96, LKVS97, Was91]. Limits [Ada96b, MDM94, Rom92, PL93]. LiN [SK91, YK97]. Lincoln [Str93]. Line [Min94b, Eng92, SE93a, CLZ95]. line-shapes [Eng92]. Line-Then-Plane [CLZ95]. Linear [AM92, Ang93, AFTM95a, AFTM95b, AFO+97, AFTM98, BBMM99, CDDM96, Eg96, GR95b, GGSA98, GH92, Hii98, IK94, Jas94, Löw93c, Löw96c, Mat99, NY98, OI98, PP95, Pie93, RR94, SB95a, SB97a, Sh96, St93, SV95, Wil96, Yan97, AFZ+99, BJA99, CT95, D93, For92b, GL96, hJH97, KYW95, LP99, NYKY98, NH98, Par92b, TKW98, TN96, TBW90]. linearization [DM97a]. Linearly [Mey94, Mey97]. Liner [GR96b]. Lines [HA93]. Lineshape [PLBB99]. Link [PS94a]. Linkage [GSSD+96]. Linked [KBL95, BKL98, KL93b]. Linking [CCE+93]. links [DM99]. Lionel [Ano99c, Ano99g, Ano99h, Ano99o, Ano99n, Kas99]. Liouville [NY98, NYNY99]. Liouvillean [RB95]. Lipid [J95, WP91, W98]. Lipids [CDV93]. lipoxygenase [ARB95]. Lippert [Dun96b]. Lippmann [DJ12, CG95, DJ95]. Lipscomb [Ano91-27, Ano91z]. Liquid [CT96, GS97a, JCA96, Kry98, MLR+98, OMTS97, TT98, Wal94, Cor92, FDD95, KY91b, Mar97c, MR92a, SB95b, SCP95]. Liquids [HL93a, HM97c, Mar94c]. List [Ano92q, Ano93k, Ano95r, Ano96-31, Ano96-29, Ano96-30, Ano97a, Ano99i, Ano99j, Ano99k, Ano99m, Par94c, Tri98b, Zer98b, Ano90a, Ano90b, Ano91a, Ano91b, Ano92a, Ano92b, Ano93a, Ano93b, Ano94a, Ano94b, Ano94c, Ano94d, Ano95a, Ano95b, Ano96a, Ano96b]. Lithiated [RM96, TSRP99]. Lithium [FDF97, GKKM96, JR96, KTT97, KJ93, MSC95, MMD96, RSD97, YK97, BLC95, BK97, K94, LK94, MES93, SK91, SP91, LBL98]. Lithium-Cation [GKKM96]. Liver [CAK+96]. LiX [SL93]. LM [GRK96]. LM-Conjugated [GRK96]. LMO [Sur94]. LMSS [Ran93]. LMTO [MNGK95, Spr93, WTS97]. LMTO-ASA [MNGK95]. Ln [Bou96, Bou96]. Ln=Pr [Li93]. LnBa [Li93]. Local [ADB96, BP93e, BMP93, CGR+94, CA97, Cze99, Day95, GR94, GD94, HMG93, H97, KLL98, KS94a, K95, L97a, LBL97, LBK98, LBL98, LBK98, LBK98, LBK98]. local-density [DA91, Min90b, YB99]. Local-Exchange [KLL98]. Local-Scaling [LB97, LBK98, LBK98, LBK98]. Local-scaling [W92]. Locality [HH97, MA99a]. Localization [BBK90, Fue98, HR95, HS92c, M97, PM97, PV98]. Localization-Consistent [PM97]. Localized [KBT94, KK90, KKE+96, MYN+96, MCM98, PBB94, PV94, RH95a, RH95b, RH96a, RMPR98, SBIP97a, Spr96, Ste96, Sur94, Ter97, K91, DRGC90, För92a, KBB+90, KH96a, MAC96]. locally [CA92a, KH96a, NE95]. Locate [BLRD92]. Located [Kov98a]. locations
Magnetism [MC97a, MC97b, PEBS97, Mar94c]. magnetoresistance [Nes94]. Magnets [MC97b, Mat99, MNT96]. Main [DKM97, BCLS94].

Main-Row [DKM97]. major [XSA+92]. Making [OOD96]. Maksić [Cal90d]. malarial [TCZ91]. maleic [HMK99]. malonaldehyde [LS93b]. Malononitrile [ET97]. malononitriles [METHH94]. Manifestations [ZH99b]. manifolds [Ada91a, CCS98, DDN95, Man99]. Manipulation [BB97b, TP94]. Mann [MHN98]. Mannich [LX95, MKK98]. Manuscript [Ano93i, Ano93j, Ano92o]. Many [Ber96c, BD94a, BD94b, CBG94, Cim96, IK97, JOC97, KBT94, KNN96a, KZVG97, Koh95, Lin96b, LFD94, Mar96, Mar99a, MMH95b, MS93b, Muk96, NNY+96, NMKP94, NB97, Oht98, Pie93, SAR96, SD96a, SN98, Sta93, SPL97, SKS98, TC98a, TM93, VVS94, YAD95, Ano92l, Ano93g, AGH91, BD95a, Cam92, DWM90, HC96a, HC96b, HC96c, HC96d, Ish92, Jor92, KSF91, KL90, Kry96, MM95a, MUMH97, Muk92, Mur90, Pos91, PK92b, SH90a, SCE92, SD91, VCML90, ZC99, ZP90].

Many-Body [BD94a, BD94b, IK97, JOC97, KBT94, KZVG97, Lin96b, LFD94, MMH95b, NB97, Pie93, Sta93, SPL97, SKS98, VVS94, Cim96, Ano93g, BD95a, HC96a, HC96b, HC96c, HC96d, Ish92, KSF91, MM95a, MUMH97, Muk92, Mur90, SH90a, SCE92, VCML90, ZC99, ZP90].

Many-Center [MS93b, SN98]. Many-dimensional [Ber96c].

Many-Electron [KNN96a, Mar96, Muk96, NMKP94, Oht98, SAR96, SD96a, SN98, TC98a, TM93, YAD95, Mar99a, Ano92l, Cam92, DWM90, KL90, Kry96, PK92b, SD91]. Many-electron-wavepackets [NNY+96]. Many-Fermion [CBG94, Jør92]. many-particle [AGH91]. Many-Photon [NMKP94]. MAPLE [McD97, Pie93, TP94, Lai94]. Mapping [MKM93b, MM98, KM90c, KBM92, SM94]. Maps [AP96, MK99]. Masao [Ohn95]. Mass [Ara94, MMP+94, MG93a]. massively [Ken93]. Masten [Ano92n]. Master [BG95]. Masthead [Ano90k, Ano90l, Ano90m, Ano90n, Ano90o, Ano90p, Ano90q, Ano90r, Ano90s, Ano90t, Ano90u, Ano90v, Ano90w, Ano90x, Ano91k, Ano91l, Ano91m, Ano91n, Ano91p, Ano91q, Ano91r, Ano91s, Ano91t, Ano91u, Ano91v, Ano91w, Ano91x, Ano92r, Ano92s, Ano92t, Ano92u, Ano92v, Ano92w, Ano92x, Ano92y, Ano92z, Ano92-27, Ano92-28, Ano92-29, Ano92-30, Ano92-31, Ano92-32, Ano92-33, Ano92-34, Ano92-35, Ano92-36, Ano92-37, Ano92-38, Ano92-39, Ano92-40, Ano92-41, Ano92-42, Ano92-43, Ano931, Ano93m, Ano93n, Ano93o, Ano93p, Ano93q, Ano93r, Ano93s, Ano93t, Ano93u, Ano93v, Ano93w, Ano93x, Ano93y, Ano93z, Ano93-27, Ano93-28, Ano93-29, Ano93-30, Ano93-31, Ano93-32, Ano93-33, Ano93-34, Ano93-35, Ano93-36, Ano93-37, Ano94j, Ano94k, Ano94i, Ano94m, Ano94n, Ano94o, Ano94p, Ano94q, Ano94r, Ano94s, Ano94t, Ano94u]. Masthead [Ano94v, Ano94w, Ano94x, Ano94y, Ano94z, Ano94-27, Ano94-34, Ano94-35, Ano94-36, Ano94-37, Ano94-38, Ano94-39, Ano94-40, Ano94-41, Ano94-42, Ano94-43, Ano931, Ano93m, Ano93n, Ano93o, Ano93p, Ano93q, Ano93r, Ano93s, Ano93t, Ano93u, Ano93v, Ano93w, Ano93x, Ano93y, Ano93z, Ano93-27, Ano93-28, Ano93-29, Ano93-30, Ano93-31, Ano93-32, Ano93-33, Ano93-34, Ano93-35, Ano93-36, Ano93-37, Ano94j, Ano94k, Ano94i, Ano94m, Ano94n, Ano94o, Ano94p, Ano94q, Ano94r, Ano94s, Ano94t, Ano94u].

[Coh97, DJF98, SB96, Mar94c, Tos95, YNNR97]. **Mathematical**

[DB99, PV94, Ano91g, CDB99]. **Matrices**

[CB94b, FBKD97b, Gin96a, HH97, HM97b, KSG93, KBWJ96, Maz98, Mez97b, PRTV97, PK96, Sam97, SFM94, Spr96, Zap95, Cal90a, CES87, Ell92, GL96, Hol98, HMK96, Mar95a, Mar99a, MHH95, MYPL90, MP91, NZ92, PC99]. **Matrix**

[Bad95, BM96, BG98b, BG98c, BG98d, ČHM95b, DV98, DKBB97, FBKD97c, Gin98, Gin99, GMI95, Iga95, JBT+95, Kin96, KA95b, KMM96, LY98, LBM95, Mik94, Mor93b, Pal93b, Sch95b, Tit92, Tit93, TCM98, TNM97, WT98, ZWZ96b, ZARB96, BCD91, DW90, Ell91, FL91, For92b, FJR96, ITC91, JRS99, Kov90b, MD99, NM94, NE95, PAC90, PAC90, PN994, PK92b, SN99, SP90, SG96a, Sch95a]. **Matter**

[Ino96, Lü90c, Mar94b, BCD91, CDB90, Lü91a, Lü91b, Lü91c, Lü91d, Lü92b, Lü92d, Lü92a, Lü93a, Lü93b, Lü94b, Lü95c, Lü95f, Lü95d, Lü95b, Lü96b]. **Maxima** [Che96]. **Maximum**

[AYAZ95, AZAC97, CC91b, GH96a, TSP97, WG94, ZZ91, Zha92a, MP91, pea95, Zha92b]. **Maximum-Entropy** [AZAC97, AYAZ95]. **May**

[Cal90d, FG96, JPP87, Kar93, Bha99]. **MBHO** [HZ94]. **MBPT**

[GR95a, GS97b, KBB+90]. **McClelland** [She90c]. **McGraw** [Str92]. **McGraw-Hill** [SGB98]. **MCI** [SNH99]. **MCM** [AT99]. **McMurtrie** [JGP91]. **MCC** [SG96b, SGB98]. **MCP** [PSAU89]. **MCSCF**

[BBS91, FG99, JR96, KSIH92, NÁJ91, NÁJ92]. **MCSCF/MCLR** [NAJ92]. **McWeeny** [CS96b]. **MD** [FVN98, LSGS91]. **MDG** [SJB90]. **Me**

[Sta95b, CRK+91, GAR97]. **Mean** [ADB96, Gui98, Mez94a]. **Mean-Field** [ADB96]. **meaningful** [Ada91b]. **Means** [Gin98, LBPL97, LBKLC98, LBLK98, MBA97, MS93b, BMA90, MS92, SO97]. **Measure**

[Mez97a, NP96a, BR92, MM99a]. **measured** [Hal91]. **measurement** [Kar93, CPW92]. **Measures** [HM97a, HSS95, Mez97a, Mez97b, MFAT98, SMO+96, BBSS96, CC92a, CC92b, HSWS95, Mez94b]. **Measuring** [BCC99]. **Mechanical**

[AY92, AM97, ALRP96, BLBP97, CDC98, ECHB96, FLRV97, GDI98, JDJP99, KL97b, NFVM94, RL94, TNN98, TTK99, Tch96b, Tch96a, VB92, Val94, Wen96a, ZWPJ94, Ano96-31, Ber96b, BV93, CBL95, DV96, FNS99, Fer91, FG96, KJL96, KS94c, Lan95, NOY98, NPL90, NGM+95, OM91, SH90a, SR99, Wen96b, YUS99]. **mechanically** [GS96]. **Mechanics**

[BLBP97, Emc97, O’C96, Pri95, RKN97, WHo94, Wlo95, Wlo94, Adl95, BD95c, Chr98, Deu96, Gar95, Gin91, GZ97, GZ06, LCP+91, LU92b, MA99a, Mic96a, Pos91, PK92b, RTKP95, RS90, SR93, SR92, Sch94, SN97, Wha96, WP90, Car96, Str91]. **Mechanism**

[DDP96, FF94b, HBB98, LX95, OSA+97, AKCS91, BBTU97, BP90, ...
CLOFR98, DV91, DD99, FMS+99, FF92, FF96, FWZ97, GWB97, JUG90a, KO91, NOY98, DZB92b, SBZ92d, TF92, TCA+91, ZH99a. Mechanisms [BAK96a, BAK96b, Cha95, ECBH96, Sak97, Sak98, BH99, BDP+92, CH91, DRGC90, KZW98, MV92, Nes94]. mechanistic [Ano96-58].

method [Duc90, Fau92, FNSV99, Fer92, FZZ92, FW92a, FHHE90, GHB + 99, GRTR96, GB90, Hag96, Har94, HZ91a, HZ99, HK97, Ish92, JM96a, hJH97, Jun92b, Kal90, KGN96b, KF96, KY92, KB92, LO93, LK90, LK99, LH94, LP97d, LP98, LJS94, LH90, MRC99, MHS95, MFH91, MHY98, MB93, MW90a, MRT95, MR97, MC91a, MC91b, Moh92, MAPLB92, MPP92, NSTFC94, NNY + 96, NKS + 96, Nag96, Nes94, New97, N92, Pai92a, PSAUS90, Par90a, Pau92, PCO + 94, PL91, PTL90, PZ92, RAI99, RRC94, Réa90, Rin96, Roc99, Rom92, RL97, RK92, SG96a, SW + 99, SP90, She90c, SS92d, Sin92, Sme92, STM96b, TSY99, TR91, Tho96, Tit96, VR90, WS92, YITY93, ZM95, Zha92b, Zho93].

methodological [GDB98].

Methodology [BPL97b, Del92].

Methods [ASP97, BIM97, BLE96, BBS + 97, BLRD92, BF94, BL92b, CCM + 96, DRB96, DZO97, GD96, HS92b, Her98, HS91, HS92d, Jug96, JM96c, Jur97a, Jur97b, Jur97d, Jur97g, L92, Löw99, Mar95c, Nic99, PM + 92, PTH + 97, RL94, RHC96, RWT92, Roz97, Sab90, Saw97, Sch95c, SRM98, Sim97, SAL + 94, SG97, SGB97, SGB98, Sta93, SATP94, Sza95, UWB94, VFHL93, WR96, ZON + 96, ZZZY96, ANB94, ACAT92, Ano90g, Ano90i, Ano93g, BMA90, BBV97, Bo90, CZ93, CMA + 99, DS90, DSS90, FG96, FG92, GL92, Gut99b, Hag92, Hag95, HK95a, HC96c, HSES94, Iac92, Jak93, J94, Jer92, JK92a, KK99a, KLO + 98, KL92, L91, LS92b, MG97, Mku92, PAF91, RPT90, RWT91, RC92b, SGCC99, SSC92, Sim95, Sim99c, SES93, SG96b, WGP99, YBZ92, ZF92, BBSS96].

Methoxy [HS99]. Methoxyidazoxan [HS92b].

Methyl [MZ93, NSS + 95, PSCZ97, BH92, CMG92, HDY + 91, MJLL99, PVF + 92, RT99, STS95, SCJK90, VS95, SSM + 99].

Methyl-Ethyl [NSS + 95].

Methylacetamide [TT98].

Methylamine [AMKS93].

Methylated [VDD96, HWB97].

Methylation [FW92c].

methylcopper [CPN91].

Methylene [Oli99].

Methyleneimminium [MKK98].

methylenimine [FF92].

Methylformamide [TT98].

Methylglyoxal [VC92].

Methylpyridones [RM96].

methylthio [SSM + 99].

Metiamide [MTP + 98].

Metric [Löw96c, Me97].

meV [Eng92].

MFI [MBML91].

Mg [BZQ95, NBS95, Cs96, FR93b, Pro94, Pro95, YDD92].

MgAl [BILA95].

MgC [DDC95, DTA + 96].

MgF [LG96].

MgI [MBG90].

MgO [LXWZ99, AMT + 99, FP96, PCB92, YNNR97].

MH [SNH99, SM96a].

Mimet [SWK90].

Mimic [LZ91].

Minic [Cha96, Gre98].

minima [SCH92a].

minimal [PCD99].

Minimum [FP94, Pai97, PL98, KM99a, Pai91, Pai99, WP91].

Midgap [TYY91, TYY91].

Midpoint [Mar94a].

midrange [Tos95].

Mills [EMMHP92].

Mimics [LJ95].

mind [Cha96, Gre98].

Minimization [FP94, Pai97, PL98, KM99a, Pai91, Pai99, WP91].
Minimum-Energy


Model [AT99, AMO+96, ATI97, Ara94, BE95, BE98, BC96b, Bra97a, CLSI94, CA90a, CMFA93, CB96b, COL97, CPA95, CS97, DDD+96, DL92, DMB97, EMMK94, FT97b, Fru94, GC94, GMS98, HU96, JK94, JM95, JKRW98, JGR98, JMR98, JSG97, KBWJ96, KPR97, KPTS97, Kon94, Lah92, LCL095, LB95, LEA+94, MF93, MHH95b, Mat99, MAD98, MA95, MPV94, NA94, NM95, OK98, PW97, PPP97, PTC94, PS94b, RP9M95, RAZ94, RML97, RG96, Sak98, SB98, Sch99a, Sch99b, SBIP97a, SLS91, ST96b, SFGW96, TSPK96, WBP98, WI96, YO92, Zha92a, AEJ91, AC92, AD92, BOA95, BPH96, BL91, CT95, CPV90, Con92, CF99, DV93, Del90, DDA92, DCK92, EZ92, FKR92, FM92a, GPSM93, GWB97, GJ97D97, GL96, HFM91, JM96a, JUG90b, KR91, KF96, KSH92].
Modeling AT99, AMO+96, ATI97, Ara94, BE95, BE98, BC96b, Bra97a, CLSI94, CA90a, CMFA93, CB96b, COL97, CPA95, CS97, DDD+96, DL92, DMB97, EMMK94, FT97b, Fru94, GC94, GMS98, HU96, JK94, JM95, JKRW98, JGR98, JMR98, JSG97, KBWJ96, KPR97, KPTS97, Kon94, Lah92, LCL095, LB95, LEA+94, MF93, MHH95b, Mat99, MAD98, MA95, MPV94, NA94, NM95, OK98, PW97, PPP97, PTC94, PS94b, RP9M95, RAZ94, RML97, RG96, Sak98, SB98, Sch99a, Sch99b, SBIP97a, SLS91, ST96b, SFGW96, TSPK96, WBP98, WI96, YO92, Zha92a, AEJ91, AC92, AD92, BOA95, BPH96, BL91, CT95, CPV90, Con92, CF99, DV93, Del90, DDA92, DCK92, EZ92, FKR92, FM92a, GPSM93, GWB97, GJ97D97, GL96, HFM91, JM96a, JUG90b, KR91, KF96, KSH92].

Modern [Amo96, CTG97, KGC+96, Lów97b, Oli99, SP95, TC98b, GZ97, GZ06, Kla93, Kry96, Sém96a, Tri96]. Modes [KC98a, KC98b, PP98b, BZMR92, HZF+91, HW91, JDB99, KLC98b, WD91].
Modification [DD90b, FW92a, GRT96, GRTR96, Gin91, Iva96, Iva97].

Modifications [Sta98a, ZZW96]. Modified [BE95, Fue98, MPP95, MK99, NM94, Pec93, Por99, RL92, SWMB94, Tag97, Was91, ZARB96, BGS97, FHHE90, Hol98]. Modified-Hartree [Hol98].

Modifying [ZZZY96, ISOA99]. modulated [Lin91]. MoF [FAV92]. Molecular [AEAO99, AP96, AC94, Ano92j, ATI97, AM98b, Art96, Art98, BKR97, BC96a, BSB94, BM96, BCMO97, BLBP97, BSHP97, BG98a, BBLK94, BR94, BFH96, BMP93, Cal90d, CCM+96, CC92a, CC92b, CMMC96, CFB97, CC97a, Cio94, CG96, Coo94, Cor92, Csi82, DR92, DE92, DP93, DM96, DTM96, DN96, DBF+96, DZF93, Dun98, ESHP99, Enk97, ECBH96, Fan97, FM92b, FWT+96, GBVM93, GVK99, GJ95, Gho95, GRT96, Gin99, GT93, GPD94, GGP97b, GGHP94, GLBM96, GW98a, Gus98, GLLY94, HW04, HAEMA92, HS92b, HGC93, HL93a, Her97, IYF99, JM96b, Jon94, Jos97, KUN+98, KFS92, KPD93, Ken97, Ken98, KKB92a, KM91, KE91, Krui97, KPB99, KL97c, LB96a, LJ95, LZ96, LF97b, LLC+94, LPD93, Lip91a, Lip91b, Löw99, LH90, LTY92, LL92, LU92b]. Molecular [Lun92, LB96, Mar90, Mar94d, Mar95b, MHA98, MKM93a, Mar95c, MC97b, Mat99, MR99, Mez90, MK99, MAI95, MH98, MCS95, MK97b, MK98a, MK98b, Mor97a, MV99, MSC92, MAAP+98, NK96a, NY92, NP96b, OMTS97, OOD96, OSA+97, PC92, Pen96, PVU+93, PC95, PAAM98, PJ96, RK97, RD98, RWT92, RV98, Ro96, SM98, SM96b, Sch95b, Sch95c, SNMB97, SCP95, SS99b, SRS92, SG94, STM97, SGGMGFS96, SMO+96, SM92b, SH96, Ste96, SP94, Sul97, Suz99, SBZ92a, TMSI98, Tal93, TMP97, TD96a, The96, TC98b, TNM97, TD96b, US97, US96, UWB94, VFHL93, W594b, Wan94, WP90, Wil96, WGR+94, WP92, Wu94, YTY97, Zha92b, Zha92a, ZLHZ94, ZM96, ZM97, Ägr91, ARD92, ACAT92, An90i, An96-1c, AM90a, AM90b, Alt93, Ata94, AD92, Avi92].

molecular [BBSS96, BJ92, BKL92, BKM90, BV91, BV92, BM93, BMFP92, BJMK92, Cal90f, CM99, Chr89, Clio91, Con92, CA90b, CB91, CE90, DS99, DCK92, DRGC90, DO94, DQ90, FMR91, FMD+96, Geg91a, Geg91b, GJDD97, GP91b, GG84, HSWS95, HDB+95, HOF+97, Iac92, JO94, JEO90, JOn92b, KDB90, KKK90, KJ91, Kin93, Kin94, KH96a, KKN99, KW98, KA99, Kov90a, Kov90b, KJ90, Kry96, KSW98, KSK+99, KKM99, KL92b, KJ90, LYL95, LAV92, Le99, LF99, LHL91, Les92, LV97, LTY90, LU90, LCP+91, MD92a, Mar92a, MT90b, ML99, MM94, MCA92, Mez94b, MK94, MK95, MK96, Mun92, MSC92, MP99, NKS+96, NMN+99, NY99, Nal92d, DZB92b, NL96a, NL96b, OKY+99, PBP90, Pic92, RTKP95, Rau92, RFC90, RWT91, REU+91, RK91, RK92, RC99, RCW94, RAM91, RF90, Sa92].

molecular [SCA93, SX96, Sch95a, SC96, SGGC99, SCP91, SOK+98, SCJK90, Sla92, Smi96, SKR90, St91, TTM99, TH90, TYY91, TW90, TW92, TCB99, The94, Tom91, Tuh91, UBA92, VES+99, WM92, WLB+94, WW97, WGP99, Woo99, AEHM91, AHM97, Bir94, Bra98b, KMR92, KN99a, SK99a, SH94, Mic97].
molecular-electronics [Sla92], molecular-orbital [Mar92a].
molecular-state [KSW98, KSK+99]. Molecule
[AS96, BBC+94, BvL96, CWX93, CCB+97, DB99, Del96, Gin98, GV93,
GY97, Hbl99, JCÁ96, KM92, Kon94, KA95a, LD95, MB98, Mon99c,
MTD96, MP98, PVLG93, PLA98, Pie93, PTC94, RGT95, SG93, SZ98,
TKN96, TMSI98, VDBP97a, YTYS97, BSS+97b, CrsP93, CCC+95b,
CRK+91, CWJ+99, Coo92, DDC95, GSM90, GJPZ97, HGL99, Ike99, LLI92,
MRRSN92, MHM95a, MUMH97, Nak92, Na91, Na92c, NWG+99, OTS+95,
PGM95, Ran93, Rec91, SOK+98, SG92, TGS99, TG96, XSA+92, Zha91].

Molecule-Surface [GYDY97]. Molecules
[AHI96, AZAC97, BBOR96, BKM93, BEJ98, BZQ95, BK98, CT96, CAY+96,
CC95, Che97, CL94, DTA+96, DIP99, DHC95, DWM97, DKE97, FCFL98,
GG97a, Gra97a, Har96, HP97, HIl98, HHH99, IP93, JCM+92, JAG95, J96c,
KL96, KMM95, Kup98, LGMA96, LKMCVT95, LKMCVT96, LTP96, LN96,
LSC98, Mar94b, Mar98b, MRL99, MR92b, MKM96, MK97, ML+96, Mor93a,
MP93, NK98, Pa97b, PBB98a, PDC96, PP97, RPI96, R98, RL98, RABZ94,
RS97a, Rye94, SC97, Sch98, SD96a, SF96, Sh96, Sta96a, Su93, Suk95,
Sup99, TNS+94, TDO97, VFD96, VHFL93, WP93, WS95, WZ96, YDFS98,
ZWJP95, ZZCSE94, A99, BZ92, BZMR92, BK99, BJ96, BL91, Bro95b,
BPVP92, BLG95, Cal90d].
molecules [Cal90e, CCWCF96, CTF92, CXFP99, CS99, CRL95, CLGW95,
CTC95, Csi76, DKE97, Den98a, DA91, DT96, DBF+92, EMS92, E92,
FLHT90, GFS92, GS92a, GSPSM93, GL99, GS91, GDY97, GDF92, GS90a,
GS90b, HS95, HZ9+91, IL95, hH97, JY94, KM90a, KPTS+93, KY92, KT95,
Kov98b, Lu92a, LSC98, Mar93b, MKDL93, MSMR99, MH95, MKP91,
MB92, MW90b, Min90b, MC91a, MC91b, Mol92, MKBP97, MAAP90,
MPP92, MJLL99, MIW91, MBS90, NE95, O91, OS92, PY89, PAR99, PK94,
Rat92, RF94, RD90, RTS91, RSCP92, Sar90, SM99, SC91, Sco90, SP90,
Sin92, SM90, SKRK90, SLDB91, SN90b, ST91, TFS95, Tit96, TKK+90,
VA90, VPS+90, W90a, WMW92, WZ96, Y99, YKN+99, ZB92, ZM90,
D89, Mak87, Ágr90, Ca93, Lin96a]. Molin [Kra96]. Møller
[Cim96, HC96d, Hir92, KLO+98, Kir95, KSY97, MJS93, Pra97, SAS99,
Suh93, VCML90, vDV9799]. Molten [BPL97b]. Molybdenum
[Boe98, CF96, TGDS97]. Moment
[Far92, Gus98, K93, MS98, Mc97, MK98b, RDF98, Sut99b, ZZ93].
Moment-method [Far92]. Momenta [Kru92, YPC97]. Moments
[BOX94, CJA94, KBW96, KY93, MZ94, Mon98, SPS96b, DOPS91, GB90,
KS91, LBG97, PS090, PTL90, PNB94, SSC92, SKKR90, TP90, TK92].
Momentum [AZAC97, AH96, AHWA96, BDNT96, BDNT97, Can97, DDD93,
HSS+95, Mar96, MAC96, OLS96, Pa99b, Sch94, TP90, TK92].
Momentum-Space [AI96, MAC96, Sch94]. monitoring [MBM92].
Monkhorst [Jér92]. Mono [Bér77, Cha97, GL97, WSTB90]. Mono-
[Bér97, Cha97, GL97, WSTB90]. monobridged [OTS+95]. Monocarbides
N [CEM +96, Eri92, Kor90, Kum93b, MM94, SP91, SSM +99, Str92, WYW96, YK97, ZC96, IP93, KSN93, Tit92, AEA99, ABDM94, ASM91, BMA90, CLGW95, DSS90, DOPS91, DZ97, Eva97, FDC92, GV93, Hir92, HB95, Kal90, KBGE97, LC93, MK90, MZ95, PGM95, FGS97, RK95, SK99a, SP92a, SW95, SSM +99, SES93, STC96, Tew94, Tew97, Yam90], N- [LC93].

N-Acetyl-2 [RK95]. N-band [Yam90]. N-Sulfinylanilines [AAO99].


N-Acetyl-2 [RK95]. N-band [Yam90]. N-Sulfinylanilines [AAO99].


N-Acetyl-2 [RK95]. N-band [Yam90]. N-Sulfinylanilines [AAO99].

Kov90b, MAI97, MT96, VHFL93, CTC95, CGMG92, KP92, Min90b, OYN98, Sch92b, TTM99, ZA95]. **Optimizations** [TJ95, VFHL93].

Optimize [Sir99]. **Optimized** [Ada91a, BC97b, EBG95, GG97b, GvLB96, Huz96, MKM96, MS93b, Nag98b, PG94, Pen93, Pen96, RSGC96, Sch95b, WBP91, GV92, HZF+91, MM99b, MS92, TC98c]. **Optimized-Basis-Set** [Pen93, Pen96]. **Optimum** [FB90]. **Options** [MPR97]. optoelectronics [Mun92]. Optogalvanism [YM99]. Orbit [HBL99, KMVA95, RI92, SFG+98, BG98b, BG98c, BG98d, ERC91, JRS+99, KLO+98, KRZ91, Man95a, Man95b, Man99, PW91, TSY99, Tit92, VAI+92].

**Orbital** [AEA099, And90, ATN97, BR94, BFH96, BEJ96, Bro93, Cio94, DE92, GBVM93, HAFMA92, HS92b, Hl99, IYF99, JKRW98, JGR98, JMR98, JZ95a, JZ95b, Jur96a, KUN+98, LP97b, MH98, MGC95, Mor97a, NS95a, NS95b, Ney95a, Ney95b, OSA+97, PS96, SRS92, SGGMFS96, Sta96a, Sta97, Sta98a, TMS98, TMP97, TD96b, Wan94, Zha92a, ZLHZ94, AEHM91, AHM97, Ada91a, Cio90a, CA90b, DO90, FMR91, GV92, HS92c, KDF90, KH96a, KCL95, LMM93, LO90, LTY90, Mar92a, MKDL93, MLI99, MCA92, NE95, OKY+99, PC92b, Pau92, PP90, RK91, RMR90, SCA93, SX96, SCJK90, SKR90, Sta95, Sta96b, Sta98b, Sta98d, Sta98e, SS98, TTM99, TH90, TYY91, WB94, WL90, WP92, Zha92b]. orbital / molecular [RK91]. **Orbitally** [GWCT97, NM92, Na92b]. **Orbitals** [BW97, Bro93, BJLK98, Coo96, DTS97, DDD93, EBC95, FG93, GM94, GVC96, Gia95, Gin99, GY95, GJ96, Gus98, GOAY98, Her97, HO94, Huz96, Ish96, Jon97, Jur97c, LLL97, MYN+96, MBA97, Mey94, Mey97, MR92b, MS93b, NMM97, NU95, PBB94, PGH95, RSGC96, RMPR98, Spr96, Ste96, TV92, WZV96, BKK90, BJA99, BP93d, Bud92, BFW92, CKB91, Cio90a, CC91b, Cio91, DM94a, DRGC90, EJ93, För92a, HS92d, HOF+97, JE90, JEB92, Jon92b, Jon93, KKN99, Koll90, KKL91, KM97, KMR92, LLY90, LMM93, LO90, LTY90, Mar92a, MKD93, MLI99, MCA92, NE95, OKY+99, PC92b, Pau92, PP90, RK91, RMR90, SCA93, SX96, SCJK90, SKR90, Sta95, Sta96b, Sta98b, Sta98d, Sta98e, SS98, TTM99, TH90, TYY91, WB94, WL90, WP92, Zha92b]. **Orbital** [K91]. **Organic** [ASP97, AR93, BBS91, BS94, BP96b, CV94, CB94b, DM96, DB94a, DM94b, DMB97, Eid99, FR93b, HM97b, KSY97, KD95, LS93a, LFS94, LJN+98, Mor93b, Ort89b, Sam97, Sie93, Sim93b, Sim98, SP94, SATP94, SPL97, TD96a, VVS94, VK98, VFHL93, ZO95, Ada91a, Ada91b, BSS97a, BKL91, BCD91, Cio91, DM94a, DRGC90, EJ93, För92a, HS92d, HOF+97, JE90, JEB92, Jon92b, Jon93, KKN99, Koll90, KKL91, KM97, KMR92, LLY90, LMM93, LO90, LTY90, Mar92a, MKD93, MLI99, MCA92, NE95, OKY+99, PC92b, Pau92, PP90, RK91, RMR90, SCA93, SX96, SCJK90, SKR90, Sta95, Sta96b, Sta98b, Sta98d, Sta98e, SS98, TTM99, TH90, TYY91, WB94, WL90, WP92, Zha92b]. **Orbit** [K91]. **Organic** [ASP97, AR93, BBS91, BS94, BP96b, CV94, CB94b, DM96, DB94a, DM94b, DMB97, Eid99, FR93b, HM97b, KSY97, KD95, LS93a, LFS94, LJN+98, Mor93b, Ort89b, Sam97, Sie93, Sim93b, Sim98, SP94, SATP94, SPL97, TD96a, VVS94, VK98, VFHL93, ZO95, Ada91a, Ada91b, BSS97a, BKL91, BCD91, Cio91, DM94a, DRGC90, EJ93, För92a, HS92d, HOF+97, JE90, JEB92, Jon92b, Jon93, KKN99, Koll90, KKL91, KM97, KMR92, LLY90, LMM93, LO90, LTY90, Mar92a, MKD93, MLI99, MCA92, NE95, OKY+99, PC92b, Pau92, PP90, RK91, RMR90, SCA93, SX96, SCJK90, SKR90, Sta95, Sta96b, Sta98b, Sta98d, Sta98e, SS98, TTM99, TH90, TYY91, WB94, WL90, WP92, Zha92b]. **Orbits** [Ols96]. **Order** [ASP97, AR93, BBS91, BS94, BP96b, CV94, CB94b, DM96, DB94a, DM94b, DMB97, Eid99, FR93b, HM97b, KSY97, KD95, LS93a, LFS94, Ljn+98, Mor93b, Ort89b, Sam97, Sie93, Sim93b, Sim98, SP94, SATP94, SPL97, TD96a, VVS94, VK98, VFHL93, ZO95, Ada91a, Ada91b, BSS97a, BKL91, BCD91, Cio91, DM94a, DRGC90, EJ93, För92a, HS92d, HOF+97, JE90, JEB92, Jon92b, Jon93, KKN99, Koll90, KKL91, KM97, KMR92, LLY90, LMM93, LO90, LTY90, Mar92a, MKD93, MLI99, MCA92, NE95, OKY+99, PC92b, Pau92, PP90, RK91, RMR90, SCA93, SX96, SCJK90, SKR90, Sta95, Sta96b, Sta98b, Sta98d, Sta98e, SS98, TTM99, TH90, TYY91, WB94, WL90, WP92, Zha92b]. **Orders** [R94, RT90]. **Ore** [Us96]. **Organic** [Jen99, KM97, Mor93a, Sta97, TMD98, An92j, Ano93b, An96-58, AI99, BLC95, BHH92, Csi76, Csi77, CD81, FCA91, FKR92, FS99, GFS92, HS95, KMR92, MKK96, Mar93b, MAAP90, MPP92, OCK99, Pár98, PSBL98, SP90, Sm96, Sta98b, Yam90, MKP91, Eri92]. **Organization** [Lun92, TD03]. **Organized** [AR96]. **Organomagnesium** [OSA+97].
Organometallic [DDH+96, DRBE96, Tch96a, ARDP92, BDPS97, CEZ+99, KR91, Yam90].
Organonickel [TB95]. organophosphorus [Kin94]. orientation [CL90, Tew97]. Orientation [Kry98, MV92]. Oriented [SWF93, WP95].
Origin [BDT96, MBA94, Sak98, TBBE98, TI94, ZH99b, KMP+90, Le 97, Pop90].
Origin-Shift [BDT96]. origins [Par90a, Cio93]. Orientational [Kry98, MVB92]. Oriented [SWF93, WP95].
Origin-Shift [BDT96]. origins [Par90a, Cio93]. Orientational [Kry98, MVB92]. Oriented [SWF93, WP95].
Origin-Shift [BDT96]. origins [Par90a, Cio93]. Orientational [Kry98, MVB92]. Oriented [SWF93, WP95].
Origin-Shift [BDT96]. origins [Par90a, Cio93]. Orientational [Kry98, MVB92]. Oriented [SWF93, WP95].
Oscillations [ANB96, DMB97]. Oscillator [CB93a, Coo94, DBB94, KMP97, LDGA96, Lef97, MS97b, Pal93b, Pal97b, Pal98, RJ97, SB97a, SB97a, AR92, BRL92, BADM97, DOPS91, DW90, KSF91, LC90, ML92, MK90, PR9S92, Pal91, PV91, RÉ9a0, SP90, YBZ92]. Oscillators [NYLBN97, RDF98, SB97b, TZ97a, DB94b, Fan90, WN90].
OsO [NS91]. Other [CCE+93, CRK+91, FLWZ90, Hag92, HC96d, SPM+96, SKM99]. Our [Löw97b]. Outlines [Lad97a]. outlook [KK92b]. Outperform [JCM+92].
Overcoming [Rey90]. Overcomplete [Per98]. Overlap [Day95, Day96, GI96G, GOAY98, HO94, HS92f, Jon97, MMD96, NS95a, NS95b, NE95, Ney95a, Ney95b, VR95, Zha92a, ACZ91, BZ92, EZ92, Jon92a, JEB92, MRC99, NITFC94, ZZ91, Zha92b]. Overlapping [GV92]. overtone [KSF91]. Overture [Bal96]. overview [TCM99].
Ovomucoid [NK96a]. oxepins [Tri98c]. Oxford [Cal90f, Cal93, Den96, JER92, Kla93, Kum93a, Kum93b, Lin93, Lin96a, Mic96a, Str93]. oxidase [RC99]. Oxidation [NN97, BBB+95, LC93, PHBB94, YNST99]. oxidative [HDB+95]. Oxide [HLS94, JZ95a, Jur98a, Bro95a, GW97, KCP90]. Oxides [BK94c, ETV94, Jur96b, SDE94, MS93a, Nor91, Yam90]. Oxidized [TTK99]. Oxirane [KMVA95]. Oxo [GL97, MRT97]. Oxo-aminotautomers [GL97].
Oxohydroxy [MRT97]. Oxohalides [CCG+96]. Oxohydride [RKG96]. Oxygen [BvL96, GMR+93, JM96c, KFS92, LV98, MGNK95, Min96, RP98a, SFG96, UWB94, YNMT98, YTS97, CSH99, FEE+98, Kha91, Li97, ML94, OS92, SAB+97, SM92a, SKC99, SW92, BB93]. Ozone [RRS97, BH99, NJA91, NAJ92].
P [BKL97, Brä98a, Brä98c, BCY95, BZQ95, CRaP93, Eri92, Kar93, Kor90, SPFL93, SP91, SJÖ96, Str93, TIPM96, TR96, BLK97, DWR99, LB94, MEP90, BRL92, Man99, Mar97b, P WL98, RSCP91, SC95, STC96, WGC94, PAT93].
p-phenylenevinylene [DWR99, LB94]. P450 [CL90, KKS99, LC93].
PS94a, PB95c, PJ96, Pon97, Pon98, ROSM96, SP94, WS94a, ZH99b, AS95, BHV96, EKI94, FL95, GDF92, Ish92, KSIH92, LK90, MRD92, PCD99, PB99, Roe91, TGS99, TG96, Zie96, FW92c. Pair-Density [PEBS97].

pair-excitation [KSIH92].

Paired [KSG93, GT97, Pau92]. Pairing [DMB97, May97, Pon98, She90b, Ukr94, KŽ90, LRM93, PS99, Tas94].

Paireon [CYY95]. Pairs [BL92b, Br¨a93b, CD93, HNB92, KV96, SM98, ZL98, AGNS92, LM91, LJS94, RFG99].


Parameters [BDD93, EMMS97, GIA96, MM98, NG95, Por98, TV92, DLF99, MSS99b, NL96b, PACO90, Por97, Por99, SC96, WA94, WZ99]. Parametric [MK98b, R97, SRM98, HDB +95, YG90].


parnassum [And93b]. Parr [Cal93, Ano90z, Ano94i, Ano94-37, Iva96, Iva97, Par94a]. Parrinello [Kry93]. Part [DPP ++94, MDS98, GVB96]. Partial [Kat97, LB96b, MTT93, Ort97, RH96b, GZD97, Kat91, Lin92, SN99, VA90].

Partially [GVC96, GV92, PK90]. participants [Ano90a, Ano90b, Ano91a, Ano91b, Ano92q, Ano92a, Ano92b, Ano93k, Ano93a, Ano93b, Ano94a, Ano94b, Ano95r, Ano95a, Ano95b, Ano96-31, Ano96-29, Ano96a, Ano96b, Ano97n, Ano99i, Ano99k, Ano99l, Ano99m, Zer98, Ano96-30, Ano99j, Tri98b].

Particle [Bla96, DP97, Ino96, Lev97, MPOG99, ZW96b, AGH91, BMDM99, CC91a, LC90, LLL91, NM94, NS92, Sch92c, SD91, SZ92a, WA94].

Particles [BMFPV92, GSM90, KSIH92, KSW96, Mar93b, OM91, Woo99]. Partition [RW92, Kin94, Luk92, RW92].

Partitioning [Cio90b, IY99, JKK +92, KS90, MR99, Muk96, SKS98, MG93a].

Partitions [FJRS97, PM97]. Partner [MPOG99]. parts [Ska92]. Path [BA91, CB94, KNA94, KNN96a, KNN96b, KKN97, Mar94a, Min94b, NONY97, Okt98, Pon97, BA92, Hei95, Mat97, Nag96, RD97, ZB92].

path-integral [Nag96]. paths [AM90a, AM90b, CE90, LAM91, LAM92, MBM92]. pathway [SHF94, WJC +98, WJC +99]. Pathways [Fir94, FK98, LB93, CF99, TCB99].

PBE [MSMR99], PC [NSÅS⁺90], PCM [AGAP98, TCM99], PCO [HZ91a].
Pd [BYE⁺97, CCB⁺97, SZC97, SCS94, XKB⁺99]. PdO [BYE⁺97].
peculiarities [BSS⁺97b]. Peel [FHHE90, HE90]. Peierls
[AT97, Kup94, LN96]. [Pet92, MTD93]. 1 [Boč90]. 6-31 [FL95, Les92].
Adsorbate [NNMH96]. Alumina [SWMB94], blood [BPHB96]. bond
Dissociation [Moi97]. endo [SLG⁺96]. FCP [DKWM97, DKM97].
Pentacoordinated [DBG92]. Pentadentate [BBOR96], pentamethyl
[NAK95, PFMC97, SKJ98, WHF92, Jac92, JGCJ96, KM99a]. Peptides
[PFMC97, NMSJ99, PVU⁺93]. Percival [Kar93]. Perfluorodimethyl
[DD⁺93]. Performance [AH96, JG95, Mar95c, RA99, BDPS97, CLGW95, GJPF92, Gut99b, Ken93].
Peircyclic [Pon97, JK90, OS90, PS92b]. Perimetric [LKB97]. period
[Cle92a]. Periodic [ANB96, GKS99, LV98, MCM98, NNMH96, NK96b,
NB97, PSBL98, ZY95, For92b, LO93, VZ92, ZWD98a, ZWD98b]. periodically [FS95a]. Periodicity [Har98a]. periods [Kor90]. Peripheral
[MZ93, GVV⁺90]. permanent [KY91a, KY91b]. Permanganate [DZ96a].
Permethylation [RM99]. Permutation [KSG93, SAR96]. permutations
[Che92]. peroxidase [CL92], peroxide [MS99b]. peroxy [BHGC99].
Personal [Par94a]. Perspective [Rin94, SS92e, TD99]. Perspectives
[CCM⁺96, Mos98, SC97, Hei95, Roo93a, Mat97]. Perturbation
[Ada90, Ada91b, Ada96b, Ada99, AR93, Ång93, CJA94, CZ93, CB93a,
CJ98, Gin98, IK97, KBT94, Kir95, KSY97, KD95, LD94, MH95b, MV98b,
RDF98, SG98, SAFK97, SAS99, Su93, SPL97, SJ91, TBCP95, W98,
vDvLR99, Ada94, Ada96a, Cim96, Fer92, GL95, HC91, HC96a, HC96b,
HC96c, HC96d, Hn92, Hol98, Ish92, KSF91, KLO⁺98, LC90, MH95a,
MUM97, MRD92, MD92b, Suh93, SO97, VCML90, ZC99, ZP90, Suh92].
perturbational [TFY91]. Perturbations [ANB96]. Perturbative
[Gho95, LB99, SB95a, ZON⁺96, HIG95, MD99, SS98]. Perturbed
[AE9999, DP97, LB98, MD93a, Nc99, Su94, ABCM93, BILA95, PM92].
PE5 [Ei991]. PEt [BUZ94]. PF [FAV92]. PH [SC99, PS93, WW99].
Pharmacophores [MBV⁺98]. Pharmacophoric
[LBEB98, TBE97, GV⁺90]. Phase
[BDT96, Boe98, BMP93, BZ95, CM96a, CT96, CCZ97, DBB94, ET99, FY95,
FD96b, HPSC97, Her98, JG95, J´CA96, Mar97b, MS99a, MLR⁺98, Oku98,
SM98, Sim97, Sim98, Sd91, VUB99, VZ93, W94, W95, ZL98, BKL92,
Cab96, CFMA95, DNN99, DLF99, FSW⁺91, Har90, KFK91, Mez90, Sas90,
Sim95, Sim99c, TKO+92, TTOY93, TCS+90, VX99, WSM+94, ZDO96.
**phase-fitted** [Sim95]. **phase-lag** [Sim99c]. **Phase-Shift** [Sim98, KFK91].
**Phase-Space** [DBB94, Wlo94, Wlo95]. **Phases**
[Mar94b, Mar97a, Lei99, NMN+99, NWT92, Lunn92]. **PhD** [Ano99n]. **Phe**
[Lu92b]. **Phenanthrene** [CR96a]. **Phenol** [SC98a, HWB97a, WI96].
**phenolic** [PHBB92, PBHB95]. **phenols** [BP90, BHPB93, HB94, VES+99].
**Phenomena**
[IK94, MA96, O’C96, Kum93b, Tom91, ZJ89, ZJ93, ZJ96, ZJ02, Kum93a].
**phenomenological** [DBM99]. **Phenomenon**
[GMMH97, TMM97, AC92, BR92, SBZ92c]. **phenoxypropanolamine**
[WTD+94]. **Phenyl-** [MH98]. **Phenylene**
[JKK+92, Lah92]. **phenylenevinylene** [DWR99, LB94]. **phenylethynyl**
[TSRP99]. **PHGLF** [WD95]. **Philadelphia** [Mon93]. **Phloroglucinol**
[MCE+93]. **Phonon** [BS93, KCP90]. **Phonons** [LMAK93].
**Phosphatase** [K˚A99]. **Phosphate** [FLRV97, KJL96].
**Phosphorus** [CCG+96, GBL97, PD93]. **phosphoesterase** [KK99a].
**Phosphodiester** [BV93]. **Phospholipid** [CPGC99]. **Phosphorescence**
[FSHC99]. **Phosphorus** [CCG+96, GBL97, PD93]. **phosphotriesterase**
[KK99a]. **Photo** [Ano99o, NMN+97, NMN+99]. **Photo-induced**
[NMN+97, NMN+99]. **photobiology** [ESTM95, Kra96]. **photocaged**
[RC92b]. **Photochemical** [DHL+94, FK98, Kha91]. **photochemistry**
[CPN91, SCM93].
**Photochromic** [MRRA92]. **Photodecarboxylation** [FY95].
**Photodesorption** [DDH+96, YBM97]. **photodetachment** [MCB99].
**Photodissociation** [DDH+96, Man99, MY99, GL96, IF94, MIW91].
**photoelectrochemical** [KPM+90]. **Photoelectron**
[DZOR98, Gin95, KM90a, LFD94, MKBP97, NVR+91, NV97b, TKK+90,
KIJ96, Ort97, PVF+92, YJL92]. **Photoemission** [BS96].
**Photoenolization** [SC94]. **photoexcited** [TYY91, TYY91].
**photofragments** [MIW91]. **Photoionization**
[CM96a, DC97, LD94, LEA+94, SLD95, DD96, DD95]. **photoisomerization**
[Er90]. **Photon** [NMP94, Hag99b, OB95, PSO90]. **photonic**
[MKP91, Eri92]. **photosynthesis** [DM97b].
**Photosynthetic** [DTM96, SKTN97, CMSF93, STKN90]. **phototransfer**
[LMA91]. **Phthalocyanine** [GBVM93, HE90]. **phycoerythrocyanin**
[SCM93].
**Phyllosilicates** [NTL96]. **Physical**
[BDD93, HSS+95, WK90, Del90, HYS91, JKG99, Pea95, SS92e, DS99].
**physicist** [Roo93a]. **Physicists** [Mon99c]. **Physicochemical** [RVL97].
**Physics** [Deu96, HWB95, Löw90c, Löw94c, BLK92, Brä95, Brä98b, CVW91,
HW84, HW87a, HW87b, HW92, HW94, HW96, HW00, HW04, Hei90, Kry96,
Lad94, Löw91a, Löw91b, Löw91c, Löw91d, Löw92b, Löw92c, Löw92d,
Löw92a, Löw93a, Löw93b, Löw94b, Löw95c, Löw95f, Löw95d, Löw95b,
Löw96a, Löw96b, Rau02]. **Phytochrome** [GDB98]. **phytohormone**
[RTKP95, RT99]. **Phytohormones** [RT98, RTKP96]. **PI** [DD90b, AH92a].
**Pi-electron** [AH92a]. **Picture** [AH96, KS98, PS94a, BD95c, Car96]. **Pike**
[Deu97], Pilar [Str92], pilocarpic [KE91], Pilocarpine [EK94, KE91], Pilot [ZM95], Pines [Dun99], Pinnacle [WP95], pinocarveol [PRB96], piroxicam [BD95b], pitfalls [DV93], pK [MK95], place [WI96], plan [Ari92], Planar [JM96b, Jur98b, RHR95b, KH96c, MFC94], Planarization [Tri98c], Plane [PM95, BK97, HK95a, LTSL96, WM92, CLZ95], plane-wave [HK95a], Planes [Mar97a], planning [FG96], Plants [ML97], Plasma [YM99], plasmas [Mar90, WYZ+92, ZW96a], plastoquinone [MD94, MD95], Platelet [DBF+96], Platelet-Activating [DBF+96], Platinum [BC97a, Boc96, MA99b, SFG+98, TSS97, SBPH92, SC96], Platinum-Centered [Boc96], Playground [BA97a], pleated [Suh91], Planum [Ano93g, Mon94], Pleiset [Cim96, HC96d, Hir92, KLO+98, Kir95, KYS97, MJS93, Prn97, SAS99, Suh93, VCMLL90, vDvLR99], plicies [Löw95c], PM [BHKK93], PM3 [DZ96b, GKKM96, LJS94, MAL96, MC94, NSS+95, HS92b], PMO [SBM97], PNA [ITT+94], Point [AL95, LMR94, Mey94, Mey97, Sta91, And93a, AH92a, BA92, FCMB99, GKM90, KDB90, LF90, Mar92a, Mez90, PC99, Sm90], Points [AB97, BLB95, BLRD92, KPA95, CE90, HR99, Mez90], Poisson [PW98, LP97a, PTH+97], Polar [HP97, Mor97b, PRC98, BKY99, Ert90, KY92, RWT91], polarity [DR92], Polarizabilities [BSB94, BP93c, Can97, CMCR96, C294b, CMFA93, CA96, DT96, KSY97, LL92, SS92b, SO94, AD92, BP93b, CA90a, CA92b, CMA93, Har94, JCA97, SDO91, SSC92], Polarizability [G97a, MRL99, TSR99, CP99a, DBF+92, MFC94, MCA95b, Par92b, PN94, SGCG99], Polarizable [FM92a, JCA96, PRC98, CT95, Cor92, MCT99, TCM99], Polarization [AP96, AO93, CMFA93, DD93, GJ95, KL93a, MB98, OS91, SO94, DMR96, DD90a, DRGC90, JMP99, RC92a, Res99, SDO91, Sm99, WWFR99], Polarization-Induced [MB98], Polarized [Boe93, BS94, GR94, KLI92, McH91], Policies [Löw90c, Löw91e, Löw91a, Löw91d, Löw92c, Löw92d, Löw93a, Löw93b, Löw94b, Löw95f, Löw95d, Löw96b, Löw91b, Löw92b], Politzer [Tri96], Poly [DWR99, Lah92, BL92a, GT97, LB94, GT97, LUG92a], polyacènes [GK90a, G90b], Polycetylene [DD97a, GP97, LRM96, LRM97, MI93, RML97, VZ93, AKS+90, CMA93, CP99a, DY96, LTY92, xLTY92, Sas90, Sta98e, TIA+92, TTY91, TTY93, WL90, YLY90, YLY93], Polyallyl [Che93], polyamides [ITT+94], Polyatomic [BLBP97, DQ97, KDP93, LDG96, WP93, Cal90c, CTF92, DD98, FLHT90, ZM90], Polyatomic [MSD95], polyazamacrocyclic [HBGR99], Polycation [Lah92], Polycentric [Wil96], Polycyclic [LL92, RL94, BBL94, KM90c, LYS95, VRR92], polycycloalkanes [DD96], Polyelectron [FK94], Polyene [Mat99, CA90a, PP92, PP91, PC92], Polyenes [ATI97, BEG94, BE95, BE98, BC95, BC96b, GP97, IK94, JCA97, KBT94, KBGE97, LP96, RR94, ST93, KKL90, Kur90, LRM98, LP99]
NNH98, Suh92, TWK98, MD92b. Polyethylene [Gin97, And90, CA92b]. polyethylenes [DO90]. Polyhedral [MFAT98]. polyhexapeptide [LU90].

Polyiodide [Sta97]. polyisocyanates [RBT99]. Polymeric [CMFA93, And90, BL92a, Dia99, FADC91, MFC93, MCA95b].

Polymerization [Sak97, BT96, Jug90a]. Polymers [˚AGL97, ASI94b, CA ¨O96, IAN +94, JSKC95, MAI97, NV94b, Ott94, PB97a, Sta96a, SL98, TMDB98, AMH93, Art94b, Art96, CA90a, CA92b, CFMA95, För92a, CJDD97, HZ91a, Kir92, LO93, LB94, Nob99, PK94, Sta98e, Suh93, TYY91, TYTY91]. polymethine [BBS90, Rep96]. polymorphism [CDM +94].

Polynomial [BˇC96b, ˇCB96b, LKLBD98, NS97b, SYZ96, TZ97a, ZW96b]. Polynomials [Gin96b, KL93c, CA92b, CFMA95, F¨or92a, GJDD97, HZ91a, Kir92, LO93, LB94, Nob99, PK94, Sta98e, Suh93, TYY91, TYTY91]. polynuclear [ML97].


Potential [ASP97, AL98, AP93, AP96, AR99b, AK97, ABLA97, AD97, BBOR96, BR97, Bla96, CGLP96, Coo94, CL95, DFDK99, DREW98, DD93, FT95, FP96, PCVL98, GPH90, GBS +93a, GG97b, Gra97a, GvLB96, GVB97, GSM98, GW98b, HM97b, HWS92, Huz96, IP93, Jas94, Jur97e, Ju98a, KLL98, KY93, KLL97, LB97, LX95, Lio92, LC90, LBM95, MB93, Mez94a, MTD93, Min94b, MPR97, MK99, MM98, MPV94, Mor96a, MTL97, Nag98b, NK96a, OSS95, Pai97, PL98, PLA98, PPSK96, PPK97, QS98,
RRS97, SS92b, SGK+95, SR96, ST93, SS97b, SATP94, VH96, XR94,
ZARB96, ACB+99, ARBB95, AGNS92, AKCS91, AR99a, ALS+91, BCLS94,
BJM+94, Ber96c, BKL91, BML98, BFW92, CDM91, CCS98, Cor92, CEM+96,
Dav90, DFR+96, FT97a, FDD95, Gao93, Gec91a, Gec91b]. potential
[Hag95, Hag96, Hag99b, HS93, Hir92, KR93, KY92, KL92, KM90c, LLL92,
LM92, MD92a, MCOS94, MV97, Mez90, MR92a, MPSLB91,
MGLBP95, Mur90, NOYF92, NM91, Na92a, Nes94, NÅJ91, NÅJ92, Pai91,
Paï99, PW91, RSCP91, R96, RR92, RAM91, SF90a, SP92a, SM92a, SM94,
SPS96a, STS95, SN90a, Ska92, Sla92, Sm99, TNS99, TCS+90, TM99,
TSPKM94, TC98c, VAJ+92, VVO98, WDS97, ZP90, GZSvD99, SES93].
Potential-Barrier [MPV94]. Potential-Derived [KY93, KY92].
potential-energy [AGNS92].
Potential-Derived [KY93, KY92].
potentials [BP96a, BMP93, CDDM96, Coo95, Coo94, CRG+94, ECBH96,
FLRV97, FD96a, Jur97d, KMM95, LG95a, LKMCT95, LKMCVT96, MG93b,
MKM96, MKM97, MPOG99, Mor94, MPJ98, MTL97, MM95, MSCP92,
MAAP+98, NKUS97, NC95, Nüüs4a, PG94, Pie93, RABZ94, ROM96,
STMR97, Sie93, Taq96, Taq96a, TE96, TSPK96, WR96, YY96, Zit94,
Ano96-31, BC97b, BMP92, CA92a, CB99, DGMW90, DDA92, DSW93,
ERC91, GW91, KL92, KLO+98, KCLI95, KKM99, LRR92, MD94, MD95,
MH98, MD94, MEP90, MRSP90, MB91, MIP99, Nag95b, PO91,
Rey95, SP90, SLL+91, SS95, Van96, WBP91, YNNR97].
Power [De 97, Ino96, Por98, Sie93, Por97, Por99, WTS93]. Powerful [Val96].
Powers [PZW93]. pp [Ano92i, Ber96b, Brä95, Brä96b, Brä96c, Cal93,
Dun96b, Kar96, Mic96a, Str91, Str92, Str93, Kum93b, Kum93a, Str92].
PPAR [Bl99]. PPO [LAM92]. PPP [Bal90, BEG94, BE95, BE98, BC96b,
CR96a, CPV90, CB96b, Del90, FHHE90, HE90, H90, Jug90b, MAAP90,
Par90a, PCE90, PVN90, Pop90, RPT90, SM96b, Sas90, SP90]. Practical
[Pan95, CC92b]. practice [Ci76]. Prasad [Eri92]. PRDDO
[DKM96, DKWM97, DCMK97]. PRDDO/M [DKM96, DKM97]. PRDDO/M/FCP
[DKWM97, DKM97]. Precision [Csa92, KL97b]. precrystalline
[EZ93]. precursors [CF99]. Predict [Far97, Fir94, DO90]. Predicting
[TSS97, CMA+99, Gut99b, MG93a, VVO98]. Prediction
[AST95, GL97, HIJ94, BDF+92, Mez90, SP92a, Sco90, TGDS97, Woo98].
predictions [GS97b, PWL95, SKM99, TFSZ95]. Predictive
preferred [LE92]. prefixed [GV92]. Pregnanolones [KG99]. Preliminary
[FDD+93, HDY+91, JTZ+96, PIP97, SH96, MG91, MG93a, KY91b, PW98].
Prentice [Str92, Wha96]. Prentice-Hall [Str92]. preparatory [Cle92a].
Preparing [Ano93i, Ano93j, Ano92o]. Presence [OK96, Sch97, Lás93].
Present [Dav98]. Present-Day [Dav98]. Press
[Cal90f, Cal93, Deu96, Jör92, Kla93, Kum93b, Kum93a, Lin93, Lin96a,
Mic96a, Mon93, Mon94, Str93]. Press/Gordon [Mon93]. Pressure
[MSS99a, Bar90]. Pressure-Induced [MSS99a]. Price [Cal93]. Primary
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Q [DM97b, CMSF93, DM97b]. QCISD [Bau98]. QCISDT [HKC96]. QCT [TUK90]. QDPT [LD95]. QED [Lin96b]. QM [BLBP97, Tho96]. QM/MM [Tho96]. QR [BB97a]. QR-SCMEH-MO [BB97a]. QSAR [BBE95, Rom92]. Quadratic [HKC96, Shn96, CCG96, Fau92, HC91, KMR92, PSO90, Par92b, SN90a]. Quadrature [DW97, HS91, HS92e, DD97b, SH90b]. Quadratures [Sch95b, SS92a]. quadruple [L92, TKSH93]. Quadruply [PTF95]. quadrupolar [S1C96]. Quadrupole [BOX94, BP93c, BP93b, FV96, PVC+90, VPS+90]. Quality [NP96a, Ros96, SS92f]. Quanta [Atk91, HWB95, Brä95, Brä98b, HW92, HW94, HW96, HW00, Str93]. Quantal [CSG99, HM97c, LLL91]. Quantenphysik [HW87a]. Quantification [Mar94a, WK90]. quantiques [GK90a, GK90b]. Quantitative [BBSS96, HB94, AM90b, BTKVG99, HZ91a]. Quantities [Nal94, Chu99, Nal92a]. Quantization [BK94a, GMI95, K92a, SR99]. Quantum [AV92, AM97, AR96, ALS+91, AAS93, ALRP96, BW97, BLBP97, BBC+94, BBC+96b, BSHP97, BHX96, BG95, BBRT94, BG98a, BR94, BVV91, BVV92, BFY+93, BBE95, BYGA99, Cal90b, Cal96b, CCM+96, CCC93, CCC98, CMG92, CB93b, CB94a, Cha92, CEP98, CD93, CBL95, Con92, CDC98, DHL+94, DBB94, Deu98b, DD98a, DD98b, Dun98, ESP98, EP98, Emc97, Enk97, ECI96, ET94, Fa97, FI97, FLLZ90, FNSV97, FLRV97, FS99, GKM90, GDID98, GPMML91, GJOV97, GJLA99, GZ98, GLBM96, GW98a, Gur99, Hag92, HMK99, JCA96, JDJP99, JPP87, KSKJ94, KPD93, KS94c, Kir95, KTK97, KL97b, KY91a, KY91b, Lan95, LBM94, LB98, LGT94, Löw90c, Löw91a, Löw91b, Löw92b, Löw92c, Löw92d, LZ92, Löw93a, Löw93b, Löw94b, LZ94, Löw95c, Löw95d, Löw95b, Löw96a, Löw96b]. Quantum [Löw99, MUL99, MKDL93, Mar99b, MHK95, Maz98, Mz97b, MZ99, MLT+96, MDS98, Mos98, NY98, NFVM94, NS95a, NS95b, Ney95a, Ney95b, Nic99, NV94a, NV94b, O'C96, Den97, PZ95, PS94a, Pop98, Pr95, RL94, RB95, RT99, RM99, Rid82, Rid88, Rid93, Rid99, RW99, Ry94, Ry99, S90a, SKJ98, SB95a, SB97a, SB98, SR93, SR02, SDE94, SN97, SMO+96, SS97a, SES93, Sfr97, SFGW96, TNM98, TTK99, Tch96b, Tch96a, Tob99, TSS97, VR95, VdV96, VBV92, Wn96a, Wl94, Wl95, Wl94, Zer99b, ZZ96, ZWPJ94, ZJ89, ZJ93, ZJ96, ZJ02, Ada94, Adl95, Ano90g, Ano90i, Ano96-31,
Ave89, BZ90, Bha99, BX94, BS91c, BSP98, Brä96b, Brä98b, BD95c, BMVV93, BV93, Cal90g, Cal90e, CDB99, CC92a, CC92b, Car96, Chr89, Coo05, CPW92.

quantum [DVJ93, DV96, Deu96, DD95, EC96, EVSN92, Fer91, FG96, FL95, GSN90, Gin91, GB90, GZ07, GZ06, GL96, HZ93, Hag94, Hag96, HW84, HW87a, HW87b, HW04, HL96, HZ91b, Hin88, JY94, Kar93, KC93, KJL96, KTC93, KH95, KH96c, KSH92, LMMK93, Lei99, LTSL96, LZ91, Löw91c, Löw91d, Löw91e, Löw92a, Löw95f, MD94, MD95, Mat96, MA99a, MB97b, MCB99, NPL90, NE95, NR97a, O95, OM91, Pan95, PS95, Pos91, PK92b, Qui02, RS00, Rey90, RSCP91, SPS96a, SHB+96, Sil95, SR99, SJ96, SMH92, Str91, Str92, TIA+92, TMA97, UBA92, WJC+98, Wen96b, WP95, YUSM99, CPW92, Löw91e, Löw95f, Löw95b, Ber96b, Kar93, Kla93, Kum93a, Sta90, Str92, Tay91, Wha96].

Quantum-Chemical [GJPMML91, GJLA99, VdV96, FLWZ90, HZ91b].

Quantum-Classical [GLBM96, JCÁ96, Ry99]. Quantum-Mechanical [GJ96].

quantum/classical [GL96].

Quartet [Jur99b].

Quartic [DBB94, MS97b, SB95a, Ta96b, AR92].

Quasi [CC91a, CJA94, Gin96a, GP94, JG95, KSY97, LP97c, LD94, MHM95b, NMCK92, SZL95, Spr96, ZYY95, BL92a, BMDM90, KSF91, LO93, MM95a, MM93, MRD92, Spr93].

Quasi-Degenerate [CJA94, JG95, LD94, MHM95b, KSF91, MM95a, MRD92].

Quasi-Energies [LP97c].

Quasi-Energy [KSY97].

Quasi-One-Dimensional [Gin96a, Spr96, ZYY95, BL92a, Spr93].

Quasi-particle [CC91a, BMDM90].

Quasi-Relativistic [NMCK92, SZL95].

Quasi-Spin [GP94].

quasi-symmetric [MM93].

quasidiabatic [Nob99].

Quasienergy [CJH98].

Quasiparticle [VCML90, Egu96, GNF90, ORt97].

Quasiperiodic [ANB96].

Quasispin [Vin92].

quaternionic [Adl95, Deu96].

quinoid [GJDD97].

quinone [MD94, MD95, Rey95].

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Quintet [BS92, BS94].

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R2R3 [JTZ+96].

rôle [GK90b].

Radial [KTT97, ST96a, Sim97, TZ97b, TN96].

Radiation [Brä98c, TNS+94, BK97, CH91, Hag99b, PS95, WA94, Deu97].

radiationless [SLS91].

radiations [WK90].

Radial [KTT97, ST96a, Sim97, TZ97b, TN96].

Radiation [Brä98c, TNS+94, BK97, CH91, Hag99b, PS95, WA94, Deu97].

radiationless [SLS91].

radiations [WK90].

Radial [KTT97, ST96a, Sim97, TZ97b, TN96].

Radiation [Brä98c, TNS+94, BK97, CH91, Hag99b, PS95, WA94, Deu97].

radiationless [SLS91].

radiations [WK90].

Radial [KTT97, ST96a, Sim97, TZ97b, TN96].
RBB+94, ZP92b, Mon94. **Raphson** [ZA95]. **Rapid** [Cul95, DV94, Ish96, MBV+98, JS91]. **Rare** [GD96, PP98a, GL96, KSK+99, MK90]. **Rare-Gas** [GD96, PP98a]. **ras** [YSJ94]. **Rate** [Chr94, Chr97, FF94a, Lu95, Ni97, RZ96, Sch93, Chr92, TFT+91]. **Rates** [LMR94, Oku98, DM97b, EBMS92, GS90a]. **Rational** [De 97, ZCT98, RSCP91]. **rational** [BH96]. **Ray** [˚AGL97, DC97, Mar98a, TNS+94, ACHT95, BKS97, DD96, GGHP94, WS94b, Brä98c]. **Rayleigh** [Ada91b, Ada96b, ´Ang93, Gin98]. **Rb** [KSW98]. **Reactant** [NOYY94]. **Reaction** [AT99, ADPS98, BCS96, CN94, CPA95, CF99, DZ94, FF94a, FF94b, FY95, FK98, FB96, Gre94, Jur98a, Jur99b, KTK+90, KO95, LMR94, LX95, MKK98, MB98, MD93a, Min94b, Oku98, PBB92, Pon97, Pra97, RZ96, RD97, RW92, Sak98, SKTN97, Sch99a, SPM+96, TKN96, TMP97, VdV96, VC92, XY95, YNST99, YTYS97, AM90a, AM90b, BA91, BH99, BHGC99, BP90, BS95, BYGA99, CLOFR98, CRsP93, CR96b, CB93b, Chr92, CMSF93, CE90, DGMW90, FF92, FF96, FEE+98, FNSV99, He95, HZ91b, JCS90, LJ90, LLM99, LAM91, LAM92, MBM92, Mat97, MRT95, MV92, Nag96, NOY98, NH90, OYNY98, STKN90, TKT+91, TFFF91, TP92, TF92, TMA97, UJS90, VR90, WJC+98, WJC96, XFD96, YSH97]. **Reaction-Field** [MB98, LKM99]. **Reactions** [ART94a, BPL97b, Bra97b, BZQ95, BK98, CR93, CCT98, DHL+94, GLBM96, Jen94, Jur97a, LL94a, LL97, MV98a, NOYY94, PMM97, Pon97, RC97, Sch93, WR96, ABSW95, BBSS96, BS91c, BCY95, CDB90, CWJ+99, ELMY96, EZ92, JK90, KK99b, LM91, LAM91, ML99, NOY92, OS90, PB95b, PHBB94, RK91, SLG+96, TLTL92, TUK90, WY99, WY95, WP92, WZ96, ZM90, Deu98a]. **Reactive** [KEG+97, HS95, LGBL94, Nal98]. **Reactivities** [RL94]. **Reactivity** [ET99, FSF96, MV98a, Mon93, MM95, Nal95a, Nal97, TKN96, Tch96a, WDC97, BBB+95, Cas91, FS99, GRTR96, MCA92, PS92b, RFF90, Yu95, An92]. **Reagent** [LX95]. **Reagents** [OSA+97]. **réaction** [GK90b]. **Real** [Bad94, Bec97b, BBS+97, BP93c, BP95, NV94a, NV94b, ZW96a, BOL+90, BP93b, BRV90, BW90, NV97a, NZ92, YB99]. **Real-Space** [Bec97b, BBS+97, BP95, NV94a, NV94b, NV97a]. **realistic** [BL91]. **Reality** [CG97b]. **realization** [LP92, SN99]. **Rearrangement** [KW92, Mic94, PRB96]. **received** [An98a, Zer98a]. **recently** [Csa90a, Csa91]. **Receptor** [GJLA99, MTD93, PW97, ARBB95, Bla99, CML92, CPGC99, FMS+99, GHH+99, PVM+93, VL91, WD91]. **receptor-bioligand** [CPGC99]. **receptor-G** [FMS+99]. **Receptors** [GJOV97, PW97, GVV+90]. **Reciprocal** [TSP97, BBLK94]. **Recognition** [Mar95c, BD9+92, FV9+90, DZ92b, PV9+93, Rig92]. **Recollections** [Hal99]. **recombination** [GL96, LM91]. **Reconciliation** [KLI92]. **Rectifier** [MBV+98]. **Recurrence** [AM98b, FS93b, Kt93, Pa97a, Ka91]. **Recursion** [LDP93, DW90, MGLB95]. **Recursive** [Mik94]. **redistribution** [TP92]. **Redox** [BDH+97, CDBKZ99, WWFR99]. **redox-active** [WWFR99].
Redshifts [Her93a, Her93b]. Reduced
[CYY95, DQB97, Fer96, MPKR94, Maz98, Mor93b, PRTV97, Sam97, VDBPR97a, YNT98, BCD91, Hud99, Kat91, Kat98a, Kov90b, KPM+90, KG98, MHN98, Sim99c, VDBPR97b, YNST99]. Reduction
[BP92b, FBKD97b, ZW96b, GWB97, MD94, MD95, PBBH93, WSW96]. Redundancy
[CYY95, DQB97, Fer96, MPKR94, Maz98, Mor93b, PRTV97, Sam97, VDBPR97a, YNT98, BCD91, Hud99, Kat91, Kat98a, Kov90b, KPM+90, KG98, MHN98, Sim99c, VDBPR97b, YNST99]. Reduction
[BP92b, FBKD97b, ZW96b, GWB97, MD94, MD95, PBBH93, WSW96]. Redundancy
[Sta91]. Reference
[GR95b, JKJ94, JKJ95, JKRW98, MCM98, Nal97, NU95, PPP97, LP93, WB94, ZP90, GR96b, HFM91]. Reflecting
[Nal97]. Reflections
[Hal99]. Reflective
[GSPSM93]. Regime
[TMM97]. Regimes
[CSG99]. Region
[AP93, NMN+97, NMN+98, KL93a, VRR92, VS95]. Regional
[GSM90, Tac96, Zou92, GS92a, TNSM99]. Regions
[CW97, MPR97, WP93, GK90b, GK90a]. Regular
[Cal00a, LNT99, vvBS96, NYKY98]. Reimann
[BDZ94]. Riedel
[Cal90c, Cal90a]. Reinterpretation
[Sah95a]. Related
[BHPB95, DZB92a, FT95, KM92, LEA+94, Mez97a, MFAT98, MK99, PBB92, RHHR94, TVP93, FT96, FT97a, FEE+98, FLWZ90, FLLZ91, Gal98, JY94, KTCN93, LSS96, LW92, MEP90, Na92a, PAC90, RC92a, Tom91]. Relating
[JDB99]. Relation
[AMKS93, Aon98, Coo94, JBT+95, Mar98a, See97, WTS97, AMH+92, Kat91, MS91, Mar94c, MNT96, Mar99a, MBP91, PMS94]. Relations
[DM92, FS93b, HM97a, Kat93, Kin99, LG99a, Pa97a, BS91a, CSH99, DW90, GSM90, GS92a, GS92b, NM92, Sch92c]. Relationship
[GG97a, HSS+95, Mon98, RF94, SM94]. Relationships
[BMP93, GJ97b, BTKVG97, HB94, Khu92, KMB92]. Relative
[BB9+95, HPSC97, KSN95, WR96, AGA97, BKEMM94, BDFS97, Jur99d, MSRP90, Zha91]. Relativistic
[AO93, AAS93, Boc96, Boe98, BJJK98, Del98, EKI94, FBKD97a, FBKD97b, FBKD97c, Flo97a, HCRR94, Ish92, IK97, KS98, KLT97, LMK93, LBM94, LKB97, LLZ98, Lin96b, MDS95, Mey94, Mey97, ML97, NKUS97, NG96, NCM92, PG94, RP98b, SZL95, SZ97a, SRW96, SB90, SM95, SO97, WS92, XKB+99, vvBS96, BSS97a, BC97b, Boe90, Boe97, Bro95b, BL95, ERC91, Flo97b, Ish91, KLO+98, SN99, TM99, VAVN91, WP91, Boe90, EKI94]. Relativistically
[Loh91]. Relativity
[DN96]. Relaxation
[GH96a, Her98, TD96a, ACL96, Sim99a, Sim99b]. Relaxed
[CF94b, relaYr90]. release
[SH94]. Relevant
[RL94, VDBPR97a, VDBPR97b, BH99, SJ91]. reliability
[MVS97]. Reliable
[MK90, VCCM92, FG99, RCB+99]. remark
[Ber96a]. Remarks
[GL94, Ino96, Loe93d, Kys90, Loe90d]. Reminiscences
[McW96, Pau97, Mat92]. Removal
[vYMvL97, AM93]. Renner
[Pet92]. Renormalization
[Her96, KSH94, BK95, CDG04, KUM93b, SME92]. Renormalized
[Ort91, RDF98, ZDO99, Ada96a]. Reorganization
[BZQ95, BD+97, LRM96, MB98, FON97, BCY95]. Reorientation
[HHP99]. Replacements
[NK96a]. Report
[FG96, Har97a]. reports
[Lun91]. Representability
[Mor93b, Sam97, Har90]. Representable
CC95, SFM94, CCWCF96, KLM91, KL92a. **Representation**

[CBC94, KSG93, KBT94, KKE96, KO95, KMM96, OLC96, Ryl99, VJ95, VJ97, WM92, Wk94, WZ94, AS95, AH92a, BRV90, CC92a, CC92b, CEd94, HCC93, KBB90, KH95, MM91, MPSLB91, Na91, Na92c, RCB99, Sh90c].

**Representations** [CB95, FL97a, LKLBD98, PZW93, RP96, SAR96, Wk95, WFK97, Fl97b, DJ12]. **Representative** [ART94a, BF95]. **Representing** [AFT95a, AFTM95b, AFO97, AFTM98, AFZ99]. **repressor** [KRRB99]. **reproduce** [GKV99, GV92]. **Repulsion** [Che93, FS93b, Ish96, US97, GJP91, MT90b, MHS95, MFCA93, SH90b, TN96]. **requirement** [OYL91]. **requirements** [CML92, Iva96, Iva97, WI98]. **Requisites** [Jou97]. **Research** [Kar93, Kas99, BTKVG99, Cle92a, GZ97, GZ06]. **Resemblance** [Löw93d, SC96]. **Reservoir** [Del96]. **Residue** [Mik94, NK96a, LS99]. **Residues** [SK98, BOL90]. **Resistance** [LNT99, BBLK94, MD93b]. **Resolution** [AFTM95a, AFTM95b, AFO97, AFTM98, LVL93, AFZ99, TWWC91, WO92]. **Resolutions** [BG95]. **Resolved** [GWCT97, LM91, Na92b, NM92, PL91, YCML91]. **Resonance** [BT95, IK94, KLT97, Mio97, Ran97, RG99, SSP98, AS99, BW90, Eng92, Hags99b, HBGR99, MCT99, Me91, MM94, WO92]. **Resonance-Stabilized** [SSP98]. **Resonances** [BR97, Brä93a, PE993, Sim97, And93a, HS99, MM94, MTTS93, ZZW94]. **Resonant** [RG96]. **respect** [YG90]. **Response** [CDDM96, CJH98, CB94b, Gho95, Hag98, JBT95, Jas94, KK94, LG95b, LNN98, Na97, NS93b, PP95, PO97, SV95, TCM98, BBS91, CT95, DB94b, Eg96, Hag96, KMR92, Kic97, KK91, KY95, LKM99, MCT99, Pal92a, PSO90, Par92b, Par92, Ra92, SM99]. **restraining** [KS95a]. **Restricted** [AB97, GT93, JEB92, Kol97, Nu95, SE97, SBIP97b, VDL95]. **Restrictions** [PS96, W199b]. **Results** [AOH96, CR96a, Dat95, KP97, KWT95, Pra97, SBM97, TV92, BF92, KY91b, LG96, OS90, OS92, PC92, RDY95, UBA92]. **retards** [TW90, TW92]. **Retrospective** [KK92b]. **Returning** [BM93]. **revealed** [AS99, ITT94]. **Reversal** [Mey94, Mey97]. **Reverse** [ZL99, DZ92b]. **reversed** [BS91b]. **Reversible** [SCMF93, BMFP92, KL93a]. **Review** [Ägr90, Ano92a, Ano92b, Ano92c, Ano93g, Ano93h, Ber96b, Brä95, Brä96b, Brä96c, Brä98a, Brä98c, Ca90g, Ca90d, Ca90f, Ca90c, Ca90e, Ca90b, Ca90a, Ca93, Car96, Deu96, Deu98a, Dun96b, Eri92, Gre98, Jen99, Jer92, Kar93, Kar96, Kla96, Kra96, Kurn93b, Kurn93a, Lin93, Lin96a, Lin91, Lin92, M1at97, Mic96a, Mic97, Mon93, Mon94, Deu97, Sjö96, Sta90, Sta93, Str91, Str92, Str93, Tay91, Tri96, Woa96, Zer99b, Deu98b, Mic99, Mon99a, Mon99b, RKS99, Tri99, Zer99a, Deu99, Pan99, Jer92]. **revised** [MSMR99]. **Revision** [TGS99]. **Revisited** [GR94, JK94, KTT97, MM95b, C93, DT96, PL93]. **Revisiting** [CEM96]. **Rh** [NG95, SM96a, SC99, EZ92, EZ93]. **RHF** [BE98, FDF96, FMD96, FDF98, FADAC90, GJDD97, RT98]. **rhodium** [CCC95b]. **RI** [FKHD97]. **ribbon** [NMSJ99]. **Rich** [WZW96]. **Ridley**
[Sta90]. Right [PFMC97]. Right- [PFMC97]. rigid 
[FKR92, KY91a, KY91b, WLB+94]. rigidified [Tho96]. Rigorous 
[Cio93, The98, Geg91a, Geg91b, RPY95, KY91a]. Rigorous [Kry93]. Ring 
[ACP98, Bla96, JZ95b, KVMÅ95, LN96, MZ93, MK99, MJS93, RMP98, 
SF96, BJM+94, CAM+97, DD90b, KLW92, LAM91, MMCC99, Yu95]. 
Ring-Opened [KVMÅ95]. ring-opening [CAM+97]. Ring-Shaped 
[Bla96, LN96, KLW92]. Rings [BT95, GBL97, Tri98c, DV99, Les92, Ran95]. 
Rn [HBL99, MTL97, RP98b]. RNA [PS99]. RNase [KW98]. RnXe 
[RPM98b]. RO [BHGC99]. Robert 
[Deu98a, Mic97, Ano90z, Ano94i, Ano94-37]. Robust [Dav98]. ROHF 
[LG96, LBG97]. Role [BP96a, DL92, GDID98, GRFR94, LRM98, Li97, LZ94, 
Mar94d, Min96, PFMC97, Sak97, SM98, SC94, SH96, Cas97, CMSF93, DV91, 
MS94, PTM92, RC92a, SBZ92a, SB92b, LBBK91, LSGS91]. Roothaan 
[CC97a, GRT96, KMP+90, Mar93a]. Rostoker [Fau92]. rotamers 
[WBH90]. Rotating [Loh96]. Rotation [BW99, Bue96, Che97, PO97, VJ97, 
Aon99, BVF94, CTF92, Gx98, MJLL99, ST91, TS92, WFS93, YX96]. 
Rotation-Vibration [VJ97]. Rotational 
[AST93, GH99, HMGP93, Jou97, LKMCVT96, RBT99, YLD97, MIW91]. 
Rotationally [GYD97, CF93, She90d]. Rotations 
[Pal97b, BRV90, CLZ99, HRRBL97, LÖw92a]. route [CB99]. Routes 
[PSCZ97]. Rouvary [Mon93]. Rouvray [Ano92k]. Rovibrational 
[XY98, FV96, PVC+90]. Rovibronic [YLLJ96]. Row 
[BA97a, Can97, Dat95, DLG95, DKM97, Jur97d, KJ93, PDT97, Ros96, 
WFK97, YDFS98, ACZ91, Bro96, DS90, JF92, Lon99]. Roy [CS96b]. RP 
[FG99]. RPA [GARC97, PP95, Per93]. RPA-AM1 [GARC97]. Rps 
[CMSF93]. Ru [SBIP97b]. Ruben [Zer99b]. rubredoxins [SZ95]. Rudolf 
[Ano90y]. Rudolph [Ano90-27, Ano90-28]. Rule 
[PKM93, A99, Gut99a, MPP+97, Nor91, Par99, Le99]. Rules 
[AMH93, Kat97, DD97b, She90a, SR99, SS92g, VV91]. Rumor 
[KRZ91, LP92, SA96]. RuO [NS91]. rupturing [CR96b]. Ruthenium 
[BC97a, SBIP97a]. Rutile [RHC96, Bre99, HSSL92]. Rydberg 
[CBT93a, KSK+99, MBG90, MKDL93, MCL95, RL98, TGS99]. 
Rydberg-like [CBT93a]. Rydberg-valence [TGS99]. Rys [SS92a]. 
S [Ano92l, Ano92-45, Ano92-44, Ano93h, BUZ94, Ber96b, BP93b, BCY95, 
BZ95, Crs93, Cze99, JH90, Mon94, MNC95, Deu97, RNS93, SES93, 
TIPM96, BRL92, BP93b, BGS98, CG97b, GS90b, HJ94, HS92b, HZ99, JL91, 
JH90, KRZ91, LC93, LK94, Man99, SP92a, VG90, WBD97, WY99, ZGPS97]. 
S-2-disisopropylaminoethylmethylphosphonothiolate [HJ94]. 
S-containing [LC93]. S-Type [BGS98, JL91]. SA [BBS91]. SAC [NS91]. 
Sachs [HK97]. Saddle [Mar92a, Smi90]. Saddle-point [Mar92a]. Sahni 
[SS92b]. salicylaldehyde [CSH99]. Salt [LX95, MKK98]. salts 
[PBBH93, Sta98d]. Salvetti [FGM90, Mor93b]. Same [GIA96, Sta98a]. 
Sample [VM92]. Sampled [BBC+96b]. Sampling [CDC98]. Sanibel
Second-derivative [Sem96b].
Second-harmonic [Lev94].
Second-Neighboring [Gin97]. Second-Order [ASP97, AR93, CV94, CB94b, DB94a, FR93b, KSY97, KD95, Mor93b, Ort98b, Sam97, Sim93b, SP94, SATP94, TFYY91, TRP99, VVS94, VIK98, YNY99, YNNY99, ZM95, Ada91a, Ada91b, ACZ91, BP92a, BP93b, BCD91, Bro96, CPA98, CP99a, Cin96, DS90, DBF92, FT96, GFS92, JF92, KMR92, KLO98, Kor90, LYS95, Lev94, NYNY99, Nor91, Sem96b, Str93, VAJ92, VCML90, WKP95, ZC99].
Second-Row [DLG95, Jur97d, KJ93, PDT97, ACZ91, Bro96, DS90, JF92].
Section [CM96a, CHMA95, CCS98]. Sections [RH96b, SLD95, WS94b, KSW98, SK99a, WM92]. Sectors [HK95b]. Secular [Gin96a, Gin96b], Sediments [ML97]. see [TD99]. Selected [MC94, WN90, UBA92]. Selection [RPJZW96, Par99]. Selective [BF96, GBS93b, GWB97, MM99b, VL91]. selectivity [Bla99, KO91]. Self [AGNS92, AR96, BG95, BKM93, BZQ95, CV94, CM94, CE90, DM94a, DTM96, Fer96, Huz96, KSKJ94, KNNY99, Kok97, KE93, MHN98, MB98, MRT95, Pan93, RM99, Sch95e, SG98, SMO+96, Ste96, TKMA92, VVS94, VFBP96, Wlo94, Wlo95, BBS91, BZMR92, BHGC99, BCY95, Con92, FCMB99, FEE+98, FNSV99, GRTR96, Ish90, KL92a, MC91a, MC91b, Moh92, NSTM84, TC98e, TD03, ZWD98b]. Self-adjoint [KE93].
Self-Trapping [KSKJ94]. Semiclassical [DPP+94, Her98, Mar94a, SG98, Sie93, YLD97].

Semiconductor [Mar97a]. Semiconductor
[DKBB97, Kox98a, LRM97, SD98, Bat92, GDF92].
Semiconductor-Insulator [Kov98a]. Semiconductor-Metal [LRM97].
Semidirect [ZO94, ZO95]. Semiempirical [BBD97, BLRD92, BL92b, BS95].
SPC96, SR96, Was96, BFP93, BG98b, BG98c, HVS98, KMP+90, KM90b, KF96, KS90, LP98, MHG95, MC91a, MC91b, Moh92, MCB99, Pal92a, PMDM97, PZDM97, PMDM98, PZDM98, VDL95, YOT93, ZY90.

**shell-structure** [BFP93]. **Sheells** [KPTS97, PAT93]. **Sheppard** [DQB97].

**Shepard-Type** [DQB97]. **Shevelko** [Br¨a98a, Br¨a98c].

**Shepard-Type** [DQB97]. **Shevelko** [Br¨a98a, Br¨a98c].

**Shielding** [SZ96, SZ97a, GR95a, GS97b, KH96a, RN96, Tos95].

**Shift** [BDT96, Sim98, BZ92, BJMK92, BG98c, FNSV99, KFK91, XSA+92].

**Shifting** [RS98, CA90b].

**Shifting** [Mon98, NN94, PRC98, See97, Sim97, TMP97, BRS95, DO90, VG90].

**Shiotani** [Lun92].

**Shock** [KDHW90, TBW90].

**shocked** [SCP95].

**Shopping** [PB96].

**Short** [GVB97, CLC90, Per93].

**Short-Range** [GVB97, Per93].

**Silicon** [DBG92, DJF98, HU94, LV98, Mar97a, PB97a, TIPM96, Tri97, Boe96, GKM90, KPW+95, MD92a, PDO92, SBL+94, Suh93].

**Silica** [NNMH96].

**Silicon-based** [Suh93].

**Silole** [YY96].

**Silver** [KSN95].

**Silverman** [Sj¨o96].

**Similar** [MRL99].

**Similarity** [HM97a, Mez97b, MFAT98, SMO+96, SP94, AM90b, BBSS96, CC92a, CC92b, CC91b, Kn93, LM92, LAM92, MM99a, Mez94b, PS92b].

**Simon** [Lin93].

**Simple** [CCE+93, Hoo94, Iva96, May97, PPP97, PZW93, PP98b, RC97, ROL+90, Ros96, Sch99b, TSY99, US96, ZWP99, ZZCSE94, Ada94, AI99, BE93, Bra¨96b, GSPS93, Ken93, LLL91, PT99, PA99, YTY91, Iva97].

**Simplified** [HWS92, KLL97, SPF96, Cio91, DCK92].

**Simulate** [GBVM93].

**Simulated** [BLRD92, MT96, IB95, JH90, KI94].

**Simulating** [CL92].

**Simulation** [BBC+94, BPL97a, CGS+94, DHL+94, Jud96, LMC97b, LL94a, MKM93a, OMT97, PW97, SW97, BK92, Cor92, FG96, GGHP94, Jak93, Kid99, Mar97c, MR92a, NH90, OT91, PLB99, SCP95, TW90, TW92].


**Simultaneous** [TTM99].

**Simultaneously** [KM92].

**Sinanoglu** [She90a].

**Sinc** [KH96c].

**SINDO1** [JAG95].

**Single** [BR94, Cio91, GM94, Hag99b, JKJ94, JKJ95, JKRW98, KP93, KSK91, KSW98, Le97, Lev97, PPP97, Ada91a, BMA90, CS99, IHG95, LP93, MHG95, NS92, PK92a, SK99a, SD91, PMDM97, PMDM98].

**Single-active** [KSK91].

**single-bonded** [CS99].

**Single-Center** [BR94].

**Single-Cycle** [KP93, PK92a].

**Single-density** [PMDM97, PMDM98].

**single-electron** [BMA90, SK99a].

**Single-electron-capture** [KSW98].
Solutés [CCM⁺96]. Solution [AM97, Bec97b, BD94a, BD94b, Bra97a, CCT98, CV94, DZF93, Eid99, FD96b, Gin98, GH99, JI95, NOYY94, Nic96, Rod91, Ste96, Taş96b, WR96, AGAP98, AMF99, AMH⁺92, BD95b, BPVP92, CAM⁺97, CP92, CTC95, DV91, ESHP99, FG96, Gegg91a, Geg91b, Hag92, HB95, NOY98, New97, OYNY98, OM91, PP91, RBB⁺94, SWK90, Sim99c, TK9⁺92, TTOY93, Tom91, WO92].

Solutions [BDNT97, EDF⁺98, JM93a, JKJ94, JKJ95, Sad97, YO92, Ada90, Brä95, BMA99, CDB90, FC99, Hal93, JM96a, JGKM99, JGP91, KS92, Oz92].

Solvation [Cas91, EBMS92, OLC⁺96, PTH⁺97, RPB⁺95, AMH⁺92, CT95, CA91, FM92a, KH90, STZ96, TFT⁺91, TLTL92, TNS96]. Solvatochromism [CD⁺99, DV96]. Solved [Löw94c]. Solvent [AL95, BDZ94, CPA95, CCZ97, CDC98, Gao93, GSM98, Jug90a, MAK⁺91, MB98, MR97, NP96b, OLC⁺96, PCE95, SAFK97, SM92b, FKR92, GPMML91, MRB⁺96, MRT95, MT91, PZTPMC99, RCB⁺99, SCA93, Tom91]. Solver [RW98].

Solving [CM94, Gin96a, Hag98, IK94, MS97b, TZ97b, Fan90, Hag95, JK92b, Sme92, Kh96c]. Some [AEAO99, BP92b, BF94, BPL94, Bra96a, Brä93b, BDD93, BK94c, BMG⁺98, CL97, CDB99, Che97, CSS93, EMMK94, Ek94, FSBS⁺95, GL94, Hal93, HAEMA92, Hom93, Hsu99, Jur97d, LLL92, Löw91c, Löw93c, Löw93d, Löw94c, Löw97b, LJN⁺98, Mar97b, McW96, MK93b, MK96, PBB92, PSC97, RC97, SSK⁺92, SM96b, Sch92a, SC97, Sha95, SS97a, Spr93, TKNI96, TBB98, TSS97, UWB94, ZJS99, ZZZY96, AHM97, BS91a, BBS90, BE93, Bha99, DBM99, FLL91, FH95, GFS92, HBG99, Kan93, KR91, Khan2, Kin99, KY92, KM92, LLY92, Li92, Löw92b, LE92, MCOS94, MS90, MEP90, MRP90, OS90, Par99, PHBB92, PBH95, PG95, RAM91, SM94, SJ97, TCZ91, TG96, W91, K91, RDY95].

MK97b, NV97b, Par97, PÅS+97, SAFK97, SBIP97a, SBIP97b, STM96a, TL98, TZCT97, TT98, TDO97, YXX99, YLLJ96, ZJS99, AEHM91, AHM97, CB96a, DHDP92, DD96, DM98, FLHT90, FLWZ90, FLLZ91, FHHE90, FL95, GX95, HS99, HS95, Kar90, Kha92, KLC98b, MKBP97, NAJ91, NAJ92, NVR+91, OSS95, PVF+92, PLBB99, RCWN94, SE92, SJ97, SZ95, TLC98, TST+99, TFSZ95, TBP99, WK+95, WBS99, YJL92, ZFZ92].

Spectral [AT93, AFTM95a, AFTM95b, AFO+97, AFTM98, BG95, FJI97, Gij96b, KBWJ96, RPKM95, TFP+97, AF+99, CA92a, DB93, DOPS91, S890b, LMV92, Lin91].

Spectrometric [MG93a].

Spectroscopic [BS94, CWZ98b, DFlb90, Gal96, GMR+93, MCOS94, MRST95, WBS99, ZH99b, Brã98a, Dù96b, LG92, LM95, MSS99a, OS91, She97, SSM90, SZ97b, Sut99b, RC92b].

Spectroscopical [BPL94].

Spectroscopies [TN96, Agr91].

Spectroscopy [CSZ97, EB97, FWT+96, GDID98, KPD93, KW98, Sta93, Sul97, Ano93g, BBZ91, G9k2, KM90a, McH91, Muk92, T9K+90, W902, YCML91].

Spectrum [BJ98, CCZ97, DZ96a, KLT97, MDD93, Nic99, Tas93, Tas96a, Zit94, BDZ94, G9eg91b, KL92b, NE95, Ort97, RSCP91, SP92a, Sme92, SZ97b, SCC91, V9X99, VCEL90].

speculation [Tr98c].

speech [Rig92].

Sphere [BZQ95, BDH+97, RH96a, SD97, BCY95, HFM91, MFH91, ZBL99].

Spherical [A995, FS93b, HR97, J9on94, SF95b, A.95, Brã98a, D9w92, YCMLL90].

Spherically [SAW97].

Spheroidal [BPL94].

Spin [AO93, BH96, B9e93, Bra96a, B9S94, C9CC93, CDDM96, C9e93, C9T96, C9S97, EE9L97, FBKD97b, FBD97c, F9ko97a, FWC+93, FJR96, G9R4, G9L99, GVC96, G9Pe94, HBL99, I9g98, JFP95, K9SG93, KFS92, KBJ96, KPR97, KS95b, K9MV95, L9w96c, M9PK94, M9T96, M9CM98, M9A96, M9A99b, NM+97, N9g94, N9U95, O9Li99, PM93, Pen93, Pen96, PB997, PTV97, PG96, P9TP95, P9W91, P9GH95, PSS97, R9SG96, R9F99, RPKM95, R9P96, RL92, S9FG+98, SZ97b, S9ur97, T9D96a, T9D96b, V9DBP97a, W9M+98, A999, B9G98b, B9G98c, B9G98d, C9e92, C9EZ+99, C9e99, D9W90, D9RG99, E9RC91, Fl9ob7, J9R+99, K9S92, KLO+98, K9R91, KL92, L9P93, L9w92h, L9BC97, Man95a, Man95b, Man99, Mar99a, M9HY98, M9M99b, M9D99, M9W90a, M9NC95, O9C99, P9A9US90, Per93, Pet92, R9BT99, R9GO94, SG9K9].

spin [Sir99, TSY99, TFR99, Tit92, V9AJ+92, V9DBP97b, WS92, W9It99b, LF97d].

Spin- [BHX96].

Spin-Adapted [C9D9M96, JFP95, KPR97, M9PK94, N9U95, PTV97, P9TP95, RPKM95, V9DBP97a, J9RS+99, L9P93, M9D99, V9DBP97b].

Spin-averaged [SZ97b].

Spin-Catalysis [MA96].


Spin-Dependent [F9K97c].

spin-extended [MW90a].

Spin-Free [WWW+98, FJR96, M9a96].

Spin-Independent [K9S92].

Spin-Mediated [NM+97].

Spin-multiplet [PG96].

Spin-Orbit [HBL99, K9M9A95, RL92, S9FG+98, PW91, B9G98b, B9G98c, B9G98d, E9RC91, J9RS+99, KLO+98, K9R91, Man95a, Man95b, Man99, TSY99, Tit92].

Spin-Paired [K9G93].

Spin-Polarized [B9e93, B9S94, G9R4, KL92].
Spin-Projected [Iga95]. Spin-Spin [AO93, DRGC90]. Spin-Unrestricted [CCC93, PGH95].
spionaphthoxazines [MRRA92]. Spline [DLV95, FGS92, DBLV94]. split [Sta98d]. Splitting
[PM95, She90d, CB96a, KBBK90, ROL+90, She90c, SC98b, PL91]. Splittings [STM96a]. sponsored [Biz94]. Spontaneous [SW97].
spontaneously [RVF92]. spore [HB94]. Springer
[Brä95, Brä96b, Brä96c, Car96, Dun96b, Sjö96, Str91]. Springer-Verlag
[Brä95, Brä96b, Car96, Dun96b, Sjö96, Str91]. Square
[HM97a, NG95, WM92], Square-Cell [HM97a, WM92]. Square-Pyramidal
[NG95]. Squared [MSRSP93]. Squares [BBC+95b, DBLV94]. Squeezed
[MSRSP93, Pal97a, PSM94]. Squeezing [Fan90]. SSCH [SLL+91]. SSH
[SSL+91]. ST [PTP95], Stabilities [RGHH94, KP96]. Stability
[Boe98, BMG95, CAJ95, GD96, HU94, KSN95, LN96, PHBB94, RKG96, SL93, SM98, YNMT98, AS99, AGA98, BREMM94, CPF91, Cio93, FAV92, LaF90, LAM92, MW90b, Moc99, PBB95, SPR94, TFO92, WYZ+92].
Stabilization [HP98, BB93, BHGC99, LRM98, YAD92]. Stabilized
[SSP98, VBF95, BF93, VFBP96]. Stabilizing [PFC97]. Stable
[Can97, FT95, Hag98, HOS95, LAS93, Su93, FT96]. stacked
[Sta98b, She90c]. stacked [CEZ+99]. Stacking [MAI95]. Stages
[Hoo94, SL93]. staggered [Pal94]. Standard
[DRBE96, She91, ZL98, DBF+92, MD94, MD95, VCCM92]. Stands [SL93].
Stark [ABDM94, HHHP99]. starting [AA92]. State
[ABBB93, Ale95, BF96, BEG94, BLB95, BK94b, Bra97a, CSL94, CGLP96, CAJ95, DTA+96, DLV95, DMB97, FSBS+95,Fri93b, GFRR94, JKR98, JMR98, KA95a, KMM96, LCL95, LZ92, Mar98b, MM99b, MTD93, NYY+96, Na94, Nic96, N93b, Pan93, RS94, RW92, SE95a, SIM93a, SGGMGFS96, SD97, TBCP95, TT98, WT98, ARDP92, Ano90g, Ano90i, BBSS96, BBS91, BRL92, BP93b, Boe95, BSS+97b, BMA99, CCS98, CEZ+99, DDC97, EJ93, FV96, GH96b, G91, Gut99b, HR99, KA96, KSW98, KSK+99, K90, KB99, LKM99, LZ91, LS93b, MUL99, MG97, MLB92, MHM95a, MB93, MW90a, NM91, New97, NOS94, OYY98, Ort93, PY92, PFK99, RR95, RA96, RK92, SK99a, SM92a, SKC99, SE95b, SW95, SSM90, STM96b, SN99, TWH98, TG96, Tri98c, TNS92, UJS90]. state
[VX99, WI96, WW97, YTTY93, ZA95]. state-averaged [BBS91].
State-Selective [BF96, MM99b]. State-Specific [Nic96]. State-Universal
[JM98]. States [ART94a, BKL97, BLK97, Bec97a, BR97, BC96b, BS94, BGS98, CX93, Cai93, Cai94, CBT93a, CLZ95, CLSI94, CR96a, DTA+96, DD97a, Dan94, FSBS+95, FS95c, Gre94, GSJS97, HHKM95, HML98, Jac97, JM95, JK95, JG95, Kan93, KBGE97, KS95b, KN99b, K98a, MSRSP93, MM95b, MB98, MR92b, MR94, Nag95a, Nam98a, Nag98b, NMP94, Nic96, NK98, Nie99, Nii94b, Pal97a, PS93, PCC93, RDF98, RL98, RSD97, Sch98, SC97, SC98b, SG93, Sim93b, SGB98, Sza95,
TPR96, TG95, The97, The98, TC98b, TCM98, TD96b, VJ95, VJ97, VZ93, WS95, WD97, WBD97, Was96, BGS99, BOL+90, Bar90, BFRN90, BS92, BFV+93, Camb92, CBT93b, CWZ98b, CLZ99, Cede94, CB99, CC91b, Cio91, DDC95, DWM90, FKK92, GDS99, HC93]. states [IHG95, Jac98, JKGM99, KP92, KD92, KN99a, xLTY92, LK94, MCOS94, MH95, MLL99, MV90, MAAP90, MPP92, MDM94, MSS99b, NS91, NNH98, Nob99, NAJ91, NAJ92, N94, OMK90, ORt91, PVČ+90, PSM94, PZ91, RVP92, RB93, Roc99, REKP92, SE93a, SHB+96, SPFL93, SFD+99, ST97, SC92, SRR90, TGS99, Wil90]. Static [ABDM94, BA97b, CZ94b, Gho95, JCA97, MFP96, Ols96, SS92b, SB95a, SO94, Voj96, CP99a, DBF+92, DB94b, MFC94, MCA95b, Pal92a, MCB99].

Stationary [AL95, AMKS93, AB97, BLB95, BLRD92, Gho95, KPA95, BA92, HC93].

Statistical [AB97, CAK+96, DCD95, DDP96, ST96a, DD99, FNSV99, STS95, Tit96, TSS95].

Stephen [Deu96].

Step [AB97, CAK+96, DCD95, DDP96, ST96a, DD99, FNSV99, STS95, Tit96, TSS95].

Stepwise [Fir94].

Stepwise [Fir94].

Strain [LS96, LMAK93, DD90b].

strained-layer [MW92, MSPS90, Tri98c].

strained [MW92].

Strativated [CV98].

stratospheric [BH90].

Strategic [Avi92].

Strategies [Enk97, Sae92, SN90a].

Strategy [CTG97, Jon97, WWM98].

Strengthened [DS93].

stretching [DS93].

strictly [Sur94].

String [TFT+91, TFYY91].

Stripped [DD98b].

strips [Dia99].

Strong [Che93, FU197, KL97a, Pal95, RS94, RS97a, Sch97, SC97, Sch98, KCP90, SC91, BMDM90].

Strongly [CM98, BOL+90, Che92, Mar94c, PCP92].

Structural [Ali99, Ana96-58, AFTM95a, AFTM95b, AF97, AFTM98, AF97, Bae98, BJA99, CML92, DS96, DJF98, GV+90, JL95, KBA96, KEMM93, LL99, MPSF97, PCF94, Suh92, ZYY95, ZC95, AM90b, Cas97, CZ94a, CCS99, DFGB99, FDC92, HGL99, JMF99, KPW+95, MEP90, PAC090, RA91, RBB+94, Sn92, TTO93].

Structure [AL95, ATP+96, AH97, ALRP96, BKWL97, BS91b, Bec97a, BBS+97,
BTN98, BFH96, BCD95, BS94, BJL98, BK94c, CCC+95a, CAK+96, CXL97, CFMR96, Che93, CCT98, Cio94, CG96, CM94, CSZ97, CF96, DZB92a, DWB98, DL92, EDF+98, FFD98, GP95, GD96, Gin95, GV93, GJOV97, GJLA99, GvLB96, GP97, GLLY94, HNB92, HL93b, IAN+94, Ino96, Kan93, KGC+96, KEG+97, Khu92, KM97, KS96, KGVM97, KG97, KG99, KL97c, LB96a, LMC97a, LRM96, LY98, Les91, LEG+94, MRL99, MVV+97, MW90b, MK97b, MK98a, MC95, Mor96c, Mor97b, Mor98a, NvM+98, NAK95, Nic96, NC95, NS97b, PW97, PV93, P94a, P96, QS98, RHC96, RW98, RKE95, RKG96, Sah95b, SD96a, SC98a, SST93, SBIP97a, SS97b, SA+94, SG97, SGB97, SC95, SPR94, Sz99, TWK98. **Structure**

[TH97, TIPM96, VR95, VR92, VHFL93, Wil96, Xu96, YN99, YK97, ZL98, ZY94, ZM96, ZR97, Agr90, ANB94, Ano92j, BTKVG99, BL92a, BILA95, BUZ94, BBZ91, Ber96b, BJM+94, Boe93, BFP93, Bro95a, VD90, Cal90d, Cal90e, Cas91, CJX+92, Co92, Csi82, DR92, DD92, DS95a, FLW90, FLL91, FMD+94, FKR92, FS99, Gal98, GK92, GS91, GL92, GDB98, Gur99, GH92, Gth99b, HS93, HB94, Iac92, JDB99, JMS95, KK99a, KTK+90, KH90, KJL96, KW98, KT95, Kov90a, Kov90b, KG98, KMB92, KL92b, LMC97b, Lan95, Lip91a, Lip91b, LDF99, LT92, Mak87, MW92, ML992, MM99, MS93a, MB92, Min98, MK96, METH94, Muk92, NSS92, NMS99, Nor91, OTS+95, PTM92, Rat92, RRC94, RE92, RK91, RCW94, SM94, SX96, SBAD90, SK91]. **Structure**

[SST94, SKM99, SLDB91, SG96b, Sh91, TJ97, T96, VRR92, VM97, W94, Wil90, WL92, Woo98, XCY98, XKB+99, XSA+92, Xu99, YLY90, YS95, ZGPS97, IT+94, Kar90, MK95, Pul90, She91, Sta93, Ano93g, L91]. **Structure-Activity** [GJOV97, BTKVG99]. **Structure-Affinity** [GJLA99].

**Structures** [AMKS93, ADPS98, BK98, CL97, Coo95, EMMS94, Har96, Jur96a, KGv93, Lad97b, L95, LRM96, LS92a, LS93, LF95, Loh96, M93, MA95, NOY94, PV99, RW92, Spr96, TZCT97, AKS+90, And90, ABCM93, BL99, BS99, BB91, BJM+94, BT96, BCD91, Dia99, EZ93, FLL91, FB90, FMD+96, Fra99, GJDD97, Hal91, IBS95, JK90, KP96, KSN93, KSSG95, K94, LO93, Li97, MEC97, Min94a, NM92, PS99, PMS94, Sch92a, SZ99, SLDB91, TST+99, TFS95, W99, XSG97, BHC99, K97]. **Strumian** [AH92b]. **Students** [Ano99n]. **Neither** [FW+96, PIG94, RHC96, Ry94, SAF97, TNS+94, GZSvD99, hJH97, LSG91, NS91, ZY94].

**Studies** [ART94a, AK97, BKL97, BZ995, BCS96, BDH+97, Cal93, CL97, CCC+95a, CBR+98, CXL97, CDC98, EZ92, FF94a, FF94b, FT95, FB96, FLF96, GBVM93, GJLA99, Har97a, HS92b, HIKM95, H98, I90, Jur98b, KR95, KS99, KN92, LKM99, LX95, MZ95, MR92b, MZ93, MK99, MC95, Mor98a, NNHM96, NOY97, NH97, Pau92, PV93, PBB94, PS94b, RKPE95, RKG96, Sak97, SA96, Sta98a, S98, TZCT97, TSPK96, T95, TD96b, WO92, YXX99, YTM97, ZY95, BJM+94, BH99, BD95b, BH92, CPBC95, CLGW95, CP99b, DB97, DBL+90, DP96, FT96, FF96, FT97a, GY+99, GL96, HCCR94, Hag99a, HWW97b, HWW97a, JY94, Kar90, KL92b, LYS95,
LSS96, Les92, LC93, LB94, LUU90, LCP+91, MFCA93, NMN+99, Nak92, NAJ91, Nov92, NL96b, PVN90, PCF94, Rat92, RTS91, REKP92, RC99].

studies [SS90, SP92b, SCP93, Ska92, SSM90, Spr93, TCZ91, Tri98c, TNS92, VRR92, WJC+99, WY95, WP92, YOTY93, NÅJ92]. Study

[AL95, AKD96, AP93, AMT+99, AHI96, AMKS93, AR96, ADPS98, BA97b, BBD97, BBOR96, BTTS97, BJ98, BEG94, BLE96, BBC+96a, BSP97, BSHP97, BHX96, Boe96, BP92b, BjH97, BAK96a, BAK96b, BAK97, BCR94, BPL97b, BRA+99, Bra97b, BHPB95, Bue96, BDD93, BK94c, BvL96, CBAM97, CWX93, Cal94, CdBKZ99, CCB+97, Che96, Che97, CA97, CC97, CD81, DS96, DD97a, DN96, DB94a, DZ96a, DZ97, DD93, Dun99, ESP98, EMMK94, ET97, ET99, EDF+98, FY95, FLRV97, FD97, FDD+93, FWBT94, Gal96, GG97a, GD96, GL98, HZ91a, HP97, JK+92, JKRW98, JGR98, JMR98, JDJP99, Jur96b, Jur97f, Jur99b, Jur99a, JSKC95, KW92, KH96a, Kry98, KGVM97, KG99, KRN7c, LV93, LJ95, LMV92, Li92, LH94, Lio92, LFD94, LSC98, Lu99, LBG95, MKK98, MRT97, MAL96]. Study

[MTP+98, MDD93, Mav98, MB98, MG93b, MRL99, MDT93, MDJ98, MY99, MK99, MC94, MK96, Mor97a, MBP97, NSS+95, NN94, NF9M94, NM95, Ol99, Pan93, PM97, PP98a, PHH94, PFMC97, PLV92, PPP97, PM93, PBB92, PZ95, RL95, RC97, RH94, RF98a, RK95, Roz97, RMS96, SE93b, SE95a, SKTN97, SL93, SNMB97, SZC97, SPS96b, SDE94, SR96, SGGMFS96, SGB97, SGB98, SHC+98, Sta97, SC95, STC96, SFGW96, TTK90, TB95, VDBPR97a, VDD96, VB92, VC92, VZ93, WYW96, XLW+99, Yam97, YW92, Yur95, ZJS99, ZL98, ZW95, AEHM91, ADB95, AG99, ANB94, AKCS91, ABCM93, ABSW95, AH92a, AD92, BL99, BMA90, BL95, BHL+99, BJ92, BAR94, BOA95, BTOU97, Bat92, BILA95, BCLS94, BBM99, BH92, BH92, BHGC99, BR99, Bre99, BHPB93, BV91]. study [BV92, BMV93, BYE+97, BF98, BS95, BSG95, BLY98, BZ98b, CLOFR98, Cas92, CPN91, CRP93, CCB+95, CAM+97, CW+99, CS99, CSH99, CCS99, CMA+99, CL92, CDP+99, CF99, DD90a, DB+96, DSS90, DD96, DI95, DV91, DLF99, ESH99, EVSN92, Ext90, Eva97, FMS+99, FF92, FEE+98, FWZ97, FNSV99, FV96, FMD+94, FGM90, FL95, FR92, Fra99, Gal98, GE92, GPS90, GX98, GJDD97, GBS99, GS90a, HK95a, HDY+91, HGR99, HPP99, HZ91b, HGL99, HHP99, I94, J95, J98, J99, J99, KK93, KSN93, Ki94, KA96, Kha92, KC93, Kor90, KC97, LC92, LHK99, Les91, LHL91, LST94, LCS98, L94b, LB97, MLL99, MG97, MG90, MRRA92, MK96, MC94, MB90, MKDL93, MMRR92, MMCC99, MAL93, ML98, MMR99, ML99, Men99, Mil97]. study

[Min98, ML99, MBML91, MCA95b, MRBM91, NF92, NHH98, NL96a, OTS+95, PBC92, Pal94, PČ90, PB95b, PB99, PHM+91, PHBB92, PHBB93, PBB95, RF99, RIK96, RBT99, Ré90, RCB+99, RD97, RK91, RCW94, RK+98, SCL96, SE93a, SM96a, SDP+95, SAB+97, SC98, SM92a, SRP+98, SC93, SX96, SP91, Sem94, ST97, SEKE98, SCJK90, SW92, SCS94, SW95, SLS91, SBO97, SLL+91, Sta98b, SC98b, SC99, SLG+96, SBZ92d, TIA+92,
Studying [CL94, KKE96, SKS98]. Sturmian [AHWA96]. Sturmians [Ave00]. Stuttgart [Brä95]. Styrene [RW92]. sub [KDHW90]. sub-nanometer [KDHW90]. Subgraphs [ZW96b]. Subgroup [PC99]. Subgroup-chain [PC99]. subject [KKWT99]. Subjected [Bla96]. Submission [Ano95f, Ano95g, Ano95h, Ano95i, Ano95j, Ano95l, Ano95m, Ano95n, Ano95o, Ano95p, Ano95q, Ano96h, Ano96i, Ano96j, Ano96k, Ano96l, Ano96m, Ano96o, Ano96p, Ano96q, Ano96r, Ano96s, Ano96t, Ano96u, Ano96v, Ano96w, Ano96x, Ano96y, Ano96z, Ano96-27, Ano96-28, Ano97a, Ano97b, Ano97c, Ano97d, Ano97e, Ano97f, Ano97g, Ano97h, Ano97i, Ano97j, Ano97k, Ano97l]. Subsets [WBD97, GS92b]. Subshell [GM94]. Subspace [GW98a]. Subspaces [GM93, Ban91]. Substates [GSSD+96]. Substituent [CV99, CC96, FLF96, KZ94, KN92, HZ91a, Tew97, PHBB94]. Substituents [DWR99, Jay92, JM94, KPTS+93, XSA+92]. Substituted [Bra97b, MZ93, RL95, SSMK93, Shu96, BHPB93, HB94, KBM92, PHBB94, RC92b, SLG+96]. substitutes [BBS90]. Substitution [Gra97b, KK99a, LE92, MZ91, PHM+91]. substitutional [RD90]. substitutions [DGMW90, MHG95, MBML91]. substrate [TNS92, WMW92]. substrate-free [TNS92]. Substrates [SD98]. subsystems [GSM90]. subtilis [HB94]. Subtle [Mar95b, GVK99]. Subunit [CMFA93, SCMF93]. Success [DVJ93]. successive [LP97d]. succinonitrile [WBH90]. Suited [Ada99]. Sulfides [Jur97b, Mor98a, CMB95]. Sulfinylanilines [AEA099]. Sulfones [Mor98a]. Sulfur [AH96, LS92a, MV98a, BVV92, FWS97, Les91, SLG+96]. sulfur-bridged [FWS97]. Sulfur-Centered [MV98a]. Sulfur-Containing [AH96]. Sum [Mar98b, Kat98a, MPP92]. Summation [LS93a, CVW91, TW90, TW92]. Summations [Har98a, FDAC90]. Sums [KP93, Kat93, Kat97, Kat98b, Sie93, CFMA95, FAC91, PK92a]. suosan [SM94]. Super [NV94a, NV94b, AMH93, CDG04]. Supercell [EDF+98]. supercells [NV97a]. supercluster [Cze99]. Superconducting [Fri93b, LK99, LG95b, Bar90, GK91, Tac92]. Superconductivity [BS93, Fri93a, Fri93b, SBZ92d, SBZ92e, WL99, AS95, Mat96, MNM+99, SBZ92a, SBZ92b, LRM93]. Superconductors [BS99, CL97, CG97a, DMB07, Li93, Min96, MNM+97, MNM+98, Suk95, BB91, DBM99, JMS95, KCP90, MS94, Min94a, Yam90]. Superdirect [DM94b]. superlattice [MW92]. superlattices [BL92a]. Superposition [CSS93, E192, FW92a]. superstrong [RR95]. superstructures [BDP+92]. Supersymmetric [Bla96]. Supersymmetry [DJ95, DJ12]. suppressants [GX95]. Surface [ASP97, AT99, AP93, Art98, BMP92, BMP93, DP94, FP96, GMR+93, GDY97, GBJMA94, Jur97c, Jur98a, KM99a, KO95, LCL95, Min94b, MPR97, MA95, MBP91, MAAP+98, NTL96, NMB+98, NHH97,
OMTS97, PLA98, PM93, Sch99a, See97, SATP94, SFGW96, TNM98, WG95, YNMT98, CDM91, CEM+96, EDH+92, Eng92, FMR91, Gao93, GE92, GL92, GRTR96, GZvD99, JWG95, KR93, Kie97, KK92a, LMC97b, MD92a, MLT98, Mii97, MD91, MPIP99, Nak92, NF92, OYN98, PCB92, PSBL98, RK92, SAB+97, SCS98, SM92a, SRP+98, SBPPH92, ST95, Ska92, SS95, WY95, YNST99, MKRW99. *surface-molecule* [Nak92]. Surfaces [AMT+99, BBOR96, DDH+96, GW98b, Hea97, Jugu96, JSG97, LL94a, LL97, Lio92, MAL96, MD93a, MPV94, NTL96, PPS96, PPK97, PAM98, RK97, Sch97, SS97b, WGR+94, X94, AGNS92, Ber96c, BDK90, GPS90, HS93, LV97, Löw90, LM92, MV97, Mez90, MD93b, MPP90, N91, N92, OSS95, PBPN90, PTL90, RAM91, SM99, SX96, SW92, SN90a, Sut99b, VBD+98, WG92, ZP90]. *Surprises* [LS96]. Surrounding [SKTN97]. survey [OCK99]. *susceptibilities* [GFS92, Lev94]. Susceptibility [KM97, LFS94, SSK+92, DCK92]. *Susceptibility-reduced* [Kov90b]. Symmetry-adapted [CLZ99, LV97, PC99, ZWD98a, ZWD98b]. Symmetry-reduced [Kov90b]. Symposia [Alt96, The97, The98, Alt92, KZ90, Lin93]. Symmetrized [Ada96b, CW93a, ZWD98a]. *Symmetrizing* [CC98]. Symmetry [BKB98, CC98, CGG96, GS94, GLM91, GKS99, Her97, HC96e, JBS97, Kup94, Kup98, Mey94, Mey97, Mez97a, SM96b, Sen96, SW97, TMB98, WT98, Y92, Zha92a, ZW96b, ZMB97, And90, CLZ99, Coo92, Kov90a, Kov90b, LV97, Mez90, MJLL99, Nob99, Oza92, PC99, Sta91, Vin92, VZ92, ZZ91, Zha92b, ZWD98a, ZWD98b]. Sympoia [Ano97o, Ano98p, Ano93a, Ano93b, Ano90a, Ano90b, Ano91a, Ano91b, Ano92b, Ano94a, Ano94b, Ano95a, Ano95b, Ano96a, Ano96b, Pul90]. Symposium [Cal90d, JPP87, LZ92, LZ94, Ano90g, Ano91, Ano92, Bil94, Cal90c, LZ91, Nan95, CES87, Ca90a]. *synchronization* [CR96b]. Synchrotron [TNS+94]. *synthase* [ARB95]. Synthesis [ASI94b, Cio94]. synthetic [PBHB95, RC99]. synthons [KP90]. *syntopy* [MM93]. System [ABB93, ANB96, BW97, BMK96, FK94, Fer95, GW98a, GKS99, KPR97, KN96a, KMP94, KMP97, M96, NV94a, NV94b, See97, SSD96, SC95, TBC95, Voj96, ZY95, AZ99, BPH96, Cas92, Eng92, KC93, Nag96, Nan92a, NV97a, OM91, PS92a, Ska92, SGW+92, Sut99a, TKO+92, TTO93, TSP9M94, TNS99]. System-Partitioning [Muk96]. Systematic [Bou94, CV99, RTK95, SZC97, ST97, Les91]. Systematics [LS96]. Systems [AT99, ADPS98, AT93, ACPR98, Ara94, AFTM95a, AFTM95b,
AFO, AK97, BMA93, BA97b, BLBP97, BG95, BGS98, BAD99, Cal96a, CBG94, CV98, CMFA93, CCE+93, Col97, Dun96a, Dun97, DQB97, EMMK94, Eng95, FS95c, FU197, GD94, Gin96a, GBRA94, GG97b, Har98a, Her98, KS94a, KSY97, Kof95, KN92, Kup94, Lad97b, Lah92, LLL97, Lin96b, LG95b, LEA+94, Mar96, MB97a, MS97b, MR99, MCM98, MK99, MA95, Mon94, MV99, NFVM94, Nal94, NM95, NU95, NB97, NP96b, OLC+96, PKM93, PV94, PAT93, PZWJC96, PGH95, Pri95, RMPR98, SE93b, SLtM+94, SPOAS97, SDW+98, SAR96, SSP98, Sch99b, SS99b, STMR97, Spr96, Suh94, Suk94, TKNI96, Tag97, TC98a, TDK+94, Ukr94, VBV92, WS94b, WD95, WD97, Wi96, YAD95, ZWPJ94, ZRNZ97. systems [Ada94, AM92, AM93, Ale95, AEJ91, AB99, AI99, AST95, AFZ+99, BOA95, BE93, BD95a, BA90, BX94, BSP98, BB94, BB95, Bon96, BB97a, BV92, BC93, Cal90c, CD92, CSG99, CPBC95, CAM+97, CB99, Che92, Cio90b, CDG04, CE90, DAA92, DW90, DO94, DB94b, FG99, FFD96, For92b, FKR92, FS92, Gal98, GPS90, GRBA92, GJDD97, GBS99, GDF92, HVS98, HK95a, HS92e, HL9j6, I'H90, JPP87, KG92, KR91, Kel97, KL90, LO93, LC90, LBB91, LMD92, LLL91, LM93, LL99, LTY90, Lun92, MB90, MECE97, MD92b, MHSV96, MCT99, MM93, MtPC+96, MFCA93, MEP90, MRD92, NSTFC94, NKS+96, NMN+99, NYK98, Nak92, Na98, NV97a, OCK99, PAF91, PA92, PM90, PDM97, PD92, PM98, PD98, PZPM99, PAC90, PACO90, RFG99, RC92a, RCB+99, ROL+90, RSCP91]. systems [SCL96, Sae92, SGK99, SG96a, Sch90, SC96, Sem94, SR99, SES93, Spr93, Suh93, SD91, SBZ92c, TP92, TCM99, TD03, VZ92, Yam90, YOTY93, YITY93, ZM95, An92, Br96b, Mon94].

[Sut99a]. Tensor [GWCT97, BRV90, Cam92, LG96, MHY98]. Tensorial
[Pal97b, ZWZ96a, Ell91, Ell92]. Tensors [GARC97, LBG95, Pal93b, Pal97b,
Pal98, SZ96, SZ97a, GS97b, HZ99, Pal91, PV91, PN94, Sen96b], tentative
[GK90a, GK90b]. teratogenicity [CLC90]. term [SBZ92a, TGS99].
Terminal [ZYY95]. Terms [AM98a, DTS97, GR95b, GR96b, Gin95, Gin96b,
Gin97, GGSA98, KBL95, KC98b, NS95b, Ort98b, HC91, KE90, KL93b,
MHN98, PCO+94, SLDB91, Sut99a, SB92b]. tert} {CAM+97}.
tert)-butylcyclopropanone [CAM+97]. Tesla [BMG+98]. Test
[AR93, KP97, Lef99, LD95, MSM96, SKN95a, SKN95b, BA91, BHK93,
LO90, KLO+98, Van96]. Testimony [ILH90]. Testing [ˇCB96b, KLC98b].
Testosterone [KG97]. tests [Bec94, KPB99]. tetracaine [DB97].
tetrachlorodibenzo [MEP90]. Tetrachloromethane [GMS97].
Tetracyanoethylene [Cio94]. Tetrafluoride [SM95]. Tetrafluorobenzene
[MSS99a]. tetrahedral [EMS92]. tetrahedrane [SPM+96].
Tetrahydrocannabinols [BjH97]. Tetrahydrofuran [KUN+98]. Tetrakis
[TSKP99]. tetramer [BB95]. tetramethylene [Jug90a].
tetranitromidazole [CP99b]. tetrapeptide [NSS92]. Tetrasilane
[Yam97]. Tetraatomic [AS96]. tetrazine [Ort97]. tetrazole [IGK+92]. TG
[SST94]. théories [GK90a, GK90b]. Theinyl-Imino
[MH98]. Their
[ADM98, BDG96, BMP93, CDD+99, Flo97a, GBVM93, Gin96b, HH92, Her98,
HSS+95, HM95, IK97, Jur96b, Löwe97b, Lu99, NK98, Nün95b, Ott94, PZ95,
SSK+92, Sch99b, See97, SGB97, SH96, STC96, YO92, AMH+92, BDP+92,
BSS+97b, Brä98a, Cea90, CS99, CBL95, CMA+99, Flo97b, GVV+90, Jur99d,
Löw91c, MRST95, MKBP97, MBP91, NNNH98, RF94, SC96, She97, TTM99].
Them [BP93c, Ber96c]. Theorem
[Day96, HWS92, KCI98, LBM95, May97, Mor94, Nag94, Csa90b, CK91,
Ell92, Gin91, GLM91, KS90, LV97, MDM94, PLS99, She90b, SN90b, DMFR93].
Theorems [AFTM95a, AFTM95b, AFO+97, AFTM98, HM95, KL93c,
Löw93d, Popp98, AFZ+99, BP93a]. Theoretic [Del98, Dom99, PMM97].
Theoretical [AP93, AMT+99, AFM99, AMKS93, ADPS98, ASI94b, BMA90,
BMA93, BKW97, BF95, BA97a, BSB94, BSP97, BH99, BD95b, BjH97,
Boe91, BDP+92, BHGC99, BZ95, BK94c, Cas92, CR93b, CPBC95,
CCT+95b, CBB+97, CBSR+98, CWJ+99, CS99, CSH99, CPD+98, CD99,
CDD93, DB97, DDC95, DTA+96, DM97b, DB94a, DD96, EK94, ET97,
ET99, Eng95, EC96, FMS+99, FY95, FWZ97, FL91, FDD+93, FB96,
FL96, Gal96, Gal98, HJ94, HWH97b, HWB97a, I19, Jug90b, JZ95a, JZ95b,
KW92, KSN93, KA96, KCI98, KMM96, LYS95, LHI91, LFD94, LRR92,
LC93, LBB98, Löwe94c, LSC98, LCS98, MV98a, MA98, Mar95c, MBG90,
MMRS92, MMCC99, MAL96, MTP+98, Mav98, MG93b, Men99, MY99,
MBM91, MPOG99, MC95, Mor96c, Mor98a, NONY97, NMN+99, NTL96,
Nak92, NF92, NN94]. Theoretical
[NNH97, NNNH98, NST94, OLC+96, Ott94, PWL95, Pár98, PP98a, RGH94,
RCWN94, RKG96, RW92, Sak98, SKT97, SL93, SP92a, SRP+98, SCA93,
Theoretically [FF90, YLLJ96]. Theoretically-derived [FF90].

theoretischen [HW87a]. Théorie [GK90b, GK90a]. Theories

Theory [BG95, KS98, Lev97, NS95a, NS95b, Ney95a, Ney95b, KDB90, NS91, NE95].

Theory [AGL97, Ada96b, Ada99, ASI94a, ABR95, And94, AR93, Ång93, Aon99, AO93, BDG96, BIM97, BC98a, BA93, BAD99, CG97a, CC95, CIA94, Cha98, CGLP96, CSP98, CDDM96, CJK98, Chr97, Coh97, CA90b, CPA95, Csi76, CB94b, Dou94, DHPC95, DZ94, DD98b, DZOR98, Eng95, EMMS97, FP94, Fr93a, GID98, GR94, Gho94, Gnh98, Gnh99, Gör98, GG79b, GG84, Gna97b, GWCT97, Hag97, HBW95, HHMK95, HB98, HY99, IF999, JG95, JM93b, JP95, JM96b, Jur96b, Jur97a, Jur97b, Jur97c, Jur97d, Jur97f, Jur97g, Jur98a, KBT94, Kar93, Kar95, Kir95, KZVG97, KYS97, Kfo95, KGH95, KGL98, L995b, Le99, LP96, Lin97, LD94, Löw90e, LZ92, Löw96c, Löw99, LBBM95, LAS+95, LIN+98, Mar95b, Mar98a, MO98, MHH95b, MC97a, MC97b].

Theory [Mat99, MV99, Mun92, NOYY94, NY99, Nag94, Nag98a, NU95, NKFP94, NV94a, Oli99, PV99, PP98a, PEBS97, PLA98, PM93, Dca97, QS98, RDF98, RL95, RB95, RB96, RZ96, RP99, RQ94, RSB92, SP98, Sah95a, SD97, SZ96, S97a, Sch93, Scu95, SB96, SG98, SAFK97, SN98, SAS99, STY+98, SH96, Sn93, Suk94, Suk95, SPL97, SV95, TK9196, Tac96, TMP97, TC98a, TG95, The97, The98, Tob99, VDBPR97a, VVS94, Wal94, Ws94, Wt95, WWM98, jYL94, YCML91, ZLHZ94, vDvLR99, Ågr91, Ada90, Ada91b, Ada94, Ada96a, Ali99, AC95, Ano90g, Ano90i, Ano92a, Ave89, B90, BAR94, BX94, BSP98, BAL95, BDS97, Cal93, CT95, CW98b, CCS98, Cha96, Cha92, Che92, CLGW95, Cm96, C91, CEM+96, Csi77, Cze99, DDA92].

Theory [DA91, DP96, EDH+92, EKI94, EZ92, Fau92, Fer92, För92a, FS99, GJFP92, GNF90, GL95, GP91b, G91, GZLD99, GW91, Gut99a, HW84, HW87b, HW92, HW94, HW96, HW90, HW04, Ha93, HR99, HC91, HC96a, HC96b, HC96c, HC96d, HLJ96, HZ92, IL95, Ish92, Jac92, JH92, Jur99d, Jur99c, KSF91, Kla93, KMP90, KM90b, KLC95, KL90, KLM91, KL92a, KK92b, Kum93b, Kum93a, KP90, LC90, LC99, LM93, Lin96a, LBL98, LZ91, Löw91a, Löw91b, Löw91c, Löw91d, Löw92b, Löw92c, Löw92d, Löw92a, Löw92b, Löw93a, Löw93b, Löw94b, Löw95c, Löw95f, Löw95d, Löw95b, Löw96a, Löw96b, LTY90, Mar92a, MS91, Mar92b, Mar95a, MN98, Mar99a, MVS97, MHH95a, MUM97, Mat96, MM99b, McW90, McW99, MB93, MCA92, MRT95, Mon93, Mon94, MAAP90, MRD92, MD92c, Na95b, OKY+99].
theory [OGK90, Ort91, Ort92, Ort93, Ort95, PL93, PV91, PY89, Par90b, PMDM97, PZDM97, PMDM98, PZDM98, PP90, PG96, Pet92, PS95, Pop90, Qui92, RVP92, Rig92, SH90a, SS99a, SB92a, SP95, Sem96a, SOK+98, SNNY99, SS91, SC99, Suh92, Suh93, SO97, SNH99, SBZ92b, SB92b, SDR91, TNSM99, TMA97, Tct93, TC98c, TGD97, Tre96, VDBPR97a, VVO98, VDL95, VCM99, WB93, WMZ98, Yor95, ZC99, ZP90, ZY90, ZY94, Zie96, ZJ89, ZJ93, ZJ96, AZ92, ZPBC97, LP98, Bra98b, Cal90b, Ano92k, Bra95, Bra98b, Gre98, Jor92, Cal90f]. Theory-Based [BDG96]. Therapeutic [WWFR99]. There [KJ95, Ada90]. Thermal [BMK96, KW92, LMR94, RW92, To99, KPW+95]. thermally [OS90]. Thermochemical [Bec94, HPSC97]. Thermochemistry [GBL97]. Thermodynamic [VH96, Chua99]. Thermodynamics [FDD95, Gar95, Mic96a]. Thermolysis [ZH99a]. Thiamin [FB96, FVN98]. Thiazole [MH98]. Thickness [MPV94, Boe92]. Thin [MPV94, Bat92, Boe92, MV90]. think [Ber96c]. thioacetone [SSM90]. Thioanisole [DOR98]. thioacetate [Pro94]. thioformaldehyde [GH96b]. thioguanine [RBB+94]. Thioxamides [KM90a]. Thiopeptide [BSB94, SL98, BL92a]. Thiopeptide- [SL98]. thioamines [EVSN92]. Third [BSB94, DM94b, LFS94, NK96a, Suh93, SPL97, VFHL93, ZO95, CJM+91, DCK92, Kor90, Ort97, PWL98]. Third-Order [BS94, LFS94, SPL97, VFHL93, ZO95, Suh93, DCK92, Ort97]. Thirty [Na95b]. Thomas [Csa92, Csa96, GC91, MK97a, MHN98, ZP92b]. Three [ABB93, ANB96, Art98, DM96, DTM96, GBL97, HS91, Hoo94, KFS92, KJ95, PM95, PPP97, Pfe93, SP98, Sta95, St96a, Sta96b, Sta98d, Sta98e, VDD96, WD95, WD97, Bud92, BFW92, D99, DCK92, GSPSM93, GDF92, ITT+94, Kin99, KE90, LL99, MGB90, MVH96, MS92, MSC92, NM91, RA91, Sta98b, NM90]. Three- [GBL97, PM95, PPP97, GDF92, MS92]. Three-Body [KFS92, Pie93, WD95, WD97, KE90, MVH96]. Three-Center [HS91, KJ95, SP98, RA91]. Three-Dimensional [Art98, DM96, Sta96a, Sta96b, Sta98d, Sta98e, D99, LL99, MSC92, Sta98b]. Three-Dimensional-Doped [DTM96]. three-electron [Bud92, BFW92, Kin99, NM96]. Three-Level [ABB93, ANB96, DCK92, GSPSM93, NM91]. three-stranded [ITT+94]. threo-ethylcarbonyl [SSM+99]. threshold [CB96a]. threoxobone [ARB95]. thylakoid [DS99]. Thymine [AKD96, LF90]. Ti [SG97, SBG98, BR95, GY+99, SG97, WB99]. Ti-doped [GBS95]. TiCH [SG97]. TiCO [hJH97, SG97]. Tight [LRM96, MA98, TR94, GL92]. Tight-Binding [LRM96, MA98, TR94, GL92]. Time [ABB93, AL98, AM97, CT96, CSP98, CJC98, CCE+93, DD95, DD98b, GFR98, HGC93, LM91, MS97a, MS97b, Mey94, Mey97, Mic96b, RB95, R97, RW98, SB95a, SB98, TC98a, TC98c, TCM98, YB99, YBM97, BFL91, BMA99, CSM98, CÅ92a, FMR91, HZ93, Hag95, Lin94, PL91, PG96, Rod91, RMF90, YCM91, SB92a]. Time-Averaged [CJH98]. Time-Dependent
[AM97, CT96, CSP98, DD98b, Gär98, RB95, RW98, SB95a, TC98a, TCM98, DD95, TC98c, YB99, BFL91, BMA99, CCS98, FMR91, PG96, Rod91, RMF90, SB92a]. **Time-Evolution** [Mic96b, RJ97]. **Time-Independent** [MS97a, MS97b, SB98]. **Time-resolved** [LM91, PL91, YCML91]. **Time-Resolved** [Mey97]. **Time-Varying** [ABB93]. **Tin** [LEG +94, RRC94]. **Titanium** [BFL91, HLS94]. **Titanium/Oxygen** [BFL91]. **Tin-Encapsulated** [LEG +94]. **Tin** [Min96]. **Tokyo** [Str93]. **Toluene** [NM95]. **Toluene** [NM95]. **Tool** [HN90, Val96, Har91, Mez90, WM92]. **Top** [HHHP99, PRTV97, Val96]. **Topic** [PDC96]. **Topics** [Lun92]. **Topographical** [SG94]. **topoisomerase** [JDB99]. **Topological** [HSES94, LLL91, MESH93, ZLM94, ZM96, VD90, HGP +92, OS95]. **Topologies** [BKL94]. **Topology** [Sch97, SRM98, SHC +98, AM90b, BFL91]. **Torsion** [VB99]. **Torsional** [GW98b, MJ99, YY96, MSS99b, SLL +91, VVO98]. **Total** [CM94, GZ97, IY99, Ort92, VV95, AH92a, Csa90a, Csa91, DWM90, GL92, GH92, LH94, LFD99]. **total-energy** [GL92]. **Totally** [IP93]. **toxicological** [BG99]. **trace** [GHB +99]. **Traces** [PRTV97, Val96]. **Track** [BJ92, WA94]. **trans** [MG97, DSB99]. **trans** [BBF97, BCS96, BAD90, CAK +96, CLS94, CR93, DTM96, Del96, GL98, HP98, MIK94, N94, PK90, RML97, SBM97, Spr96, Sta98a, Sur95, WP98, B90, BOA95, BDM97, BK99, BC95, CDB90, CMSF93, Cdi91, DM97b, DSW93, EMS90, EBMS92, FMR91, Gao93, GZvD99, GBS99, HE90, KK99, KS95a, LBBK91, LB93, LKM99, LS92b, MM91, MK96, Na98, OKY +99, Pal92b, PMO90, PC91, PBR96, RBB +94, RMF90, SY91, Sta98b, WG99, W96, ZBL99]. **Transferability** [FSVZ97, GS91, MM98]. **Transfers** [GBS93b, DS92]. **Transform** [ABLA97, HS92e, KM97, Mez97b, MK98b, CM99, CP92, KKK90, KK91, KK92a, Kin93, Kin94, MK95, MK96, Rod91, RW98]. **Transformation** [AH97, BA93, Gho95, LLM +95, SF95b, Boe97, Fan90, GV92, LBL98, PV91, PDM97, PZM97, PZDM98, PZDM98, Üle92, Wen93]. **Transformations** [HM97a, Le97, LBPL97, LBLKC98, LBLKC98, LR94, Low96c, SP98, Wen96a, BA92, Cio90a, LOW92b, Pau92, Wen96b]. **Transforming** [ITK91]. **Transforms** [F93, MK97b, Ced94]. **Transient** [FS96, TMM97].
ART94a, ADPS98, BA97a, BC97a, BTN98, BK98, CLZ95, CAK+96, CJA94, DHL+94, DMFR93, Dun99, Gre94, HHPT91, JKR90, LRM97, MTD93, MBA94, MR94, NYY96, OYN98, PAT93, RW92, SZ97a, SPS96b, SDE94, Sim93b, SGB97, SGB98, STM96a, SDG97, Tit93, YLLJ96, ACZ91, And93a, BBSS96, BRL92, BUZ94, BCLS94, BDK90, Boe93, Bro95a, Bro96, BPVP92, CLZ99, CKM91, DY96, FZZ92, GZSvD99, KSF91, Ken93, LU92a, Mar99b, MSMR99, MAC96, MS93a, MLK94, MCCF95, Nor91, PO91, PSO90, PTL90, PZA92, ROL+90, SHB+96, STM96b, SC99, TKO+92, TTOY93, Van96, WS92, ZBL99.

Transition-Element [SGB97, SGB98].

Transition-Metal [BA97a, BC97a, MBA94, STM96a, Bro95a, Bro96, CKM91, MSMR99, Nor91, PZA92, STM96b, SC99, Van96, ZBL99].

Transition-State [NYY96, RW92, SDG97, OYN98, BBSS96].

Transitional [Luo95].

Transitions [Art97, BM96, JI95, MPR97, NMN+97, NMN+98, PSD97, TD96a, Art96, Dun96b, LMMK93, LM95, MBB90, MLB92, MKDL93, MCL95, Rep96, RBB+94, SMM+90, Sme92, WSM+94, YBZ92].

Translated [Br¨a95].

Translation [ˇCHMA95, MRC99].

Translational [Jou97, TW90, TW92].

Transmission [DRGC90, Hag99b, TWK+92].

transpolyacetylene [DYD96].

Transport [Ara94, DY96, DP93, DM96, DS99, Ino96, Khu92, Mar94c, MK96].

Trapped [RM99].

Trapping [KSKJ94].

traversal [HZ93].

treat [Mar99a].

treated [LK90].

Treatment [AMRT94, AAO99, BMA93, BLBP97, BXZ95, Bla96, BP93e, GY95, HAEMA92, Kry93, LCL095, MM94, MH98, SKT97, SCH95c, TM98, VBUS99, AHM97, CF93, FL91, FR98, Hir92, KRZ91, KY19a, KSK+99, MD94, MD95, NSTFC94, NKS+96, SS98, ST91, TFY991, TT999].

Treatments [MCM98, SP+96].

Tree [JM96b, JGP91].

tree-search [JGP91].

Trees [JM96b, TMH94].

Trends [MM95, SL98, Tay91].

Triads [SBM97].

Trial [Gui98].

Triation [Kup98].

Triatomic [NFVM94, RABZ94, Su93, BZMR92, HZF+91, MIW91, ST91, Sut99a, MKDL93].

triatomics [Pet92, TS92].

Triazole [PGS97].

tribute [An96-58].

tricyclic [CMA+99].

Tricyclo [Lu99, XSA+92].

Tricyclohexane [Gal96].

Tricyclopentane [Gal96].

triadiagonal [NZ92].

triexcited [CPV90, LP98].

trifluoromethyl [KH97].

Trifluoromethylvinyl [KH97].

Trigger [PW97].

triglycerides [CDM+94].

Trimer [CCB+97, Fou94, GW98b].

trinitroimidazole [CP99b].

trioxane [BJM+94].

Tripeptide [MK98a].

Triphenylphosphino [Boe96].

Triple [CS98, PG94, WB93].

Triple-Excitation [CS98].

Triple-Zeta [PG94].

Triples [HK96, NU95, WB94].

Triplet [BS94, CG97a, GV93, HHKM95, Jur97c, KBBK90, STM97, Gut99b, KD92, LM91, LS93b, SC98].

Triplet-singlet [KBBK90].

triplex [ PWL98].

Triply [PTP95, RSD97, HOF+97].

TRIPOS [WHF92].

Trisnitrooxymetaphenylene [TD96b].

tromso [Fuk90, Löw90d].

tropolone [WB599].

Trotter [Lun91].

Trp [LU92].

Truncated [Sad97].

tryptamine [DB93].

Tryptamines [HAEMA92].

TST [JC90].

TTF [Sta98b].

TTF-2 [Sta98b].

TTF-DNCQI [Sta98b].

TTF-TCNQ [Sta98b].
Tungsten [DFDK99, FDD95, LMC97b, LFD99], Tunnel [EMS90], Tunneling [BS96, BCS96, CR93, Hag98, NBS95, SB97b, SC94, CMG92, DVL+91, EBMS92, Hag92, HZ93, Hag94, VBD+98], Turkey [Yur95], turn [SJB90], Twentieth [JPP87, Cal90c], twist [RK96], twisted [MFCA94], Twisting [M93, MGK99], Two [Bal90, BBC+94, BMS98, Chr94, Chr97, DTA+96, De 97, DP97, DQB97, FK94, FS95c, FWT+96, GJP91, GY95, HBL99, Har98a, HO94, HS92e, IY99, IP94, LS93a, LMR94, LR94, MT90b, MBA97, MRL99, NMM97, NPL91, NYLBNS97, Pan95, PO90, PM95, PMN+92, Ple93, PAT93, RML97, RDK97, SB97b, SSD96, Ta96a, TE96, TZ97b, Val96, VBUS99, WG95, WFK97, YO92, ZW96b, vvBS96, AS91, BSS97a, Budd92, BFM92, BMA99, BG98b, BG98c, CB99, Cio90b, CE90, Dav90, DW98, DW90, Fan90, FR98, GP91a, GDYY97, GDF92, HR99, HW91, IIT+94, Jon93, KG92, KlW92, KM99b, KTCN93, LLL91, LDJ90, LDH92, LM92, MH98, MBG90, MA99a, MS92, MGLBP95, MD93b, NM91, NM94, NV97a, PTL90, PZ91, RDK02, SB95b, SB92b, TG999], two [Tit96, WDS97, YKN+99], two-body [FS95c, YKN+99], Two-Body [FS95c, YKN+99], Two-Center [GY95, HO94, HS92e, IY99, LR94, MBA97, Pan95, MT90b, Bud92, BFM92, Cio90b, DW90, Jon93, MGLBP95], Two-Component [HBL99, vvBS96], two-coordinated [ASM91], Two-Dimensional [BBC+94, FWT+96, Har98a, LS93a, SB97b, SSD96, TE96, VBUS99, WG95, YO92, GDF92, HR99, LLL91, LM92, NV97a, SB95b], Two-Particle [ZW96b, NM94], Two-Particle-Hole [DP97], Two-photon [PS90], Two-Point [LMR94], two-proton [MA99a], Two-Row [WFK97], two-shell [BG98b, BG98c], Two-Site [RML97], two-state [BMA99], two-step [Tit96], two-valence [MBG90], Two-Well [Ta96a], two-one [BSS97a], two-one-component [BS97a], Type [AM98b, BR94, BF96, BEJ98, BG98, CB93a, DTS97, DQB97, FFD98, GY95, GIA96, Gus98, GOAY98, HO94, HS91, HS92e, Ish96, JZ95a, JZ95b, Jur96a, Jur97c, KL97a, MBA97, PR97, SZ97a, Sim97, Sur95, Wil96, Boe96, BJA99, BDPS97, Bud92, BFM92, CS91, Ell91, EJ93, FDC92, FM92b, GS92b, HB1+92, HS92f, J91, J90, JEB92, J92b, Jon92b, Jon93, Jon97, KKT97, MHS95, NMC92, RAA94, SMM+90, SH90b, VL91, YC98, ZZ93, ZF92], type-IV [FDC92], Types [Chr94], typical [RRC94], Tyr [LU92b, TWK+92], tyrosine [KÅ99].

U [MECE97, Tit92], UB [Loh91], UBC [Loh91], ubiquinone [CMSF93], UC [Loh91], UF [DN96], UFe [MECE97], UHF [NM96], UK [Str93], ultimate [WP90], ultime [GK90b], ultra [Boe92], ultra-thin [Boe92], Ultrastar [ESTM95, YCML91, Kra96], Ultrahigh [SS97a], Ultrasharp [FSHC99], Ultrashort [MY99], ultrathin [AST95, WTSN94], Ultraviolet [MK97b], Unambiguous [BCL98], uncoupled [CMA93]. Uncoupling
Valence-Bond
[Har97a, JG95, JGR98, JF92, KFS92, KGC+96, KZVGB97, LP92, LP96, MF96, McW90, NFVM94, NMM97, PS93, Par97, Rin94, RL92, Rot96, SR96, SBD+92, TC98b, WWM+98, DDC95, DHDP92, For92b, HB3+92, HSES94, JM96a, KJL96, KT95, MBG90, McW99, MAAP90, NM94, NM96, Rin96, SCJK90, SLDB91, TGS99, WG99, YJL92, Rot97, Sta98d].

Valence-Shell
[JM93a, JM95, JG95, JGR98, JM96a].

Valence-split
[SBD+92, For92b, McW99, SLDB91, WG99].

Valence-Universal
[JM93a, JM95, JG95, JGR98, JM96a].

Valencies
[CPTR96, ETV94].

Valency
[SGK+95, SG90].

Valent
[CC96].

valid
[Sch94].

Validity
[Ada96b, Csa96].

Valproic
[CLR+93].

Valpromide
[TBBE97, TBBE98].

Valuable
[HNB92].

Value
[JM93b, EMP92].

Values
[KS98, NS93b, Núñ95a, Sie93, JJ96].

Vanadate
[KW98].

vanadium
[GWB97].

Vapor
[CL95].

Variable
[AH97, ST96a, VJ95, VJ97].

Variable-Step
[ST96a].

variables
[YG90].

variants
[FV96, KRRB99].

Variation
[DDD93, DC95, KG92, LG92].

Variation-Iteration
[DDD93].

Variational
[CG95, CT96, CMCR96, CJA94, CJH98, CTG97, CLKMTA95, HZF+91, HW91, Rot96, Ryc94, TMSI98, Tit93, TSP97, WN90, Wh94, ZB92, ACAT92, C293, Csa90a, Csa90b, CK91, Fer91, FR98, KDB90, KS92, LV97, MRD92, Rot97, SGCC99, TTM99, Wil99a, BBMM99].

variety
[LS92b, ZW96a].

Various
[BLRD92, BAK96a, DP93, IAN+94, JM95, Löw93d, BHGC99, CLGW95, DSS90, JM96a, WW97, WP90].

Varying
[AB93, DPP+94, PB95a, Hug95].

VB
[CTG97, KSR95, LP97d, MZ95, Oli99].

VBSCF
[CWZ98b, DV99].

VCO
[CF97].

Vector
[FCVL98, PZA92].

Vectors
[Alt96].

Verlag
[Brä95, Brä96b, Brä96c, Car96, Dum96b, Sjo96, Str91].

Version
[Amo96, Fue98, LLBM+95, CGMG92, LBL98].

Versus
[Cha97, SBIP97a, EMP92, MCB99, MCCF95, OCK99, PZDM97, PZDM98].

Vertex
[MD93c].

Vertex-Alternation
[MD93c].

vertical
[MYH98, ZM95].

Very
[DKWM97, D MKH97, Koh95, MLT+96, SPOAS97, Sul97, D KM96, NSTFC94, New97].

VI
[TGD97, CF99, ERC91].

VI
[LRM97].

Via
[CR93, Aks+90, AFTM95a, AFTM95b, AFO+97, AFTM98, AFZ+99, CSZ97, D97a, GGS98, JBT95, KM97, LZ96, LKMVT95, LKMVT96, Mar95a, MK95, MK96, MK97b, MK98a, Sah95a, SN99, SD98, SE95b, SE97, FF96].

Vibration
[GSSD+96, LT99, TL98, VJ97, CTF92, FR93a, ST91, TS92].

vibration-rotation
[ST91].

Vibrational
[AML+95, AMD+97, ABDM94, BKWL97, BZMR92, Bau97, BCMÖ97, Cha97, FSH99, GD98, GH99, Hea97, Her98, Hua92, JDJP99, JAG95, Kal90, KV99, KC98a, KLC98a, KC98b, KC97, KMM96, KLM97, LKMCVT95, LKMCVT96, Pa93b, RABZ94, SM96b, STMR97, TCL98, TT98, VX99, VJ95, WD91, YBM97, Ali99, AH92a, BFL91, CD91, FLHT90, FB90, FL95, GZD97, HS99, HZF+91, Kar90, KLC98b, KLM97, LTY90, MHL94, Mch91, NL96b, OSS95, RCWN94, SE92, SBZ92b, TLTL92, TBP99, WBS99, Zha92b].

Vibrational-Rotational
[LKMVT96].

Vibrationally
[DDH96, BJ92].

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Anonymous:1991:Mh


Anonymous:1991:Mi


Anonymous:1991:Mj


Anonymous:1991:Mk


Anonymous:1991:Ml

REFERENCES


Anonymous:1992:SSLb


Anonymous:1992:Aa


Anonymous:1992:Ab


Anonymous:1992:Ac


Anonymous:1992:Ad


Anonymous:1992:Ae


Anonymous:1992:AP


Anonymous:1992:BN


[Ano92q]


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