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Title word cross-reference

\((1s)^2(2s)(2p)\) [Tat73], \((1s2s,3S)\) [RM79]. \((ns)\) [CH74]. +
[FM78a, JZ79a, Koc74, PK71, RM74, RW75, RM79]. 1/z [Lin70]. 12
[HLMV77]. \$18.10 [Cal77b]. 1:1 [SP71]. 1s [Lec76a, Lec76b]. 1s2p3s [SA77].
1s2s3 [LAM71]. 1s3d [AC70]. 1s3p [AC70]. 1s3s3 [LAM71]. 1s2(2p)2 [Lar78b].
1s2s2p n [HT75]. 1sσ [AM77a]. 1σσ [AM77b, TS72]. 2 [Han70a]. \$22.50
[Gos78a]. \$24.95 [Mär78]. \$29.95 [Sab75a]. 2d [Chu77]. 2l + 2 [Mos73]. 2p
[Tat73]. 2pπ [SHI73]. 2πσ [AM77a]. 2pσ σ [TS72]. 2s [GB72]. 2sσ [AM77a].
\$30.00 [Shu77a]. \$38.50 [Ano78c]. 310 [Meh79]. 3π [AM77a]. 3σσ [AM77a].
\$43.00 [Cal76b]. \$48.50 [Dun78]. \$49.50 [Shu77b]. \$56.00 [Sti79]. 5 2 0
[Lin73]. \$69.50 [Lar78c]. \$74 [Ahl77a].
\(<2^{2N/2-S}, 1^{2S}>\) <\(2^{N_1/2-S_1}, 1^{2S_1}>\) ⊗ <\(2^{N_2/2}-S_2>\) <\(1^{2S_2}>\) [SD79b]. +
[BB70, BS70, Doo78, HL79, HG75, HT75, KP71a, Kol76, KJ78, LH74, Lar75,
Lar78a, Lar78b, LV71c, PK71, Pul74, PPB78, RS79, SD78, TS77]. ++
π [Bra75, Bra79a, ČPP75, HTG77a, JPTM78, KTO+78, KJ75, KT76, KL79, Loc77d, MCST72, MK75a, Mic76b, MK72, NT79, PN76, San72, SPČ79, SIM75], π → π [DRCT78], \( r^N y_M^A (\theta, \varphi) [SF75, ST70] \), \( r_{12}^{-1} \) [SR72a, Sal73]. \( r_\varphi [WRS70] \rightarrow [FM78a, JZ79a, PK71] \). \( \Sigma \) [SIM75, BB72c, GBS70, HTG77a]. SU(2) ⊃ D\(_\infty\) ⊃ D\(_4\) ⊃ D\(_2\) [KG77]. T ⊃ C\(_3\) ⊃ C\(_1\) [BW76c].

\* [DRCT78, NT79].

- adrenergic [Dav77b, KVSG79]. -adrenomimetics [ZG79].

-alkynitrosamines [TPC77]. -band [MGM78]. -bonds [BCL79].

-Berechnungen [BKWK75]. -bonds [Loc77d]. -completeness [KK76b].

-Electron [Bra75, Mic76b, Bra79a, Gal74, JPTM78, MK75a, PN76, SHI73, San72, SPČ79, SIM75, Gal72a, Jun78]. -electronic
[ČPP75, KJ75, MK72, SPČ72]. -electrons [SIM75]. -expansion
[Lin70, MW75c]. -fermion [Per78]. -fold [Lét74]. -functions [Sha76].

-glycine [RRS75]. -helical [VU79]. -hybrid [DF76]. -ionized [KTO+78].

-Lactam [Boy77]. -line [Kot76]. -matrices [Han70a]. -matrix [Kij72].

-method [DC73]. -molecule [GS70a]. -monosubstituierten [FJP70].

-monosubstituted [FJP70]. -orbitals [FGV77, RS78a, Tat73]. -particle
[Col78, Mat74a]. -Picolins [BKWK75]. -radicals [KT76]. -Representability
[Col71, Col70, Kum77, LD71]. -scattered [BB75]. -state [Mat79b].

-structures [BCL79]. -Substituted [Boy77]. -systems [BB72c, GBS70].

-technique [MSKM77]. -type [LS72, LGR73].

/2 [ZR78]. /3 [ÅFL78, LBÅF78]. /VRDO [KPPH78, PK77a].

1-fluoroacetic [BL75]. 10-epoxide [LPP78]. 10.50 [Com77a]. 11-
[WMB75]. 12.00 [Com77a]. 128K [Spa78]. 134 [Cal77b]. 14th [Pub79b].


1971 [BP72, Mar73b, Sla71b, Cal76b]. 1972 [BP73, Cal73b]. 1973
[Slå73b, Sab75a]. 1974 [Cal75c]. 1975 [Lar76]. 1978 [Pub78b, Sti79]. 1s
[ÅSW77, DY73, GMZ73]. 1st [Tho76]. 1st-row [Tho76].

2 [DMS+78, DD71, KPKC73, SL73, Wel71, ZBH+78]. 2-benzeyne [MPS70].

2-matrix [MSL73]. 2-particle [LD71]. 20-parameter [BS71]. 225 [Cal76a].

240 [Cal73a]. 2nd [Cal79b]. 2s [DY73].

358 [Sab75a]. 378 [Lin73]. 3G [ZSR79].

5-fluorouracil [GJP79]. 5-hydroxyindole [WO77].

5-trifluoromethyluracil [PLSL78].
8-dihydrodiol-9 [LPP78]. 8-tetracyanoquinodimethane [DT75].

a-growing [Lak76]. Ab-initio
[KPP77, Meth79, PKT73, ZSR79, HKP79, KPKC73, Kau79b, RL79]. ABH
[TG76]. abnormal [KHH79, KKP77]. abortifacient [KD79b], above
[Enz73]. absolute [CZ79]. absorber [Sch71b]. absorbing [BBT71].

Absorption [HMV77, HMV78, AeAs78, BMD70, Bow71, BHL78, GPC+71, LGM77, NT79, Sch76b, Sch71c]. Abstract [Eig78]. Academic
[Com77a, Com77b]. acceptor [DSM+78, ZV79]. acceptors [SRE+79]. account [MCF+70]. accuracy
[JTR77, MR73]. Accurate
[DS74, MH72, PO77, RS79, YG77, Bar70, CA72, JM73, HS79].

Absorption [HMV77, HMV78, AeAs78, BMD70, Bow71, BHL78, GPC+71, LGM77, NT79, Sch76b, Sch71c]. Abstract [Eig78]. Academic
[Com77a, Com77b]. acceptor [DSM+78, ZV79]. acceptors [SRE+79]. account
[MCF+70]. accuracy [JTR77, MR73]. Accurate
[DS74, MH72, PO77, RS79, YG77, Bar70, CA72, JM73, HS79].
antisymmetric [Sim72]. antisymmetrization [Lin77a].
antisymmetrized [Lya78]. antitumor [Gab76]. Anwendung
[PTUK69, Cal73a]. any [KD79a]. applicability
[DCS77, KP71a, KSP78, SM76b, SM76a]. Application
[APC77, CD74, CSY ±74, Kla78, KR78, LB73b, MMR74, Ner75, Nir75,
OJB77, Pai71, PAC77, Ros78b, Tru73b, ANR75, BBA73, CE73, ES73a, Ell73,
Gra77, Hal75b, DV79, JM76b, JMP78, KL75, Lar79, NI70a, PLYM78,
PGQ77, PKSB78, Rei76, RC70, RC71, RC72, RPK78, SW77, VK74, Bur72,
Bur77, BW76c, Goo76, GL74, LH74, LG75, LGR73, Mel78, NI70b, PNJB78,
PTUK69, RKE79, SPC79]. Applications
[ERW75, Jor75, Lan77, Roe73, Sun75a, WO76, BO73, Chr79c, DL75, HST70b,
Jan76, Joh73, JM76a, KKW73, MS76a, Na78, Pea74b, WO75, BR78, Csi77,
JL70, LG77, MK75a, SDM74, Lar78c]. applied
[BEF78, CS73, Dav77b, EB74, Lar78b, LV71b, LV72, SK71, SC73, Spe73]. Approach
[Ave79b, AB79, Ave79a, Har71b, OJB77, AC76, AM72b, Ave79c,
Boy72b, CPP75, CP77, Csa77b, Del73, DC75, DDD70, ES79, FU76, FBL79,
Fis74, Gab76, Gin78, Har70b, Joh70, Kau76, KKP77, KE79, Lat76, LB79b,
LÖ77, Lin78, Nir75, Pal75, PW79, Pop79, Rout9, SCP79, SP75a, Sha77b,
Sha78b, TB78, TOED79, WP79, ZF76, ZF77, Ano76e]. approaches
[APC77, CL73, Kau77, PAC77, Rat78]. approximant
[CPP75, CM78]. Approximants
[GB71, GBL ±73, Røe73, Røe75]. Approximate
[Csa79a, KP78, NN74, Sco74, SC78a, Abs72, BDP73, CA78, Cas79, CZ75,
DY76, JTR77, JPTM78, KP71a, MDC79, NN77, Nor75, PN76, Sam75,
SWP77, GZ72a]. approximately [KPP77]. approximating
[GG79]. Approximation
[LP74c, OL78, Ara78, BA78, BBP71, BBL72, Bow79, Bre73,
CM75a, CL76, CESW70, Dav72, DF76, DLG79, Ess77, ES70, FFCB79, Fis70,
GP79, GLS79, HLGC73, HNT78, HTG77a, HT77b, KT77, KM76, Lar75,
LV71b, LV72, Läz79, Lin71, Mel78, MLM75, Nol79, NMS77, OL79a,
NC+78, PW74a, RL77, Rat71, SM77, Sco71, Spe73, SS77b, SO77,
Tru73b, Van70, WO76, Wil74]. Approximations
[Kas76, Spe72a, DR75, 1ve74, JW76, Lan74, PK75]. April
[BP70, BP71, BP72, BP73, Pul78b, Sti79]. APW [BK75c, Koe74]. aqueous
[Tal77]. arbitrary [BF70, BW76b, But76, BW76c, CM72a, KK77b, SP75b].
ARCANA [AM73, CAM71, KPK73]. ArF [SD78]. arginine [DAP79].
arising [HT75, Tat73]. Aromatic [LSB+79, BOP76, DEE+75, Her74,
KPP78b, Kl75, LP79a, Mem79, Nec75, PD77, Pul77a, SG77a, Sha78a, UP71].
Aromaticity [BP71]. aroms [Su77]. arrangements [JM76b]. Array
[BL77b]. Aspects [KPP78c, SL70, BS75a, BP70, DEC78, ED79, GSE78,
HC78, KC73, LP79a, SW78, Vol79]. ass [MKT77]. Assessment [Mag79].
associated [EL73, Pop71]. astronomical [Lay77]. Asymptotic
[Kut78, Ra76a, BS71, CS78, DMM75, WB76]. Athylenen [FJP70]. Atkins
[Gos78b]. Atom [Nes75, OJB77, AM74, BK75a, CM72a, CSH74, CH74,
CH75, DCS77, Goo76, JG72, KP76, Kle74b, KL77b, LA70, LKH77, MMS70,
PS73, Pol79, RB77, Rei72a, Sco70, WC75a, WK72, WJC70, WAL71, vDR79].
atom-diatom [KL77b, LKH77]. Atom-molecule [Nes75]. atom-pair [KP76]. atomes [Mar73a]. Atomic [Fla79, GJP79, Lud77, SDS73, Thu75, WM79, Ada73, Ahl77a, BS74a, BS76a, BN74, BT71, BP75b, BEH77a, BEH77b, BL77d, BB77, CL76, CP71, CM78, CA72, CA73, Fis74, FKS76, Fri72, GF76, GBV77, GK76, GL74, GRM75, HKM71, Hea71, Höj79a, Höj79b, IS75, JMM71, JS70, JNZ72, JL74, Kar70a, KZ73, Lan77, Lar79, LG75, LAM71, MMM71, NN72, NN74, PK72, PD78b, Raf75, Rou79, RGM75, SK72, SP79, Sch72, SDD72, ST70, Sim72, SH75a, SHR76, Sl7a1a, SJH79, Sol71, SR72c, SW77, SW78, TGG79, TS71, TNB79, YJ76, JBG70]. atomic-integral [Rou79]. Atoms [Nes71, AZ72, Ave72, BM74, BK76, BW73, BB73, Cal73c, Cal74, CP70, CW77, CL78, Csa75, Csa77b, Csa79b, Dah78, Dea72, DY73, DCS77, DDD70, GGJ75, GB75, GB72, Jak76d, Jam70, JBP76, JP73, Jun78, KM74a, KP72, Koc74, Kol74, Kol75, Lin73, Mar73a, Mi71, MS76b, Mor78, MI78, MDS75, MSM70, MBM71, NS72, Nes70, Nes77, NY76, OK75, PF74, Raf75, Rob71, Rob72b, RS79, RK76, SHO71, ST72, SDJ79, Sin73b, SJH79, Spe71b, Wel77a, Wel77b, Wei79, WR70, WS79, YD75]. attachment [Nes77, SL79]. attack [HPK79, PLSL78]. attempt [BCR +78]. attention [WV74]. attenuation [PP71]. attraction [LR77]. Attractive [GBTB78]. Attractive-dominant [GBTB78]. aufbau [Nov73]. Auger [TNB79]. augmented [ML76, WFS77]. augmented-plane-wave [WFS77]. auramine [BZSD79]. Author [Cal76a, Cal77b, Lar76, Lin73]. Authors [Cal73a, Sab75a]. auto [TGL70]. auto-cohérente [TGSL70]. auto coherent [Gou73]. autodetaching [Sim78c]. autoionization [Naz72]. autoionizing [MCW78]. Automatic [BSZ78]. autonomiterque [BP79]. auxiliary [Gri70, LA76]. Auxin [BCL77]. average [KZ73]. Avery [Lin73]. Axial [Han79, BM71b, RS78b]. axis [Lét74]. aza [Sha78a]. aza-aromatic [Sha78a]. azulene [JL70].
Dah78, DRCT78, DPGC79, ES79, Eue71, Fa79, FGV77, Fin73, HS70a, Hög79a, Hög79b, Hur77, KB77, KMO77, KPO76, LSC77, Lec76a, LCK76, Lev78a, LGR73, LPT+74, Mal71a, Mar73a, Mcd79, MYCT77, MDC79, NI74, OKM74, Pel77, PAM75, RPK78, SNP78, SM74a, SJ79, SC78b, SSH78, TB74, Van74, Wel76, Wel77b, Bur77, DLG79. bath [HMV78].

bathochromic [MP71a].

be [SH75a, Bun77, GF76, Jak76b, RS79, SP75d, SBD+70]. beam [SMMA73].

BeCH [RMB78].

BeF, [SLJ78].

BeH [GG79c, Mul71a].

Behandlung [FJP70].

be [SH75a, Bun77, GF76, Jak76b, RS79, SP75d, SBD+70]. beam [SMMA73].

Behavior [BG76, DMM75, Kut78, Tal77].

bem [KBA76].

bends [BCL79].

beneath [VH75].

benzaldehyde [LM72].

Benzene [SPˇC72, AB73, HG75, KP76, NI70a, NI70b, NT79, PLMB73, San71].

benzene/H [HG75].

benzenes [MR72].

benzenoid [SG77a].

benzo [HKP79, KPPH78, LPP78, LP79c].

Benoz [HG75].

Benozol/H [HG75].

benzomorphans [RW79].

benzocoumarin [MK72].

benzylic [KKM70, NN74].

benzene [MP70].

BeO [SBD+70].

Berechnungen [BKW75].

Bergmann [Cal73b].

BERKELEY [BS78c].

Berlin [Cal73a, Cal79a, Cal77b, ZL78].

Berlin-Heidelberg-New [Cal77b].

Bernard [Shu77a].

Berthier [RCE79].

Beryllium [BS78b, GBV77, Tat73].

Besançon [RMB78].

Berechnungen [BKW75].

Bessel [SW77, SW78].

Best [Jak76a, Jak76b, Jak76c, Jak76d].

Between [Gal72b, Sim77a, AMSS79, Bas78, Cas79, Cha71, CL78, Col79, Con70, Csa77b, Dah78, DCC77, DD72, Dea72, ED79, FM72, Fin73, GJP79, Hal71, PK79, Hg75, Kib75b, KC74, Koc74, Kof74, Kol75, KL73, Kum77, LPP78, LB77, LR77, MM72a, NY76, PLY78, PCL78, PW79, Rob71, SF76, SRE+79, SD79, SE79, Sin73a, SKS77, SS78b, SP71, Suy77, SO77, TTS71, Tie79, WK72, WB76, WV74, WM77, WP79, ZG79].

Beyond [Wil74].

BH [LL72, BS74a, BS76a, EL73, GG79c, MHA70, Mul71b].

Bibliography [RWF571, Sab75a].

bicyclic [BBG79].

bielecronic [Rue79].

Bifluoride [LS79].

big [KSP78].

bimolecular [Ch77].

binary [DV79].

Binding [L78, SL78, CZN70, CD74, CT79, CV73, DAC+79, Eins77, GJL75, Han79, KPD78, Lak75, NKK79, NTT+79, Pul74, PPG76, PP77, PD79, RKE79, SS79, ST78, TNB79, UP71, WRF73, ZL78, KD77].

biocatalytic [JM76a].

Biochemistry [Pul78b, Sti79, BP70, Cal73b].

bioenergetics [Dav79].

biogenic [KM72].

biological [Bai74, BP73, BL79, Cho79, Chr79c, GH79, Hos78, MPMK79, Pau78, PBC74b, SJ79, SLO79, Tal77, Urr78, WCK+76, WOE78].

biologically [BB79, DSS79, Kla78].

biology [Cal76b, Com74, Hal79a, Mar73b, Pul78b, Rei70, Ros74, Sti79, Sun75a].

biomacromolecules [AMJS79, SAM79].

biomembrane [Urr77].

biomolecules [KPP79a, SA79a, PP77, Pul70, RC78].

Biophysical [Har75].

biopolymer [Kho79].

biopolymers [AMJS79, FB72, Lad76, LSS78, Pul78a, Sun74b, Sun75b, ST78, ST79b, Dun78].

Biorthonormal [Dah78, Lat77].

biphenylene [JPTM78].

bipolar [Sal73, SF75].

birefringence [Loc72].

biréfringence [Loc72, DQ77].

birthday [Cal75b].

bisglycinato [RRS75].

bisglycinato-Cu [RRS75].
BISON [WBKL70]. Bloch [Kun78a, KOW78, Kun78b, Wan79]. blocking [KVS79]. BN [SBD+70, ZF77]. body [Bal78, BS74a, BS76a, BWS77, BP78, BFH78, CJCM73, DDD70, Feu77, KBA76, Lev78a, LR77, Lin78, LRJ73, MMM75, Ner75, NY75, Per78, Ros78b, SM70]. Bogoliubov [Cli73]. Bond [Bur77, Del73, Gal72b, Par72, SS71b, Ada77, Bas78, DBBJ76, DMS+78, GN77, Gin78, Hal75a, HR79, JJ78, KHI79, Kle79, Kle70b, LS72, LS79, MPS70, NG73, OK75, Pe77, PNC+78, RTS74, RS76, Sri77, TRS73, TS77, TS78, TS79, TTNT6, Wój76, Woj78, Lar76]. bond-length [TTNT6].

bond-length [TTNT6]. bonded [AM72b, BS75c, CP70, Cho79, Loc77c, TP77a, Wel77a]. bonding [AMC73, ACG74, Bai74, BL75, CP70, Cur77, DS76a, DMS+78, ES73b, GH72b, Har71a, HR79, Mel79, Nir75, PDE79]. bonds [BV072, BK75b, Coo79, Gin78, Loc77d, Sab71, SDD+77]. Book [Ahl70, SC76a, Ahl70, Gra77, LWA74, RCE79]. boundaries [SP75b]. boundary [WO75]. Boundaries [AB73, BL77c, LVDC74, Sin73a, WM79]. boundary [WO75]. Bound [Abd71a, Abd71b, Bur73, LL70, TL79, BR75a, BBK76, BR72, Gra77, JW76, JP73, Lin70, RE70, Vog79, WW71].


Butterworths [Már78]. bytes [Sp78].

C [Com77a, Com77b, SBD+70, PDT77, CV73, ETF79, ED79, GG79c, GBT79, HLYC77, HT15, JKH6b, KP71b, NN72, RAM78, Ros78a, SMP77, Tru73a]. C-C [SMP77]. Ca [KD79b]. cage [Ave75]. Calais [Shu77b]. calcium [AD77, LB79b, NTN+79]. Calculated [KW76, AB73, BL77c, LVDC74, Sin73a, WM79]. calculating [Gin78, HS77, ML76, Nam75, PLYM78, Spe73]. Calculation [BFH74, BW76a, But76, BW76c, Cas79, Com72, FB76, HH77, HNT78, KPO76, Li76, LP74c, LA76, LW76, Loc77a, Loc77b, LL70, Mon77, RR72, SK71, SP75a, SLB77, SH74, Sve79, ANR75, Ahi70, AD77, AFD+78, BNL782, BN76, BSM72, BM73, BS75c, CZNL70, CJ73a, CSFM72, CW77, Chi77, CP72, CL78, CWE71, CE73, CAMC71, CH74, CH75, DRC78, DD72, Del74, Ema74, FRM74, GZ72a, GF76, Gof79, GML77, GBM74, GRM75, Hai73, Har71c, Hos72, ICS74, JR74, Joh75, JPTM78, JS70, JNZ72, KR71, KTO+78,
KBA76, KA76, KT76, LD73, LL75, LGP75, Lin77, Loc76, Loc77d, MCST72, Mes73a, MM72b, MH72, Mu76, MSM70, MBM71, Muk74, MMM75, MS71c, Ner75, NB78, Nin75, NY76, PPK78, Pie71, PK71, PK76a, RBDV77.

**calculation** [RGM77, RPK78, SK72, Sel75, SLC78, Sin73b, SP75d, SSH78, Tru73b, WC75b, Wei71, WFS77, YL74, BCL79, FG79, MMM71, NS73].

**Calculational** [CM72a]. Calculations [Ave79b, AB79, Ave79a, BL77b, BB78, Eld73, Gal72b, Har71b, JE79, LCP76, LZ77, Mak71, PNJB78, PK76b, Sas74, Abs72, Alm74, Als73, ABD+79, Ano78c, ACD+74, Ave79c, Bal74, Bar70, BL77a, BBP71, BBL77, BB72, BK75, BEH77a, Bri73, BB73, BWRD79, CP70, ČZ79, Chr73, Cla70, CM76, Csi76, Cur77, Dan72, DCM74, DRM74, Dau74, DDH78, DE+75, DK77, ESR74, EH73, ED74, FTN77, FBL79, Fis74, FB72, FMZ70, FL79, Gar78, GG79c, GG79b, GG79a, GV77, GBS70, GPP73, GBV77, GMG75, GH72b, GJ76, GHJ77, Hal75a, HS76, Han79, HPK79, Har70b, HLGC73, HSBD78, HPK72, HU74, HCIE75, HS70a, HS70b, Höj79a, Höj79b, Höll77, HP77b, Ive74, JW76, JZ79a, Jor73, JL70, Jun78, KL78, KS73a, KT77, KTO+78, KK72].

calculations [KPKC73, Kau73, KK76a, KK77a, KPP77, KPS78, KPP78a, KPP78b, Kau79b, Kel75, KP71b, KMI4b, Kle70b, KD77, KD79b, KKK79, KL79, LD74, Lan77, Lar75, LFF79, LAV72, Lev78a, Lev70, LKH77, Loc77c, LH79, LJB75, LS74b, Lun79, MM70, MW74a, MEW70, MSDK77, Mch79, ML76, Mey71, ML72, MR72, Moh77, MMS70, MDA78, MM70, NN72, NN74, Nee75, NAR72, Nis77, NMS77, NS78, OM76, Ove73, Pai73, PPC72, PCM77, PS70, PK75, PK77a, PK71b, PGPP79, PLMB73, PK73, PPK75, PK77c, Pul70, RS76, RM77, RB77, RU76, RKO77, Roe75, RL79, RS79, RK77, Ros78b, Rout79, San72, SM73a, SD78, SN79, Sas79, Sha77a, Sha78a, Sim72, SJ79, SDB74, SC75b, Spa78, SF75, TRS73, TS77, TS78, TS79, TP78].

**calculations** [TL71, Tru73a, Van72, Vla70, WJ79, WMB75, WH75, Wei77, WN78, Wel77a, WJC70, Wit72, Wol71, WM77, YG77, DP79, LH77, May74a, NS72, SDB73, Wes79]. **calculus** [Pal75]. **calibrate** [Kau73].

**CAMSEQ** [WH75]. can [Fri72, Hal79a]. cancer [Abd76, DEC78, LL76, SG76a, SG77b]. **candidate** [LPP78]. **Canonical** [WLS77]. **canonically** [Wes73]. **carbenes** [Har71c]. **Carbon** [NT7+79, BWS77, DP79, PGPP79, SD70, WK72, Wil77b]. **Carbon-13** [NT7+79]. **carbonic** [PD79, SS79, SS74]. **carbonyl** [KJ75, ST73, VG78]. **carboranes** [PK77a]. **carboxy** [RL79]. **carboxylic** [KPP78b]. **carcinogen** [HP79, LPP78]. **carcinogenesis** [BS79, Dau77, Her74, Kau74a, Kau79b, LS78, LS79, LÖ77, Mem75, Mem77, Mem79, Pul79a, Ros75, TP77].

**carcinogenic** [HP79, KPP78]. **Carcinogenicity** [SR78, SS78]. **carcinogens** [HPK79, KPP78a, NK79, Nee75]. **carcinoma** [WLS77].

**career** [Ano76a]. Carlo [Cas78b, Col77a, CL78, Col79, RC78]. **Cartesian** [BM71a, GM73a, KOW77, SC78b]. **case** [AP77, BS78, Dmi75a, Dmi75b, Kib75b, MK75b, NRS79, PAC77, ST79a, DRCT78]. **casino** [Fox75].
[Hil79, APČ77, BNLS72, BS78b, KT77, KSP78, KPÖ76, KMLB77, KL79, Lar78a, MW74a, MLB76, ML79, Mey71, NRS79, PAČ77, PCMS77, SH75a, SHR76, Sin73b, WJ79, WMB75]. CIBS [Mcd79]. Circular [Tin79, BCL79, Dub72, MSSF79]. circumvent [LAV72]. cis [TS78, WMB75]. cis-butadiene [TS78]. C1 [Cur78, FM78a, MMR74, FM78a, PK76b]. Class [KK74a]. Classical [FM78a, Dub72, Sch71c, Sch76b, WO74]. classification [KR76, MCM73, MLM75]. Clebsch [KG76, KG77]. Cliffs [Cal76a]. ClO [FM78a, GH72b]. Closed [Hil79, CP72, DK77, Gor71, Gor72, JBP76, KC77, Lai73, MM75, SH73, Sin75, Spe71b, SO77, PAC77, SS73a]. Closed-shell [Hil79, CP72, DK77, JBP76, KC77, Lai73, MM75, Spe71b, SO77, SS73a]. closure [MMD78]. Cluster [Wes73, FCL79, GbK77a, Har77c, Kle77, KGB77, LH76, Lin78, Mat79a, Mon77, Pai73, Rob71, Rob72b, SP79, SLC78, Živ77]. cluster-type [SLC78]. clusters [HP77a, Muf76, NY75, Sin73b, Sla79]. CN [GML77, KJ78]. CNDO [CS74, DMS+78, Duk79, Kau70b, KPKC73, SL73, SS78]. CNDO/2 [DMS+78, KPKC73, SL73]. CNDO/S3 [Duk79]. CNS [BWRD79, KK75]. CNS-active [BWRD79]. CO [LB79a, FM72, EIS77, LK78, PD78a, PD79, RC72, SBD+70, Tru72, VQG78, KTO+78]. co-ordination [FM72]. Cophorpine [KTO+78]. Coarse [MF73]. cobalt [KTO+78]. code [Coo78a, FM79]. coefficient [DH73, JW78]. coefficients [Ah74, Bar79, DH78, KG76, KG77, LV71a, SD79b]. coherence [Kle74b]. Coherent [BK76, Bow72, DMM75, FM78b, Nis77, SK72]. cohérente [TGSL70]. Cohesive [Cal75a, SP75d, ZF77]. coil [Por77, Por78]. collagen [CBV79]. collection [WEH74]. Collective [Wen79, MOV75]. Collinear [vDR79]. Collision [Chr77, Fla79, Kle74b, MFR76, vDR79]. collisions [Ano79o, Ber75, BK75a, CL76, DLG79, MM72a, Mic74, Nes75, RM74, Tru76]. Colloquium [Sim79]. combination [Com77c]. combinations [Sol71]. Combined [SH75a, SHR76, ZF76, Nes75, RCE79]. Comment [Coo78a, Nov73, Pos70, WRS70, Amo71, HMC71, Sab71]. Comments [Bar77, KSL76, Kle74a, CR72, LB79a]. commonality [Kau74a]. comorosan [Bas75]. compact [BW76b, Butter, BW76c, KE79, SH75a]. Company [Ah77a, Lar75c, Sti79, Ano75c]. Comparative [Lec76a, PLYM78, TGG79, Ada78, CL78, Muk74, PD77, TWC73, ABM78, BB74]. Comparison [KPKC73, Kib75a, LCM72, SRP76, SS70, Sla75, Con70, Gin78, Har77b, MK76a, Min79, ML76, PSK77, Tho76, Con72, Fau71, May78, OMC76, RL79, Sch76b, SRP77, SC78b]. Comparisons [Lar78a]. Compatibility [Fan70]. complementarity [RCE75]. complete [Ab72, CLP79a, CLP79b, Sol73]. completely [Sal73]. Completeness [KB77, Dal79, KK76b, LCK76]. Complex [Bar78, CHH+78, Com78, Doo78, Hen76, Jun78, MCW78, Bar70, BFB78, CG78, DT75, FHB77, Hen74, Hen77, Hil79, Joh73, JGT2, KTO+78, Kib75a, MH74, NH0a, NH0b, NB78, Nut78, PLYM78, Re76, RRS75, Sim78a, SP71, Sun74b, Sun75b]. Complex-coordinate [MCW78]. complexes [AMC73, BR78, BV73, BV76, 2000c].
KKW73, Kle70b, LG77, Meh78, MM72b, MSM70, MBM71, MMM71, ÖL79a, Sco74, Sel75, SLC78, TGL70, Vla70, VK74, ZF76]. constant [AB73, BR72, IM73, KL77c, Men71, PGPP79, SEW73]. Constants [TPM70, Csa76, Csa78b, GPP73, JE79, LZ77, Laz79, LG71, Mak71, SP75d, TB74, Tic79]. constituent [KR76, Kla78]. constituents [PGPP79].

constrained [Mor78, MI78, NI74]. constraint [Sch78, CM72b]. constraints [Mor75]. constructed [Ra76b]. constructing [PW74a]. construction [Blo72, Blo73, Jor75, MS75, Pau77, Sab73, MMB70]. contact [HB79, Sim78b]. contacts [Jeh73]. contained [Sur71]. containing [DCS77, Mar79, MM74, SN79, TK78, WRF73]. content [HL78a].


Convergence [Ahl77b, BG76, BK71, DSY74, Sal73, AM77b, AM77a, CJ777, Csa77a, Euw71, FP77, JSC78, KS75, LAV72, TRP77, Ahl70]. convergent [PW74a]. converging [SH73]. conversion [Plo79]. convex [Col77b]. convulsant [AJ79].

CoO [WJ79]. Coordinate [Spe72a, AMC73, Jun78, LV78, MCV78, Na78, Spe71a, Spe71b, SP79]. coordinated [JMP78]. coordinates [CH78, KOW77, Rei76, WRS70]. coordination [RBD77]. Coplanar [GMZ73]. copolyamino [SWF79].

Core [CE73, SHI73, BFS73, KZ73, San72, TP78, YD75]. core-electron [BFS73]. correct [SK71]. correction [Csa79b, Han77a, RB75b, YD75].

Corrections [BMM75, CFHS77, CT77, DC73, Mal71a, Mal71b, PT78, PPI73, YJ76]. correlated [BS70, GL74, Hn78, KM74a, LG75, Meh73a, Meh73b, Pet77, PNC78, Rob71, Rob72b, Sim72, WV74]. correlating [SBD70].

Correlation [BF73, BS74a, BS76a, BL77d, CP71, CPH74, CP75, Con77a, GTBB77, Nes71, Nes77, PCH74, SPC79, Spe72a, Aro78, BB70, BBD73, BP78, BN74, BS76b, CEK72, FU76, Fis75, GL74, Hur76a, Hur77, JMM71, JMP79, JZ79a, eAJ76, KM74a, Kau70a, KP78, KKK77, Lan73, LG77, LG75, Lud71, MW75a, MNN75, MMM75, NES70, Ove71, PA75, PT78, Pet77, PBS76, PKSB78, Res78, Rob71, Rob72b, Rue79, SDD72, Sha77b, Sha78b, SJH79, Spe70, SL70, SW71, SO77, Tat76, WK72, LB73b, RK77]. correlations [BC75, Ran78, Sin73b, SS78]. corresponding [Bur72, RC78].

Cosmic [Fox75]. Cotton [AB73]. Coulomb [AM77b, BK74, Eng72, KKK79, LH74, Lar78b, LC77, SL71, Sur71, TL79].

Coulombic [AF78, PD78a]. couplage [TGS70]. Coupled [BSM72, BM73, GBM74, GRM75, Har77c, HDG71, MM72a, RGM77, BP78, BM75, CP71, HMV77, HMV78, HEB78, Hun74, JZ77, Lin78, Mat79a, Mon77, SPC79, Vog79, Ziv77]. Coupled-channel [MM72a].

Coupled-cluster [Har77c, Lin78, Mat79a, Mon77, SPC79, Ziv77].
coupled-pair [BP78, ČP71]. Coupling
[GO68, HL79, BOP76, BAA73, GPP73, Hal75b, IMN79, JE79, KK74b, KK77c,
Laz79, LRD+77, LRD+87, Mak71, Men71, Shu77c, TGLS70, TB74, GOJ+73].
couer [JM76b, TBB70]. covalent [Ada77, FCL79]. CR [BFH74]. CrF
[KL78]. Crick [Sun77]. Cristal [DQ77]. cristallins [JM76b]. criterion
[JTR77, LCK76]. Critical [BG70, Hub71, BBK76, BS78b, ČZ79]. cross
[Bar79, BG78, Chi77, Fac79, ML76, SSM75]. cross-sections [ML76].
crossing [NB72, Pop71]. crossings [BR75b, BF78]. Crystal [Ave79b, AB79,
Ave79a, Bal71, Loc76, SW71, WN71, AD77, Ave79c, Bow71, Ell73, HP77a,
LFF79, MME79, MCM73, RW74, RT77, SLC78, SW70, Sol73, SS77b, Wol71].
crystal-field [RW74]. crystalline [BL70, CKI75, Euw71, JM76b, Kar78, VK74].
Crystals [Jul78, Sl70a, BF71, Cal75a, DS70a, Dav72, DF76, GMG75, HKM71, JPM78,
Kho79, Kun78a, KOW78, Kun78b, Lip72, Loc77b, MCM73, Sch71d, Spe73,
SM70, TW77, Wö76, Fan70, Cal79a]. Csizmadia [Ano78c, Lar78c]. Cu
[KD77, RRS75]. Cubic [KOW77, Kun78a, KOW78, Kun78b, SS77b]. CuCl
[FWJ+79, KWC79]. cumulene [Ukr72]. current [Löw77]. curve
[Liu71a, MVB75]. Curves
[HL79, Gub79, GBBK77b, Jor75, May78, NS73, PK71, Wil77b]. cut [CM72b].
cut-off [LC77]. Cyanide [Mof79]. cyanogen [Mof79]. cyclic
[Bar77, Kar78, LV71b, LV72, ME78, Ra76a, Sun74b, Sun75b, ST78, ST79b].
Cyclo [RSK+78]. cyclobutane [KC79]. cyclohexapeptide [RSK+78].
cyclopropane [LG77]. cysteinyl [PPC72]. cyt [Han79]. cytochrome
[Har77a, LK77, PL79, RL79]. cytosine [CLP79b, KD77, PZP79, ZR78].

d [AS78, Cal73a, Cal73b, Sti79, AC70, AJK78, MS71b, Rit76, Ros78a,
TP77b, Wei76]. d- [AJK78]. Dancoff [HU74, Lar78a]. dans
[DQ77, TGLS70, TBB70]. Darboux [BG72]. data
[CFMO73, FKS76, SKW72, WEH74, Ahl77a]. dC [PPP79]. decade [Van71].
decay [BYB79, HLMV77, HF72]. decaying [HMM77, HMM78].
decomposition [Jor77, KM76]. Decoupled [NS72, NS73]. Decoupling
[WZ70]. defects [FL79, Lar75, PBPL78, Rou78, SC79]. defining [Fin73].
definite [KR73a, KR76]. definition [Wil79b]. Definitions [Spe71a].
Deformation [Ave79b, AB79, Ave79a, Ave79c]. degeneracies [LG71].
degeneracy [Eng71]. degenerate
[BEF78, BY76, CSA78a, Dmi75a, Dmi75b, IS75]. délocalisation [JM76b].
delocalization [EL73, JM76b, KPP78b]. delocalized [Loc77d]. delta
[CB72]. delta-function [CB72]. demonstrating [RU76]. demonstration
[RR72]. Densities [BHM75, BW73, CG79b, Hen78, HYL78, Lim75a, NN72,
Pai73, Pau78, RR72, Sch73a, Sha77a, Sha78a, Sin75, SM70]. Density
[Ave79b, AB79, Ave79a, Gar78, HS79, Har71b, KL75, LS71, LL70, MW75b,
SL70, SJH79, Spe72a, Spe72b, SS77a, Ada72a, Ada79, AM72b, Ano75d,
Ave79c, BG75, Bun77, CM72b, Ci73, CMF73, Col78, CH77, CES70,
Csa77a, CM75b, DC73, Del74, DD77a, DR75, FM78b, GF76, GH78, Gäs71,
GY75, GP79, GJLL75, GJ76, Han75, Har70b, Har77b, Har79a, ICS74, Ive74, Kau73, KKA78, KP71b, Kry77, Kry78, KR73b, LS70, Lar73, Lar78a, Lar78b, Lar79, MSL73, Pea74b, PS75a, Ros78b, SP75c, SLC78, Spe71a, Spe71b, SC73, SM71, TB78, TW77, YL74, ZF76, ZF77, KOW78, Kun78b, SDB76.

density-matrix [Cli73].
derpendance [TBB70].

Dependence [Bow71, DRCT78, FN73, MDC79, AZ72, Csa75, Fog71, HF72, KMLB77, MP71b, NB78, Nor75, RS78a, RS78b, RS78c, Sco71, Tal77, Tan74, TBB70].

Dependent [MK78, Sch71e, Ahl74, AMSS79, Bre73, Cli73, CESW70, CEK72, Gol73, Han70b, Har77a, HU74, JL70, Kar70a, Kar70b, Kar70c, KFY71, Moc73, RGM75, Sch71b, Sch71c, Sch71d, SM73b, VU79, WA71, Jam70].
depolarization [Urr77].
deprotonation [HL78b].
depsipeptides [Pul74].
derivation [Ada75b, Man77].
derivative [PKSB79, Col79, PW74a].
derivatives [BSZ78, BS79, MPN79, SB75]. derived [RE70].
Desargues [Ran79].
describing [CSDV78, Gos75, PP79].
Description [Koc74, Ada77, Car75, ESG79, GSE78, Kau74b, KN79, LH74, Lar78b, SM77].
descriptions [FM72].
design [Kau79a, ME78, WH75].
detachment [SL79].
detected [MSSF79].

Determination [BS77b, BS78a, BCL79, Boy70a, HE77, JW72, JMP78, KZ73, OJB77, Ben72, LP74b, Pal73, RK77, WB73, BJ73, BJ73].
determining [CD74, CSFM72, MCF+70, MCM73, Sol73].
deux [TBB70].
Development [SC78b].
developments [Mes73b, Mic74, Mic76b, Pai73, PHL+76, Pul79a, Sal79, Tri77].
dG [PPP79].
d'hydrogène [Lei74].
diagonal [Erd78a, ST79a].

Diagram [KE79, Man77, Pau77].

Diagrammatic [SL70, Wil77b, BS75a, WS79].
diagrams [PCH74].
diamagnetic [Ema74, GZ72a, GZ72b, Hal73].
diamagnetism [SM73b]. diamond [SEW73, WESW73, ZF77].
dianion [MW74a].
diatom [KL77b, LKH77].
Diatomic [Jai70, AM77b, AM77a, BR75b, BFR78, Dav72, EB74, FW75, Gia76, Gin78, GJ76, Hal75b, HE77, Hen79, KD79a, Li76, Na78, NS73, PK75, SM73a, S71b, SD+70, Wo76, YG77, vDR79].

Diatomics [NS79b, Dv78, Moh77, Pul78a].

Diatomics-in-molecules [NS79b].
diatoms [CB72].
dibenzo [CT79].
dibenzo-p-dioxins [CT79].
dibenzo furans [CT79].
dichroism [BCL79, Dub72, MSSF79, Tn79].
dielectric [Bre73, Bre75, Csa76, Csa78b].
diene [Par72].

different [Hat71, JS70, Sj77a].
different [CL73, HMV77, Kut78, MK76a, May78, SRP76, SRP77, TB74].

Differential [HTG77a, BKW75, HBE78, PK75, SSM75].

Differences [AJK78].
Difficulties [ML79, BK71, LA72].
diffraction [CFMO73, FM78b, MPW75].
diffusion [Ta77, WRF73].
difluoride [RTM77].
dihydrides [LB73a].
dihydrodiol [LPP78].
dihydrouracil [GJP79].
dilated [Bal78].
dilemma [Kat72, KD74].
dimension [Ada72b].
dimensional [CK73, FY79, RW75, Red79].
dimer [ACG74, BS78b, Dau74, MO77, MHW78].
dimerization [EL73].
dimers [Sch71c, WZ70, Cur77, Wel77a].
dimethyl [LCPP79].
dimethylphosphate
E. [Sla73b]. earth [PBG76, RW74, LB73a]. easier [Col77a]. Easy [Gia73].
Eckart [Jør78]. economic [Bil72]. ecosystem [BCL77]. Ed
[Lar78c, Sti79, Cal79b, Dun78]. edifices [RS78c]. Edited
[Cal73b, Cal75c, Cal76b, Shu77a]. Editorial [Sab75b]. Edward
[Lon73]. Effect [JMM71, KGP79, LRJ73, MK72, NMS77, Nor75, San71,
SSM75, SS77a, SH75b, Tat73, Ave75, Bas75, BN74, BMM75, CHH+78,
ČPH74, DY76, Han71, HT75, JVM78, KN79, KKBČD78, LCPP79, MSSF79,
MG77, PK72, Rei76, SHO71, VHI75, Vol79, YR76, GZ72b, Sch71e]. Effective
[BW76a, Bra75, GJC73, MW75c, ST79a, TP78, TOED79, Wes79, Bra79a,
CW77, Jor77, KK74a, SL79, Wes73, WJC70]. Effectiveness [Sas77, Jak76c].
Effects
[ST73, BBB73, BS79, BL77d, ČPH74, ČPP75, CJCM73, DN75, DBJ74, Han79,
HPW79, KC73, KC77, Klc74b, LC77, Lun77, Mat73a, Mat76c, MVN75,
ME78, Nes77, PCH74, PP74, RKE79, RM72, TP77a, TDB77, WC75a, Wen79].
efficient [GJ76, Koe74, PD78a, ROn79]. EHF
[May74a, MK75b, MK75a, May78]. eigenfunction [HL78a, KD79a].
eigenfunctions [BB73, GTG76, MS75, RB75a]. Eigenproblem [Kun78a].
Eigenspace [ACH72, Car74]. eigenstates [Bri73, Gol79]. eigenvalue
[LA70, KK77d, KKK79, KPˇO76, Lad74a, LH74, LP74a, LG77, Lim76b, LE72, LS74a, LÓ77, LBÁF78, LB73a, LG75, LPT+74,
Lun77, LAM71, MMB70, MW74a, MS71a, Man77, Mar79, MM74, Mat76b,
Mat79a, May74a, May74b, MK75b, MK75a, May78, MLB72, Moh77, NN74,
Nes77, NB78, PCL78, Pau78, Pet77, Pet79, PN76, PBS76, PK77c, PÖ77,
RL77, Rat78, RC70, RC71, RC72, Rob71, Rob72b, RJ73, RB75b, RK76,

effect [ST73, BBB73, BS79, BL77d, ČPH74, ČPP75, CJCM73, DN75, DBJ74, Han79,
HPW79, KC73, KC77, Klc74b, LC77, Lun77, Mat73a, Mat76c, MVN75,
ME78, Nes77, PCH74, PP74, RKE79, RM72, TP77a, TDB77, WC75a, Wen79].
efficient [GJ76, Koe74, PD78a, ROn79]. EHF
[May74a, MK75b, MK75a, May78]. eigenfunction [HL78a, KD79a].
eigenfunctions [BB73, GTG76, MS75, RB75a]. Eigenproblem [Kun78a].
Eigenspace [ACH72, Car74]. eigenstates [Bri73, Gol79]. eigenvalue
[LA70, KK77d, KKK79, KPˇO76, Lad74a, LH74, LP74a, LG77, Lim76b, LE72, LS74a, LÓ77, LBÁF78, LB73a, LG75, LPT+74,
Lun77, LAM71, MMB70, MW74a, MS71a, Man77, Mar79, MM74, Mat76b,
Mat79a, May74a, May74b, MK75b, MK75a, May78, MLB72, Moh77, NN74,
Nes77, NB78, PCL78, Pau78, Pet77, Pet79, PN76, PBS76, PK77c, PÖ77,
RL77, Rat78, RC70, RC71, RC72, Rob71, Rob72b, RJ73, RB75b, RK76,

effect [ST73, BBB73, BS79, BL77d, ČPH74, ČPP75, CJCM73, DN75, DBJ74, Han79,
HPW79, KC73, KC77, Klc74b, LC77, Lun77, Mat73a, Mat76c, MVN75,
ME78, Nes77, PCH74, PP74, RKE79, RM72, TP77a, TDB77, WC75a, Wen79].
efficient [GJ76, Koe74, PD78a, ROn79]. EHF
[May74a, MK75b, MK75a, May78]. eigenfunction [HL78a, KD79a].
eigenfunctions [BB73, GTG76, MS75, RB75a]. Eigenproblem [Kun78a].
Eigenspace [ACH72, Car74]. eigenstates [Bri73, Gol79]. eigenvalue
[LA70, KK77d, KKK79, KPˇO76, Lad74a, LH74, LP74a, LG77, Lim76b, LE72, LS74a, LÓ77, LBÁF78, LB73a, LG75, LPT+74,
Lun77, LAM71, MMB70, MW74a, MS71a, Man77, Mar79, MM74, Mat76b,
Mat79a, May74a, May74b, MK75b, MK75a, May78, MLB72, Moh77, NN74,
Nes77, NB78, PCL78, Pau78, Pet77, Pet79, PN76, PBS76, PK77c, PÖ77,
RL77, Rat78, RC70, RC71, RC72, Rob71, Rob72b, RJ73, RB75b, RK76,
SHI73, San72, SM73a, SM76b, SM76a, SD78, Sar75, SPČ79, SM71a, SM71b, SM71c, SLJ78, SMH77, SG77a, Sha77b, Sha78b, SS73a, SS73b, SM75, Si7l, ST70, Sin73b, SS71a, Sla70b, SJH79, SR72c, SBM70, SMW71, TS71, TNB79. electron [TOED79, WMB75, WRS70, WV74, YL74, ZV79, SL79, SDS73, Com77a]. electron-atom [CM72a]. Electron-conformational [VGS79a]. electron-density [CFMO73]. Electron-intramolecular [LRD+77, LRD+78]. electron-lattice [CS72]. electronegativity [Joh77, MR72]. Electronic [AFL78, BT78a, CT79, CSR79, Chr79a, Duk79, EP71, Fau71, Fau76, FWJ+79, GPC+71, GML77, GL74, KMO77, KWC79, LSS78, LF77, LGM77, LM72, LG75, LV71c, MW74a, MHWC78, MH78, MOV75, Nes70, Nes71, Pet78, Pop71, Rit76, RL79, SM79, SM79, Sto71, Ukr72, AeAs78, AN75, Ada75a, AMS79, BF71, Boy72a, BS78c, Bur77, Car75, CSFM72, CS76, ČPP75, CR72, CL78, CK74, CS78, De 78, DD77a, DM72, Fin73, FBL79, GP79, GK75, Har78, HS70a, Hin77, Hop78, HT75, HR76, JR74, Joh75, JW72, JG72, Kau74, KR71, Ke75, KJ75, KL77a, KC74, KD79a, KU70, KS79, Lad75b, LL76, LVDC74, LP79a, LFF79, LKK+79, LE72, LÖS73, LK78, LS79, Lud71, Lud75, MP79, MS72a, MS74, MCF+70, MCM73, Mic76b, ME78]. electronic [MR72, NS75, NT79, Pai71, Pal75, PH77, Pet77, PNC+78, RM79, SHO71, SP74, SP75b, SLB77, SLC78, Spe73, SWP77, SG76a, TB74, Tho76, Tr73b, Tr73a, VG78, WS79, ZF76, LL72, PLSL78]. Electronic-structure [KMO77]. Electronically [FM75, BS75c]. électronique [LL72]. Electrons [JBC70, TW77, AL71, BKW75, Col77b, GGJ77, Hil79, KMLB77, Lin71, MK76a, SM75, SK77, SM73b, Tat76, TL71, Wan79]. Electrophilic [Men75, Mem79, HG75]. Electrostatic [CM75a, CFHS77, HKP79, NS79a, SS73c, DRCT78, GPP79, Kih75b, OMC76, PPP79, PT75, PPP78, PD77, PZP79, SBB79, GJP79]. Elektronenpaars [BK75]. elektrophilen [HG75]. element [Sha78b]. elementary [Bra79b, Cz79, Lan74, Re70]. Elements [Gal72b, HL79, Sas74, DD72, Dav74, HBB77, HLGC73, KR73a, LS74a, Nis77, Oda73, PW79, PN76, Pos78, RCE75, Sur71, Tr72, WG74, Wt76, WP79]. Eleventh [Pul78b, St79]. elliptical [LGR73]. Elsevier [Ahl77a, Ano78c, Lar78c]. elucidation [Pul77]. embedded [Dmi75b]. embedding [BHL78]. emergence [Pae74a]. emission [GK75]. emitted [He71]. empirical [BBL77, CAMC71, HLYC77, LÖS73, NMS77, San71, San72, SM77, SG77a, WJC70]. End [RBDV77]. End-on [RBDV77]. endowed [KMT77]. energetic [KC77]. energetics [VU79]. énergie [BJ73, BPTLM73, eAJ76]. Energies [OJB77, Abd71a, Abd71b, BM74, BJ73, BP75b, Cal72, Cal73c, Cal74, CM72a, Cas79, CJ77, CP72, CR72, CAMC71, CV73, DGC77, DCM74, DMR74, Dau74, GJP79, GBT79, GLS79, Gln78, Hal75a, Har77c, HE77, Jak76d, JMP79, JSC78, KZ73, Kau70a, KPCK73, Med79, Mey71, MDS75,
Muk74, MMM75, Nir75, PT78, PNC78, Rit76, SHO71, SBBM72, SP75d, SO77, Tai77, TNB79, Tru73b, Tu75, Tu78, WJ79, ZR78, ZBH78. **Energy** [BG75, CD76, DL75, Dau72, DF76, FY79, HF72, Jia70, KKA78, Lad70, Lad76, LL70, LB73b, OK75, Sch71a, SW71, TC70, Wan79, AF73, BBS73, BA78, BS74a, BS76a, BNL72, BZSD79, Bor70, Bor74, BPTLVM73, BEF78, BFH74, BWRD79, CZN70, CB72, CJ73a, CJ73b, Cha71, CL76, Col74a, CESW70, CEK72, CH74, CH75, CZ75, DMS78, DEC78, EL73, EH73, Eng71, Euw71, FN73, Gar74, GTBB77, Gra77, GBK77b, HS76, Han77a, HSS75, Hen79, Hol77, JTR77, JZ79a, Jor75, eAJ76, KS73a, KP71a, KP76, KM76, KDD79b, KBK72, KP78, KKK79, KMLE77, Lad74b, Lar78a, LV71b, LV72, LW77, Lin77, LG70, Lip72, MP71b, Myn78, MDA78, Myf76, NY76, PT78, PCC72, Pet78, PK71, PD78b, Ppop71, RU76, RKOU77, RE70, Rue79]. **energy** [San71, SP75a, Sco71, SDD72, SW70, SB78, Spe73, Sri77, SP77, SK79, SL73, SO77, TB78, TTS71, TDB77, Vog79, WK72, WS75, Wei77, WN78, We176, Wel77b, WS79, WFS77, WM79, ZSR79, CT77]. **Energy-band** [Lad76, Pet78]. **Energy-based** [TC70]. **energy-dependent** [CEK72]. **energy-localization** [Eng71]. **Energy-shifted** [CT77]. **energy-spectrum** [WFS77]. **England** [Com77a, Com77b]. **Englewood** [Cal76a]. **Enhanced** [Ave75]. **enhancement** [Gol70]. **enhancements** [BC76]. **enol** [ZR78, ZBH78]. **ensemble** [BHLM78]. **enthalpy** [BCR78]. **entropy** [HˇCZ79, Pri75, Sch76a]. **environment** [ST73]. **Environmental** [TP77a, PP77]. **environments** [Boy70a]. **enzymatic** [BCR78]. **enzymatically** [LHK77]. **enzyme** [Gol70, LP79b, VGS79a, WEH74, Ano76c]. **enzyme-catalyzed** [WEH74]. **enzymes** [AMSS79, LKK79]. **epieptic** [Wal77]. **Epoxide** [PDEB78, LP77, LP79c]. **epoxides** [LP79a, PDE79]. **Equation** [Lib70, TN73, Ada73, Amo71, Bie75, Csa79a, ESG79, Fro79, Hen77, Koe74, LA70, LWA74, NS75, Nor75, PW74b, PW74a, RL77, SII73, SII71, VB72, WA71, We70, Wel71, WZ70, WAI71, Woo72, YL74]. **Equations** [FG79, HY78, Ada78, BEH77b, Cal79c, Cli73, DSY74, DR75, FW75, HS78, HBE78, JMI73, Kar70a, Kar70b, Kar70c, KF71, Lai73, Lan73, Lim74a, MLB73, May74b, MK75b, Mes79, Ner76, SA77, SIM75, SS71a, SD74, Živ77, Sim77a]. **Equations-of-motion** [FG79, DR75, SIM75]. **equilibrium** [DN75, Sim78b, SP75d]. **Equivalence** [JD74, HT75, SHO71, SDB76]. **Equivalence-restricted** [JD74]. **Equivalent** [GÓ69, GÖ77, Sch77b, BS74b, DN75, PW74b]. **Erich** [Ano77, Par77]. **Errata** [GZMM73, GÖ77]. **Erratum** [Mey75, PA77, SRP77]. **Error** [LTR74, BS77b, BS78a, Col77a, JW76, KA76]. **Errors** [HS76, SP77]. **ESCA** [BL77c, Con72, WK73]. **ESR** [MS71b]. **esters** [Kla78]. **estimate** [CS74]. **estimated** [JZ79b]. **Estimation** [BYB79, LSOC77, PT78, DMS78, LB73b]. **état** [BJ73]. **états** [BJ73]. **ethers** [DBB76, GBS70, GBS70]. **ethidium** [PL77, RKE79]. **ethyl** [MEW70, OMC76]. **ethylating** [HPK79]. **ethylcarbonium** [TWC73]. **ethylene** [CSR78, FWF77, FJP70, HMC71, MMD78, PDEB78, Rat71, Rou74, TS78, WC75b, Wes79]. **etiology** [Kau74a]. **Etude** [DQ77]. **etudié** [TGSL70]. **europium** [Fog71, Liu71b, SKS77].
evaluate [PD78a]. evaluated [SHI73, Sla79]. evaluating [Jet73].

Evaluation [BR78, Che71, DDH78, BOP76, BSG77, Col79, eAJ76, Sha78b, ST70, PAM75, Pos78]. Evaluations [Sha76]. even [Raf75, Sar75].

even-tempered [Raf75]. evidence [Feu77, Oda73, Pet78]. evidenced [Lar75]. Evolution [Sun74a, BF75, DS79]. evolventibus [BP79].

Examples [BG72]. Exchange

[GMZ73, SW71, AM77b, BYB79, CJ73a, CJ73b, CESW70, CEK72, Csa75, Dan72, ES70, Hit70, Iye74, Kle70a, Lin71, LPT+74, Ove73, Pie71, Sco71, Si71, SW70, Sl71a, SC78a, Suz77, Tat73, SJH79]. exchange-correlation [CEK72].

Exciton [Par72].

Excitons [MBMM79].

Expectation [BSG77, BL77d, SK71]. experiment [BP72, Ber75, Gin78, IZZ+77]. Experimental [Rob72a, Con70, Coo78a, Nes75, Sin75, Feu77]. Experimentalist [WBKL70]. explicitly [Sim72]. explore [PBC74b]. explore [SDD+77].

Expansion [Dal79, Ada72a, Ada79, Csa77a, Ema74, FB76, GPP79, Gra77, HNT78, Lin70, Man77, MHPS70, Mat71a, Mcd79, MW75c, Rob71, Rob72b, RK79, SR72a, Sal73, SR72b, SP79, WS79, You75].

Expanded [Ber73].

Faraday [Ave75].
[Sab75a]. fast [TS71]. FCC [KOW78, Kun78b]. FCO [TB74]. Fe
[BMD70, GML77, MSSF79, Har77a]. features [RU76]. Feenberg [GS70b].
Fehlerminimierung [KA76]. Fermi
[Csa79a, GY75, Goo76, YG77, Bie75, Csa77b, Csa79b, DH76, GGJ75,
Han70a, Han7a, HB79, KW76, Lun75, PN71, SKW72, SC73, WC75a].
Fermi-like [GGJ75]. Fermion [Col71, Col70, GH78, Per78]. fermions
[Bow72]. ferrimagnetic [Fog71]. ferroelectric [CHHS74, HCIE75].
ferromagnetism [MCP73]. ferrous [LK78, RL79]. Feshbach [LKH77].
Feynman [CD71, NRS79, TG76]. FH
[Lei74, ST72]. Fibrous [GK78]. Field
[GO68, G ¨OJ +73, Sla70a, AD77, Bal71, BKS79, BM73, Bow71, CE73, DS74,
DL79, El73, Gou73, Gra77, GL74, Hac74, Hal78, Har71c, HP77a, HDG71,
Hor71, JL74, KK73, KK74b, KK77c, LGP75, LG77, LG75, NaN78, Nir75,
PS75a, RW74, SF76, Sch71a, Sch71b, Sol73, TGSL70, WN71, Wan79, Wol71].
fields [DL75, G ¨as71, LL73, MGM78, NaN78]. Fifth
[Ano78d, Boy70b, BM71a]. Fifth-rank [Boy70b, BM71a]. Filled [Bee76].
filling [Kau79b]. final [Rot73, Tru76]. Fine [BK77]. Finite
[HB79, BF70, Blo72, Blo73, ES79, Fae79, FW75, FU76, KE79].
finite-difference [FW75, FU76]. First [CH74, JBP76, Lip72, NRS79, Bun77,
Cal74, Coo79, CH75, DGC77, Gou79, GL74, Hs76, Lan73, LF77, Lazz78, LZ79,
MCST72, Moc74, NG73, RB77, ST72, SC73, Van71, Wel77b, Raf75]. first-
[Moc74]. First-Order
[JBP76, NRS79, Coo79, HS76, Lan73, LF77, Lazz78, LZ79, SC73].
first-principle [CH75]. First-principles [CH74]. first-row
[Cal74, DGC77, NG73, ST72, Raf75], five [AMC73]. five- [AMC73]. fixation
[NPL +79]. fixed [KM74b, Loc77a]. flexible [DSMM79, LJB75]. Floating
[AM74, HP77b, RMB78, TL71, AF73, AM72a, ADDLG76, RR77].
fluctuation [Bra79b]. fluorescence [AZ72]. fluoride
[AD77, Lei74, ST78, VG78]. fluorides [PK77c]. fluorinated [KR73b].
fluorine [SDD72, WRF73]. fluorine-containing [WRF73]. fluoro [BL77c].
fluoro- [BL77c]. fluorooxacetic [BL75]. fluoronium [Lei74]. fluorosulphate
[HS70b]. fluorouracil [GJP79]. fluoruro [Lei74]. fluxional [TB73]. FNO
[HR79, MG77]. Fock [BR78, Bre73, Cli73, MM73a, SS71a, SD73, BMM72,
BM73, BMM75, BEH77b, BK71, Bur72, Bur73, DSG74, FW75, FS70, FS74,
GHS79, GMG75, GBM74, GRM75, HKM71, IVE74, Jam70, Jor73, JL70, JL74,
Kar70a, KKA78, KM76, KT76, KBK72, KMO77, Lai73, LS70, LS71, LS75,
Laz78, MHP70, MN79, MLA73, May74b, M279, Mes73b, MW74b, Mes78,
Mes79, NN72, NN74, NS72, NS73, OKM74, PCL78, PS73, PS70, PKSB79,
RS79, RGM77, SA77, SH73, SLB77, SD79, SDB74, SDB76, SB78, Spe71b,
SP75d, SEW73, TTN76, Tru73a, Van70, Vog79]. fold [L ´et74]. folding [PF79].
follow [BCR +78]. fonction [BPTLVM73]. fonctions [eAJ76]. fundamental
[BJ73]. forbidden [TH78]. Force [MM78, CJCM73, KP71a, NaN78]. forces
[Abd71a, AM77b, Bri70, Cla71, FY71, GK78, Jeh73, KKW73, MAL71a,
Mal71b, Pie71, RM72, RM73, RMP71, WB76]. forcing [JSC78]. form
Formaldehyde [DRCT78, LED73, Tan74].

Formal [Bra75, Bra79a].

Formalism [ADDLG76, ACD+74, Car74, CDEO76, Com77c, CE73, Feu77, GP74, GJLL75, GJ76, KP72, Min79, Mor75, Sac72, TC70, ZF76, ZF77].

Formalisms [Mic76a], formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formamide [PK76b, LB˚AF78, OSL77, OSL77].

Formation [BB70, HČZ79, Kho79].

Forming [Mor75].

Forms [GPC+71, Kob78, KL79, LH76].

Formula [CA78, JW78, MHR76, Tu77, Tu78, WW71].

Formulas [BSG77, BSZ78, CM78, Gor71, Gor72, Har77a, Hos72, KE79, Spe71a].

Formulation [Cli73, HST71, KPJM70, Lar79, Mat74a, Mat76b, Mat79a, MW74b, Nel79].

Formulations [KC74].

Formic acid [SP75c, SJH79, SMW71, TB78].

Formaldehyde [DRCT78, LED73, Tan74].

Formalism [ADDLG76, ACD+74, Car74, CDEO76, Com77c, CE73, Feu77, GP74, GJLL75, GJ76, KP72, Min79, Mor75, Sac72, TC70, ZF76, ZF77].

Formalisms [Mic76a], formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].

Formalism [Bra75, Bra79a].

Formally [NG73].
Lim76a, Loc77a, Lud75, Lud77, Meh73a, Meh73b, MDC79, Moc74, MK76b, MM72b, Mos73, MSM70, MBM71, NaL78, Ner75, Pau77, Pol79, Pop71, RWFS71, Rob71, Rob72b, RK76, Sab75a, SDD+77, SH73, Sch78, Sch72, SC76a, Sco74, Sha76, SS73a, SS73b, Sim72, SH75a, Sha70b, SC78b, SW77].

**functions** [SW78, SWP77, SSH78, Tan74, Tru72, Tru73a, Urr78, VB72, VF76, Wel76, Wel77b, Wit76, WV74, Mos73, Pos77]. **fundamental** [HPK79, Kau79b, Ful74]. **fundus** [JG74].

**Future** [Sla73a, Ost79].

G [Ano78c, Cal76a, Cal79b, Lar78c, Mår78, Sab75a, IMN79, Nam75].

**Galerkin** [Jan76]. **gallium** [Fog71].

**gallium** [JG74].

**Gaussian** [AF73, ADDLG76, BBP71, BP74, BSG77, DPGC79, EUW71, GM73a, GM73b, Hal76, HS70a, HP77b, JP73, KC72, KC77, KSP78, Lec76b, Lo75, LA76, MEW70, Mat71a, Mat73a, Mat76c, MYTC77, NY76, OK75, PAM75, Pos77, RA75, RR77, RMB78, RM72, RS78a, RS78b, RS78c, SBB79, SC78b, TB74, TL71, Van74, Van70]. **Gaussian-Lobe** [RS78a, RS78b, RS78c]. **Gaussian-type** [Lec76b, Mat73a, Mat76c, NY76].

**Gaussians** [FHP70].

**Geminal** [SPˇC72].

**geminals** [Lya78, LB73b].

**genealogical** [GTG76].

**General** [ADDLG76, KSP78, Gar74, Hac74, Jak76a, JG72, JNZ72, KR73a, Kau74b, Kib75b, PW74a, Rob72b, SP75a, ACD74, BS78, BS78c, Car74, Kle77, Lar79, N70a, Rob72b].

**Generalization** [GHS79, K73b, SL79, DSG74, Ste77]. **Generalized** [CGRC74, Car72, Hal78, Hal79b, Joh70, LG70, RT77, RK76, Sch76a, Suz77, Ahl77b, CW76, FM79, LA70, LWA74, Lev78b, MW74b, Pet77, PNC78, RC70, RC71, RC72, SB75, SL70, Tu75, Tu78, Van74, WAL71, Woo72, SC76a].

**Generalized-molecular-orbital** [Hal78]. **generated** [BW76a, HKP79].

**Generating** [Wit76].

**Generation** [GTG76, BL77a].

**generator** [LV78].

**generators** [Lar75, PW79, WP79].

**genetic** [Coo78a, Coo78b, FM79].

**Geometric** [BB71, HT77b, L79, Har77b, HTG77a].

**geometries** [Z78, ZBH78].

**Geometry** [Har79a, JZ79b, AF73, AMSS79, BS78, CD71, CL79a, CL79b, FWFM77, JR74, LK78, TT70b].

**gerichteter** [BK75].

**German** [Ahl70, BKW75, FJP70, HG75, KBA76, KA76, PTU79, Sch73b].

**giant** [Cal79a, Jul78].

**Gly** [G68, G73, KML77, May78].

**Glauber** [GLS79].

**globular** [MME79].

**Gly** [BWRD79, CB79, RSK78].

**Gly-Pro-Pro** [CBV79].

**glycin** [DEC78, RRNS75, RRS75, RC78].

**Glycosyl** [SY77].

**glyoxal** [DEC78, DAP79, ED79, LDP79, OS77].

**glyoxalase** [SWF79].

**glyoxals** [Abd76].

**glyoxylase** [LP79b].

**Goldstone** [LH76].

**Gordan** [KG76, KG77].

**Goscinski** [Shu77b].

**Gradient** [Gar74, CE73, LGP75].

**gradients** [RPK78].

**Graph** [Ran78, RW79, Sh77b, Ran79].

**Graph-theoretical** [Ran78].

**graphical**
[APČ77, LH74, Lar78b, PAČ77, PW79]. graphs [Ran79].
[CSH74, BSS78, BKST79, BBA73, CP72, HR76, LD71, LF77, Lau79, MHRST6, MHRST77, Ner75, PBPL78, Rat71, Sco74, VB72, WFS77]. Ground
[Bra79b, OL78, SDT73, Spe72a, ADDFL71, BWBS77, BJ73, BS70, BP75b, Bun77, Cal72, Cal74, DRCFT78, Fis75, GL74, IVE74, Kol74, KÖT71, Kut78, LH74, Lar78a, LEC76a, LEC76b, Lin77, LG75, Man77, MCTST72, Mul71a, OL77a, PS70, RB77, RS79, RS78b, SK71, SK72, SM+,79, SH75a, Sin73b, SD70, SDB74, Tan74, Tat76, WKT3, WRS70, Wil77b, WB73, Hal79b].
ground-state [IVE74, Sin73b, WB73].
Group
[BDT77, CSFM72, Hub77, KR76, MCF70, MCM73, TB75, BDT79, BF70, Boy72b, Boy72c, Cor72, ES73a, FMZ70, JS70, Kle70b, LP74a, Mat74a, Mat76b, Mat79a, Meh73b, Meh78, MM77b, Nel79, Nov73, Oda73, Pal75, PW79, PTUK69, PS79b, Rei72b, SDD+77, Sha77b, Sha78b, ST73, TP77b, WP79].
group-function [Meh73b]. Group-theoretical [CSFM72, MCF70].
Groups
[Gal72a, Blo72, Blo73, BW76b, But76, BW76c, Flu72, Gal74, GP72, KG76, KG77, KE79, KK77b, LP79c, Lét74, Lim77b, Ros78a, SAM79, Sin73c, ST73c, SLOKP79]. growing [Lak76]. growth [BC75, MDA78]. gruppen
[Wyb73b]. Gruppentheorie [Cal73a, PTUK69]. guanine
[HPK79, KD77, LPP78, PLYM78, PZ79, ZBH+78]. GVB [PNC+78].

Hamilton
[TL72]. Hamiltonian
[AC76, Abs78, CK74, DD72, Feu77, HL78a, Jør73, KS72, KK77d, ML75, MMM75, WJC70]. Hamiltonians
[BW76a, Bra75, Bra79a, CS78, Han70b, Rei72a, Sac72, Wes73, Wes79].
Hammerstein
[PW74b, PW74a]. Handbook
[FKS76, Atk74, Atk91, Gos78b, Ahl77a]. handed [SY77].
handedness
[DS79, SY77]. hard [GH72a, Wei76]. hard-sphere [GH72a, Wei76].

H
[Bur77, DY73, GG79c, HG75, HLYC77, JŽ79a, KP71a, Koc74, Lar76, RR77, RW75, RKOU77, Sab75a, Sla71b, TG76, SY77, ASW77, ÅS71a, Adä78, Ada73, Ada77, AM72a, AM74, AM77b, And79, BB74, BC79, BDT77, CJ73a, CJ73b, Doo78, EHT3, FMZ70, GG77, HNT78, HG75, HP77b, JTR77, JE79, JP77, KR71, Kat72, KSP78, Koc74, Kut78, LB79a, Lec76a, Lec76b, LTR74, LG77, Liu71a, LG73, MS71b, MM72a, MG77, OSL77, RW75, RS79, ST72, SHR76, Spe72a, SW77, TS77, TBB70, TG76, Tru72, Tru73b, Tru73a, TS72, WB73, You75, TBB70]. H-like [AM72a, AM74]. haemoglobin
[Har71a]. Hafner
[Lar76]. Half
[SD73, SDB74, SB78, SDB76].
Half-Projected
[SD73, SDB74, SB78, SDB76]. halide [Fla79, Moh79].
halides
[BB72c, CKD73, JM76b, LVDC74, LR73, LPT+74]. Halkjaer
[OL79b]. Hall
[Cal76a]. halogenated
[DBBJ76]. halogens
[Hall75b]. Halogénautes
[JM76b]. HAM
[AFL78, LBAF78]. Hameka
[Lar76].
Hamilton
[TL72]. Hamiltonian
[AC76, Abs78, CK74, DD72, Feu77, HL78a, Jør73, KS72, KK77d, ML75, MMM75, WJC70].

Handbook
[FKS76, Atk74, Atk91, Gos78b, Ahl77a]. handed [SY77].
handedness
[DS79, SY77]. hard [GH72a, Wei76]. hard-sphere [GH72a, Wei76].

hardcover
[Gos78b]. harmonic
[Bas78, DR77, Hun74, RB75a, WO75, ST79a]. harmonics
[KOW77, Sch77b, SR72c, SF75]. Hartree
[BR78, Har78, Jam70, Jør73, KKA78, KMO77, PS70, SD73, BBK76, BSM72, }
BM73, BMM75, BEH77b, BK71, Bre73, Bur72, Bur73, Cli73, DSG74, FW75, Fis70, Fis74, GHS79, GMG75, GBM74, GRM75, HKM71, Iv74, JL70, JL74, Kar70a, KM76, KT76, KBK72, Lai73, LS70, LS71, LL75, Laz78, Lim74b, Lim75a, Lim75b, Lim76b, Lim78b, MPH70, MN79, MLB73, May74b, Mcd79, MBB73a, Mes73b, MW74b, Mes78, Mes79, NN72, NN74, NS72, NS73, OKM74, PCL78, PST3, PKSB79, RS79, RGM77, SA77, SH73, SLB77, SDJ79, SS71a, SDB74, SDB76, SB78, Spe71b, SP75d, SEW73, TTN76, Tru73a, Van70, Vog79]. 

Hartree-like [Har78]. Having [Lét74, SP75b]. HBCh [RMB78]. HBeCH [RMB78]. Having [L´et74, SP75b]. HBF [TB74]. HCl [PK76b]. HCO [TB74]. He* [RM79]. He-like [BS71]. He-sequence [MMS70]. Heats [GTBB77, GBT79]. Heavier [HLGC73]. Heikes [GTBB77, GBT79]. Heidelberg [Cal77b]. Heisenberg [GbK77a, SHI73, SK73, SL70]. Heitler [Aba72, Ada77, Ano77-28, LP74a, LP74b, Wil77a]. Heitler-London [Ada77, LP74a, LP74b, Wil77a]. Held [BP70, BP71, BP72, BP73, Pul78b, Sti79]. Helical [IZZ79, KP79a, SY77, Urr78, VU79]. Helices [VBC78]. Helium [BG70, LP74e, AC70, BK74, CL78, DD71, HG78, LA70, MC78, SK71, SK72, SE79, Spe70, Tat76, WAL71, YD75, Pel77]. Heliumlike [Lin70]. Helix [CC79, DS79, Meh79, PPP79, Por77, Por78, PZP79, SY77]. Helix-coil [Por78]. Hellmann [CD71, NRS79, PF74, TG76]. Hellmann-type [PF74]. Helmholtz [SF75]. Heme [DAC79, Eis76, Eis77, LK78]. Hemoglobin [Sal72]. Hemoproteins [MSSF79, KN79]. HeNe [SBD70]. Hertmann [HC72]. Hermitian [Gou73, Han75, Hen77]. Hermitien [Gou73]. Heteroatoms [SN79, SG77a]. Heterocycles [KRKS78, Rou73, Rou74]. Heterocyclic [BP70]. Heterogeneous [Sal79]. Heteronuclear [AM77a, Tyu78]. Heteroorganic [Hil79]. Heuristic [HSDB78]. HFS [HC72]. HgI [HLGC73]. High [Mal71a, Mal71b, KTO78, Lib76, Sch76b]. High-spin [KTO78]. Higher [RB75b, SB75, GbK77a]. Highest [FG79]. Highly [He78, KH79, SC76a]. Hilbert [Lan77]. Hill [Lin73]. Hindered [DMS78]. Hirschfelder [CJS77]. Histamine [MHH74]. HKS [Har79b]. HL [CSMF72, FM72]. HNO [HR79]. Hoffmann [Mat76a]. Hole [BFS73, BK74, Cs75, LD71, LH74, Lar75, Lar78b, MW77, Rat71, Wen79]. Holes [Csa78a, Res78]. Holland [Sti79]. Homogène [Mar73a]. Homogeneous [Mar73a]. Homonuclear [vDR79, Tyu75]. Homopolymers [FB72]. Homopolynucleotides [SL73]. Honour [Cal75b]. Hoping [Fro79]. Hormone [MDA78]. Hovi [Cal75b]. HP [LL72]. Hubbard [FN73, Mat76a]. Hückel [Mat76a, AM72b, Als73, Ano77a, BRS75, CFH77, EB74, Han79, KPK73, Par77, SDM74, SS74, Tri77]. Hulthén [Cha77, GB72]. Human [Har75, WLS77]. Humanities [Cal73b]. Hund [Ano77a, Par77]. Hurle [Com77a, Com77b]. HY [SH75a, SHR76]. Hybrid [Lec76b, Loh76, DF76, Eng72, MI78, Pol70, Sil71]. Hybridization [Ran74, ACC76]. Hydration [LCPP79, LDP79, PP74, PA74]. Hydrazines
[GPC\textsuperscript{+71}]. hydrazyl [GPC\textsuperscript{+71}]. hydride [Bur72, DCS77, MVN75, SDB74]. hydrides [DGC77, DSC\textsuperscript{+77}, KC77, NG73, PK77a, PK77c, Swi71]. hydrocarbon [GBTB78, Her74, KT76, NN72, GG79b]. hydrocarbons [BOP76, BK71, CPH74, DDBJ76, DEE\textsuperscript{+75}, GBT79, LP79a, Mak71, Mem77, Mem79, Muk74, NMS77, NS78, PCH74, PD77, Pul79a, SG77a, SR78, TP78, TTN76, TSE76, UP71]. hydrodynamic [SE79]. Hydrogen [ACG74, BL75, BK75b, PPI73, YR76, AM74, AM72b, Bai74, BR\textsuperscript{+75}, Bas78, BS75c, BFH74, Cho79, Coo79, CSH74, Cur77, DDBJ76, DMS\textsuperscript{+78}, Dea72, GZ72a, GZ72b, GGCK79, HKM71, Koi74, Koi75, KMO77, KGB76, Lei74, Lib76, LS72, Loc77c, LS79, Mal71a, Meh79, MO77, MS76b, Nir75, OKM74, OK75, Pie71, PDE79, PGM79, Rei76, Rit76, Sab71, Sch77c, SL78, Sti78, SH74, TP77a, Wel77a, Wil77a, Woj76, WO78, Woo72, Zer74, CP70, GGCK79]. hydrogen-bond [DMS\textsuperscript{+78}]. hydrogen-bonded [BS75c, Cho79]. Hydrogen-like [PPI73]. hydrogen-molecule [BR\textsuperscript{+75}, MS76b]. hydrogenic [JP73, Lau79, WG74]. hydronium [MS71b]. hydroquinone [SP71]. hydroxyapatite [WRF73]. hydroxyindole [WO77]. hydroxyl [MK72, WRF73]. hydroxylation [PL79]. hydroxymethylcarbonium [TWC73]. Hylleraas [BS71, CL78, Jol79]. Hylleraas-type [BS71, CL78]. Hyper [LS71, BM72, LS70]. Hyper-Hartree [LS71, LS70]. hyper-polarizabilities [BSM72]. hypercycle [Eig78]. hyperfine [BNLS72, IM79, LL75, Lun79, Men71, NN72, NN74, PPI73, TB74]. hypersurface [HG75]. hypervalent [ST72]. hypervirial [Cas78a, Gop76, ST79a]. hypervirial-scaling [Cas78a]. hypochromic [Vol79]. hypothesis [HS71]. hypothetical [PS70].

I. [KA76]. Icosahedral [BO73, Boy72a, BS74b]. ideal [SKL79]. ideas [Tho75a]. idempotent [Hen78]. idempotents [Sch71a]. Identification [DSM79]. identity [Lat77]. IETS [Feu77, Feu77]. II [Har77a, KD77, MSS79, RRS75, Abs78, AP\textsuperscript{+77}, AM77a, AB79, Bar79, Blo73, But76, CW78, CD78, CSFM72, CSR79, Coo78b, CH75, DSC\textsuperscript{+77}, DMR74, Dmi75b, DDD70, Fan76, GZ72b, GL74, HH77, HS79, HR79, Hj79b, Jak76b, KC73, KG77, KBA76, KOW78, LZ79, LP74b, MBB70, Mal71b, MM74, May74b, MK75b, MHR76, MVN75, N70b, NS73, PCH74, FW79, PHL\textsuperscript{+76}, Pet77, Pos79, PS75a, Ran79, RC71, Rob72b, Roe73, RS78b, Sch71c, SG77a, SP\textsuperscript{+72}, SM74, SS73b, SH75a, SDB74, SCY77, Spe71b, SC73, ST78, Tu78, Wel77b, WAI]. III [AM72b, Ave79c, Ave79a, BB72c, BW76c, CP71, Dau74, DH78, FB72, G\textsuperscript{+78}, Har70a, Har79a, Jak76c, Kun78b, LB\textsuperscript{+78}, LG75, MW74a, MK75a, MHR75, Med79, CMC73, ML72, MDS75, PP74, RC72, RS78c, SP75c, Sch71d, Spe72a, Spe73, ST79b].

imaginary [BR72]. imidazole [KRK\textsuperscript{+78}]. imidazolium [WO77]. imino [ZR78, ZBH\textsuperscript{+78}]. imino-enol [ZBH\textsuperscript{+78}]. immunity [Ram78]. Impact [Wil77b, BK76, PS79b]. impacting [HG78]. Implications [KK70, Kob78, Cho79, Van75]. Importance [EH73, BP78, CW77, JM76a, RR72]. improve [Kau74b]. Improved
improvements [ESR74, Sla74].
improves [Ram78].
impurities [JVM78].
Impurity [Fan70, Ada72a, AD77, BHLM78, CD78, Csa76, Csa77a, Csa78b, DT72, KGP79, MCM73, SLC78].

impropriety [Cla71, Feu77].

incluant [JM76b].

incluant [BM79].

Incompletely [Kun78a, KOW78, Kun78b].

increased [Har71a].

increased-valence [Har71a].

increases [MK76a].

increases [Kun79b].

incoherent [BK76].

incomplete [Mcd79].

incomplete [Kun78a, KOW78, Kun78b].

incorporating [PBS76].

Increased [Har71a].

Increased-valence [Har71a].

independence [KB77].

Independent [Meh73a, Coo74, GGJ75, GK76, Lud75, Man77, Sol73, TGG79].

independent-particle [GBK76, TGG79].

indicate [Kau79b].

indices [SS78b].

indirect [Cal79c].

INDO [BL77c, FG77, Kau70b, KP71a, KP72, KPKC73].

Indolealkylamines [WCK+76].

induced [BC76, INY+71, Lar73].

inelastic [Fau77, MM72a].

inequalities [GH78, Gol73].

infinitesimal [Han70b].

Influence [FSV79, eAJ76, MGT79, NT79, BKW75, Sal72, SP77, eAJ76].

influences [Kau79a, NG73].

Information [Ber76, HL78a, Lar73].

Information-theoretic [Ber76].

infrared [W´oj76, Woj78].

Inhibition [SWF79].

inhibitor [MDA78].

inhibitors [SS74].

inhibitory [Gab76].

inhomogeneous [GOK79].

initial [GPC+71].

initio [Alm74, Bai74, BP74, BP75a, BCR+78, BVR78, ČZ79, Chr73, Cla70, CDEO76, Cur77, DCM74, DM74, Dan74, DEE+75, ED74, FBL79, GG70c, GG79b, GG79a, Gv77, GCP79, HO73, Ha74, Hal73, HKP79, HPK79, HS70a, HS70b, HL78b, JZ79a, JR74, Joh75, KR71, KTO+78, KPKC73, Kau73a, Kau74b, KP77, KPP78a, KPPH78, KPP78b, Kau79b, Koc74, KPD78, KP79b, LSOC77, LS74b, Meh79, MDC79, OM76, OSL77, PCMS77, PT75, PPK78, PN76, PK71, PK75, PK76a, PK77b, PP74, PGPP79, PLMB73, PK73, Pul74, PA74, PB76, PB77, PP78, RST74, RWFS71, RBV77, RL79, Rou74, Sab75a, Sel75, SD79, SL78, SPA78, TS73, TS77, TS78, TS79, TB74, Tru73a, WJ79, ZSR79, BS75c, LD73, MBM73b, Tru73b].

injection [VH75].

Inner [GB71, Löw71a, Ahl77b, BÖ78, GB79, GBL+73, Löw70].

inorganic [MS76a].

insertion [JZ79a].

instabilities [FMRG75, TTN76].

Instability [Mes79, Mes78, NS78, SN79].

Instrument [WB71].

insulating [Lip72].

insulator [DD77b].

insulator-to-metal [DD77b].

insulators [Bra76].

Integral [Ban74, BL77b, Kau76, TG76, BS75b, GC73, JW76, KT77, Lan74, PGG77, PK75, PW74b, PW74a, RSS75, Ron79, San72, Tat73].

Integrals [Ave79b, AB79, Ave79a, BH17, GMZ73, Mos73, RB75a, Th75, TL79, Abs72, AT75, Ave79c, BL77a, BB71, Bt72, CH77, Cc71, Cof74a, Eng72, Gru70, HLGC73, Jet73, Kau70a, KZ73, KM74b, Lo75, LA76, MM74, Mat71a, Mat73a, Mat76c, PAM75, PPI73, RW74, SH73, SR72b, Sha76, Sil71, SWN78, ST70, SR72c, SP77, Van74, GM73b].

integrated [Bow71].

integration [BEH77a, DD72, Hur77].

intense [Sch71b].

intensities [BL77c, MS71c, Sch76b, Sve79, WJ79].

intensity [BS71].

Inter [JS70].
Inter-level [JS70]. interacting
[CS72, DT72, DDD70, GHS79, Mal71a, Meh78]. Interaction
[BB74, Bas78, CC79, DEC78, HöI77, RM74, Sas74, SO77, TTS+79, TL79,
Abd77, AMJS79, ACK+75, BS77b, BS78a, BP74, BK75c, BR72, BS78c,
CJS77, Cha71, ČPH74, Cof74b, Dah78, DD72, Dav77b, DMS+78, Dea72,
DY73, DAP79, ESR74, ED79, FY79, Fis70, GHS79, HB79, HSBD78, HPK72,
JMM71, JSC78, JSK75b, Kap79, Kau74b, Kau79b, KL77b, Kob78, Kol74,
Kol75, Kol76, KD77, KKM70, KKK79, LED73, LD74, LL75, LB79b, LS+79,
MCP73, MCF+70, MSF79, Moh79, NY76, OK75, PW79, PS77, RSR72,
Roe75, SD79a, Sas77, SRP76, SRP77, SDJ79, SE79, SMB72, SR78, SDB76,
SS77a, TS71, TH78, Tru73b, Wei76, WV74, WP79, YW73, You75, Mal71b].
Interactions [BKW75, KL73, SKS77, TBB70, Abd76, AFD+78, BR+75,
BB72a, BB72b, BP75a, CW78, CW77, DY73, DY76, Dun78, FL79, GJP79,
GCP79, Hö77, KM76, Kle70a, KMT77, KR78, KPP78c, LB79b, Lim74a,
LW76, Loc77a, Loc77d, LR73, MME79, MGT79, MHR76, MHR77, MP75,
MS76b, OCRMLR+71, FLYM78, PD78a, PDE78, Pol79, PBJ76, PGDM77,
Pul78a, RKE79, RM73, SRE+79, SC78a, SBM70, Sun74b, Sun75b, ST78,
ST79b, Sus77, VGS79a, VGS79b, Wei75, WO77, Wes73, WMV77, Ano76e].
interative [HR76]. Interatomic [RMP71, DY76, FY71, GKT78, Kle70a].
intercalation [PL77]. interest [KG76, KG77, Mos73, Ran79]. interface
[FBL79]. interfaces [Joh77, PBPL78]. interference [HLMV77].
Interfragment [VGS79b]. interhalogen [SM73a]. Intermediate [Rei72a,
Ste74, BL79, BKW75, CL76, GLS79, Kol74, Koll75, Kol76, KK74b, Sac72].
intermediate-energy [CL76]. intermediate-field [KK74b].
intermediate-range [Kol74, Kol75, Kol76]. intermediates [Tho76, TPC77].
intermetallic [Gin78, PTN71]. Intermolecular
[Ar78, BB72a, Cho79, CGP79, MME79, MS76b, Pul78a, AM77b, BB72b,
Brä70, Cla71, DCM74, DMR74, Dan74, FL79, HSBD78, Jeh73, Kap79,
Kle70a, KR78, LW76, Loc77a, Loc77d, MGT79, Pol79, PGDM77, RKE79,
RM72, RM73, SC78a, WB76, Dun78]. Internal
[Bor71, GPT2, MEW70, TBB70, WC75b]. International
[Cal76b, BP70, BP71, BP72, BP73, Pul79b, Ede70]. interne [TBB70].
intracellular [CODM77, GZ72b, Mui74, Zer74]. Interpolation
[Thu75, Sha71]. Interpretation
[LBÄF78, DBJ74, Feni77, INY++71, JJ78, Kor76, Wij78, JJ78, BFE78].
Interpretive [SLM70]. Interrelations [AMSS79, HYL78]. Interscience
[Cal75c, GOS78a]. intramolecular [Bri73, LRD+77, LRD+78, Pol79, Rat78].
intrinsicly [BMD70]. Introduction [Ano78a, Chr79b, Hur76b, Löw71b,
Löw78, Slà1b, Slà73b, Bar78, JW76, Com77b]. Introductory
[Nau77, Nau78, Wij78]. Invariance [SP79, FG77, Kob78, NN77]. Invariant
[CA72, Hal73]. invariants [BM71a]. inverse [Ste77]. inverses [Ra76a].
inversion [SK72, SMM73]. Investigation
[Csa77a, AŠW77, Coo78a, Ema74, KJ75, LÖS73, LAM71, MP71a, MPN79,
MM72a, SLOK79, UP71, VBC78]. investigations [TPC77]. involvement
[WLS77]. involving [Ald75, DY73, RM73, Wel77a]. Ion [GRB74, CJ73a, CSH74, GZ72a, GZ72b, GGCK79, Goo76, HS70a, INI71, JS71, KKK70, KP71a, KSP78, Kol76, KD77, KD79b, LH74, Lar75, Lar78a, Lar78b, Lei74, LS79, MFRE76, MBR73b, PK71, RR77, Sun74b, Sun75b, Tal77, TWC73, Urr75, Woo72, Zer74, CJ73b, DT75, ST77]. ion-molecule [PK71]. ionic [GRB74, CJ73a, CSH74, GZ72a, GZ72b, GGCK79, Goo76, HS70a, INI71, JS71, KKK70, KP71a, KSP78, Kol76, KD77, KD79b, LH74, Lar75, Lar78a, Lar78b, Lei74, LS79, MFRE76, MBR73b, PK71, RR77, Sun74b, Sun75b, Tal77, TWC73, Urr75, Woo72, Zer74, CJ73b, DT75, ST77]. Ionization [Hun75b, Mey71, ASW77, CSDV78, Con72, Gos75, Hal79b, HLGC73, HYL78, MN75, MK72, Ner75, PT78, PK77c, PO77, RM79, SMH77, SG77a, TS79, DH78, Jak76d, MDS75, TS78]. ionizations [Ner76]. ionized [KTO78, PLMB73]. ions [AMJS79, BFS73, BT78a, Bar79, BS71, BM73, Cal73c, Cal74, Col79, CS74, Csa75, Csa76, Csa78a, Csa77a, Csa77b, Csa78b, Csa79a, Fro79, GGJ75, Joh75, KR71, Lin70, MH78, MMS70, MM72b, PA74, PBC76, RW74, RGM77, Sim77b, ST77]. isethionic [CS74]. isocyanate [Mof79]. Isocyanide [Mof79]. Isoelectronic [Mar73a, NJ77]. isolated [Dmi75a, NJ77]. isomer [GML77, Kot76]. isomeric [JE79]. Isomerism [A79]. Isomerization [BBG79, GP78, Mat78, Mof79]. isomers [Mof79, PLMB73]. isopotential [NS79a]. isotopic [Hal71]. isotropic [BM71a, Mal71b, TB74]. isovalent [AAC76]. Israel [Pul78b, Sti79]. Iteration [BE77b, Gia73]. iterations [KÖ71]. Iterative [Cas78a, JW76, AM72b, Als73, BEH77a, Gol79, TRP77]. IUCHF [Vog79]. IV [BL77c, CP70, CT77, Hir70, Hos72, Jak76d, LCPP79, May78, PK77a, RTM77, Sch71e, SHR76]. IX [KPP78, TS78].


L [Cal75c, Sab75a, Shn77b, RRS75, AJK78, BP75a, Fae79, Mem77]. l-alanine [RRS75]. L-region [Mem77]. L-shell [Fae79]. L-Thyroxine [AJK78]. LaB [ACK75]. Lactam [Boy77]. ladder [HBB77].
Ladungsverteilungen [BKW75]. Laguerre [Mos73]. Landau [Csa78a]. lanthanide [NTN+79]. lanthanide-substituted [NTN+79]. Laplace
[MKF77, SF75]. Laplace-type [SF75]. Large [ACK+75, CSM71, Chr73, DM72, DEE+75, Duk79, Hat75, KHP77, NS79a, OMC76, PLYM78, PCMS77, PK75, Ra76a, RSR72, Rob72a, Sas77, Tin79, WCK+76]. laser
[Enz73, MHRS76, OCRMLR+71, CJCM73, CS72, KOW78, Kun78b, SP75c, Sch71c, SP75d, SEW73, TTN76]. LCAO
[Abs72, Kau70b, LS74b, ADFL71, BR78, BDP73, BBL72, BBL77, Bil72, Del73, Del74, DCS77, FTTN77, KS73a, Kar70a, KT77, KTO+78, LSOCC77, LAV72, Min79, NIT0a, NP70b, PPK78, PD78a, PK76a, PK77b, SLC78, Spe72a, Spe73, SW78, Vla70]. LCAO-calculations [FTN77]. LCAO-CO
[PD78a]. LCAO-MO
[SLC78, SW78]. LCAO-MO-SCF [PK77b]. LCAO-X
[DCS77]. LDH
[BC76]. LDH-pyruvate [BC76]. lead [YR76]. learn [Fri72]. least
[Aad73, BT71, HS75]. least-squares [HS75]. Lebenslauf [Ano77m]. Lecture
[Cal79a]. left [SY77]. left-and [SY77]. length
[Kob78, Sin73a, TTN76]. Lente [BP79]. Lenz [Loh76]. Leu [BWRD79]. leurs
[Mar73a, TBB70]. Level
[BT78, HU74, SH73, JS70, Sim77a]. Level-dependent [HU74]. levels
[CH74, CH75, Csa78a, Dmi75a, HP77a, San71, TDB77, Wen79, WM79]. Levi
[Ran79]. Levy [RCE79]. Lewis [LL72]. Li
[Bar79, BS70, BS76b, Fis75, GS70a, Jak76b, KP71a, LL75, LE72, MM72b, MDS75, RM74, RS79, SP75d, SBD+70, ZL78]. Li-like [Bar79]. liaison
[JJ78]. Liapunov [SB75]. LiCH
[RMB78]. Lie [Wyb73a]. LiF
[Fai71, SBD+70, ZF77]. life [Con73, SG76b]. lifetimes
[BNLS72, BOP76, HE77, Naz72]. ligand
[Bal71, Han79, LB79b, PBG76, PGM77, SF76, Sch71a, Van72, WN71, LK78, PD79]. ligands
[AMSS79]. Light
[Sch76b, Sch71c, TS71]. LiH
[BS74a, BS76a, BS76b, HH77, LG77, MM70]. like
[AM72a, AM74, Bar79, BS71, GGJ75, Har78, PPI73, YD75]. limit
[Kat72, OKM74, Ra76a]. Limitations [CAA+75]. limited
[APC77, CPH74, KMLB77, NRS79, PAC77, WJ79]. limits [Wei71]. Linda
[ÖL79b]. Linderberg [Shu77b, KSS73]. line
[BMD70, Fog71, HMV77, HMV78, Kot76, WEH74]. linéaire [TGSL70]. Linear
[Han77a, BBA73, BB771, Com77c, DN75, GbK77a, Hur77, KB77, KL73, LR77, Liu71a, Nor75, Sol71, TK78, TGSL70, KA76]. Lineare
[KA76]. linearly
[Sol73]. linkage
[Boy74, Har77a]. linked
[LH76, Man77, SMP77]. linked-cluster
[LH76]. linked-diagram
[Man77]. LiNO [HR79]. Linus
[Ano78f, Ano78u, Eyr78]. LiOH
[NS79b]. LiON [HR79]. lipophilicity
[Tic79]. lipoprotein
[Har75]. liquid
[Col79, HK74, DV79, Kho79, Nrr75]. liquids
[DV79]. lithium
[AST8, Bur72, CS73, RB77, Rei72a, SA77, SC73, Spe73, SBD74]. little
[Gia73]. living
[MBMM79, SGM78]. Lobe
[Pos77, RS78c, Ron78, SC78b, RS78a, RS78b, RS78c]. **Local**
[CKI75, Ivo74, SMW71, ZF77, EH73, GSE78, HS75, HK74, JTR77, MR73, Sco71, TW77, ZF76, LB73b, PS75a]. **local-mode** [GSE78]. **Localization**
[SFC72, BO79, Eng71, LB77, Lvd71, RC72, Wen79]. **Localized**
[De 78, GH72a, SS77b, Car75, Cof74b, DGC77, DSC77, DD72, DS70b, Del73, DC75, GbK77a, GC77, Kau74b, Kle77, KGB77, LAV72, Lin71, Lvd77, MMB70, MI78, Pol70, RPK78, SS77a, SK79]. **localized-site**
[GbK77a, Kle77, KGB77]. **logarithmic** [PW74a]. **loge**
[ACD74, Lud71, Lud77, MDC79, SDD77]. **London**
[Com77a, Com77b, Lar76, Lin73, Mar78, Sab75a, Shu77a, Ada72, Ada77, LP74a, LP74b, Mal71a, Mal71b, Moh78, Wil77a]. **lone**
[BKW75, DSC77, Kau74b]. **Long**
[AFD78, DY73, Kle79, Kol74, Kol75, Kol76, SBD72, Abd71a, Cha71, Dea72, FY71, GPP73, KPI71a, KL73, MOV75, PD78a, SZ76, Uke72, WMV77]. **Long-range**
[AFD78, DY73, Kle79, Cha71, Dea72, FY71, GPP73, PD78a, SZ76]. **longitudinal** [HDG71]. **look** [Tho75a]. **Low**
[Hen79, AMJS79, ACK75, Boy70a, ČPH74, DM72, GLS79, Han75, KTO78, KG79, MSSF79, PCH74, PCMS77, Tan74]. **low-energy-electron** [Hen79]. **low-lying** [PCH74, PCMS77, Tan74]. **low-molecular** [ACK79]. **low-order** [Han75]. **low-spin** [ACK79]. **low-temperature** [ACK75, MSSF79].
**Löwdin** [Sch77a, CGLÖ76, Cro77, De 76, Duf71, Gra77, Jan77, JW78, KS73b, LCK76, Sco73, Ste77]. **Lower**
[JP77, Lin70, LL70, BBK76, JP73, LTR74, SMB79, TTS79, Wei71, Gra77]. **lower-bound** [LTR74]. **lowest**
[FG79, JZ79b, Kol76, Mul71b, Pie71, SHR76, TTS79]. **LSD**
[RG74, WCK76, WEOG78]. **LSD/serotonin** [WCK76]. **luminescence** [BYB79]. **lying** [ČPH74, PCH74, PCMS77, Tan74].
M [Alh77a, Cal73a, Cal79b, Cal75c, Cal76b, SS78a]. **macromolecules** [BV072, BL79, KGP79, NGR77]. **macroscopic** [Fog71].
**Magee** [Cal75c]. **magic** [CA78]. **Magnesium** [LB79b]. **magnetic** [Ada75b, BMD70, Bow71, DL75, Fog71, HDG71, Hor71, JVM78, LL73, LZ77, Loc72, MF73, MSSF79, NTN79, PGPP79, Pul78b, PPI73, RKO77, SKS77, Sti79, Wan79]. **magnétique** [Loc72]. **Magnetism** [Mat72a, Mat79b].
**magnetization** [Hub71]. **Magneto** [DR77, IM73, SH74, SH75b].
**Magneto-optical** [DR77, IM73, SH75b]. **Magnon** [Liu71b]. **main** [MOV75].
**Mainly** [BB73]. **manmary** [WLS77]. **manganese** [Han79]. **manifolds** [Dal79]. **manipulation** [ACH72, Car74, NGR77]. **Many**
[BP78, CJCM73, DDD70, Fen77, Gás71, Lev78a, Lim76b, MVVM75, AC76, Abs78, BS74a, BS76a, BWS77, BHF78, BB73, CHD71, ČP71, Dav72, DF76, FP77, Gru70, JMM71, JBP76, KL75, Lim74a, LR77, LO77, Lin78, LRJ73, Lun77, MRT7, Man77, Mat76b, Mat79a, MK75b, MMM75, Ner75, NB78, RK76, Sha77b, SS73a, SS73b, SL70b, WW74]. **Many-body**
Many-centered [MVM75].

Many-electron [CJCM73, Gás71, Lim76b, AC76, Abs78, BP78, BB73, CHD71, ČP71, JMM71, KL75, LÔ77, Lun77, Mán77, Mat76b, Mat79a, MK75b, NB78, RK76, Sha77b, SS73a, SS73b, Sh70b, WV74].

many-neighbor [Dav72, DF76].

many-particle [Lim74a].

many-points [MR73].

many-shell [FP77].

mapping [TC70].

March [BP70, BP71].

Markoffian [SM77].

Marois [Cal76b].

master [ESG79].

Masthead [Ano70l, Ano70f, Ano70g, Ano70h, Ano70i, Ano70j, Ano71a, Ano71b, Ano71c, Ano71d, Ano71e, Ano71f, Ano71g, Ano71h, Ano72a, Ano72b, Ano72c, Ano72d, Ano72e, Ano72f, Ano72g, Ano73a, Ano73b, Ano73c, Ano73d, Ano73e, Ano73f, Ano73g, Ano73h, Ano73i, Ano73j, Ano74a, Ano74b, Ano74c, Ano74d, Ano74e, Ano74f, Ano74g, Ano74h, Ano74i, Ano74j, Ano74k, Ano74l, Ano75a, Ano75b, Ano75c, Ano75d, Ano75e, Ano75f, Ano75g, Ano75h, Ano75i, Ano75j, Ano75k, Ano75l, Ano76a, Ano76b, Ano76c, Ano76d, Ano76e, Ano76f, Ano76g, Ano76h, Ano76i, Ano76j, Ano76k, Ano76l, Ano76m, Ano77a, Ano77b, Ano77c, Ano77d, Ano77e, Ano77f, Ano77g, Ano77h, Ano77i, Ano77j, Ano77k, Ano77l, Ano77m, Ano77n, Ano77o, Ano77p, Ano77q, Ano77r, Ano77s, Ano77t, Ano77u, Ano77v, Ano77w, Ano77x, Ano77y, Ano77z, Ano78a, Ano78b, Ano78c, Ano78d, Ano78e, Ano78f, Ano78g, Ano78h, Ano78i, Ano78j, Ano78k, Ano78l, Ano78m, Ano78n, Ano78o, Ano78p, Ano78q, Ano78r, Ano78s, Ano78t, Ano78u, Ano78v, Ano78w, Ano78x, Ano78y, Ano78z, Ano79a, Ano79b, Ano79c, Ano79d, Ano79e, Ano79f, Ano79g, Ano79h, Ano79i, Ano79j, Ano79k, Ano79l, Ano79m].

Masthead [Ano79a], Mathematical [CA78, SW78, KN79].

Matrices [Gal72a, LL70, SL70, Spe72a, Ano78d, DB75, GH78, GP79, Han70a, Han75, Har77b, Har79a, ICS74, KP71b, Kry77, Lar73, Lar78a, Lar78b, Ra76a, Spe71a, Spe71b, Wel70].

Matrix [Dav74, Gal72b, HBB77, HLT79, Har71b, KR73a, LS71, LS74a, MW74b, PN76, Sas74, Sha78b, Spe72b, Ada72a, Ada79, BG75, Bun77, CM72b, Cli73, CFM73, DD72, Del74, Fox75, FM78b, GF76, Gar78, Gol79, Har70b, JW78, KL75, Kij72, Kry78, LS70, MHT71, MHR77, MW75b, MSL73, Nis77, PW79, Pea74b, Pos78, Ros78b, Soc73, SDB76, SCD73, Sur71, Tru72, WG74, Wit76, WP79].

matter [Lay77, PS75a], Mavroyannis [Cha71].

Maxima [MI78, DL75, Mak71, Ran74, Sch78].

Mayer [Cal79b].

MBPT [BS78b].

MC [KS72, KS75, KK77d, Lev70].

MCD [JPTM78, MSSF79].

McGraw [Lin73].

McGraw-Hill [Lin73].

MCHF [Fis75].

McIver [TB75].

MCSCF [BS76b, Gar78, RD79, RCE79].

mean [TL72].

means [ETF79, Fin73, LG71, MI78, Nis79, Nor75, Pol79].

Measurement [BW73, Con74].

measurements [KK70].

mechanical [CBV79, Che71, Coo74, DAP79, FJP70, GJ76, HS79, HS79d, Hos78, KKK79, MP71a, MK77, PP74, PG77, PS75, PC76, Pul77, RW75, TPC77, Wal77, Wei71, WO74].

mechanics [Col77a, Con73, GP74, GT75, Hun75a, MM77a, NB72, PTUK69, PP71, Pul76, SE79, Shu77a, TL72, Van71, Wil79b, Wil79a, Cal79b].

Mechanism [PF79, BYB79, Dav79, HG75, KKK74, KK75, LP79b, PL79, Pul79a, Sal79, SM79, SLOK79, TPC77, UPT1].

Mechanisms [KKKP79, Pet79, BDT77, MSS78, TB75, Urr75, WO77, WOE78].
Mechanismus [HG75]. media [BBT71, Chr79c]. medium [HLMV77, KPP77, Sim78b]. mediums [HMV77]. Meeting [Pul79b].
melting [KGP79]. membrane [Sun74b, Sun75b, ST78, ST79b, Urr77, Van75]. membrane-active [ST79b]. membranes [BK75b, Fro79, GH79, Hos78, Mar79, Urr75]. memory [Spa78].
meperidine [LJBN75]. MERGE [HKP79, HPK79, KPPH78]. Metabolic [NKKY79]. metabolism [ME78]. metabolites [HKP79, KPPH78, NKKY79]. Metal [Ber73, Swi71, BR78, BFS73, CS73, CHHS74, CS74, DD77b, DC577, FN73, JW72, Joh77, KD77, KGB76, LVDC74, MS72a, MS74, Moh77, MM77b, SC73, Spe73, Sto71, Van72].
metal-ferroelectric [CHHS74]. Metal-to-nonmetal [Ber73]. metallic [KMO77, OKM74]. metalloporphyrins [DAC+79]. metals [CJCM73, CM75b, De 78, FMRG75, KW76, LB73a, MGM78, PK77c, Sch77c, SKW72].
metastable [DD71]. metastables [KSP78]. Methadone [LJBN75]. Methane [Dan72, DPGC79, HSB78]. methionyl [PPC72]. Method [Hen74, LS71, Rei76, Aba72, AFD+78, BR78, BB75, BBL72, Bil72, BK75c, BFH74, Bur72, CS73, CK75, Cas78a, Cas78b, CD74, CODM77, CS74+79, Cla71, CSH74, DC73, DRCT78, Eps77, FFBC79, FG79, FRM74, FHB77, GH579, GB75, GML77, GL74, GJ76, GH77, Hal78, HS77, Har77c, HC72, Hen76, Hen77, HCT78, Jan76, Jet73, JW72, Joh73, JM76a, Joh77, JM73, JS70, JN72, KK71, Kau73, KSP75, KA76, KR78, KU70, KK77d, LS70, LVDC74, LV71a, LV78, LP74a, LP74b, LFF79, LG77, Lim74b, Lim75a, Lim75b, Lim76b, Lim77b, LG75, Loc76, MK77, Mak71, Mat71a, May74a, MK75b, MK75a, May78, MCF+70, MS76a, Mes73b, Mes78, MW75c, Mon77, Mor78, MMR74, MS75, Nam75, NIT74, Pa71, PD78a, Ran74, Rob71, Rob72b, RH79, RK77].
method [Rue79, RP78, Sa72, Sam75, SF76, SM76a, SH73, SC76a, SIM75, SKL79, Shu77c, SBM72, Sl73a, Sl74, SC76b, SC73, Spe73, Sri77, TGL70, Tru73b, Van70, VK74, WE74, WK73, WA71, We74, We76, YJ76, ZR78, ZBH+78, ZF76, DCM74, KS72, LB73b, We76]. méthode [TGL70].
Methodology [BW76b]. Methods [Chi77, CFMO73, GMZ73, Shu77b, SBD+70, Tur74, AP77, Ano79, BG76, Bar70, BNL72, BBL77, BS78b, BL77c, BS78c, CGL76, CSFM72, CP71, Cof74a, DS76b, DCS77, Ell72, Ema74, Fau71, Gar78, GV77, Har77b, Har78, Kar70b, Kar70c, KFY71, Kau70b, KK74b, KK77c, KVSG79, Lar78a, Lev78a, Lun79, MK76a, May78, MCM73, MW74b, Min79, ML76, NS72, NT73, PLY78, PAC77, PCL78, PBPL78, PSK77, Pos79, RW77, Sin73b, SS70, Sla75, Vog79, WFS77, Cal76a].
methyl [BS79, Kla78, ML72, MK72, RRNS75, Sha77a].
methylimidazoles [KRRK78]. methyltransferase [SS78a]. Metric [Mor78]. Metric-constrained [Mor78]. Mg [PPB78]. MgO [KGB76]. microelectronics [Ost79]. microscopic [Coo78a]. microwave
migration [FY79]. Milne [YL74]. MINDO
[Boy77, SL73, ZR78, ZBH+78]. MINDO/2 [SL73, ZBH+78]. MINDO/3
[Boy77]. minicomputer [Spa78]. minimal [Cur78, KPÔ76, Mal71a, RPK78].
mimic [BJ73, Muk75]. minimization
[BJ73, HS75, Jol79, KS73a, KA76, KBK72, Wed76, Wed77b]. Minimum
[GY75, HH70, JŽ79a, MI78, You72]. mixed [ACG74, Euw71]. mixing
[LV71a]. mixtures [GH72a]. MO [Ano78c, BBL72, BBL77, Csi77, KT77,
Kau70b, KL79, Lar78c, LAV72, MW74a, NN77, PCM77, PPK78, PK76a,
PK77b, Vla70, WMB75, MM77b, Abs72, Bil72, CA78, CSFM72, Cof74a,
Csi76, Del73, FTK77, FM72, Hi79, H3I79, KS73a, Kar70a, Kar70b, Kar70c,
KFC71, KTO+78, LS74b, M3KM77, MR72, Moh77, NI70a, NI70b, Sam75,
SD78, SMH77, SG77a, SS74, SLCT78, SW78, WRF73, ZR78, ZBÔ78, BFH74].
mode [DBBJ76, GSE78]. Mode
[KL77b, LLP78, LP79a, PD79, SPÇ72, AF73, ADDLG76, AÔ+79, BS77b,
BS78a, BL70, BFR78, BK71, Bra79b, CB72, CD78, Cho79, ÇPP75, CE73,
Coo74, Coo78a, Coo78b, Coo79, CZ75, Dov77b, Dec70, Doo78, Duk79,
ER75, ED79, FCL79, FH78b, Gb777a, GOK79, Goo76, GGJ75, Hal75b,
Han77a, HB79, HC78, ICS74, JS71, JVM78, JL70, JM76b, Kib75b, Kl79,
KBK72, Lar75, Lar78a, LP79c, LP79b, LW77, LB73a, LK78, LPT+74, Lud75,
Mal71a, MCP73, May74a, Mic76b, PLC78, Par72, Per78, Pet77, PNC+78,
PP74, Por77, PP79, RSS75, RR77, RM78, RC70, RC71, RC72, RL79,
SM76b, SPÇ79, Sch71a, SP75a, Sha77a, Sha78a, SB78, SL70, St78, Tal77,
TP77a, WN78, Wo76, Wei76, YJ76, Sch71d, SPÇ72, YD75]. modèle
[JM76b]. Modelling [SKL79]. modelling [FHP70]. Models
[LHK77, PA78, Wo77, AM77a, ÇPH74, GK76, Hõl77, JPM78, Lad74a,
LS74a, Löw77, Mag79, PL79, PCH74, PBS76, TW77, Urr77, WEÔ78, SK73].
Modern [Kap79]. modes [BDT77, Hor71, SLOK79]. Modification
[Bee79]. Modified
[GM73a, GM73b, KK77d, KL79, Rue79, BSG77, Csa77b, JW78, PS73]. MODPOT
[HP79, HP79a, KPP78a, KPP78b, KPP78b, PK77a, PK77b]. MODPOT/VRDDO
[HP79, KPP78a, KPP78b, PK77b]. MODPOT/VRDDO/MERGE [HP79]. MODPOT/VRDO
[PK76b]. modulus [SEW73]. moiety [RKOU77]. MOLE [PHÔ+76]. moléculaire
[LL72]. moléculaires [TBB70, BJ73, Mar73a]. Molecular
[Ac77, Al77, BB70, BL77b, BH71, CD78, Cur78, DHT7, DL79, DK77,
E676, Ed73, FW77, FB72, FHP70, GPP73, GM73, GH77, JG74, KC73,
Kau70b, KPP78, KPP78b, KL77a, Köt76, KD77, LV78, Le70, LCR73,
MS72a, MS72b, Mat73a, Mat76c, MHA70, Mul74, MHH74, NLR+79, PP72,
P779, PK76b, PK77a, PK77b, Pul70, PZP79, SMP77, SS78a, SJ79, SR72c,
TP70, Urr75, Van72, Van74, AF73, AM74, Anô79a, BTD79, BNLS72, BL77a,
BJ73, BBP71, BV73, BVS76, BT71, BT78b, BV78, Boy70b, B78c, BS77,
Cal76a, CM75a, CW76, Cas79, CSDV78, CJS77, CSM71, Chr73, Ç71, CR72,
CDE076, CM76, Com77c, Con72, CAMC71, CSH74, CD71, CZ75, CA72,
DGC77, DSC77, DRCT78, DT75, DEE75, Ell73, Eng71, FTM77, FCL79].

**molecular**

[Fla79, Flu72, GGCK79, GG79c, GG79a, Gia73, GC77, GPP79, HO73, Hac74, HH77, HHR70, Hal78, Hal79b, HLMV77, HKP79, HLGC73, Hen74, Hen76, Hen77, HLYC77, HL78b, Hos72, HTG77a, HTG77b, IS75, JSC78, Job70, JS71, JP77, KR76, KTO78, Kau70a, Kei75, KM76, KK77b, KPG79, KPD78, LL72, Lan77, LGAM79, LP74a, LP74b, LFF79, Lev78a, Liib76, Lo75, Loc77b, Loc72, MBB70, MEW70, MS74, Mat71a, ML76, MDC79, Mic74, Mic76a, MHWC78, Mil74, Nal78, NB72, Nec75, Ner75, OMC76, PH77, PCMS77, PT75, PPK78, PK75, PGP79, P75a, PBC74b, Pul76, Pul78b, Pul79b, PO77, RR72, RWFS71, RK77, Rou78, Sab75a, SM73a, SD79a, SPC79, SP75a, Sch72, SLB77, SLJ78, Sel75, SMMA73, SDM74, SBB79, Shu77a, Sil71, Sim72].

**molecular**

[Sla71a, SC76b, SC78a, SC78b, SF75, SP77, SS73c, Sti79, SWP77, TBB70, TNC79, TP77b, TH78, Tur74, Tu75, Tu78, ULM76, VBC78, WO77, WOE78, WJC70, Wij79b, Wit72, Wij76, Woo72, Fan70, KD79b, Mar73a].

**Molecular-orbital** [Van72, BTD79, CSDV78, Joh70, JS71, KPD78, KD79b].

**Molecule** [OJB77, Ada78, AF73, BRS75, BWS77, BG78, DN75, ES73a, FSV79, GZ72a, GZ72b, GGCK79, GLS79, GS70a, HH77, Hen79, HK74, IM73, JZ79b, Jør78, KPT1a, KSP78, KD79a, KL73, LD74, L78, LE72, MS76b, Min79, Nes75, Pie71, PK71, Rit76, SH74, TDB77, TOED79, WO76, Wil77b, Wil77a, Zer74, vDR79].

**Molecules** [Jai70, KM74b, Nes71, AM72a, AM74, AM77b, AM77a, Als73, AMJS79, Ave72, Bar77, BB74, BJ73, BBP71, BP74, BP75a, BSZ78, BP73, BR75b, BFR78, BS76b, BBG79, BW73, Boy74, Boy72a, CK75, Cha71, CSF72, CW77, CS71, Chr73, CR72, Ciz76, DN75, DSMM79, DTM72, Duk79, DCS77, ER75, EB74, FB75, Fox75, GP72, GP78, GB75, GJ75, GJ76, Hal71, Hal73, HE77, HF72, HRBB76, Hilt9, Hur76a, Hur76b, Hur77, IM73, IM7N9, ICS74, JBP76, Joh73, Jul78, Kla78, Kle70b, Koc74, KBK72, KL73, LL72, LL73, LCP76, L77, Li76, LR77, LM72, Lin73, LG73, MBB70, Mal71a, Mal71b, MCST72, Meb78, MCF70, MLM75, ML72, MOV75, Moh79, Mor78, MI78, Mun76, NI70a, NI70b, NS73, NS79b, Nes70, OMC76, PLY78, Pau78].

**molecules** [PK72, PCMS77, P79a, P80, Plo79, PF74, PK75, Po70, RR72, RS72, RT74, RM73, Rob72a, Rob71, Rob72b, Sam75, SM73a, SM76b, SM76a, SD79a, Sas77, SP74, SP75b, Sch73b, SG77a, Sim79, Sim78, Sla75, S76, SBD70, Su77, SH75b, TGS70, Tin79, TB73, Ty75, V78, VG79a, VG79b, WCK76, Wen79, WS79, WM77, BJ73, LL72, Loc72, Kle70b, Com77a, Com77b, Ano78c, Cal79a].

**Molecules-in-molecules** [KM74b].

**Moleküle** [Sch73b].

**Møller** [BP75b, PKSB79].

**Moment** [Ell77, AAC76, Als73, CAT72, DSC77, Fac79, KP71a, MMD78, Tru72].

**Momentum-polarized** [Ell77].

**Moments** [OJB77, CAMC71, DH76, EFT79, HH77, Lar78a, L79, Li76, RR72, SMW71].

**momentum** [BS70, BBT71, BW73, But76, Cro77, CM75b, GN77, WESW73].

**Monday** [Sla71b].

**mono** [Har77a, INI71].

**mono-negative** [INI71].
Monocyclic [Boy77]. monoelectric [BSG77]. Monographs [Gos78a].
monolayers [VH75]. monomer [AZ72]. monomolecular [Chr77].
monographs [Gos78a]. monolayers [VH75]. monomer [AZ72].
monomolecular [Chr77]. monoxide [BWS77, SD70, Wil77b, WFS77].
Monte Carlo [Cas78b, Col77a, CL78, Col79, RC78]. more-electron [Sin73b].
Mössbauer [GML77, Kot76]. motion [DR75, FG79, GP79, LG71, SHI73, SIM75, SD74, SLOK79, SH75b, Web74, Sim77a]. motions [Bri73].
Mott [Bra76]. Mouton [AB73]. moving [DR77]. MS [GML77, BFH74, Con72, CG79b, KC79, Kau73, PKK75, PK77c, WC75b].
MSW [SP75a]. MSX [RK79]. MT [CD78, KC79, RK77]. muffin [DC73, FFCB79, FRM74, GHIJ77, Pai73, Sla74, Wil74]. muffin-tin [FFCB79, GHIJ77, Sla74, Wil74].
Multilayer [CM75a, CA78, Kau70b]. Multi-configuration [MM70, Hac74, NI70a, NI70b]. Multiconfiguration [Har71b, SC76a, BG76, BS78, BK79, Fis74, GB75, Hal78, Har70b, JS77, KKW73, PNC74].
Multiconfigurational [GBV77, Gre71, KK76c]. multidimensional [BF78, LG71]. Multimolecular [Sla79].
Multiple [AD77, Dav77a, Wil74, BL77c, CW76, CW78, Dan72, DC73, FFCB79, GGC79, Gin78, KL78, KCI75, LVDC74, Li76, MMR74, RK77, WK73].
multiple-scattering [Dan72, FFCB79, Li76]. multiple-scattering-X [DC73]. multiplet [BFS73]. multiplets [LP74b].
Multipole [CJ73b, DH76, GPP79, MM72b, SP79]. muons [Fri72]. muscarinic [Kan74].
muscle [Dav71, SP79, NTN79]. Musher [An76n, Cus75]. mutation [GRE77].
mutations [Coo74, Coo78b, RCE75]. Mutually [Abs72]. my [SG76b].
myosin [BZSD79].

N [PK71, RKO77, SY77, AAC76, Bur77, DEC78, Har70a, HLYC77, KPÖ76, ML76, PL79, PK71, RNS75, RC71, SBD70, Tru72, WK73]. N-acetyl [RRNS75]. n-h [SY77]. N-hydroxylation [PL79]. N-methyl [RRNS75].
N-methylacetamide [DEC78]. N3 [ME78]. Nakajima [HLMV77].
nalorphine [KK77a]. Nanosecond [GC75]. naphthalene [BOP76].
naphthalene [KT77]. narcotic [KK72, KKK74, KK75]. narcotics [KM72, KKK74, KK75, LJB75]. native [FSV79].
Natural [BS70, BC79, KT71, SD74, EIG78, RCE79, SDB76, TRPB77, ICS74]. Nature [KBKCD78, Sim78c, BVO72, BM71b, MPS70]. Naturel [DQ77]. Nb [MM77b]. near [De 78]. nearest [SS77a, SS77b].
nearly [BL70, BSE78, LB73a, SM73b]. necessary [Kun77]. necessity [Kau79b].
necessity [Kau79b]. need [Del74]. negative [BB78a, Csa77b, Csa79a, I171, KSP78, Sim77b].
neighbor [Dav72, DF76, MHR76, MHR77, OCRMLR71, SS77b, WJC70].
neighborhood [KL73]. neighbour [SS77a]. Neon [Fae79, NY76]. nerve [BK75b, NM77].
nerve [BK75b, NM77]. nested [MHPS70]. networks [KHI79]. neuroleptics [KK74a]. neurotransmitter [Kau76, KPP79]. neurotransmitters
[GRB74]. neutron [MPW75]. next [SS77a, SS77b]. next-nearest [SS77a, SS77b].

NH

[Bai74, BWRD79, CE73, FMZ70, HNT78, KC72, LV71c, RC70, RC71, Bai74].

Ni [JR74, LB79a]. nickel [CZNL70, DCS77, SDJ79, SLC78]. NiH [GBK77b].

nitric [KÖ71]. nitrite [HCIE75]. Nitrobenzene [GBK77b].

nitric [K¨O71]. nitrite [HCIE75]. Nitrobenzene [GBK77b].

[n'] [JSK75b, JSK75b]. NMR [JE79, KVSG79, Pul77]. NO [PK71, Cal73a, Cal76a, Cal77b, Lin73, Sab75a, Cal79a, KKK70, LK78, MSSF79, Cal75b]. noble [BM74, Csa77b, MHW78, NY75, Sto71]. noble-gas [MHW78].

Non-applicability [KP71a]. Non-Bloch [Kun78a, KOW78, Kun78b].

nonalternant [Lai73]. nonbenzenoid [SG77a]. Nonbonded [Sun74b, Sun75b, ST78, ST79b].

Nonclassical [Urr78]. Nonclosed [SS73b]. Noncompact [Sin73c]. Nondegenerate [Hor71].

Nonempirical [HPK79, ABD79, KPP78a, KPP78b].

nongeometrically [DN75]. nonlinear [CK75, Wel75].

Nonlocal [Ove73].

nonmetal [Ber73]. nonmetallic [JMP78]. Nonorthogonal [JSK75a, JSK75b, Lya78, Meh78, Wel76, Wel77b].

nonorthogonalized [KR73a]. nonplanarity [RKOU77]. nonpolar [SAM79]. nonradiative [HE77, HF72].

nonreactive [Ber76, Tru76]. Nonrigid [DN75, TDB77, EST3a, GP78, PST9a].

notensor [Bri73]. Nonzero [PBC74a]. Normal [KKP77]. normalized [Nal78]. notation [KL77c].

Notes [FM78b, Cal79a]. nouvelle [JJ78]. novel [FLB79].

Nuclear [RKOU77, TB73, Boy72a, Bri73, GP79, Laz79, RMP71, Pul78b, Sti79].

nuclei [LZ77, PGPP79]. nucleic [AMJS79, DS79, FB72, IZZ79, KD77, KL79, LP79c, LS87, NKKY79, PL77, Pol79, PGPP79, SD77, SMB79, SRE79, Sun74a, UPT1, VBC78].

nucleic-acid [FB72]. nucleophile [PDEB78]. nucleophilic [PLSL78].

nucleoside [KP79b, PB77, SPP77]. nucleosides [GPP73, KP79].

nucleotide [Lak75, ME78, SW79]. nucleotide-binding [Lak75]. nucleus [HB79].

number [KL77c, KMLB77, MW77, MK76a, Res78].

numbers [GCJ73, Har79b, ICW74]. Numerical [GMZ73, KP71b, TH75, BEH77a, CHS77, DD72, GJ76, RS79, Sur71, WA71, BBL77, DD72, ES79, TW77].
Nutrition [Web74].

0 [BMD70, FM78a, Har70a, Har77a, LGM77, Shu77b, ASW77, BZSD79, Bur77, CV73, DMS+78, FM78a, FMZ70, Gub79, HL79, Han79, HNT78, HPK72, LG77, LE72, LK78, MS71b, MG77, PK71, Ros78a, ST72, SS78a, TTS+79, Tru73b, WK73]. O-methyltransferase [SS78a]. O [Jan77].

Obituary [Löw73]. observables [Kun78b, ML79]. observations [GK76]. obtained [BB75, CESW70]. obtaining [Cas78a, CFMO73, CH74]. occasion [Cal75b]. occupation [Har79b, ICS74]. occurring [DDH78]. octahedral [LVDC74]. octupolar [MMS70]. Odd [May74b]. Odd-electron [May74b]. odorant [LM72]. off [LC77, Mil71, ST79a]. off-diagonal [ST79a]. OH [Cur77, LV71c]. Öhrn [Shu77b]. old [Tho75a]. Ole [OL79b]. Olov [CGLÖ76]. on-line [WEH74]. One [BSS78, BDP73, BH71, Eng72, SBM70, TNB79, Ada72b, AM72a, AM74, AM77b, AM77a, AT75, CB72, CD78, CP77, CM76, Dah78, DSG74, Dec70, FY79, Fri72, GC77, HNT78, Hen78, Hos72, HR76, Jak76a, Jak76b, Jak76c, Jak76d, JM73, KZ73, KS72, KK77d, Lét74, May78, MVM75, MLM75, SS73b, ST70, SBM72, SR72c, MM74]. One-band [CD78]. One-body [SBM70]. One-Center [Eng72, AM74, AT75, CM76, HNT78, MM74]. one-centered [MVM75, MLM75]. one-centre [AM77a, KZ73]. one-densities [Hen78]. one-dimensional [FY79]. One-electron [BDP73, TNB79, AM77a, CB72, CP77, Dah78, Dec70, GC77, Hos72, HR76, Jak76a, Jak76b, Jak76c, Jak76d, JM73, KS72, KK77d, May78, ST70, SR72c]. One-particle [BSS78, DSG74]. only [Lét74, MPW75]. onto [MHP70]. Open [CGRC74, APČ77, BS78c, GHS79, GBM74, GRM75, HP77b, JD74, KBK72, Lin78, MMB70, MW75b, MLB72, MM72b, MDS75, MMM71, Muk75, Nel79, Nes77, PT78, RGM75, RGM77, SPČ79, SM77, CDEO76, Hen76]. open-shell [BS78c, GHS79, HP77b, JD74, Lin78, MMB70, MLB72, MDS75, Muk75, Nel79, Nes77, PT78, RGM75, RGM77, SPČ79, CDEO76, Hen76]. Opening [Ede70, Lon74, Lon75, Lon73]. Operator [BL72, Mic76a, Mor75, BBK76, CE73, Dal79, DC75, HBB77, KK74b, KK77c, Nee76, PSS5a, Sur71, WG74, Sim77a]. Operator-Level [Sim77a].

Operatoren [KA76]. operators [Bal78, BS77, BFH78, Col78, CEK72, Cro77, Gos75, KA76, Lar75, Lar79, Lim75b, MK78, MW75c, SL79, Sch71a, Sol73]. opiate [LJB75].

Oppenheimer [CL78, Col79, Ess77]. Optical [PS79a, BBT71, DR77, GML77, INY+71, IM73, Lip72, Mes73a, Sch71e, SH74, SH75b]. optically [Cha71]. Optimal [Raf75, Ra76b, Abs78]. optimisation [Muk75].

Optimization [BT71, Gia73, ABM78, BSZ78, Bur77, CLP79a, CLP79b, Gar78, Jak76a, Jak76c, LS74b, MK75b, RCE79, Sun75a, Wel75, BPTLVM73]. Optimized [Sol71, Jak76a, Jak76b, Jak76c, Jak76d, JP73, LTR74, SBB79, SBD+70]. optimizing [KK76c]. Optimum [Cas78b, Pol70, ZR78, ZBH+78, CHD71].

OPW [VK74]. Orbit [BOP76, Lo75, MSSF79, BP74, BP75a, BK75c, Hal75b,
JSK75b, LA76, MM74, MCF+70, SM71a, SM71b. **Orbit-orbit** [Lo75].

**Orbital** [ABM78, Ave79b, AB79, Ave79a, BL72, GMZ73, HRBB76, MVN75, Muk75, Abs78, AeAs78, AF73, Ald75, ADDLG76, Ave79c, BTD79, BBP71, BT71, BC79, BVR78, BS77, Cal76a, Cas79, CSDV78, CR72, Cof74b, CDEO76, CM76, Con77c, CAMC71, Cur78, DHT3, DEE+75, FB72, Gar78, GPP73, GC77, GH72b, GHJ77, HO73, Hal78, Hal79b, HLGC73, Hen76, HLYC77, HL78b, HP77b, Joh70, JS71, JG74, Joh77, KC73, KTO+78, KPKC73, Kau79b, KSL76, KL77a, Kot76, KD77, KPD78, KD79b, KØ71, LV71a, LB77, LGR73, LS74b, Mar73a, MEW70, MHA70, MH72, MG77, MHH74, NPL+79, Nee75, NG73, PPC72, PK75, Pop71, Pul70, PBC74b, Raf75, RR77, RMB78, SM73a, SMP77, Sch73b, SRP76, SRP77, SD74, SS78a, SM73b, TRP77, Tur74, Van72, VBC78, Vla70]. **orbital** [WJC70].

**orbitales** [BJ73]. **Orbitals** [Bee79, Gal72b, GMZ73, Kas76, Thu75, AC76, Abs78, BS74a, BS76a, BJ73, BP74, BS70, BZ78, Bur72, CW77, Cof74b, CM76, CA72, CA73, DGC77, DSC+77, DD72, Des72, DT75, Eng71, FGV77, Gia73, GB72, Hal73, HLGC73, Hen74, Hen77, Hos72, HTG77a, ICS74, JP73, JP77, JG72, JSK75a, JSK75b, KR73a, KT77, KP72, Kau74b, Le76b, LAV72, LGR73, Lo75, Loh76, MBB70, Mar73a, MS72b, Mat73a, Mat76c, MK75b, Mcd79, MI78, Mul74, NN72, NN74, NS72, Pa73, PS73, Po70, PAM75, Ra76b, Rob72a, Ros78a, RS78a, RS78c, Rou78, RCE79, RPK78, SR72b, SD79a, SBB79, ST70, SC76b, SDB76, SD74, SR72c, SW77, SW78, Tat73, TP77b, Tu75, Tu78, Van72, Wyb73a, JBG70]. **Orbitalstruktur** [Sch73b]. **orbiting** [SSM75]. **Order** [JBP76, OJB77, SLM70, WS79, Abd71b, BBB73, BWS77, Bun77, Coo79, HS76, Han75, HBE78, KD74, Kle79, KP78, Lan73, LF77, Lz78, LZ79, Moc74, Mos73, NR579, PLMB73, RM73, SK71, SKL79, SC73, TTN70, Vog79, You75]. ordered [PN71]. **ordering** [AS78]. orders [KHI79, Mal71a, Mal71b]. **ordination** [FM72]. organic [Ano78c, Csi76, Csi77, RD79]. **Organization** [GH79, Eig78, Pea74a]. **organo** [MYTC77]. **organo-silicon** [MYTC77]. **organometallic** [RMB78]. **orientation** [TBB70]. **Orientation** [Fuk70, Jør78, Cal77b, Eno76, Fuk75, TBB70]. **Origin** [Sur71, GRE+77, CA78]. **origins** [PL77]. **Orthogonal** [CH77, Gal72b, JBG70, JG72, MS75]. **orthogonality** [RS76]. **Orthogonalization** [KS73b, Ra76b, LB77, Sco73, Ste77]. orthogonalized [CWE71, ML76, NN72, NN74, NS72]. **orthonormalisation** [Lat76]. **orthonormality** [MI78, NI74]. **orthonormality-constrained** [MI78, NI74]. **Orthorhombic** [Jør77, Jør78, Sch77a]. **Oscillator** [WG74, AC70, BHL78, CM78, GBV77, Lar78a, RB75a, ST79a, Sin73a, W075, Wit76, WM79]. oscillators [Bas78, BBA73, BHL78, HM77, HM78, Hun74]. **other** [Boy74, Har77b, Jan77, KKK74, KK75, LDP79, RU76, SM71a, SM71b]. **outer** [Des72, GB77]. **Overlap** [Thu75, BB72a, HK75, DL75, DY76, GPP79, KP76, Ki75b, LV71b, LV72, Mak71, MI78, NC78, PK75, Ra76a, RR72, Ran74, RM72, Sch71a, Van70, WW71]. overlapping
overlapping-sphere [SC76b, YJ76].
overlaps [Nis77].
overview [Sim78a].
Oxford [Ahl77a, Ano78c, Gos78b, Sab75a].
oxide [KÖ71, PDEB78].
oxocomplexes [BL77c].
oxopyridine [KPP78c].
oxopyridine-water [KPP78c].
oxopyridines [CLP79a].
oxopyrimidines [CLP79a].
oxo [RL79].
oxopyridines [KPP78c].
oxopyridine-water [KPP78c].
oxygenases [Har77a].
oxyhemoglobin [Har77a].
ozone [Bur77].
ozonides [Rou73, Rou74].

P
[AC70, GL74, Har77a, LL75, LG75, MSH71, SH76, TTS71, Tat73].

p-450 [LHK77].
P-450-dependent [Har77a].
p-benzoquinone [MK72].
p-methylation [SS78a].
p-quinones [NT79].
P. [Jan77].
P-O. [Jan77].

panels [KL76, DAC79, Har71a, HK74, IM73, KC77, LG79, Sal72, TH78].
oxygenases [Har77a].

P450 [Han79, PL79, RL79].

pair-correlated [WV74].
pair-correlation [Lan73, MMM75].
pair-potential [Meh73a].
pairing [JPTM78, Kle79, MW77, Mat79b].
pairs [BM74, DSC77, GRE77, Jan76, Kau74b, KKK79, Sun77, ZV79].
pairwise [Pet77, PNC78].
pairwise-correlated [PNC78].

parametric [Kar70b, Kar70c, KFY71].
Parametrization [LV71a, Kib75a].

parametrizations [Gia73].
parent [KK70].
parentage [KK77b].

Parr [JL70].

Partial [Bar79, AM77b, AM77a, RK79, Wel71].

Particle [Lar75, WA71, Ada79, BSS78, Col78, DR77, DSG74, GJ75, GJ76, Hen78, LD71, Lim74a, Lud75, Mat74a, Rat71, TGG79, MW77].

 Partial-hole [Lar75, LD71, Rat71, MW77].

Partners [GB70].

parvalbumins [NTN79].

particularly [Abd71b].
partition [DH78].
Partitioning [Mil74, MSL73, SDM74, BB71, BF78, GGCK79, GS70b, LG71, MMM75, Ner76, Roe73].

partners [TBB70].

path [JZ79a, Lei74, PGQ77].

paths [TH78].

pattern [KP76, Pal75].
Pauli [Kij75, RL77].
Pauling
phthalocyanine [MS72b], phthalocyanines [MS72a, MS74]. Physical [GB71, GBL+73, HL78a, ML79, Pea74a, Pet77, Coo78b]. Physicochemical [KK75, KK774, Kau79a]. Physics [GB71, GBL+73, HL78a, ML79, Pea74a, Pet77, Coo78b]. Physicochemical [KK75, KKK74, Kau79a]. Physics [Gos78a, Cal76b, Ess77, Fri72, DV79, Mar73b, Sin73c]. phytochrome [SCYB77]. pi [NN72]. picoline [BKW75]. Picolines [BKW75]. picture [CSDV78]. pigment [Kli79]. pigments [MP71a]. pigment [Kli79]. pigments [MP71a]. Pioneers [Par77]. planar [Tan74, CSR79]. plane [CWE71, Euw71, KMO77, ML76, OKM74, WFS77]. plane-wave [CWE71, KMO77]. plane-wave-Gaussian [Euw71]. plant [BC75]. plasma [AJK78, Har75, Hor71]. plasmon [HDG71]. Plesset [BP75b, PKSB79]. plethysm [MCM73]. plethysms [MVM75, MLM75]. plots [SY77]. PNC [Tho76]. PNO [Bur77, Mey71]. PNO-CI [Mey71]. Point [BG70, FCL79, MM77b, SC79, ACD+74, CB72, CPP75, Flu72, Kib75b, KK77b, LP74a, Lét74, PBPL78, RCE75]. point-charge [Kib75b]. Point-group [MM77b]. points [BF78, MR73]. Pointwise [Lev78b]. Poisson [Sil71]. polar [Jor77]. polarisability [Sri77]. polarity [PS79b]. polarizabilities [HTG77b]. polarizabilities [ANR75, Ahi74, Ahi77b, Bar77, BSM72, BM73, CG79a, ETF79, GBM74, HH77, HS77, HTG77a, KK774, LCP76, LG70, Mal71b, MM72b, MMM71, RB77, RB75b, SH78, TSE76]. Polarizability [LP74c, BR72, MCST72, NAR72, RGM75, Zer74]. Polarization [BK789, DM72, Hal71, HCE75, OJB77, Sti78, Boy70b, CJ73a, CJ73b, KC77, Kle74b, KBKC78, LW77, ML72b, SSH78, YD75]. polarizations [RG77]. polarized [bor70, Ell77, Fis70]. pole [CG78]. Poly [PPP79, VU79]. poly-[VU79]. polyamino [NFJ+77]. polyanionic [BP74, BP75a, CSFM72, HF72, Jor78, Kle70b, LCP76, LZ77, MMB70, MCF+70, ML72, Mu76, Plo79, RR72]. polycyclic [Mem77, Mem79, PD77, SR78, UP71]. polycytosine [LSOC77]. polyelectronic [KPM70]. Polynene [AL71]. polyenes [KH79, LV71b, LV72]. polylignane [KL77a]. polyhedral [PK75]. Polyhedric [RT78c]. polycions [RKE79]. polymals [Pos78, Pos79]. polymer [DD78]. polymers [ADFL71, ADDLG76, AF+78, AB+79, BP73, Del74, DD77a, Par72, PD78a, SKL79]. polymethines [FTN77]. polynomials [Ra76b, Ra76b]. polynuclear [DHE+75, NT79]. polynucleotide [SY77]. polynucleotides [KP79a]. Polypeptide [Urr77, ULM76]. polypeptides [Kar78, KL77a, PPC72, Urr78]. polypolar [SF75]. Pople [JL70]. population [Kau70b, KPKC73]. populations [KP76]. porphin [Alm74]. porphine [KTO+78]. porphins [MW74a]. porphyrins [Han79, MW74a]. portée [TBB70]. Position [Csa75]. positive [BT78a, Csa77b, Sco73]. possibilities [IZZ+79]. Possible [Tic79, WLS77, Coo78a, Gol70, HPK79, HK74, Kau74a, LSS78, SY77, Wei74]. potassium [CD74, Sun75b, Sun74b]. Potential [BR75b, Cof74a, Gu79, GBK77b, HL79, HG75, Kau70, Liu71a, AŞW77, ABD+79, BA78, BLN72, CL77, CL78, Col79, CG79b, CH74, Csa76, Csa77b, Cs78b, DR77, DRCT78, DSG74, DEC78, Gá71, HS79, HKP79, HSBD78,
HC78, Jor75, KP71a, KD79a, LC77, May78, Meh73a, MVN75, MO77, MS76b, MK72, Moh78, Moh79, NS73, Nee75, OMC76, PPP79, PT75, PPK78, PK71, PD78b, Pol79, PKS78, PZP79, Rue79, SP75a, SBB79, SB78, SS71b, TN73, TP78, TOED79, WJC70, WM79, MVN75, Wil77b]. potential-energy [BA78, Moh78, PD78b, SB78]. Potentialhyper߬ache [HG75]. potentials [Ban74, CM75a, CK73, Con72, DMS+78, DH78, Ell77, FRM74, GPP79, Hal79b, HLGC73, Hun75b, Hal78, Ner75, Nis77, Ove73, Pal73, PD77, PK77c, PÖ77, RM74, Sab73, SM77a, SH79, SMB70, TGG79, TS78, TS79, Wei74, WO75]. pour [Mar73a]. Pouvoir [DQ77]. Power [Lau79, BG72]. powers [Boy72c, RB75a]. pp [Ahl77a, Com77a, Com77b, Sti79, Cal79a, Dun78, Lar78c, Mår78]. PPP [BK71, ČPH74, ČPP75, FTN77, KBK72, Mic76b, PČH74]. PPP-type [FTN77]. practical [SMMA73]. practice [Ano78c, Csi76]. prealbumin [AJK78]. precision [Del74]. Predicting [MP75]. prediction [BDT77, IMN79, KK74a]. predictions [Tru76]. predictors [DH78]. predissociating [HE77]. predissociation [BFR78, BEF78]. Preface [CG77, Löw79]. Preliminary [BCR+78, BS75c, BS77, LDP79, BCL77, Meh79]. Prentice [Cal76a]. Prentice-Hall [Cal76a]. presence [Abd71a]. Present [DS70a, Ost79]. Press [Com77a, Com77b, Lar76, Sab75a, Slu77b]. pressure [Bor71, Lib76]. Price [Ahl77a, Cal76a, Cal79b, Cal76b, Cal77b, Com77a, Com77b, Dun78, Gos78a, Lar78c, Lin73, Sab75a, Slu77b, Slu77a, Sti79, Ano78c, Gos78b, Mår78]. primary [MP75]. Primitive [Hir70, Kut78]. principal [GCJ73]. principle [CH75, Csa76, Csa78a, DR75, Eig78, HHR70, Lim76a, Lip72, Moc73, PBC74a, RCE75, Sre75, You72]. Principles [Rab77, CH74, GY75, Lud75, Sun74a, Gos78a]. prior [Cof74b]. Pro [CBV79, RSK+78, BWRD79]. Pro-Leu-Gly-NH [BWRD79]. probabilities [BR75a]. probability [Ada75b, AC70, Ave75, Hun74, Hun75a]. Probing [SY77]. Problem [Gal72a, LL70, Aba72, AC76, Abs78, Ada72a, AFD+78, AMJS79, BP78, C674, Com74, DRM74, ES73a, FU76, Gop76, KPM70, KBA76, KK76b, LR77, Lud71, Mal71a, MHPS70, Mat74a, Mat76b, Mcd79, MV75, MLB76, MFRE76, Nor75, Pal75, Per78, RST6, RE70, Sha77b, Sha78b, SMMA73, Shu77c, Slp70b, Ste77, West79, ZF76]. Problems [Loc77d, AM74, ČP71, Com78, DL75, DSY74, FBL79, Gás71, Kal79b, SC79, Ste74]. procedure [ADDLG76, BB71, B71, But76, CM72a, Fis75, GCP79, HS70b, Jak76a, Kau74b, Kuc74, Lan77, PD78a, PK75]. Procedures [PK76b, BB74, KPP78, KPP78b, KS75, LB77, MR73, PK77a, PK77b, TRP77, Wei75]. Proceedings [Cal76b, Sti79, BP70, BP71, BP72, BP73, Csi77, Mar73b, Pul78b]. processes [CSDV78, Chr79c, Fla79, GP78, Kle74b, Plo79, Rat78, Rei70]. processing [Bil72]. prodines [LJBN75]. produce [KKK70]. Product [Meh73b, Ada73, Bri73, Lya78]. Production [BS77a]. products [Lét74, MHT2]. Professor [Sla71b]. profile [KK77a]. profiles
program  
[BF71, CAMC71, HC72, Jech73, KSP78, Lin77, SP75c].  Progress  
[Lae78c, Dau77].  project  [Nes75].  Projected  
[May74b, SDS73, Hur77, LL75, MLB73, May74a, MK75b, MK75a, May78,  
PCL78, SLB77, SDB74, SDB76, SB78, Van70, SDS73].  projected-unrestricted  [SLB77].  Projection  
[BL72, Fin73, CHD71, Cro77, LKH77, CE73, KGB77].  Projections  
[GB71, Löw71a, Ahl77b, BÖ78, GBL+73, Löw70, Sar75].  promazine  
[PPK78, PK76a].  proof  [Rei72b, You72].  propagation  [LV77].  Propagator  
[OJB77, KPÔ76, PÔ77].  Properties  
[BL72, Fin73, CHD71, Cro77, LKH77, CE73, KGB77].  Projection  
[BL72, Fin73, CHD71, Cro77, LKH77, CE73, KGB77].
quadruple [BP78], quadrupolar [MMS70, SR72a]. Quadrupole [ETF79, BM73, Boy72b, Kot76, LK78, RR72, Tru72]. Qualitative [CPH74]. quality [DPGC79, GG79c, GG79b, MYTC77, MDC79]. Quanta [Atk74, Atk91, Gos78b]. quantal [Ber76]. Quantenchemik [PTUK69, Cal73a]. quantitative [Loc72, DQ77]. Quantitative [Pop79, Pur75, BBL77, DBJ74]. quantities [BW73, GMG75]. quantization [KL77c, SL79]. quantizing [HDG71, Hor71]. Quantum [And79, Bul71, CBV79, CGLÖ76, Cal73b, DAP79, FL79, GP74, GT75, Her74, Hos78, KK72, KKK74, KK76a, Kau79a, LH75, LW77, LJB75, MPN79, PP74, PS75b, Pul76, PC76, Pul78b, Ric77, Sti79, SLOKP79, TPC77, Wäl77, WMV77, Ave72, Cas78b, Che71, CP71, Col77a, Con73, Fox75, Gol73, GM73a, GM73b, GCJ73, GJ76, Hal75a, Hal79a, HS79, HSBD78, Hat75, DV79, INY+71, Jan76, KK75, KG76, KG77, KB77, KKK79, LPP78, LP79a, Lin73, MP71a, Mat72a, MF73, MSP73, MCP73, MPW75, MW75a, Mat76a, Mat76b, MWY77, MW77, MK78, MKT77, Mos73, NB72, Par77, PH77, PG77, PTUK69, PT75, PGPP79, PS75a, PP71, Pul77, Pul79b, RW75, Red79, Rei70, Ros74, SP75c, Sch71b, Sch71c, Sch71d, Sch71e, Sch76b, SE79, SJ79, Sl79a, Sre75]. quantum [TP77a, TL72, TWC73, Tho75a, Van71, Wei71, Wei75, WO74, WO76, Wi79b, Wi79a, Wyb73a, BP70, HG75, Loc72, MN79, Sch71c, Lr76, Mår78, Sh77b, Shn77a]. Quantum-Chemical [FL79, SLOKP79, MPN79, LPP78, SJ79]. Quantum-mechanical [DAP79, Hos78, PP74, PS75b, PC76, TPC77, HSBD78, KKK79, MKT77, PGPP79, Pul77, Wei71]. quartets [GH79]. Quasi [BBL72, BBL77, MMB70]. quasi-localized [MMB70]. Quasi-relativistic [BBL72, BBL77]. Quasiclassical [Tru76, Ber76]. quasidegeneracy [Wes79]. quasimolecular [MFRE76]. quenching [AZ72]. quinone [SP71]. quinones [NT79].

R [Sab75a, MM74, WRS70, FWFM77, You75]. Rabalais [Gos78a]. Radial [AAC76, Gru70, JB70, BS70, Ben72, CA72, JG72, JKK75a, JKK75b, RW74]. radiation [Cal75c, Hea71, Kob78, Sch71b]. radiationless [Plo79]. radiative [Bar79, BOP76, LH75, SZ76]. radical [Cla70, DT75, HS70b, KR73b, KKM70, Sha77a, Sha78a, TS78]. radicals [CDE076, GPC71, KT76, KU70, MMB70, MS71b, MLB72, NN72, NN74, SG77b]. radii [Ra76b]. Raman [DH73, MS71c, Sve79, WS75, WLS77].

Random [LP74c, OL78, And79, Lar75, Nel79, NMS77, OL79a, SO77, Tru73b]. random-phase [Nel79, NMS77]. randomness [NJF+77]. range [Abd71a, AFD+78, Cha71, Dea72, DY73, FY71, GPP73, JBP76, KP71a, Kae79, Kol74, Kol75, Kol76, MCP73, PD78a, RMP71, SKL79, SM72, SZ76, WMV77]. rank [Boy70b, BM71a]. Rapid [Euw71, SBB79]. rapidly [PW74a]. rare [Fla79, LRL73, LPT+74, MS76b, RW74, TW77]. rare-earth [RW74].
rare-gas [Fla79, LRJ73, MS76b]. rare-gas-halide [Fla79]. rat [JG74]. rate [Bar79, BC76, ČZ79]. rates [Mat78]. rational [Gab76]. ratios [Ber75]. ray [BS71, CFMO73, FM78b, GK75, GML77, HYL78, Mes73a, TS71, PNJB78]. Rayleigh [Amo72, Car72, CJSS77, Cla71, Sre75, WB76]. rays [Dec70, MFRE76]. Re [MRR74]. reaction [BC76, BCR78, BDT77, GTBB77, GBT79, JŽ79a, LPP78, Mag79, Nal78, PK71, PDEB78, PKSB78, Sal79, TB75, TH78]. reactions [ČZ79, CS79, Chr79c, FM78a, GBTB78, RW75, TC70, WEH74]. reactive [Ber75, Ber76, Hi77, Mic74, Mic76a, Nes75, RW77, Red79, Tru76]. Reactivity [WCK78, CW78, ES73a, Joh77, LP79a, LP79c, Sal72, SS78b]. real [Bre75, Fau76, Gol79, Lad75b, We77b]. realistic [FRM74]. reality [Živ77]. realization [SP75c]. Rearrangement [RB75b, BM75]. rearrangements [BVR78, BDT77, CSR79, TG76]. Rebane [WW71]. received [Ano70d, Ano70e]. Receptor [Ano76e, CT79, Dav77b, Höl77, JG74, Wei75, WCK+76, WO77, WOEG78]. receptors [CS76, SCYB77]. recherche [Mar73a]. recombination [Bar79, Gu79]. reconstructed [DS70a]. recurrence [JW78]. Redirection [ČPT]. redox [LKK79, DAC+79]. Reduced [AC76, Abs78, Bun77, Col78, JTR77, Kry78, LL70, SLM70, Spe72a, SW78, Ano78d, BB71, KP71b, Kry77, Lar79, MW74a, NS75, Spe71a, Spe71b, SW77]. Reduced-density-matrix [Kry78]. reduction [Per78]. reference [BS78, BKS79, Lar73, Lar78b]. Refined [RD79]. Reflections [Ano76a]. region [BB72a, Mem77, PZP79]. regions [ZL78]. Regularities [Plo79]. Regularity [CS78]. regulation [BC75]. regulations [SG77b]. related [BW73, NN74, OMC76, Wol71]. relation [Abd76, CBV79, Cas79, DEC78, KSS73, KC74, LD71, Liu71b, ST79a, WV74, Rob71]. Relations [BM75, JW78, Kau79a, Lan74, ST79a]. Relationship [LB77, ZG79, BCL77, DGCC77, Kum77, PCL78, PW79, WB76, WP79]. relationships [PD78b, Pur75, SJ79]. Relative [AS78, BKW75, CS74, JM76b, WJ79, ZR78, ZBH+78]. Relativistic [CW76, DS70b, Des72, ES70, MBM73a, RW74, Ros78a, TP77b, WC75a, BBL72, BBL77, BK75c, Cha71, CWE71, Ell77, Koe74, Mat73a, Mat76c, PPI73]. relaxation [MG77, SM77, Sch71d, Sch71e, Wen79]. relay [TP77a]. relevance [Urr77]. relevant [TPC77]. Remark [INY+71, Be75, Bra70, BF75]. Remarks [CS75, Rei70, Sin73c, Sis74, SC76b, Wei71, AT75, BV76, Bry74, Han77b, KSS73, Kau74a, Mar76, Nau77, Nau78, San72, Sch78, SG77c, Exe74, Wij78]. Reminiscences [Con73, Pul79c, Tho75b, Van71, SG76b]. Removal [CHS77, HT75, SHO71]. Renner [PK72]. repeat [RU76, RKOU77]. repetitive [CBV79]. replacement [Mil74, SDM74]. replication [Coo74]. report [BS75c, BSB77]. Representability [Col71, Erd78b, LL70, Col70, Kuml77, LD71]. Representable [Lar73, Lar78b]. Representation [Spe72a, BS76b, BT71, Bow72, LH74, NM77, Nis77, PGQ77, PS75a, SP75c, Spe71a, Spe71b, SL70, ST71].
representations [BF70, Blo72, Blo73, Boy72c, Cor72, HS79, Lét74, Rei72b, RM72, SS73c]. Representing [Gal72a, Lar79]. Reproduction [GCP79]. repulsion [AT75, HLGC73, JBP76, MM74, Si71, WN71]. repulsive [Csa77b, GBTB78]. repulsive-dominant [GBTB78]. requirements [NN77]. research [Nes75]. residues [PPC72]. Resolvent [Røe75, BÖ78]. resonances [Sim78a, BFH78, Doo78, FHB77, Jun78, KSP78, LKH77, MCW78, NB78]. resonant [CG78]. respect [KMLB77, SP79]. response [Han77a]. responsible [BL79]. Restricted [Mes78, CDEO76, JD74, Spe71b]. restriction [HT75, Kij72]. restrictions [Kau79b, SHO71]. Results [Col71, Fau76, SK72, BCL77, CS73, Col70, Doo78, GCP79, HKM71, JL74, Min79, PT75, RTM77, Red79, Sch76b, SBD70, Wei76]. retarded [MP71b]. retention [BKW75, PK75]. retinal [WMB75]. retinol [GC75]. reunification [Bul71]. reversal [VF76]. Review [Ahl77a, Ano78c, Cal73a, Cal76a, Cal79b, Cal79a, Cal73b, Cal75c, Cal76b, Cal77b, Com77a, Com77b, Dm78, Gos78b, Gos78a, Lar76, Lar78c, Lin73, Mar78, Sab75a, Shu77b, Shu77a, St79, DS70b, CS73]. Reviews [Ano74c]. revisited [Kle77]. RHF [SP77]. rhodium [AMC73]. ribonucleic [Sun77]. Riccati [PW74b]. Richards [Mar78, Sab75a]. Riedel [St79]. right [SY77]. right-handed [SY77]. rigid [GP72, Gra77, Meh78, MO77, SW79]. rigid-rotor [MO77]. rigorous [FRM74, KPP77, Sim78a, KMO77, SP75c]. Ring [Spe72a, NT79]. RNA [MP75]. Roby [CAA75]. Role [HC79, KD79b, KKK79, GK78, Har79b, KBKCD78, Lar79, Lin77a, Mem77, Per78, PDE79, Ross74, LW77]. roles [ULM76]. root [Sco73]. rotamers [BL75]. rotating [DLG79]. rotating-wave [DLG79]. rotation [CK75, Cor72, IM73, KD79a, MEW70, WC75b]. rotation-vibration [KD79a]. Rotational [FGV77, Ber76, HP77a, SH75b, Web74]. rotationally [HE77, MM72a]. rotations [Gia73]. Rotatoire [DQ77]. rotator [Gra77]. rotor [MO77]. row [Cal74, CP70, DGC77, KP72, NG73, Raf75, ST72, Tho76, Wel77a, Wel77b]. Rowe [SD74]. RPA [Bre75, Jor73, Lar78a, NS78, SN79]. rule [NB72]. rules [CPH74, CD71, HBB77, Hur77, Mat76a, Res78, TB75]. Runge [Loh76]. Rydberg [FWFM77, Hos72, Mil71, Rob72a, TTS79]. S [Ahl77a, AS78, Cal76b, OS77, RS79, BS70, BM73, BK74, DD71, LG75, LM71, SHR76, Spe70]. S-state [BM73]. S. [Par73]. S3 [Duk79]. Sagamore [Sm79]. salts [AMJS79, DT75, Sal72]. same [HMV78]. sampling [EH73]. Sanibel [Sla71b, Sla73b]. Sasaki [Ste77]. Satellite [BL77c]. satisfying [Kij72, Sch78]. saturated [Rou73, Rou74]. scaling [Bar78, BFH78, CG78, CG79a, Cas78a, Cas78b, Com78, Doo78, Gás71, Gop76, HS71, HTG77a, NB78, NG73, Nut78, Sim78a]. scattered [BB75, Joh70, JST71, JW72, Joh73, JM76a, We74, YJ76]. scattered-wave
[Joh70, JS71, JW72, Joh73, JM76a, Wei74, YJ76]. Scattering
[Ada72b, Bal78, Nut78, AD77, Ano79o, BG78, Ber76, BW73, BL77c, BY76, CM72a, CW76, Com78, DH73, Dan72, DC73, Dav77a, Dec70, FFCB79, GGCK79, Gia76, GLS79, Hen79, HYL78, KL78, Kel75, KL77b, LVDC74, Lev78a, Li76, LKH77, Mic76a, Mil71, MMR74, Nes77, PBPL78, RW77, Red79, RK77, SK72, SMMA73, TS71, TOED79, WK73, Wil74].

scattering-theoretic [PBPL78]. SCF
[KT77, KTO +78, KL79, LS74b, ZBH +78, Abs72, ACH72, BB72b, BDP73, BBL72, BBL77, BPTLVM73, CGRC74, CP70, Car74, Cas79, DS76b, DSY74, DK77, Eld73, FP77, GML77, Hil79, HS70b, JD74, JW76, JS77, JS71, JW72, Joh73, JM76a, Kau70b, KPKC73, Kau73, KSP78, KS72, KS75, KK77d, LSOCT77, LAV72, Lev70, Lim74a, Lud77, MW74a, MS76a, MR72, Moh77, MG77, MM70, NN77, PCMS77, PPK78, PS70, PK76a, PK77b, PK73, PBG76, PPB78, Sam75, Vla70, WRFT73, WMB75, YJ76, ZR78]. SCF-MO [MR72].

SCF-MO-CI [PCMS77, WMB75]. SCF-MO-LCAO [BBL72]. SCF/CI [KSP78]. scheme [Aro78, BEH77a, Gol79, HR76, JG72, KT77, KM76, KK76c, MG77, Nov73, RK79]. schemes [CSFM72, Kau74b, Kut78, MSL73, RC72]. Schiff [WTB +76]. Schrödinger [Ada73, Amo72, Bal78, BFH78, Car72, CJS77, Cla71, KA76, VB72, WA71, Wel70, We171, WB76]. Schrödinger-Operatoren [KA76]. science [CGLÖ76, Pul79b, Shu77b]. Sciences [Cal73b, Bul71]. Scientific [Ahl77a, Lar78c, Ano76n, Ano78c, Jan77, Par73]. scientist [SG76b].

SCOPW [Sco71]. Scott [Sab75a]. screened [AM74, TN73, WM79]. Screening [TPM70, Csa77a, Nec75, Sel75, SIM75, SL7C73, YW73]. screening-charge [Csa77a]. SCRPA [Lar78a]. Se [Sch73a]. search [Mar73a]. Second [KL77c, OJB77, SL7M0, Abd71b, BBB73, CP70, HS76, HBE78, KPT2, Lau79, MHR76, MHR77, Moc74, OCRMLR +71, PLMB73, RM73, SK71, SL79, Vog79, We177a, You75, KD74]. second-neighbor [MHR77]. Second-Order [SL7M0, Abd71b, BBB73, HS76, HBE78, Moc74, PLMB73, Vog79, You75, KD74]. second-row [KP72]. secondary [BCL79, MP75, Meh79, RU76]. section [BG78]. sections [Bar79, Chi77, Fac79, ML76, SSM75]. secular [Amo71, Hen77, Koe74, Nor75].

Selected [Hat75, Moh77, SM73a, SD78, DGC77, SM76b, SM76a]. selection [DLG79, HBB77]. selective [Tel77]. selene [YR76]. selenium [Ald75, VK74]. Self [BBP71, Bor70, CWE71, Kar70b, Kar70c, KFY71, Kle70b, Meh78, MM72b, MS70, MBM71, Sla70a, BKS79, BK75e, DS74, Eig78, Gou73, Hac74, Hal78, JL74, KKW73, KS75, LG77, MM71, Sco73, Sco74, Sel75, SL7C73, Tel77, TGS70, Vla70, VK74, ZF76, GL74, LG75].

self-adjoint [Sco73]. self-consistence [KS75]. Self-Consistent
[SL70a, Bor70, CWE71, Kar70b, Kar70c, KFY71, Kle70b, Meh78, MS70, MBM71, BK75c, DS74, Hac74, JL74, KKW73, MM71, Sco74, Sel75, SL7C73, Tel77, TGS70, Vla70, VK74, ZF76]. self-consistent-field [BKS79, Hal78, LG77]. Self-correlated [GL74, LG75]. self-diffusion [Tel77]. self-organization [Eig78]. Semi [BBL77, WJC70, CAMC71, Dub72, LOS73, NMS77, PK75, ...]
semi-ab [PK75].
semi-classical [Dub72, Sch76b]. Semi-empirical [WJC70, BBL77, CAMC71, LÖS73, NMS77, San71, San72, SMH77, SG77a].
semi-infinite [RT77]. Semi-quantitative [BBL77]. Semiclassical [Ada75b, FL79].
semiconductor
semi-infinite [RT77].
Semi-empirical [WJC70, BBL77, CAMC71, LÖS73, NMS77, San71, San72, SMH77, SG77a].
semi-infinite [RT77].
Semi-empirical [WJC70, BBL77, CAMC71, LÖS73, NMS77, San71, San72, SMH77, SG77a].
semi-infinite [RT77].
Semi-empirical [WJC70, BBL77, CAMC71, LÖS73, NMS77, San71, San72, SMH77, SG77a].
semi-infinite [RT77].
Semi-empirical [WJC70, BBL77, CAMC71, LÖS73, NMS77, San71, San72, SMH77, SG77a].
semi-infinite [RT77].
Semi-empirical [WJC70, BBL77, CAMC71, LÖS73, NMS77, San71, San72, SMH77, SG77a].
semi-infinite [RT77].
Semi-empirical [WJC70, BBL77, CAMC71, LÖS73, NMS77, San71, San72, SMH77, SG77a].
semi-infinite [RT77].
Semi-empirical [WJC70, BBL77, CAMC71, LÖS73, NMS77, San71, San72, SMH77, SG77a].
semi-infinite [RT77].
RTS74, SPˇC79, Sch72, Sol71, SS77b, TW77, Hal78. simplest
[HPK79, VB72]. Simplification [L´et74]. Simplifications [BL77a, BL77b]. Simplified [CP70, GV77, BFR78, Rei72b]. simulate [CEK72]. Simulated [DEE+75, CDEO76]. Simulation [Bai74, Pol79, NGR+77, RC78].
[Rat71, Ada72a, Ada79, BS77b, BS78a, BM74, CC79, CM76, Grc71, Mil74, Muk75, PAM75, SD79a, SDM74, SLC78, SC79]. single-center [PAM75].
single-centered [Mil74, SDM74]. single-electron [Ada72a, BM74].
single-parameter [SD77a]. single-particle [Ada79]. Singlet [BB75, TSE76, BP75a, MW74a, MCST72, NT79, PCMS77, SMB+79, SDB74, TH78, S873]. singlets [GH79]. singly [Csa79a, LAM71]. Singularities [BG70, CHS77, CB72]. SiO [BET78]. Site
[Fhu72, AMS79, CW78, GbK77a, Hé77, Kap73, Kle77, KGB77, PD79, SS79]. sites [LK78]. six [AMC73, Jol79]. six-coordinate [AMC73]. six-parameter [Jol79]. sixth [Cal75b]. size [BS77b, BS78a]. size-consistency [BS77b, BS78a]. sizes [DG77, Kau73, MDC79]. Skillman [HC72]. skin
[SCYB75]. skin-sensitizing [SCYB75]. Slater
[BRT78, BS74a, BS76a, BS78a, BPTLM73, Bre73, Cha77, ERW75, GMZ73, LS70, LS71, Lec76b, MHT2, SR72b, Sam75, ST70, SS71a, SR72c].
Slater-type [BS74a, BS76a, BS78a]. Slow [Gia76]. Small
[Com77a, Com77b, Vla70, BB72a, CODM77, GJLL75, HS70a, Hur76a, Hur76b, KPP77, LGR73, Mul74, Pos70, Sim79]. Smooth [Thu75, Sha71]. SN
[KK78]. SOCL [GH72b]. sodium
[Ber73, Bor70, BK75b, CD74, Col79, HCE75]. software [WH75]. solid
[FBL79, DV79, LW77, Muf76, Nan75, Sla71a, SR72c, SP75d]. solid-state
[DV79, Sla71a]. solides [KMO77]. solids [ADFL71, Bor71, Bre75, Car75, Dec70, Fau76, Joh73, JPM78, PBPL78, Sco74, Sl7a, Wen79, ZF77]. Solitons
[Dav79]. Solution
[MHP70, Ada73, BEH77b, Csa79a, DS74, FW75, HS75, JM73, Koe74, KK76b, Kun78a, Ner76, Nor75, Pul77, RRNS75, SD77, WA71, ZF76]. solutions
[Cal79c, ENRM78, FG79, Fro79, KKA78, Kho79, Lia73, Mes79, Tal77, TTN76, Živ77]. Solvation [SAM79, VN78]. Solvent
[AZ72, FSV79, HPW79, LC77, PC78]. Somatostatin [MDA78]. Some
[AT75, BS75a, BS76a, ESR74, GSE78, GK76, HCT78, Jav70, KSS73, LKK+79, Lö70, Lö71a, Lö77, Mes73b, Nal78, Oda73, PD78b, San72, Sch78, Spe72a, SG76b, Vol79, We75, AMSS79, BG76, BY79, BM74, BS75c, CK75, Cha77, CL73, DDH78, Doo78, DT75, JL74, KMT77, KR73b, Kun77, Lia73, LM72, MS76a, MR72, Mor75, Mku74, NN72, Nis77, PG77, PS70, PD77, PDE79, PK77c, RM78, Ros78b, RD79, Sh77a, Sha78a, SKW72, Sim77b, Sto71, SL73, SBD+70, Th075a, TP78, WN78, DEC78, ED79, RT77, SW78]. Sons
[Cal79b, Cal75c, Dun78, Shu77a]. Space [GGCK79, Spe72b, Bee72, BS70, BS76b, Cli73, GH79, HY78, KC74, Lani77, NM77, SP75c, Sl7a].
space-dependent [Cli73]. space-spin [KC74]. spanning [Bee72]. spatial
spatially [Csa76, Csa78b]. special [Mag79, Pan77, WW74]. special-pair [Mag79]. Specific [Gol70, AMSS79, BL79, Jeh73, KMT77, Lar79]. specificity [PL77]. spectra [AeAs78, BCL79, BL77c, BEF78, CW77, DH78, GGG77, GPC71, GK75, Hal75b, Kib75a, KJ75, KS79, LV78, LGM77, LBAF78, Lun77, MS71b, MR72, MK72, NT79, PNJB78, SLB77, Sch71e, SM79, SK79, Van72, WK73, Wój76, Woj78, LBAF78]. Spectral [BH75, Boy74, BF75, CS72, Ra76b, BFH78]. Spectroscopic [Kli79, TPM70, KKK70, WB73]. spectroscopy [Bas78, Feu77, GC75, KKK70, MKF77, Mic76b, Pul78b, Rab77, Sti79, WS75, Gos78a]. spectrum [BHLM78, CS78, FHB77, GML77, HG78, HDG71, Oni79, VG78, WJ79, Wan79, WFS77]. Speed [DMs+78]. sphere [GHT2a, Kau73, SC76b, Wei76, YJ76]. spherical [AF73, ADDLG76, BHM78, CS78, FHB77, GML77, HG78, HDG71, Oni79, VG78, WJ79, Wan79, WFS77]. spherically [Csa77b]. spheroideal [SP74]. sphingomyelins [PC76]. Spin [BP74, BOP76, BK75a, Joh77, Kau79b, Kle74b, KT76, KR73b, Lin75a, MS71a, MF73, MSP73, MCP73, MPW75, MW75a, Mat76a, Mat76b, MW77, MN79, MLB73, May74a, May74b, MK75b, MK75a, May78, MK78, Sar75, SD79a, SM71a, SM71b, SM71c, SK73, SS73a, SS73b, TH78, APC77, BP75a, Bor70, BK75c, CL73, CDE706, DL75, Dav74, Fis70, GTG76, GJLL75, GJ76, Hal75b, JMM71, JSK75b, KR73a, KTO+78, KPJM70, KC74, KGB77, Kle79, LED73, LD73, Laz79, Lim74a, Lim74b, Lim76b, Lim77b, MM74, Mat72a, MCF+70, ML75, Mes73b, ML72, MS75, NN72, PAC77, Pan77, Sha77a, Sha78a, SL70, TB73, VF76, Har79a, MSP73, MPW75, MW75a]. spin-adapted [Dav74, VF76]. spin-density-functional [GJLL75, GJ76]. Spin-Dependent [MK78]. Spin-Extended [KT76, Mes73b]. Spin-forbidden [TH78]. Spin-Free [Mat76b, MW77, MN79, SD79a, MF73, MSP73, MCP73, MPW75, MW75a, Mat76a, MW77, SS73a, SS73b, KPJM70, KC74, Lim74b, Lim75a, Lim76b, Lim77b, Mat72a, MK78]. Spin-only [MPW75]. Spin-Orbit [BOP76, BP74, BK75a, BK75c, Hal75b, JSK75b, MM74, MCF+70, SM71a]. Spin-orbital [Joh77]. Spin-other-orbit [SM71a, SM71b]. spin-polarized [Bor70, Fis70]. Spin-Projected [May74b, MK75b, MK75a, May78]. Spin-spin [MS71a, SM71c, MM74]. spin-wave [CL73]. spinfree [Lim75b]. spinless [DR77]. spinors [CW76]. spins [HLM77]. split [SM73a, SM76b, SD78]. split-shell [SM73a, SM76b, SM76a, SD78]. splitting [Har71c, HP77a, Kot76, MS71a, SM71a, SM71b, SM71c, WN71, BP75a]. splittings [BFS73, BB75, LK78, NN72, NN74]. Springer [Cal79a, Cal77b]. Springer-Verlag [Cal79a, Cal77b]. Square [RS75, And79, Sco73]. squares [BT71, HS75]. stabilité [JM76b]. Stability [Lai73, MK76b, Bur77, Coo78b, JM76b, LÖ73, LRT73, LPT+74, MHA70, Lai73]. stabilization [HK74, KSP78]. stabilized [MS71b]. stable [Hat75, RS79]. staggered [Hub71]. standard [RS78a]. Stanton [TB75]. Stark [BK77, CH77+78, Ref76]. starting [ACD+74]. State
States [Spe72a, Abd71b, AM77a, AS78, ADFL71, BSS78, BK79, BP75a, Ber73, BL79, BF71, BS75c, Boy72a, BS78c, CSFM72, CPH74, CP77, CESW70, DRCT78, DS76b, DS70a, DS70b, DT72, De 78, DD77a, DC75, Dm75b, DM75, ES73b, Fan71, Fan76, GV77, GB75, GL74, Hal75b, HNT78, Hat75b, Hos70b, HT75, Hos77, IS75, KR71, KR76, KKW73, KTO78, KS78, Kol76, Km78a, Kow78, Kow78, Kow78, Kow78, Kow78, L71, Lim74a, LV71c, LS79, LAM71, MW74a, MCST72, MCF70, MCM73, MLM75, Mip71, MMS70, MG77, Mu76, Mu71b, PCH74, PCMS77, PS70, Pie71, Pop71, PLMB73, RT77, Ros78b, RT77, SM+79, SP75a, SC76a, Sim78c, SH75a, SHR76, Sin75, SDB74, SCY75, SCY77, Ste70, St71, Tat74, TTS71, Tat73, TTS+79, TNB79, TS72, Urr78, WS75, WMB75].

Static [WK73, You72, YD75, SP7C72, SD73].

Stationarity [CG78], stationary [Com78].

Statistical [MM77a, SW70, SW71, Gol73, Han75, KR78, Lin71, Cal79b].

Statistics [TB73].

Steering [KSL76], stentorin [SCY77].

Stephen [Cha71].

Stereoregular [DD77a].

Stereoselection [Fuk70, Fuk75, Cal77b].

Steric [Tic79].

Stickstoff [BKW75].

Stieltjes [Lan74, Lan77].

Stieltjes-integral [Lan74].

STO [CH77, JW78, Mar73a, Pel77, ZSR79].

STO-3G [ZSR79].

Stochastic [ESG79].

Storage [Bi72, MHH74].

Störungsrechnung [Ahl70].

STOS [We77b].

STP [Eng72].

Strength [AC70].

Strengths [CM78, GB77, L75a, Sin73a, WM79].

Stretch [SS71b].

Strip [JG74].

Strong [Lun77, KK77c, LL73, Loc77d, SRE+79, Sh77c, Pet78].

Strong-field [KK77c].

Strongly [Kle74a].

Structural [Boy74, Chr79a, Enz73, Mof79, RW79, RU76].

Structure [BC75, LL72, Lei74, AFI78, AF73, AMSS79, AL71, BT78a, BK77, BCL77, Bur77, CB79, CGL76, Car75, Cj73b, CRT2, Col77b, Duk79, EP71, Erd78a, Fin73, FBL79, Fis74, FWJ79, FSV79, FRM74, GSE78, GK75, GML77, Har78, HS70a, Hin77, HK74, Hop78, HT75, JR74, Joh75, eAJ76, KK74a, Kau79a, Kell5, KKA78, KJ75, KL77a, KC74, KU70, KV79, KMO77, Lad74b, Lad75a, Lad75b, Lad76, LSO77, LSS78, LV7C74, LP79a, Lay77, Lev78a, LE72, LM72, LÖ73, LK78, Lu75, Lu79, MW74a, MP79, MS72a, MS74, MF73, Meh79, MHC78, MH78, MR72, MOV75, Ove73, Paf71, Pul73, PN71, Pe74a, Pet77, PNC+78, Pul77, Pur77, Ran78, RL79, SMB+79, SP74, SP75b, Sch73b, Sim79, SJ79, SJH79, SR77, SCY75, Spe71b, SM79, SK79].
structure [Swi71, TB74, Tho76, Ukr72, Van75, Wil79b, Wit72, ZG79, ZF76, LL72, Lei74, Shu77b]. **structure-activity** [Ran78]. **structure-property** [Ran78]. Structures [Boy77, ABD+79, BNLS72, BCL79, Con70, FY79, GKB78, Har70a, JW72, JNZ2, Kan74, Kry78, Lad74a, NG73, Pri75, SL73, USK+79]. studied [ÄFL78, BF78, HLMV77, KVSG79, LBÄF78, MSSF79, TGSL70]. Studies [Cal75b, Hos72, LCPP79, LG71, TB78, Ald75, BK77, BCL77, Bur77, Cur78, GZ72a, GZ72b, GL74, HR79, Har75, HG75, JE79, JS71, JG74, KKK74, KK75, KN79, Kli79, KMO77, LPP78, LP79a, LG75, LGR73, Meth79, MHA70, MS76b, MCW78, MHH74, PL79, PLSL78, PKSB79, PP74, Pul74, PS75b, PBG76, PC76, PD79, RW75, RRNS75, RSK+78, Rout74, SMP77, SS79, SS74, SS78a, Sim77b, SH75a, SHR76, St78, TGG79, TW77, PCMS77]. Study [CR72, DPGC79, FFCCB79, Jai70, KU70, Res78, AeAs78, ABM78, BB74, BM74, BBA73, CBV79, CS73, CEK72, CLP79a, CLP79b, DGC77, DAP79, ES70, Fis75, GC77, HLYC77, HLT78b, KM74a, KL78, KC79, KH79, KD74, KL77a, KPD78, KS79, KJ78, KP79b, LED73, LDP79, LP79c, LP79b, Lec76a, LCK76, LE72, MMM70, MBM73b, NPL+79, NN70a, NN70b, NT79, NS79b, Nor75, OSL77, PLYM78, PKSB78, PGPP79, PA74, PB77, PGM77, PP78, RW79, RMB78, Rob72a, SD79a, SD70, SR77, SC78a, SC73, Spe73, SP71, TS71, TP77a, TTS+79, TWC73, TB74, TRPB77, VG78, WRF73, Web74, WLS77, WK73, Boy77, GML77, LCPP79]. Sub [Sim78c]. Subduction [SD79b]. **submolecular** [Sun75a]. subspace [Sre75]. subspaces [Jan76]. Substituent [BS79, KC73, Mil74, SD74, Tic79]. substituents [MK72]. **Substituted** [Boy77, DH78, Fog71, GBS70, Kp73, MR72, NTL79, PL78, Rout73, Sh77a, SS78a]. Substitution [HG75]. substitutions [KMLB77]. substrate [SS79]. **Subsymposium** [Ano79o]. Subsystem [Mil74, SD74]. subsystems [FTN77]. subunits [Fin73, Pol79]. Successive [GS70b, MK75b]. Sudden [Bow79, KKKCD78]. Suggested [Pea74b, Kau74b]. suggestion [Mem77]. suitable [BB73, Gia73]. sulfide [ES73b]. sulfides [Mat76d]. sulfur [Ald75, PB75a, KC77, TN79]. *sulphate* [HS70a, JST1]. sulphur [Cha77]. Sum [RB77, Res78]. **Sum-over-states** [RB77]. summary [KM72]. sumrule [BB71]. super [Amo71, Nor75]. super-secular [Nor75]. **super-secular-equation** [Amo71]. superconductant [PP79]. superconducting [Mat76d]. **Superconductivity** [Mat71b, Mat72b, Mat73b, Mat74b, Mat75, Mat77, Mat79b, ACK+75, CIL73, MM77b]. superdelocalizability [Mem75, Mem79]. supermolecule [GCP79, OSL77]. superoperator [BO78]. Supplement [RWF71, Sab75a]. support [BDT77]. supported [KGB76]. Surface [SK79, BR75b, DS70a, DT72, DE78, Kaul, KP71a, KW76, MO77, RT77, SKW72, SC73]. surfaces [BNLS72, BFH74, KKW73, Lin77, Moh78, PBPL78, PN71, PKSB78, Sin79, SB78]. survey [Sim77b]. susceptibilities [BBT71, Ema74]. susceptibility [Hal73, PL78]. suspected [KPP78]. SW [MS76a]. symbols [BW76b, But76, BW76c]. Symmetric [Gal72a, Csa77b, DMM75, Go79, Jor78, Kun78a, KOW78, Kun78b, Lim77b].
Liu71a, Sch77a, Sch73b, Sla70b]. symmetrical [Moh78]. Symmetries [Gal74, Mat76d, KGB77, MWY77, Oda73]. Symmetrischer [Sch73b]. symmetrized [Boy72c, VK74, Wyb73a]. Symmetry [Bee76, BB71, BH71, BB73, De 76, Eld73, GP78, GÖ68, JSC78, Kle70a, KC74, LP74a, LP74b, Ran79, Amo71, BF71, Boy70a, DM72, DK77, Flu72, GSE78, GP72, Han75, JPTM78, Kat72, KD74, Kau79b, Kle74a, Kry77, Kut78, Lar79, Laz78, LZ79, Lim76a, LG71, MK76b, MM77b, Ros78a, Rou78, Rou79, GOJ73]. symmetry-adapted [Kut78]. symmetry-lobe [Rou78]. Symposia [Cal73b]. Symposium [Pul78b, Sla71b, Sla73b, Sti79, BP70, BP71, BP72, BP73, Lon73, Ede70]. synaptic [Wal77]. synthesis [Gab76]. System [Spe72a, AM72b, BZSD79, BS75c, Bra79b, BS78c, CS72, HL79, HBE78, HG75, HP77b, JBP76, KR76, KPT7a, Laden75a, Man77, May74a, PCL78, PHL76, Res78, Sre75, SP79, TBB70, WH75]. systematibus [BP79]. système [TBB70]. systems [ACG74, AM72b, Bai74, BA78, Bar70, BB72c, BEH77a, BEH77b, BFH78, BL77d, CP70, Cho79, CP71, CP72, CPP73, CP77, CK74, CK75, CII79, ESG79, GOK79, GP74, GB70, GL74, GBM74, GRM75, HHR70, HS79, Hat75, Hea71, HG75, HR76, IS75, JMM71, JM76a, JPTM78, JS70, JL74, KL75, KPP77, KK77, KMT77, KL77c, Lai73, Lar79, Lat77, Lin78, LDR77, LRD78, LG75, May74b, MK75a, MS76a, Mic76b, Mil74, MB77, MPM79, MMM71, MM77m, NS75, NB78, Oni79, OSL77, PT78, Pea74a, Per78, PG77, RMB78, RGM75, RB75b, SN79, Sar75, SP79, SM77, SD74, SS73a, ST72, Sol71, SO77, TS71, TP77a, TL71, VB72, WOE78, YG77, SS73b, SD73]. Szent [Lak76]. Szent-Györgyi [Lak76]. T [Sab75a]. table [Oda73]. Tableau [Gal72b]. taking [MCF70]. Tamm [DS70a, HU74, Lar78a]. targets [Gia67, GLS79]. taurine [CS74]. tautomer [ZR78, ZBH78]. Tautomerism [CLP79a, CLP79b, ZSR79]. tautomers [HLYC77]. Tc [MM77b]. Tchebycheff [Lan77]. TCNQ [DT75, ÁFL78, CHH74, HRBB76, Koh75, Lad75a, LRD77, LRD78]. TCNQ-TTF [Lad75a]. Te [Sch73a]. Technique [BL72, BPTLVM73, AFD78, ABD79, BF78, CHD71, CP72, CDEO76, Dan72, GS70b, HLM77, HPK79, KPP78, LS74b, MTK77, Mil74, Muk75, Ner76, PW74a, Röe73, Röe75, SD74, Sun75a]. techniques [ABM78, Che71, DD72, FB76, GCK79, JS77, PBC74b, Pul77]. Teller [Ham71, IN71, MSSF79]. Temperature [Tal77, ACK75, MSSF79]. temperatures [AMJS79]. tempered [Raf75]. Tempering [Pos79]. template [Gab76]. ten [DSC77]. ten-electron [DSC77]. tensor [KK74b, KK77c]. tensors [Boy70a, Boy70b, BM71a, BM71b, BO73, BS74b, Ell73, IMN79]. teratogens [KPP78a]. term [Cha71, Koc74, WJC70]. terms [Ada73, AF73, CSFM72, CD71, FT77, GC77, JPTM78, MCF70, MCM73, NY75, PS75a, WS79, ZL78]. ternary [Mat77]. Test
tests

tetrahydropyrimidine

Tetrahedral

tetrahedrally

TFD

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theorems

theoretically

theories

Theory

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Thermodynamic

Thermodynamics

thioridazine

thioracils

Third

Third-order

Thomas
GY75, Goo76, GGJ75, Han70a, Han77a, Lun75, WC75a, YG77]. Three
[RW75, Bal78, CK73, HR79, Kol76, LG75, LPT+74, PLC78, RL77, Red79,
RC72, ST72, ST70, SS71a]. three-body [Bal78]. three-center
[HR79, LPT+74, ST70]. Three-dimensional [RW75, CK73, Red79].
three-electron [LG75, PCL78, RL77, SS71a]. threshold [Mes79, Sim78c].
through-water [PPB78]. thulium [AD77]. thymine [GJP79, ZR78].
Thyroxine [AJK78]. Ti [BL77c]. TiC [GK75]. TiCl [EP71]. TiCo [PN71].
TiFe [PN71]. Tight [CZNL70, CD74]. Time
[Go73, JL70, Moc73, NB78, Sch71b, Sch71c, Sch71d, SF76, BF75,
Han70b, Man77, SB75, WA71, Jam70]. Time-Dependent
[Sch71e, Go73, JL70, Moc73, Sch71b, Sch71c, Han70b, WA71, Jam70].
time-independent [Man77].
in [DC73, FFCB79, FR71, GH77, Kot76, Pal74, Sl74, Wh74, G75].
TiNi [PN71]. TiO [G75]. tissue [Je73]. tissue-specific [Je73].
titanium [ES73b]. Tm [DS74]. today [Wyb73b]. Toivo [Cal75b].
tomorrow [Wyb73b]. top [DM75]. Topological [KM72, BT78b]. Topologie
[Ch73b]. topology [Sch73b]. Torsional [BB79, SY77]. Total
[BG78, SW71, BM74, Cas79, KP76, SW70, Spe73]. traditional [CP71].
trajectories [CG78, CH77]. trans [TS78, WMB75]. trans [TS78].
transfer [BZ79, Ch79, CD76, DT75, Feu77, Lad76, LKK+79, L77,
L77, OSL77, Pet79, Rat76, RE+79, Van72, ZV79]. Transferability
[C71, SDD+, SW78]. Transferable [A79c, A79b, AB79, A79a].
Transform
[GM73, Ban74, BS75b, G75, GB72, GC73, MK77, MH72, ZF76].
Transformation
[Thu73, W74, A78, BL77a, Co74b, FSH77, Jer77, Sch78, Sh71, Sh77c].
transformations [BW76a, Co78, Han70b, SRP76, SRP77, Wit72].
transformed [We73]. Transformation [AC70, MMD78, OJ77, BR78, BF73,
BR75a, Cal77a, CH77, De 78, DR75, DCS77, FN73, GB77, G75, J77,
KP71a, KGB76, L75, Lar78a, Lar79, LD74, MM77b, Por77, Por78,
San71, Sch7c, SKW72, Sin75, SD74, SR77, S71, Van72]. transition-metal
[BR78, BF73, J77, KGB76]. transitions [BP75a, Ber73, Co79, DM72,
DD77b, Enz73, FWM77, GML77, KD74, Lar78a, Mes73a, NT79, S75].
translation [BA73, FM72]. Transmembrane [US79, V79].
Transmission [DS79, Wa77]. transport [Fr79, Hos78, KWC79, Mar79].
transversion [GRE+77]. transversion-type [GRE+77]. trapped [BA73].
treated [BK75c]. treating [FHB77, Pa73]. Treatment
[Sla71a, AM72a, BB73, BTD79, CW78, Ch77, Cla71, CSH74, Csa78b,
S70b, Des72, FP70, GS70a, Hi79, JBP76, Kau76, KMO77, MM74, ML72,
RTS74, RM79, SA77, SD79, Sh77c, SS71a, SW78, WRS70, LG71, S75].
treatments [AM74, AM77b, AM77a, CH71, TS72]. tri [IN71].
tri-phenylene [IN71]. triatomic [KK73]. tribute [CG70, Us75].
Tridiagonal [W70]. tridiagonalization [W71]. trifluoromethylicuracil
[PL78]. Trifonow [Ca73a]. trigonal [Sch73a]. trigonometric [DD78].
trimers [Moh78]. trimolecular [CW78]. triple [Kle70b, MPS70, Wei76].
trimolecular [CW78]. triple [SN79, Abd77, BB75, BP75a, IMN79, JZ79b, NS78, PCMS77, PS70, San71, SMB+79, SCYB75, TH78, TSE76]. tRNA [Pul77]. tropoelastin [KROU77]. true [LH79]. Truncated [YJ76, ML79]. Truncated-atomic-sphere [YJ76]. Tryptamine [WOEG78]. tryptamines [JG74]. TTF [CHHS74, HRBB76, Lad75a, LRD+77, LRD+78]. TTF-TCNQ [LRD+78]. Tunneling [CK73, Ada75b, CL77, Eis76, Feu77, Gol70, Wal77]. Turkuensis [Cal75b]. turn [RU76]. Turner [Cal76a]. Twenty [Lak76]. Two [BL77b, BH71, DT72, Ga72b, Höj79a, Höj79b, MSKM77, Thu75, Aba72, BA78, BB74, Bas78, BL77a, BB71, Bil72, Cal72, Cal73c, CPP75, CL78, Col79, Dea72, Eng72, GL74, HMV77, HLMV77, HMV78, Har75, Jet73, KM74a, Kij72, KBA76, Koc74, Kol74, LAM71, MKF77, Mal71b, MM74, Meh78, MH72, OK75, Pie71, Rat71, Ros78b, RB75b, Sha76, SDJ79, SS70, SJH79, SL70, TBB70, TTS+79, WRS70, JBG70, Mal71a]. two-body [KBA76, Ros78b]. Two-Center [Thu75, BA78, Eng72, MH72, Sha76]. Two-Electron [BL77b, BH71, DT72, Aba72, BL77a, BB71, Bil72, Cal72, Cal73c, GL74, KM74a, LAM71, MM74, RB75b, SJH79, WRS70]. two-matrix [Kij72]. Two-parameter [Höj79a, Höj79b, MSKM77]. two-particle [Rat71]. two-photon [MKF77]. two-point [CPP75]. two-spin [SL70]. Type [Spe72a, BS74a, BS76a, BS71, Cha77, CL78, FTN77, GRE+77, Höj79a, Höj79b, KGP79, LS72, LM72, LGR73, Mat73a, Mat76c, NY76, OK75, Pan77, PF74, PAM75, PW74a, RL77, Röe73, Sab71, SR72b, ST70, SLC78, SR72c, SF75, Lec76b].

U [Lon73, Sla73b, LB79a]. UHF [Cla70, Lun79, Sha77a, Sha78a]. ultimate [HPK79]. ultrasonic [PP71]. Ultraviolet [Gos78a, PLSL78, Ros75, Rab77]. unbounded [BFH78]. unconstrained [Muk75]. unconventional [Lec76a]. uncoupled [Vog79]. understand [KKK74]. Understanding [HP77a, Kau76]. uniaxial [Hub71]. Unified [MM74, CL73, LÖ77]. Uniform [MYTC77, BM73]. unit [CBV79]. Unitary [PH77, Mat74a, Mat76b, Mat79a, Ne79, Pal75, PW79, Sha77b, Sha78b, WP79]. unitary-group [Mat79a, Ne79]. united [CSH74]. units [HR79, Sri77]. Universal [SN78]. universe [Lay77]. Universitatis [Cal75b]. University [Sab75a]. unperturbed [AM74]. Unrestricted [NN72, NN74, PL78, SLB77, Jar73, KKA78, PS70]. unsaturated [NI70a, NI70b]. unstable [Tho76, TPC77]. Untersuchungen [HG75]. upon [DRC78, LCPP79, Sco71]. Upper [BBK76, LTR74, Wei71]. upper-LTR74. uracil [CLP79b, GJP79, KD77, ZR78, ZSR79]. uracils [PLSL78]. urea [ED74]. Uridine [PB77]. Use [Eld73, GPP79, Jor73, LAV72, BW73, Car75, CM76, Ema74, Euw71, GM73a, GM73b, HH70, Kau73, Ladv88, LZ79, MCM73, Nee75, Ne76, PT75, PAM75, PGDM77, RK77, Ron79, RCE79, Sch72, Sin72, Sol73, Sti78, Wei74, Wei71]. used [BC75, KB77, San72]. useful [LH74]. Using [JBG70, SDD77, AM77a, BS74a, BS76a, Bri73, Bur72, Chi77, Chr73, CP71,
[CP72, CL78, CK74, CSH74, Cur78, Dan72, DD72, Goo76, GHJ77, HS70a, HR76, JG72, JSK75b, KPP78, KT71b, KMO77, LF77, LGR73, Loc76, Loc77a, OMC76, OK75, PCMS77, SD79a, Sha76, SBM72, Srik77, TB74, Vla70, WN78, WRS70, WFS77]. usual [Cla71]. utility [PS73]. utilization [ST79a].

V [FTN77, HMC71, IM73, Kla78, Kle70b, KMO77, LGP75, LGM77, PPP79, PNC78, PK77b]. vacancy [SC79]. Väinö [Cal75b]. Valence [CESW70, Gal72b, Goo76, Har70a, Har77a, HR79, WJ79, AM72b, BW76a, Bra79b, GN77, Gy77, Har71a, HLYC77, Kla79, Lad74a, LS74a, MW74a, Moh77, NN74, NG73, OK75, Pet77, PNC78, RTS74, RS76, SM73a, SM76b, SM76a, SD78, SBD70, TRS73, TS77, TS78, TS79, WMB75, TTS79]. Valence-Bond [Gal72b, HR79, GN77, OK75]. Valence-Electron [Goo76, SD78, WMB75]. valence-fluctuation [Bra79b]. Valence-Bond [Gal72b, HR79, GN77, OK75]. Valence-Electron [Goo76, SD78, WMB75].

valinomycin [Sun75b, ST78, ST79b, Sun74b]. valinomycin-potassium [Sun75b].

Values [Spe72b, BBK76, BS71, BSG77, BL77d, RK77, SK71, SG77a, SP77].

Vanadium [WFS77, PNJB78]. Variable [ES79, MR72, Scl75, Amo72, Csa76, Csa78b, PK75]. variance [HS75].

Variation [BL72, BEH77b, Zer74, Eps77, GZ72a, Mor78, MI78, MMM71, NI74, PGPP79, SY77, TS72, Wei76, Wel77b]. variation-perturbation [GZ72a, MMM71].

Variational [BR75a, BR72, Bri73, Csa78a, GBK77a, Kla77, KGB77, LFF79, Lud75, PSH77, ACD74, CK75, CSH74, Csa76, Csa78b, Csa79a, CZ75, DR75, GF76, HS77, Moc73, Moc74, MK76b, NS75, Pau71, PBC74a, TK78, WW71, Wei76, ZF76].

variationally [Csa77b, LTR74]. various [BB74, Gal74, JNM66, eAJ76].


Via [GB71, Als73, FB76, GBL74, SS77b, YL74]. vibrantibus [BP79].

Vibration [CK75, BBA73, KD79a, LRD77, LRD78].

vibration-translation [BBA73]. Vibrational

[Tru72, BS77a, Bow79, GSE78, Sch71d, SR77, Ste77, Tru76]. vibrationally [MM72a]. vibronic [CI79, WZ70, TGL70]. vibronique [TGL70].

vibrotors [SS71b]. VII [Gbb77a, Lai73, SP7C79, TS77]. VIII [Con77a, FWFM77, KPP78b, KGB77].

vinyl [Cal70, MMB70, MLB72].

viral [LFS77], virial

[BEF78, BHF78, FHB77, Lev78b, Nah78, W074, WO75, WO76]. Virtual

[Beet79, Cof74b, Med79]. visual [Kl79, MP71a]. vitamin [ED79, Ram78].

vivo [Dav77b, Web74, WS75]. Vleck [Sl71b, Gor71, Gor72]. Vol [Cal75c, Lar78c]. volatile [DBBJ76]. voltage [VU79]. voltage-dependent
VRDDO
[HKP79, HPK79, KPP78a, KPP78b, PK75, PK77a, PK77b].
VRDO [PK76b].

W [Gos78b, Gos78a, Mär78, Sab75a]. Waals
[Mal71a, Mal71b, HČZ79, KK73, LH79, WMV77]. Wahlgren [LB79a].
walk [And79]. Walker [Sab75a]. wall [ULM76]. Waller
[Lim74b, Lim75a, Lim75b, Lim76b, Lim77b]. Walter
[Ano77-78]. water [AF73, ACG74, AMJS79, CC79, Dau74, Hal79b, HSBD78, HK74, KPP78c, Láz79, LB79b, Mey71, Nir75, PDEB78, PPB78, RC78, Tal77].
Watson [Sun77]. Wave [Bre73, Ada73, ANR75, Ada75a, AB73, AM77b, AM77a, Als73, ADFL71, BB75, BN76, BDP73, BS71, BC79, Cas78a, CL73, CL78, CWE71, D574, DRCT78, DLG79, DMM75, Euw71, Gal74, GN77, Gre71, H707, HH70, HK79, Hun75a, Jak76a, Jak76b, Jak76c, Jak76d, JTR77, Joh70, JS71, JW72, Joh73, JM76a, Jol79, Jor73, KM74a, KC72, KKA78, KMO77, KK76c, LF77, LTR74, Li76, Lim76a, Loc77a, Lud75, Lud77, Meh73a, Meh73b, Moc74, ML76, MK76b, MM72b, MSM70, MBM71, NS75, NRS79, OKM74, Pau78, Pop71, RWFS71, Rob71, Rob72b, RK79, Sab75a, SH73, Sch72, SC76a, SS73a, SS73b, Sin72, SH75a, SD70, Slab70b, SWP77, Tan74, Tru73a, VF76, Wei74, WFS77, WV74, Y77, Coo74, FJP70].
wave-functions [Jak76b, Jak76c, Jak76d, JTR77, KK76c, Lim76a, Loc77a, MK76b, SWP77, VF76]. Wave-mechanical [FJP70]. Wave-vector- [Bre73].
wavefunctions [OK75]. Wavenumber [SM73b]. waves [Ada72b, MSP73].
weak [Lya78]. weakly [MKT77]. Wechselwirkungen [KW57]. weighted
[DL75]. welcome [Sil74]. Welcoming
[Bry74, Han77b, Mär76, SG77c, Exe74]. well [CK73, RSS75].
Wechselmechanische [FJP70]. Weyl [HE78]. which [CEK72, KKK70].
wide [RMP71]. width [Fog71]. widths [FB76]. Wigner
[Ahl70, Ahl70, LWA74]. Wiley [Cal79b, Cal75c, Dun78, Gos78a, Shu77a].
Wiley-Interscience [Cal75c, Gos78a]. windows [BHLM78]. Within
[Spe72a, BMD70, Eps77, KM76, LB79b, LW76, Loc77a, Loc77b, Loc77d, PD78a, SDM74, WJ79, ZF76]. Woodward [Mat76a]. work [PS75a].

X [BFH74, Com77b, Con72, GML77, JW72, JM76a, KC79, Kau73, MS76a, PK75, PK77c, RK77, STS71a, WC75b, Y77, FM78b, HYLU78, AD77, BB75, BS71, CFMO73, Dan72, DC73, Dec70, DCS77, G75, GML77, HPP79, J7oh73, J7oh77, Li76, Mes73a, Min79, MFRE76, MMR74, PNJB78, PPC72, RK77, Sam75, SF76, Sla73a, Slab75, T751, TS71, TS75, W7K73]. x-ray
[FM78b, HYLU78, PNJB78, BS71, CFMO73, G75, GML77, Mes73a, T751].
x-rays [Dec70, MFRE76]. Xe [ES70]. XeF [SD78, TDB77]. XII
[AF73, MF73]. xii [Cal76a, MSP73]. XIV [LG71, MCP73]. XIX [MWY77].
XXV [CR72, MPW75]. XVI [MW75a]. XVII [Mat76a]. XVIII [Mat76b].
XX [MW77]. XXI [MN79].
years [Lak76]. yesterday [Wyb73b]. Yield [HG78, GGJ77]. York [Ahl77a, Ano78c, Cal79b, Cal75c, Cal77b, Dun78, Gos78a, Lar76, Lar78c, Shu77b]. Young [Lim75b].

Zero [Col77a, Boy70a, Har71c, Nal78]. zeta [GG79c, GG79b]. zinc [MS72b, MHH74, RTM77]. zinc-histamine [MHH74]. ZN [JMP79, KPD78]. ZnSe [CESW70, CWE71]. zum [BKW75, HG75]. zur [KA76, HG75]. Zwanzig [HLMV77]. zwitterion [RC78].

References


**Abdulnur:1971:BSO**


**Abdulnur:1976:IGP**


**Abdulnur:1977:IMM**


**Andre:1979:NMP**


**Adnan:1978:OOT**

S. S. Z. Adnan, S. Bhattacharya, and D. Mukherjee. Orbital optimization techniques: Comparative study in a semiempirical


REFERENCES


Atomic, Molecular and Solid-State Theory and Quantum Biology.


REFERENCES


REFERENCES

Almlof:1974:ICP


Alster:1973:EDM


Ali:1972:FOC


Almlof:1972:VED


Ali:1974:FOC


Ali:1977:COCb

[AM77a] M. K. Ali and W. J. Meath. On the convergence of one-centre partial wave treatments for diatomic molecules. II. Heteronuclear one-electron diatomic molecules using the 1sσ, 2sσ,


Anonymous:1970:Ma


Anonymous:1970:Mb


Anonymous:1970:Mc


Anonymous:1970:Md


Anonymous:1970:Me


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REFERENCES

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Anonymous:1973:Aa

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Anonymous:1973:Me
REFERENCES

Anonymous:1973:Mf

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Anonymous:1974:Aa

Anonymous:1974:Ab

Anonymous:1974:BR

Anonymous:1974:Ma

Anonymous:1974:Mb

Anonymous:1974:Mc
Anonymous:1974:Md


Anonymous:1974:Me


Anonymous:1974:Mf


Anonymous:1974:Mg


Anonymous:1974:Mh


Anonymous:1975:A


Anonymous:1975:Ma

REFERENCES


REFERENCES


Anonymous:1976:RSC


Anonymous:1977:Ab


REFERENCES

Anonymous:1977:Ai


Anonymous:1977:Aj


Anonymous:1977:EH


Anonymous:1977:LFH


Anonymous:1977:Ma


Anonymous:1977:Mb


Anonymous:1977:Mc

Anonymous:1977:Md

Anonymous:1977:Me

Anonymous:1977:Mf

Anonymous:1977:Mg

Anonymous:1977:Mh

Anonymous:1977:Mi

Anonymous:1977:Mj

Anonymous:1977:Mk
Anonymous:1977:Ml


Anonymous:1977:Mm


Anonymous:1977:Mn


Anonymous:1977:WH


Anonymous:1978:Aa


Anonymous:1978:Ab


Anonymous:1978:BRB


**Anonymous:1978:FCR**


**Anonymous:1978:I**


**Anonymous:1978:LP**


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**Anonymous:1978:Mb**


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**Anonymous:1978:Md**

Anonymous:1978:Me

Anonymous:1978:Mf

Anonymous:1978:Mg

Anonymous:1978:Mh

Anonymous:1978:Mi

Anonymous:1978:Mj

Anonymous:1978:Mk

Anonymous:1978:Ml
Anonymous:1978:Mm


Anonymous:1978:Mn


Anonymous:1978:PLP


Anonymous:1979:Ma


Anonymous:1979:Mb


Anonymous:1979:Mc


Anonymous:1979:Md

Anonymous:1979:Me


Anonymous:1979:Mf


Anonymous:1979:Mg


Anonymous:1979:Mh


Anonymous:1979:Mi


Anonymous:1979:Mj


Anonymous:1979:Mk


Anonymous:1979:Ml

Anonymous:1979:Mm


Anonymous:1979:Mn


Anonymous:1979:SES


Adams:1975:PTW


Adams:1977:AGM


Aronowitz:1978:ICN

REFERENCES


REFERENCES


REFERENCES

Atomic, Molecular, and Solid-State Theory and Quantum Biology.

[Barnett:1977:CES]

[Bardsley:1978:CSI]

[Barfield:1979:PPC]

[Bass:1975:CET]

[Basu:1978:IBT]

[Banyard:1970:MFE]
REFERENCES


Bartlett:1971:GSR


Basilevsky:1972:IIR


Basilevsky:1972:SPT


Bhattacharyya:1972:TCS


Bunge:1973:SES


Basilevsky:1974:ITH

REFERENCES

489, May 1974. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bagus:1975:STS


Bunge:1978:CAE


Blaisten-Barojas:1973:AGF


Bartlett:1973:TCE


Bolotin:1979:TIB


[Bishop:1979:NOA]


[Block:1977:ASA]


[Bolotina:1979:DSS]


[Bolis:1978:PAF]

[BCR+78] G. Bolis, E. Clementi, M. Ragazzi, D. Salvadori, and D. R. Ferro. Preliminary attempt to follow the enthalpy of an enzy-


**[BEF78]** Erkki Brändas, Nils Elander, and Piotr Froelich. Extended virial theorem applied to predissociation phenomena. Interpre-


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


[Blum:1975:SAE]

[Born:1975:HBS]

[Boyer:1975:SCR]

[Blum:1976:CIE]

[Beyer:1977:FSS]


REFERENCES


C. M. Bowden, H. C. Meyer, and P. L. Donoho. Theory of the intrinsically strain broadened line shape for magnetic resonance absorption within the non-Kramers doublet of Al2O3:Fe2+. 
REFERENCES


Bendazzoli:1976:SOC


Boring:1970:SCS


Borelius:1971:IPS


Boring:1974:CEG

REFERENCES


REFERENCES


REFERENCES


REFERENCES

Binkley:1975:MPT


Bartlett:1978:MBP


Buchler:1979:VSL


Bouscasse:1973:TOE


Braun:1972:VBI


Barnsley:1975:VBT

REFERENCES


Berrondo:1975:PSC


Baerends:1978:ELH


Brandas:1970:RPT


Brandow:1975:FTE


Brandow:1976:TMI


Brandow:1979:FTE

REFERENCES

207–242, February 1979. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).


Bryan:1974:WR


Benesch:1970:NOM


Benesch:1971:EAX


Bartlett:1974:CEL


Boyle:1974:AEI

REFERENCES


[Bartlett:1975:SAD]


[Bishop:1975:NIT]


[Born:1975:ICS]


[Bartlett:1976:CEL]


[Besson:1976:ASC]

REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES

Beretta:1973:DPT

Berlin:1972:NPM

Bouma:1978:IMO

Bertetta:1976:SRD

Bonham:1973:MQR

Bradford:1976:EVS
REFERENCES


Butler:1976:CSAA


Butler:1976:CSAC

P. H. Butler and B. G. Wybourne. Calculation of \( j \) and \( j_m \) symbols for arbitrary compact groups. III. Application to \( \text{SO}_3 \supset T \supset C_3 \supset C_1 \). *International Journal of Quantum Chemistry*, 10(4):615–628, July 1976. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

But:1979:CEC


Bartlett:1977:TOM


Buchler:1976:CSD


**REFERENCES**


REFERENCES


REFERENCES


REFERENCES


[Cor71] Joyce H. Corrington, H. S. Aldrich, C. W. McCurdy, and L. C. Cusachs. Dipole moments and orbital energies from ARCANA:


[Castro:1979:CTM] Eduardo A. Castro. Calculation of total molecular energies from an approximate relation between SCF orbital energies and
REFERENCES


Colbow:1976:ETP


Chao:1978:MMI


Collins:1976:SIM


Cook:1973:CMC


Collins:1972:SED

REFERENCES


REFERENCES


Costas:1979:MPS


Calais:1976:QSM


Caballol:1974:GOS


Csavinszky:1974:FPP


Csavinszky:1975:FPP

REFERENCES

Collard:1977:OTE


Chang:1971:MSR


Chandler:1977:HST


Cantu:1971:OPT


Chen:1971:ETQ


Cerjan:1978:CCS

REFERENCES


REFERENCES


Claesson:1973:MEM


Chalasinski:1977:CPR


Carbonell:1973:TPT


Collins:1974:EHE


Carney:1975:VRA

REFERENCES


REFERENCES


REFERENCES


REFERENCES


**Cooper:1974:TMW**


**Cooper:1978:CPE**


**Cooper:1978:TMI**


**Cooper:1979:PTH**


**Corio:1972:RRG**

REFERENCES

Cantril:1970:SSC


Cizek:1971:CPA


Cizek:1972:DCE


Cizek:1977:AAB


Cizek:1974:CEL

Cizek:1975:CEP


Clementi:1972:SES


Crossley:1977:LPO


Coulter:1972:SFI


Calais:1973:SAM


Cornelius:1974:CER

the International Symposium on Quantum Biology and Quantum Pharmacology.


Csavinszky:1977:VMT


Csavinszky:1978:VPL


Csavinszky:1978:VTP


Csavinszky:1979:AVS


Csavinszky:1979:NFA

REFERENCES


REFERENCES


Cheung:1979:ERD

149


Chong:1974:ADE

CSY+74


Chong:1977:PCK

CT77


Cheney:1979:EFA

CT79


Curtiss:1977:ICH

Cur77

REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES

Davies:1974:QIP


Danese:1973:NMT


Deutsch:1975:EOA


Daudey:1974:PICa


Dunlap:1977:ALX

Brett I. Dunlap, John W. D. Connolly, and John R. Sabin. On the applicability of LCAO-X α methods to molecules con-
REFERENCES


REFERENCES


REFERENCES


REFERENCES


Duprez-Quesnoit:1977:EQD


Dmitiev:1975:VPT


Datta:1977:MOP


Daudel:1978:DEM


Davison:1970:PST

REFERENCES

[Davison:1970:RTL]  

[Damommio:1974:AAS]  

[Danese:1976:CBC]  

[Davidson:1976:SME]  

[Dhingra:1979:TEH]  

[Daudel:1977:TLP]  
R. Daudel, M. E. Stephens, I. G. Csizmadia, C. Kozmutza, E. Kapuy, and J. D. Goddard. Theory of lone pairs. II. A

**Day:1974:GHP**


**Davies:1979:IBA**


**Dementev:1974:CPS**


**Davison:1972:TET**


**Dugay:1975:AMO**

[DT75] M. Dugay and J. Thomas. Alternant molecular orbitals (AMO’s) for some organic semiconductors: Ion radical salts from 7, 7, 8, 8-tetracyanoquinodimethane (TCNQ) and chloranil/para-phenylenediamine (PDC) charge transfer complex. *International Journal of Quantum Chemistry*, 9(6):1087–1095,
REFERENCES

November 1975. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).


REFERENCES


[Edenman:1970:OAI]

[Ehrenson:1973:ISL]

[Eigen:1978:AHP]

[Eisenstein:1976:MTH]

[Eisenstein:1977:DCB]


England:1972:OCC


Enoch:1976:VPO


Egan:1978:CBP


Enz:1973:LDA


Ellis:1971:EST


Epstein:1977:PTW

REFERENCES


REFERENCES


[RCC]


[WRR]


[ALP]


[NSP]


[DCM]

REFERENCES


REFERENCES


Froelich:1977:NCT


Ford:1970:MMS


Fink:1973:PBB


Fischer:1970:CIS


Fischer:1974:MHF

REFERENCES


the International Symposium on Atomic, Molecular and Solid-State Theory and Quantum Biology.

**Farberov:1972:TBM**


**Farantonis:1978:CDC**


**Frishberg:1978:NDM**


**Findley:1979:GGC**


**Freeman:1975:EDI**


**Franchini:1970:EGF**

ber 1970. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).


REFERENCES


REFERENCES


REFERENCES


REFERENCES


Godefroid:1977:MTS


Georghiou:1975:NSR


Goddard:1977:SMO


Gruninger:1973:EPQ


Gresh:1979:IIR

REFERENCES


the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Statistics.


REFERENCES


Goddard:1979:GDC


Gianinetti:1973:OMO


Gianturco:1976:SSP


Gingerich:1978:VBA


Gunnarsson:1976:SDF

[GJ76] O. Gunnarsson and P. Johansson. The spin-density-functional formalism for quantum mechanical calculations: Test on di-


[GK78] Richard Gilardi and Jerome Karle. Fibrous structures: Their character and the role of interatomic forces in their analysis.
REFERENCES


REFERENCES


Guenzburger:1977:ESC


Graovac:1973:SOM


Gardre:1977:EMD


Goscinski:1968:CEP


Goscinski:1973:ECE


Gazquez:1979:EGM

REFERENCES

Gold:1970:SEP

Golden:1973:TDQ

Golebiewski:1979:NIS

Goodisman:1976:VET

Gopinathan:1976:HTS
REFERENCES

Gora:1971:FCF


Gora:1972:FCF


Goscinski:1975:TOD


Goscinski:1978:BRBb


Goscinski:1978:BRBa


Gouyet:1973:CAN

REFERENCES

Gilles:1972:ISG


George:1974:QMD


Gilles:1978:SNM


Goscinski:1979:END


Gubanov:1971:EAS


Giessner-Prettre:1973:MOC

REFERENCES


Goldblum:1979:UOM

Grau:1977:ABL

Goodall:1974:ICN

Grein:1971:ASE

Garduno:1977:PPB


the International Symposium on Quantum Biology and Quantum Pharmacology.

George:1977:CEC


Grabenstetter:1976:GGS


Guberman:1979:PCD


Gervy:1977:SMI


Goodisman:1975:MPT


Garrett:1972:TSDa

[GZ72a] Thomas B. Garrett and Daniel Zeroka. Theoretical studies of diamagnetic properties of the hydrogen molecule ion. I. Approx-


[Hal75a] G. G. Hall. Charges and bond energies in the analysis of quantum chemistry calculations. *International Journal of Quan-
REFERENCES


REFERENCES


Harmison:1975:BST


Harcourt:1977:VFF


Harriman:1977:CGM


Harris:1977:CCM


Harris:1978:HLM

REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES

sium on Atomic, Molecular, and Solid-State Theory and Quantum Statistics.

Harris:1971:EHF


Hariharan:1979:EMP


Handler:1978:ICE


Hopkinson:1978:IMO


Halkjaer:1979:PCN

REFERENCES


[HMV77] A. Hardisson, F. Mauricio, and S. Velasco. Absorption line shape of two coupled oscillators decaying in two different medi-

**Hardisson:1978:ALS**


**Hatano:1978:CES**


**Ha:1973:PPP**


**Høj79a**


**Høj79b**


**Holtje:1977:IEC**

Hans-Dieter Hötjje. Interaction energy calculations on interactions between pharmacon models and ionic receptor site mod-
Hopper:1978:ESH


Horing:1971:NPM


Hosoya:1972:SRO


Hosur:1978:QMT


Harter:1977:BCC

REFERENCES

state Theory, Collision Phenomena, and Computational Methods.


REFERENCES

Harcourt:1979:VBS

Herman:1976:OCD

Hillier:1970:ICU

Hillier:1970:NSP

Hankey:1971:AFS
REFERENCES


[Horino:1975:ESE] Yasuyo Horino and Hiroshi Tatewaki. The electronic structure of the excited states for B, C$^+$, and C arising from the config-
<table>
<thead>
<tr>
<th>Reference</th>
<th>Details</th>
</tr>
</thead>
</table>
REFERENCES


Hyman:1978:IAX


Imai:1974:DCD


IHaya:1973:MOR


IHaya:1979:TPG


INI71

IHaya:1971:RQC


Ivanov:1975:PTD


Ivey:1974:LDE


Ivanov:1979:CPD


Jain:1970:SSP

REFERENCES

JAKUBOWSKI:1976:BOOa


JAKUBOWSKI:1976:BOOb


JAKUBOWSKI:1976:BOOc


JAKUBOWSKI:1976:BOOd


JAMIESON:1970:TDH


JANKOWSKI:1976:CPS

REFERENCES


REFERENCES

Jette:1973:CME


Jucys:1972:GSU


Johnson:1974:MOS


Julg:1978:VNI


Jorgensen:1970:TDH


Jucys:1974:EHF


REFERENCES

1978. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).


[Joh77] K. H. Johnson. Spin-orbital electronegativity, the Xα method, and reactivity at transition-metal interfaces. *International
REFERENCES


Johnson:1973:GOO


Johnson:1977:LBM


Jorgensen:1978:SEM


Johansen:1974:ICE


Jucys:1970:ILD


Johnson:1971:SMO

[JS71] K. H. Johnson and F. C. Smith, Jr. SCF molecular-orbital studies of the sulphate ion by the scattered-wave model. *Inter-
REFERENCES


Jaszunski:1977:ATC


Jeziorski:1978:SFC


Jucys:1975:NRO


Jucys:1975:SOI


Javor:1977:RLE

Julg:1978:CGM


Junker:1978:CCC


Johnson:1978:NTM


Johnson:1972:DES


Jafri:1976:III


Jones:1978:MFS

REFERENCES


[JŻ79a] Danuta Jeziorek and Bronisław Żurawski. Ab initio calculations including electron correlation for the minimum energy path of the \((^1A_1)\text{CH}_2 + (^1\Sigma)\text{H}_2 \rightarrow (^1A_1)\text{CH}_4\) insertion reaction. International Journal of Quantum Chemistry, 16(2):277–292, August 1979. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).


REFERENCES


Kapoor:1973:SPA


Kaplan:1979:MSI


Karlsson:1970:HFM


Karlsson:1970:SCPa


Karlsson:1970:SCPb


Karle:1978:FAC

Kashiwagi:1976:IAB


Katriel:1972:SLH


Kaufman:1970:BMC


Kaufman:1970:MPA


Kaufman:1973:PUC


Kaufman:1974:DRP

[Joyce J. Kaufman. Discussion remarks on a possible commonality in the etiology of chemical carcinogenesis and allergy. *Inter-
REFERENCES


Joyce J. Kaufman. Spin, symmetry, and orbital filling restrictions indicate the necessity for ab-initio configuration interac-

**Klahn:1977:CLI**


**Kleindienst:1976:IEB**


**Koutecky:1972:DMH**


**Koutecky:1978:NSP**

REFERENCES

Kari:1972:GWF


Kang:1973:MOA


Klein:1974:SAR


Kari:1977:EEG


Kai:1979:MXM


Katriel:1974:SSD


[KFY71] Göran Karlsson, Kenichi Fukui, and Tokio Yamabe. Self-consistent pseudo-eigenvalue equations in parametric charge-

**Kibler:1976:CGC**


**Kibler:1977:CGC**


**Kunz:1976:AHS**


**Klein:1977:VLSb**


**Kosevich:1979:ELM**

Kanazawa:1979:SMS


Khokhlov:1979:CFL


Kibler:1975:APT


Kibler:1975:CBP


Kijewski:1972:TMC


Kiss:1975:TIE

REFERENCES


Kryachko:1976:SCP
E. S. Kryachko and Yu. A. Kruglyak. On the solution of the
N-completeness problem. *International Journal of Quantum
ISSN 0020-7608 (print), 1097-461X (electronic).

Kuprievich:1976:CSO
V. A. Kuprievich and V. E. Klymenko. Computation scheme
for optimizing multiconfigurational wave-functions. *International
1976. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X
(electronic).

Kaufman:1977:CPN
Joyce J. Kaufman and Ellen Kerman. Conformational profile
of nalorphine by PCILO calculations. *International Journal of
IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Konig:1977:CFP
E. König and S. Kremer. The concept of fractional parentage
for arbitrary molecular point groups. *International Journal of
IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Konig:1977:ITO
E. König and S. Kremer. Irreducible tensor operator meth-
ods in strong-field coupling. *International Journal of Quantum
IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kuprievich:1977:MOE
V. A. Kuprievich and V. E. Klymenko. Modified one-electron
Hamiltonian method in the MC SCF theory. *International
CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (elec-
tronic).
REFERENCES


REFERENCES


REFERENCES


Knirk:1977:MIP


Koutecky:1977:SQS


Kai:1978:CSM


Kwiatkowski:1979:MSM


Klasinc:1978:APS


REFERENCES


REFERENCES

Kutzelnigg:1977:DEG  

Kumar:1977:ESS  

Knezevic:1977:SSP  

Kikuchi:1979:TSH  

Kouba:1971:NOI  

Kobe:1978:IGI  


REFERENCES


REFERENCES


REFERENCES

Kaufman:1978:MCNb


Kwiatkowski:1978:AOW


Kaufman:1978:MCNa


Kaplan:1971:ICE


Kaplan:1973:MEG

REFERENCES


REFERENCES

[250]

Kaufman:1978:GAB

Kapur:1973:SRL

Klimo:1976:SEH

Kashiwagi:1977:TIA

Kashiwagi:1978:IMO

Kruglyak:1970:SES
1970. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kummer:1977:ARB


Kunert:1978:ISNa


Kunert:1978:ISNc


Kutzelnigg:1978:ABP


Kulkarni:1979:CSP


Kennard:1976:CAF

Kennard and J. T. Waber. Calculated anisotropies in the Fermi surface of alkali metals. *International Journal of Quant-
REFERENCES


Kunz:1979:ETP


Karlsson:1973:DOC


Laughlin:1970:PGE


Lo:1976:CAF


Ladik:1970:EBD


Ladik:1974:AVE

János Ladik. All valence electron band structures of simple periodic protein models. *International Journal of Quantum
REFERENCES


[Lar78b] Everett G. Larson. Representable reference density matrices applied to the graphical description of the Coulomb hole in the 1s$^2$(2p)$^2$ $^1S$ state of the B$^+$ ion. *International Journal
REFERENCES


REFERENCES


REFERENCES


[Larsson:1979:BDN]


[Les:1979:MCC]


[Lindholm:1978:IES]


[Leopold:1976:SLC]

Lazzeretti:1976:CED

Langlet:1979:SSE

Larson:1971:PHC

Langhoff:1973:ICS

Langhoff:1974:CIC

Lavery:1979:PTS
Richard Lavery, Marçal De Oliveira, and Bernard Pullman. A preliminary theoretical study of the acid catalyzed hydration

**Lin:1972:SEP**


**Leclerc:1976:CSU**


**Leclerc:1976:HSG**


**Langhoff:1973:CIS**


**Leibovici:1974:SIF**

REFERENCES

Letoquart:1974:SKP


Levy:1970:MMS


Levin:1978:MBS


Levy:1978:PGV


Lewis:1978:CPM


Laurenzi:1977:ECF


REFERENCES


REFERENCES


Lindgren:1978:CCA


Lipari:1972:FPE


Liu:1971:PCL


Liu:1971:MDR


Loew:1975:QCC

REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


Lowdin:1979:P


Ledovskaya:1974:SHLa


Ledovskaya:1974:SHLb


Linderberg:1974:DPH


Lavery:1979:MQC


Lavery:1979:TMSb

REFERENCES


REFERENCES


REFERENCES


Lunell:1979:CUP


Laskowski:1971:POM


Laskowski:1971:TFO


Liu:1971:ESN


Laskowski:1972:TFO

Lathouwers:1978:MSG


Larsson:1974:ESO


Lochmann:1976:CII


Lin:1977:QMG


Laughlin:1974:BWP

Lyast:1978:APW


Lazzeretti:1977:CMS


Lazzeretti:1979:USF


Maggiora:1979:ARC


Maksic:1971:CJJ


Malrieu:1971:HOCa

Malrieu:1971:HOCb


Manne:1977:LDE


Marinelli:1973:TOM


Marois:1973:TPB


Marston:1976:WR


Maartensson:1978:BRB


REFERENCES

Matsen:1976:SFQb


Matsuoka:1976:MIR


Matthias:1976:SSS


Matthias:1977:STB


Matsen:1978:TTI


Matsen:1979:UGF


Matthias:1979:SSP


Mayer:1974:SPEa


Mayer:1974:SPEb


Mayer:1975:E


Mayer:1978:SPE


Mukherjee:1971:SCC

Mendelsohn:1973:RHF


Mortola:1973:ISP


Mishra:1979:EBE


Mcdowell:1979:IBS


Men:1970:GTM


Mezey:1979:DAI


Morrison:1975:EKT


Miles:1978:CEP


Mehler:1973:IPP


Mehler:1973:PGF


Mehler:1978:SCN

Ernest L. Mehler. Self-consistent, nonorthogonal group function approximation: Application to two interacting, rigid HF


REFERENCES

Messmer:1973:COX


Mestechkin:1973:SDS


Mestechkin:1978:RHF


Mestechkin:1979:ITP


Massa:1970:GMO


Meyer:1971:IEW

REFERENCES


607, July 1972. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Michels:1970:MOS**


**Murphy:1974:MOS**


**Marron:1970:SHF**


**McIntosh:1976:LDS**


**McIntosh:1977:LDS**

Michels:1978:ESN


Michels:1978:ESE


Morikawa:1978:MMO


Micha:1974:RDT


Micha:1976:OFR


Michl:1976:ESR

Josef Michl. \(\pi\)-electron systems: Recent developments in electronic spectroscopy and the PPP model. *International Journal
REFERENCES

Miller:1971:ESA

Miller:1974:PMS

Mintmire:1979:LMX

Mitra:1972:EMH

Mayer:1975:SPEb
[MK75a] I. Mayer and M. Kertész. Spin-projected EHF method. III. Applications to $\pi$-electron systems. *International Journal
REFERENCES


Mayer:1975:SPEa


Mayer:1976:CDD


Moiseyev:1976:SCS


Mestechkin:1978:SDO


Makhanek:1977:LTM


Moiseyev:1977:WBQ

Mohraz:1976:COP


Meunier:1979:DCP


Millie:1972:AEC


Mayer:1973:SPE


Meunier:1976:PMC


Men:1975:SCS


Maeder:1970:AEC


Martin:1978:TMC


Makarov:1979:IIG


Mukherjee:1971:SCV


Mukhopadhyay:1975:NPH

REFERENCES

[Mortola:1974:AMS]

[Moitra:1970:SDQ]

[Matsen:1979:SFQ]

[Merrifield:1977:RRP]

[Moccia:1973:TDV]

[Moccia:1974:SDF]
REFERENCES

Moffat:1979:CII


Mohammad:1977:SVE


Mohammad:1978:LPE


Mohammad:1979:IIP


Monkhorst:1977:CPC


Morikawa:1975:OFF


Morikawa:1978:MCV

Tetsuo Morikawa. Metric-constrained variation method for atoms and molecules. *International Journal of Quantum Chem-
Moseley:1973:IQC


Misurkin:1975:ESC


Mantione:1971:QMI


Meath:1971:ADR


McMahon:1975:PRS

REFERENCES

Moskalenko:1979:BCP


Markovsky:1979:QCI


Millie:1970:NTB


Matsen:1975:SFQa


Mishra:1972:VES


Majorino:1973:AMP


1970. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).


Mineyev:1979:OOI


Muftakhova:1976:CES


Mukherjee:1974:CCE


Mukherjee:1975:OOS


Mulliken:1971:GSB

REFERENCES


REFERENCES


REFERENCES


**Norbeck:1973:FRH**


**Nir:1977:DMS**


**Nakayama:1970:MCLa**


**Nakayama:1970:MCLb**


**Narita:1974:DBO**

Nir:1975:ACF


Nishikawa:1977:ECF


Nakashima:1977:TRP


Nagata:1979:MAC


Nevis:1977:SSR

Niyogi:1977:ESE


Nanda:1972:UHF


Nanda:1974:AVS


Nanda:1977:IRA


Nordling:1975:EAL


Novaro:1973:CGT


sium on Atomic, Molecular, and Solid-State Theory and Quantum Statistics.

Novaro:1976:GTB


Ortega-Campos:1971:LDS


Odabasi:1973:SEA


Oddershede:1977:DEE


Olson:1975:EIT

Oddershede:1974:HFL


Ohrn:1978:CCG


Ohrn:1979:CCG


Ohrn:1979:LOH


Oie:1976:ICL

REFERENCES


REFERENCES


sium on Atomic, Molecular, and Solid-State Theory and Quantum Statistics.


Alberte Pullman and Hélène Berthod. An ab initio study of a
nucleoside: Uridine. *International Journal of Quantum Chem-
ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Pro-
cedings of the International Symposium on Quantum Bio-
logy and Quantum Pharmacology.

M. A. Pokrant, A. A. Broyles, and R. L. Coldwell. Nonzero
temperature variational principle. *International Journal of
Quantum Chemistry*, 8(S8):403–412, January 20–26, 1974. CO-
DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Sup-
plement: Proceedings of the International Symposium on Atomi-
c, Molecular, and Solid-State Theory and Quantum
Statistics.

B. Pullman, H. Berthod, and P. H. Courriere. The explo-
ration of the conformational properties of biological phenethyl-
alamines by molecular orbital techniques. *International Journal
of Quantum Chemistry*, 8(S1):93–108, January 17–19, 1974. CO-
DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (elec-
tronic). Supplement: Proceedings of the International Sym-
posium on Quantum Biology and Quantum Pharmacology.

A. Pullman, H. Berthod, and N. Gresh. Cation-ligand interac-
tions: ab initio SCF studies of the binding properties of alkali,
alkaline-earth, and ammonium ions. *International Journal of
Quantum Chemistry*, 10(S10):59–76, January 19–24, 1976. CO-
DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).
Supplement: Proceedings of the International Symposium on
Quantum Biology and Quantum Pharmacology.

S. T. Pantelides, J. Bernholc, J. Pollmann, and N. O. Li-
pari. Green’s function scattering-theoretic methods for point


[PCMS77] J. D. Petke, Ralph E. Christoffersen, Gerald M. Maggiora, and Lester L. Shipman. Ab initio calculations on large molecules

**Politzer:1977:CAE**


**Piela:1978:EPE**


**Politzer:1978:SPE**


**Pullman:1979:MSA**


**Politzer:1979:RHB**


G. A. Petersson. The pairwise correlated generalized valence bond model of electronic structure. II. A simple physical model...

[Pethig:1978:EPP]


[Petrov:1979:MET]


[Pohl:1974:IHT]


[Ptitsyn:1979:MPF]


[Pullman:1977:UPS]


Lucjan Piela. Perturbational calculation of the exchange forces in the two lowest states of the hydrogen molecule. *International
Pipano:1971:ICP


Petelin:1972:REF


Preston:1973:ISC


Popkie:1975:TCC


Popkie:1976:ILM

REFERENCES

1976. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

[Popkie:1976:MCM]

[Popkie:1977:MCMa]

[Popkie:1977:MCMb]

[Preston:1977:MXC]

[Preston:1975:MXC]
Harry J. T. Preston, Joyce J. Kaufman, and Walter S. Koski. MS–Xα calculations of polyhedral boron compounds. *Inte-
REFERENCES


Pople:1978:ECT


Pople:1979:DSH


Pack:1977:OSS


Pack:1979:SSM


Praud:1973:ISO

[PLMB73] Lionel Praud, Bernard Levy, Philippe Millie, and Gaston Berthier. Ab initio second-order perturbation calculations for

**Plotnikov:1979:RPR**


**Peng:1978:UPS**


**Pack:1978:CSS**


**Papaconstantopoulos:1971:BSF**

REFERENCES

Pilkington:1976:MEA


Petersson:1978:PCG


Papaconstantopoulos:1978:CXR


Purvis:1977:AMI


Polak:1970:OHO

Poltev:1979:SII


Pople:1971:ESW


Popov:1979:QAC


Porta:1977:MHC


Porta:1978:TDH


Poshusta:1970:CDS


REFERENCES


REFERENCES


REFERENCES


REFERENCES

337

Petrasen:1969:AGQ


Pullman:1970:MOC


Pullman:1974:ISB


Pullman:1976:QMM


Pullman:1977:CQM


Pullman:1978:IID

Bernard Pullman, editor. Intermolecular interactions, from diatomics to biopolymers. Perspectives in quantum chemistry and

Pullman:1978:NMR


Pullman:1979:RDM


Pullman:1979:MIA


Pullman:1979:R


Purcell:1975:QSA


Pulfer:1974:HIEb

[PW74a] J. D. Pulfer and M. A. Whitehead. The Hammerstein integral equation: a general technique for constructing a rapidly con-


REFERENCES


REFERENCES

Robb:1970:GSE


Robb:1971:GSE


Robb:1972:GSE


Romano:1978:MCS


Rein:1975:EPB


Ruedenberg:1979:MOT


1972. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).


Renugopalakrishnan:1977:NMR


Rai:1977:BTT


Rohmer:1979:ESP


Riera:1972:GRC


Riera:1973:NSO


Redmon:1974:IPD

REFERENCES


REFERENCES


REFERENCES

Rosina:1978:ATB


Rouse:1973:CAS


Rouse:1974:CAS


Rouzo:1978:DMS


Rouzo:1979:USS


Ryback:1978:AMC

References


Rouzo:1978:ADGa


Rouzo:1978:ADGb


Rouzo:1978:ADGc


Roothaan:1979:ASN


Renugopalakrishnan:1978:CSC


Rabinowitz:1972:TIT

REFERENCES


REFERENCES


REFERENCES


Sack:1972:AFM


Salhany:1972:IPS


Salmon:1973:CCS


Salem:1979:MCR


Sambe:1975:ASM

REFERENCES


Schieve:1975:HTD


Smeyers:1978:HPH


Shillady:1979:DOG


Sutton:1970:MCM


Stoddart:1970:OBP


Dale Spangler and Ralph E. Christoffersen. Development of basis sets for molecular calculations. Comparison of tetrahedral Gaussian lobe functions and Cartesian Gaussian basis sets.


REFERENCES


[Sch76b] J. Michael Schurr. Light absorption at high intensities. Comparison of quantum theory and semi-classical results. *Internationa-
REFERENCES

Scharfenberg:1977:NAS


Schmelzer:1977:ESH


Schonhammer:1977:THC


Scharfenberg:1978:SRT


Scofield:1971:ASE

Scofield:1973:NLO


Scofield:1974:ASC


Song:1975:ESP


Song:1977:ESP


Siu:1970:SGS


Smith:1974:NTO

REFERENCES


[Sarma:1979:SCS] C. R. Sarma and K. V. Dinesha. Subduction coefficients for $\langle 2^{N/2-S} \, 1^{2S} \rangle \downarrow \langle 2^{N_1/2-S_1} \, 1^{2S_1} \rangle \otimes \langle 2^{N_2/2-S_2} \, 1^{2S_2} \rangle$ of $U(n) \downarrow U(n_1) \otimes U(n_2)$. *International Journal of Quantum Chemistry*, 16(6):1195–1207, December 1979. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

REFERENCES


Sambe:1976:CBX


Szent-Gyorgyi:1976:ETC


Szent-Gyorgyi:1976:SRM


Selsby:1977:SEMb


Szent-Gyorgyi:1977:PRR


REFERENCES


[Sims:1976:CCH] James S. Sims, Stanley A. Hagstrom, and John R. Rumble, Jr. Combined CI–HY studies of atomic states. IV. The four lowest \(1^1S\) and four lowest \(1^1P\) states of He and the lowest \(1^1S\) and \(1^1P\) states of \(H^{-}\). *International Journal of Quantum Chemistry*, 10(5):853–866, September 1976. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).


REFERENCES


REFERENCES

978, June 1977. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).


the International Symposium on Atomic, Molecular and Solid-State Theory and Quantum Biology.

**Sinanoglu:1973:RDN**


**Sinanoglu:1975:CDT**


**Sisler:1974:RW**


**Sklenar:1979:MSB**


**Smith:1979:DFT**

REFERENCES


[Sahni:1971:CEV]

[Sahni:1972:RAC]

[Seitz:1973:CHS]

[Steslicka:1979:SSE]

[Shilov:1979:MSR]


REFERENCES


REFERENCES


REFERENCES

Srivastava:1979:ESS

Savin:1979:ESP

Selsby:1977:SEMa

Smith:1979:SV

Sheen:1973:PIP
Saran:1977:MOS

Stoddart:1971:LME

Sannigrahi:1979:TIS

Szabo:1977:IEB

Solomon:1971:OLC
REFERENCES


Stoll:1975:HFC


Stepanov:1977:EMI


Stolarczyk:1979:IPM


Sparks:1978:ICM


Sengupta:1972:GLS


REFERENCES


Dirk Stigter and John A. Schellman. Electrostatic representations of molecular groups. *International Journal of Quantum


the International Symposium on Quantum Biology and Quantum Pharmacology.


Shillady:1973:ECE


Sundaram:1978:NIM


Sakamoto:1979:EUD


Sundaram:1979:NIM


Stenger:1974:IPE


Stepanov:1977:KSG

August 1977. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


Trindle:1978:SFR

Thomas:1975:NLS

Thomas:1975:R

Thomson:1976:ESU

Thulstrup:1975:SIF


Terasaka:1973:ESP


Theodorakopoulos:1979:OEB


Truhlar:1979:EPA


Tapia:1977:EEH


Toivonen:1977:RMO


Topiol:1978:ECP

REFERENCES


REFERENCES


[TS72] Eleanor W. Tung and William A. Sanders. Simple perturbation and perturbation-variation treatments of the $1s\sigma_g$ and $2p\sigma_u$ states of H. *International Journal of Quantum Chemistry*, 6
REFERENCES


REFERENCES


REFERENCES


REFERENCES

VanDuijnen:1974:MIG


Vanderkooi:1975:TMS


Vetchinkin:1972:GFS


Vasilescu:1978:KHN


vanDijk:1979:CCA


Vojtik:1976:TRS


Vogler:1979:IUH


Volkov:1979:SAD


Venkatachalam:1979:CEH


Weiner:1971:PMN


Woodward:1971:PGE


Walker:1977:QMT

Evan Harris Walker. Quantum mechanical tunneling in synaptic and ephaptic transmission. *International Journal of...


REFERENCES

Weber:1975:MXC


Weinstein:1976:RCL


Webb:1974:NVR


Walter:1974:LMC


Weinhold:1971:RCU

REFERENCES

Weinstein:1974:PUA


Weinstein:1975:SNQ


Weislinger:1976:NTD


Weintraub:1977:CEC


Weltin:1970:BES


Westhaus:1973:CEC


Westhaus:1979:EHQ


Wepfer:1973:EMD


Wolf:1977:VME

REFERENCES


References


Wilson:1979:EQM


Wilson:1979:DMS


Witriol:1972:CTM


Witschel:1976:GFO


Wahlgren:1979:VPS

REFERENCES


1979. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).


REFERENCES


Ulf Wahlgren, Björn Roos, and Erik Forslind. A MO–SCF study of hydroxyl binding and hydroxyl diffusion in pure and fluorine-containing hydroxyapatite. *International Journal of


Weinhold:1971:FBR


Wybourne:1973:LAQ


Wybourne:1973:GPY


Witkowski:1970:DCV


Young:1975:NCP


Yonei:1977:ATF


Yang:1976:TAS

REFERENCES


**Yuan:1974:DCE**


**Young:1972:NPM**


**Young:1975:DRE**


**Yang:1976:HEL**


**Yafet:1973:CIS**

REFERENCES

Zielinski:1978:OGRb


Zeroka:1974:VPH


Zunger:1976:CFT


Zunger:1977:LDF


Zhorov:1979:RBS


