
Nelson H. F. Beebe
University of Utah
Department of Mathematics, 110 LCB
155 S 1400 E RM 233
Salt Lake City, UT 84112-0090
USA
Tel: +1 801 581 5254
FAX: +1 801 581 4148
E-mail: beebe@math.utah.edu, beebe@acm.org, beebe@computer.org (Internet)
WWW URL: https://www.math.utah.edu/~beebe/

08 November 2023
Version 2.15

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]. $\text{\$18.10}$ [Cal77b]. 1:1 [SP71]. 1s [Lec76a, Lec76b]. 1s2p3s [SA77].
1s2s³ [LAM71]. 1s3d [AC70]. 1s3p [AC70]. 1s3s³ [LAM71]. $\text{1s²(2p)²}$ [Lar78b].
1s²2s²p³ [HT75]. 1σ [AM77a]. 1σσ [AM77b, TS72]. 2 [Han70a]. $\text{\$22.50}$
[Gos78a]. $\text{\$24.95}$ [Mar78]. $\text{\$29.95}$ [Sab75a]. 2d [Cha77]. 2l + 2 [Mos73]. 2p
[Tat73]. 2π [SHI73]. 2σ [AM77a]. 2σσ [TS72]. 2s [GB72]. 2σ [AM77a].
$\text{\$30.00}$ [Shu77a]. $\text{\$38.50}$ [Ano78c]. $\text{\$38.50}$ [Ano78c]. 3π [Meh79]. 3πσ [AM77a]. 3σσ [AM77a].
$\text{\$43.00}$ [Cal76b]. $\text{\$48.50}$ [Dun78]. $\text{\$49.50}$ [Shu77b]. $\text{\$56.00}$ [Sti79]. 5 + 5
[Lin73]. $\text{\$69.50}$ [Lar78c]. $\text{\$74}$ [Ahl77a].
< 2⁵/₂⁻ₛ, 1₂ₛ >, < 2⁷/₂⁻ₛ, 1₂ₛ >, ⊗ < 2⁵/₂⁻ₛ − 2, 1₂ₛ >, < 2⁵/₂⁻ₛ > [SD79b]. +
[BB70, BS70, Doo78, HL79, HG75, HT75, KP71a, Ko76, KJ78, LH74, Lar75,
Lar78a, Lar78b, LV71c, PK71, Pul74, PPB78, RS79, SD78, TS77]. ++
[AM77a, JP77, RS79, SW78]. +2 [KD79b]. 2 [Gub79, Hop78, SW77]. 5 [MHA70].

[Goo76, HPK72, KSP78, KPD78, KJ78, LCPP79, RS79, TTS79]. −1
[SHR76, You75]. −3 [GML77]. 1 [BS70, DRCT78, GL74, JE79, JŽ79a, MSM70, RKOU77, SHR76, TTS71, Tat73]. 1,3 [AC70]. 13 [NN72].

[RKOU77]. 1 S [Lar78b]. 1 Š [JŽ79a, Kol75, Lec76a, Lec76b]. 2
[GH72b, LL75, LG75, MLB76, RS79, Sim78c]. 2+
[KPD78]. N [JSK75b]. 0 [AS78]. Π [Rit76]. 0 Π [Rit76]. 1
[DRCT78, GBT79, JŽ79a]. 1/2 [Sim78c]. 1+ [FWFM77]. 2+
[ASW77, Ada78, Ada73, Ada77, AAC76, BT78a, BB74, BL70, BS76b, BDT77, BMD70, Bur77, BWRD79, Cur77, Cur78, EH73, FM78a, FMZ70, GG79a, GBT79, GV77, GS70a, GG77, GH72b, GBK77b, Han79, Har70a, Har77a, HLG73, HNT78, HLY77, JŽ79a, JR74, KP71a, Koc74, KPD78, KPO76, LL72, LPG75, LGM77, Lee76, Lec76b, LG77, LET72, LGR73, LK78, MM72a, Mes73a, Min79, MMR74, MG77, OSL77, PK71, PK76b, PD79, RR77, RW75, SR77, Spe72a, SBD7+70, TS77, TBB70, TTS79, TG76, Tru72, Tru73b, Tru73a, VG78, WK73, WB73, ZL78]. 3+
[BC79, CJ73b, LGR73]. + [HR79]. 2 [KD79b]. 2 [Ros78a]. 3 [Bai74, BMD70, Bur77, BW76c, CE73, Cur77, EL73, FM78a, FMZ70, FJP70, GG79a, GBT79, GH72b, HNT78, HPK72, HLY77, JR74, KC72, LL72, Liu71a, MS71b, RMB78, RC70, RC71, ST72, TG76, WN71]. 3

[HP79, LGR73]. 3 [TP77b, Wei76]. 4
[And79, EP71, FM70, GG79a, Har70a, HP77b, JŽ79a, LB79a, Mes73a, ST72]. 4 [Bai74, KR71]. 5 [BDDT77, LPG75, LGM77, MHA70, RR77]. 5 [KR71]. 6
[ACK75, BG78, BBL77, Cur78, GG79a, GML77, HP77a, Spe72a, TDB77]. 3− [KL78]. 8 [MM74]. 8 [MM74]. 9 [WRS70]. α [BFH74, Sla73a]. C13−C13
[AD77, BB75, Con72, Dan72, DC73, DCS77, GML77, HC72, JW72, Joh73, JM76a, Joh77, KC79, Kau73, Li76, Mch79, MS76a, Min79, MMR74, PKK75, PK77c, RK77, RK79, Sam75, SF76, Sha76, SSt1a, Sla75, WC75b, WK73, JY76]. α [RK77]. Be [OJB77]. β [BK75, BCL79, Boy77, Dav77b, EB74, KYS79, RRS75, RU76, VUT79, ZG79]. − [DMS+78, LL72, PPP79]. CH+ [OJB77]. d
[BS72a, CW77, FGV77, KC77, KP72, MGG78, MMS70, RRS78a]. e2 [Lin70]. f
[KC77, MMS70]. f6 [MS71a, SM71a]. f7 [SM71b, SM71c]. g [Kij72]. G(α)
[LA76]. G 2 + f1 2 [BEFF78]. γ [Kot76]. j [BW76b, But76, BW76c]. J(0)
[Kai77]. Jkr(θ, ϕ) Y (θ, ϕ) [SF75]. jm [BW76b, But76, BW76c]. K232 [Tat73]. L2 [FB76]. P (JSK75a). m [Gol79]. N [Boy77, Col70, Col71, Col78, Gal72a, Jun78, KK76b, Kum77, LD71, Mat74a, Per78, TPC77, Gal74, Lé74]. n ≥ 3 [Lé74]. ns [CH75]. OAO [CK74]. ω [MSKM77]. p [KC77, MAT79b, RS78a]. Φ
[SPČ72]. \( \pi \) [Bra75, Bra79a, ČPP75, HTG77a, JPTM78, KTO +78, KJ75, KT76, KL79, Loc77d, MCST72, MK75a, Mic76b, MK72, NT79, PN76, San72, SPČ79, SIM75], \( \pi \rightarrow \pi \) [DRCT78]. \( r^N Y^M_L(\theta, \varphi) \) [SF75, ST70], \( r_2^{-1} \) [SR72a, Sal73]. \( r < \) [WRS70]. \( \rightarrow \) [FM78a, JZ79a, PK71]. \( s^2 p^3 d \) [YW73]. \( \Sigma \) [SIM75, BB72c, GBS70, HTG77a]. SO(4, 2) [Oda73]. \( \sigma \) [DF76]. \( \sigma \) [YW73]. \( \Sigma \) [SIM75, BB72c, GBS70, HTG77a]. SU(2) [Oda73]. \( \Psi \) [DF76]. \( \Psi \) [YW73]. U(n) \( \downarrow U(n_1) \otimes U(n_2) \) [SD79b]. x [RB75a]. Z [MW75c]. \( \zeta \) [Sel75].

* [DRCT78, NT79].


-Berechnungen [BKW75]. -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].


-structures [BCL79]. -Substituted [Boy77]. -systems [BB72c, GBS70]. -technique [MSKM77]. -type [LS72, LGR73].

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

1-fluoroacetic [BL75]. 10-epoxide [LPP78]. 10.50 [Com77a]. 11-1-fluoroacetic [BL75]. 12.00 [Com77a]. 128K [Spa78]. 134 [Cal77b]. 14th [Pul79b].

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

1-fluoroacetic [BL75]. 10-epoxide [LPP78]. 10.50 [Com77a]. 11-1-fluoroacetic [BL75]. 12.00 [Com77a]. 128K [Spa78]. 134 [Cal77b]. 14th [Pul79b].


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 [PLS78].
8-dihydrodiol-9 [LPP78]. 8-tetracyanoquinodimethane [DT75].


Advantages [SW77]. affecting [AF73, CT79, Kar78]. affinities [BB87, CS74, KD79, PK77c, SMH77, SG77a]. AG [Cal76b]. agents [KK72, KK75, Pur75]. agonist [Kan74]. agreement [Sin73a]. AH [KC77]. aid [Nee75]. Akademie [Cal73a]. Akademie-Verlag [Cal73a]. Al [BMD70, Cur78, Pos70]. Ala [RSK+78, VU79]. Ala-Ala-Gly [VU79].

alkanes [BB72c]. alkanols [VH75]. alkenes [Par72]. Alkyl [BB72c]. alkylnitrosamines [TPC77]. alk- [WMB75]. All-electron [MMB70].
All-electrons [AL71]. All-pair [NS75]. all-reactive [Hil79]. All-valence-electron [MW74a]. allene [TS78]. allergy [Kau74a].
allos- [KN79]. allowed [LP74b]. allowing [HHR70]. alloys [CM75b, Fau71, Fau76, DV79, MM77b, Sto71]. allyl [TS78]. Almon [Cal76a].
AlNC [Tho76]. alpha [De 76, Duf71, JW78]. alternancy [MW77].
Alternant [DT75, BK71, CP74, CPP75, JPTM78, KBK72, KU70, PČH74, Tu75, Tu78]. Alternate [HC72, But76, HS71, SD79a]. alternations [TTN76].
Aluminum [Sco71, SC79]. am [BKW75]. Amaldi [Csa79a, Csa79b].
Ambiguities [Sab73]. amide [PS79b, RRNS75]. amine [LSB+79, VH75].
amino [Kap73, LP79c, WTB+76, Kla78]. amino-substituted [Kap73]. ammonia [JZ79b]. ammoniation [PA74]. ammonium [PA74, PBG76]. AMO [CS73, CODM77, CD78, DT75, LV71a, SC73, Spe73]. among [CP70, HY78, KM72]. AMOS [DD77b, RD79]. amphetamine [DH78, WN78]. amplitude [Hun74]. amplitudes [Hun75a, Hun75b, KPÔ76, Nut78].
anamnesis [Ahl77a, Ano78c, Lar78c]. anaesthesia [DBJ74, DDBJ76]. analogs [Han79, RSK+78, WN78, ST79b].
allogenes [Tho76]. analogy [Sch71c, SE79]. analyses [FTN77, KPKC73].
Analysis [BS76b, LS71, SDB76, Spe71a, Spe71b, Spe72a, Ada78, AAC76, AJ79, BB75, Ber76, BC79, BK75a, CK75, CS76, CL73, CA72, DSC+77, GK78, Häl75a, HPW79, Hun74, Kau70b, KP79a, LS70, Lar78a, LTR74, MG77, PD77, Ran78, RRS75, Ron73, Ron74, TC70, Wei75, WTB+76, ZL78, AF73, RS78a].
analytic [BO79, Cal72, GGJ77, JS77, KD79a, BSZ78, Doo78, ES79, GGJ75, Jor75, SK72, Wei74]. analytical [ST70, DS74]. ancient [Lak75].
anesthetics [DMS+78, KK75]. Angular [MP71b, RS78a, RS78b, RS78c, Tat76, BBT71, But76, Cro77, Kib75b, Sch71a, Sur71]. Angularly [LL75].
anhydrase [PD79, SS79, SS74]. aniline [JL70]. anion [Hin77, LCPP79, MMR74, NI70a, PGPP79, PPB78]. anionic [KL79]. anions [KPP78b, Sha77a, Sha78a, Sim78c].
anisotropic [WMV77]. anisotropies [KW76]. anisotropy [Fog71]. Annales [Cal75b]. annelation [NT79].
Announcement [Ano71a, Ano73a, Ano74a, Ano74b, Ano77a, Ano77b, Ano77c, Ano77d, Ano78a, Ano78b, Hud72]. Announcements [Ano70a, Ano70b, Ano70c, Ano71a, Ano71b, Ano72a, Ano72b, Ano73b, Ano73c, Ano75a, Ano76a, Ano76b, Ano76c, Ano76d, Ano77c, Ano77d, Ano77f, Ano77g, Ano77h, Ano77j, Ano77k]. anßtze [GbK77a]. antagonists [Dav77b, KKK74, KKK75]. anthracene [BOP76, Chr73]. anthracenes [SS78b]. anti [BP71, Slaj70b]. anti-aromaticity [BP71]. anti-symmetric [Slaj70b]. anti-binding [ZL78]. antibiotics [SMP77, SMP77].
antisymmetric [Sim72]. antisymmetrization [Lin77a].
antisymmetrized [Lya78]. antitumor [Gab76]. Anwendung
PTUK69, Cal73a. any [KD79a]. applicability
DCS77, KP71a, KSP78, SM76b, SM76a. Application
APC77, CD74, CSY74, 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, Mehl78, NI70b, PNB78,
PTUK69, RKE79, SPC79. Applications
ERW75, Jor75, Lan77, Roe73, Sun75a, WO76, BO73, Chr79c, DL75, HS70b,
Jan76, Joh73, JMV6a, KKW73, MS76a, Na78, Pea74b, WO75, BR78, Csi77,
JL70, LG77, MK75a, SM74, 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,
Fro74, Gab76, Gin78, Har70b, Joh70, Kau76, KPP77, KE79, Lat76, LB79b,
LO77, Lin78, Nir75, Pal75, PW79, Pop79, Rout79, SP79, SP75a, Sha77b,
Sha78b, TB78, TOED79, WP79, ZF76, ZF77, Ano76c]. approaches
APC77, CL73, Kau77, PAC77, Rat78. approximant [CPP75, CM78].
Approximants
BG71, GLB73, Ree73, Ree75. Approximate
Csa79a, KP78, NN74, Sco74, SC78a, Abs72, BDP73, CA78, Cas79, CZ75,
DY76, JTR77, JPTM78, KP71a, MDC79, NN77, Nor75, PN76, San75,
SWP77, GZ72a. approximately [KPP77]. approximating [GPP79].
Approximation [LP74c, OL78, Ar79, BA78, BBP71, BBL72, Bow79, Bre73,
CM75a, CL76, CESW70, Dav72, DF76, DLG79, Ess77, ES70, FC79, Fro70,
GJP79, GLS79, HLGC73, HNT78, HTG77a, HTG77b, KT77, KM76, Lar75,
LV71b, LV72, Lz79, Lin71, Meh78, MLM75, Ni79, NMS77, OL79a,
PNG78, PW74a, RL77, Rat71, SM77, Sco71, Spe73b, Spe73, SS77b, SO77,
Tru73b, Van70, WO76, Wi74]. Approximations
Kas76, Spe72a, DR75, Iv74, JW76, Lan74, PK75. April
BP70, BP71, BP72, BP73, PUL78b, Sti79. APW [BK75c, KOE74]. aqueous
[Tal77]. arbitrary [BF70, BW76b, But76, BW76c, CM72a, KK77b, SP75b].
ARCANA [AMC73, CAMC71, KPP73]. ArF [SD78]. arginine [DAP79].
arising [HT75, Tat73]. Aromatic [LSB79, BOP76, DEE75, Her74,
KPP78b, KI75, LP79a, Mem79, Ne75, PD77, Pul79a, SG77a, Sh78a, UP71].
Aromaticity [BP71]. aroMS [Su77]. arrangements [JM76b]. Array
[BL77b]. Aspects [KPP75c, SL70, BS75a, BP70, DEC78, ED79, GSE78,
HC73, K73, LP79a, SW78, Vol79]. ass [MK77]. Assessment [Mag79].
associated [EL73, Pop71]. astronomical [Lay77]. Asymptotic
[Kut76, 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, Puls79, RB77, Rei72a, Spe70, 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, BB78, CL76, CP71, CM78, CA72, CA73, FKS76, Fr172, Fro76, GBV77, GK76, GL74, GRM75, HKM71, Hea71, Høj79a, Høj79b, IS75, JMM71, JS70, JN72, JL74, Kar70a, KZ73, Lan77, Lar79, LG75, LAM71, MMM71, NN72, NN74, PK72, PD78b, Raf75, Rou79, RGM75, SK72, SPC79, Sch72, SSD72, ST70, Sim72, SH75a, SHR76, Slan7a, SJH79, Sol71, SR72c, SW77, SW78, TGG79, TS71, TNB79, YJ76, JBG70]. atomic-integral [Rou79]. Atoms [Nes71, AZ72, Ave72, BM74, BK76, BW73, BB73, Cal72, Cal73c, Cal74, CP70, CW77, CL78, Csa75, Csa77b, Csa79b, Dau78, Dau78, Dey72, Dey73, DCS77, DDD70, GGJ75, GB75, GB72, Jak76d, Jak76d, JBP76, JP73, Jun78, KM74a, KP72, Koc74, Kol74, Kol75, Lin73, Mar73a, Mil71, 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, Wen79, WRS70, WS79, YD75]. attachment [Nes77, SL79]. attack [HPK79, PLSL78]. attempt [BCR78]. attention [WV74]. attenuation [PP71]. attraction [LR77]. 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]. autocoherent [TGSL70]. autodetaching [Sim78c]. autoionization [Naz72]. Autoionizing [MCW78]. Automatic [BSZ78]. autonominator [BP79]. auxiliary [Gru70, LA76]. Auxin [BCL77]. average [KZ73]. Avery [Lin73]. Axial [Han79, BM71b, RS78b]. axis [Lét74]. aza [Sha78a]. aza-aromatic [Sha78a]. azulene [JL70]. B [Cal73b, Dun78, Sti79, CC79, HE77, HT75, Jak66b, JPTM78, Kol75, LH74, Lar75, Lar78a, Lar78b, MDS75, PPP79, PZP79, RR77, Rit76, SBD70]. B-DNA [PPP79, PZP79]. Back [LB79a]. backbone [SY77]. bacterial [KKKP79]. balance [KKP77]. Band [FRM74, PN71, AL71, ABD79, CD78, Con70, KKA78, Lad74a, Lad74b, Lad75a, Lad76, LSC77, MGM78, Ove73, Pal73, PNJB78, Pet78, Sco71, SL73, Swl71, ZF76]. bandstructure [Ove73]. bandmatrices [Wel71]. Bands [HP77a, Bor70, CZNL70, CD74, CD78, Csa78a, Dav72, DF76, Ewe71, FN73, Lar70, Lip72]. barbiturates [AJ79]. barrier [CL77, MEW70, WC75b]. base [ENRM78, FB72, GRE77, KKK79, LL72, MW74a, Mar73a, PZP79, RCE75, Sun77]. base-pair [ENRM78]. based [AM74, DMS78, FRM74, HSB78, KT77, Kau74b, Pau78, San75, SRP76, SRP77, TC70]. Basel [Cal76b]. bases [ANR75, Bri73, CLP79b, GJP79, KD77, KS79, KL79, LP79c, LSB79, MHP70, Mos73, NHK79, NY76, PH77, Raf75, Sey76, SRE79, SM79, WTB76]. Basic [Ano76e, BCL79, Spe71a, Hos72]. Basis [BL72, Kas76, Tan74, ASIC77, Abs78, Amo71, BS75b, CA78, CHS77, Cur78,
Dah78, DRCT78, DPGC79, ES79, Euw71, Fae79, FGV77, Fin73, HS70a, Höj79a, Höj79b, Hur77, KB77, KMO77, KPÖ76, LSOC77, Lec76a, LCK73, Lev78a, LGR73, LPT+74, Mal71a, Mar73a, Mcd79, MYTC77, MDC79, NI74, OK74, Pe77, PAM75, RPK78, SW78, SM72, 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 [GG79a, Mul71a].

Behandlung [FJP70].

behavior [BG76, DMM75, Kut78, Tal77].

bends [BCL79].

benzaldehyde [LM72].

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

benzene/H [HG75].

benzenes [MR72].

benzenoid [SG77a].

benzomorphans [RW79].

benzoquinone [MK72].

benzyl [KKM70, NN74].

benzyne [MPS70].

Berliner [Cal73a, Cal79a, Cal77b, ZL78].

Bernard [Shu77a].

Berthier [RCE79].

Beryllium [BS78b, GBV77, TTS71, Tat73].

berylliumlike [JL74].

Bessel [SW77, SW78].

Best [Jak76a, Jak76b, Jak76c, Jak76d].

Between [Gal72b, Sim77a, AMSS79, Bas78, Cas79, Cha71, CL78, Col79, Con70, Csa77b, Dah78, DGC77, DD72, De79, ED79, FM72, Fin73, GP79, Hal71, HP79, Hs77, Kib75b, KC74, Koc74, Koa74, Koa75, KL73, Koa77, LPP78, LB77, LR77, MM72a, NY76, PLY78, PCL78, PW79, Rob71, SF76, SRE+79, SD79, SE79, Sin73a, SKS77, SS78b, SP71, Suz77, SO77, TTS71, Tic79, WK72, WB76, WV74, WM77, WP79, ZG79].

beyond [Wil74].

BH [LL72, BS74a, BS76a, EL73, GG79a, MA70, Mul71b].

Bibliography [RWF71, Sab75a].

bicyclic [BBG79].

bielectronic [Rue79].

Bifluoride [LS79].

big [KSP78].

bimolecular [Chr77].

binary [DV79].

Binding [LK78, SL78, CZN70, CD74, CT79, CV73, DAc+79, Eis77, GJLL75, Han79, KPD78, Lak75, NKK79, NT+79, Pul74, PB76, PP78, PD79, RKE79, SS79, ST78, TBN79, 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, SLOK79, Tal77, Urr78, WCK+76, WOE78].

biologically [BB79, DSM79, Kla78].

biology [Cal76b, Com74a, Hal79a, Mar73b, Pul78b, Rei70, Ros74, Sti79, Sun75a].

biomacromolecules [AMJS79, SAM79].

biomembrane [Urr77].

biomolecules [KPP79, NS79a, PP74, Pul70, RC79].

Biophysical [Har75].

biopolymer [Kho79].

biopolymers [AMJS79, FB72, Lat76, LSS78, Pul78a, Sun74b, Sun75b, ST78, ST79b, Dun78].

Biorhitchenormal [Dah78, Lat77].

biphenylene [JPTM78].

bipolar [Sal73, SF75].

birefrigence [Loc72].

biréfringence [Loc72, DQ77].

birthday [Cal75b].

bisglycinato [RRS75].

bisglycinato-Cu [RRS75].
BISON [WBKL70]. Bloch [Kun78a, KOW78, Kun78b, Wan79]. blocking
[KVSG79]. BN [SB270, ZF77]. body [Bal78, BS74a, BS76a, BWS77, BP78,
BFH78, CJCM73, DDD70, Feu77, KBA76, Lev78a, LR77, Lin78, LRJ73,
MMM75, Ner75, NY75, Per78, Ros78b, SBM70]. Bogoliubov [Cli73]. Bond
[Bur77, Del73, Gal72b, Par72, SS71a, Ada77, Bas78, DBBJ76, DMS78,
GN77, Gin78, Hal75a, HR79, JH78, KHI79, Kle79, Kle70b, LS72, LS79,
MP70, NG73, OK75, Pet77, PNC78, RS74, RS76, Sri77, TRS73, TS77,
TS78, TS79, TTN76, Wój76, Woj78, Lar76]. bond-length [TTN76].

bond-order [TTN76]. bonded
[AM72b, BS75c, CP70, Cho79, Loc77c, TP77a, Wel77a]. bonding
[AMC73, ACG74, Bai74, BL75, CP70, Cur77, DS76a, DMS78, ES73b,
GH72b, Har71a, HR79, Me79, Nir75, PDE79]. bonds
[BVO72, BK75b, Coo79, Gin78, Loc77d, Sab71, SDD77]. Book
[Ahl70, SC76a, Ahl70, Gra77, LWA74, RCE79]. broadened
[BMD70]. Brueckner [LH76]. building [Kau70a]. bulk [SEW73]. Buridan
[MKT77]. Burton [Cal75c]. butadiene [TS78]. butatriene [TS79].

Butterworths [Mar78]. bytes [Spa78].

C
[Com77a, Com77b, SBD70, BD77, CV73, ETF79, ED79, GG79a, GBT79,
HLYC77, HT75, Jak76b, KP71b, NN72, Ran78, Ros78a, SMP77, Tru73a].
C-C [SMP77]. Ca [KD79b]. cage [Ave75]. Calais [Shu77b]. calcium
[AD77, LB79b, NTN79]. Calculated
[KW76, AB73, BL77c, LVC74, Sin73a, WM79]. calculating
[Gi78, HS77, ML76, Nam75, PLYM78, Spe73]. Calculation
[BFH74, BW76b, But76, BW76c, Cas79, Con72, FB76, HH77, HNT78,
KP076, Li76, LP74c, LA76, LW76, Loc77a, Loc77b, LL70, Mon77, RR72,
SK71, SP75a, SLB77, SH74, Sle79, ANR75, Ah70, AD77, AFD78, BNLS72,
BN76, BSM72, BM73, BS75c, CZNL70, CJ73a, CSFM72, CW77, Chi77,
CP72, CL78, CWE71, CE73, CAMC71, CH74, CH75, DRC78, DD72, Del74,
Em74, FRM74, GZ72a, GF76, Gof79, GML77, GBM74, GRM75, Hai73,
Har71c, Hos72, ICS74, JR74, Joh75, JPTM78, JS70, JNZ72, KR71, KTO78,
KBA76, KA76, KT76, LD73, LL75, LGP75, Lin77, Loc76, Loc77d, MCST72, Mes73a, MM72b, MH72, Mu76, MSM70, MB71, Muk74, MMM75, MS71c, Ner75, NB78, Nir75, NY76, PPK78, Pie71, PK71, PK76a, RBDV77.

**calculation** [RGM77, RPK78, SK72, Sel75, SLC78, Sin73b, SP75d, SSH78, Tru73b, WC75b, Wei71, WFS77, YL74, BCL79, FG79, MMS71, NS73].

**Calculational** [CM72a]. Calculations [Ave79b, AB79, Ave79a, BL77b, BB78, Eld73, Gal72b, Har71b, JE79, LCP76, LZ77, Mak71, PNJB78, PK76b, Sas74, Abs72, Alm74, Als73, ABD+79, An078c, ACD+74, Ave79c, BAI74, Bar70, BL77a, BB77, BB72c, Bil72, BKW75, BEH77a, Bio73, BB73, BWRD79, CP70, ČZ79, Chr73, Cla70, CM76, Csi76, Cur77, Dan72, DCM74, DMR74, Dau74, DDH78, DEE+75, DK77, ESR74, EHT73, ED74, FTN77, FBL79, FB72, FMZ70, FL79, Fr74, Gar78, GG79a, GG79c, GG79b, GV77, GBS70, GPP73, GV77, GMG75, GH72b, GJ76, GHJ77, Hal75a, HS76, Han79, HP79, Har70b, HLG73, HSB78, HK72, HU74, HCF75, HS70a, HS70b, Höj79a, Höj79b, Hö77, HP77b, Ibe74, JW76, J79a, Jor73, JL70, Jun78, KL78, KS73a, KT77, KTO+78, KK72].

**calculations** [KPKC73, Kau73, KK76a, KK77a, KPP77, KSP78, KPP78a, KPPH78, KPP78b, Kau79b, Kell75, KP71b, KM74b, KLe70b, KD77, KD79b, KKK79, KL79, LD74, Lan77, Lar75, LFF79, LAV72, Lev78a, Lev70, LKH77, Loc77c, LH79, LJBN75, LS74b, Lun79, MMB70, MW74a, MEW70, MSK77, Mch79, ML79, Mey71, ML79, MR72, Moh77, MMS70, M79, MM70, MN72, NN74, Nee75, NAR72, Nis77, NMS77, NS78, OMC76, Ove73, Pai73, PPC72, PCM77, PST0, PK75, PK77a, PK77b, PGPP79, PLMB73, PK73, PKK75, PK77c, PUL70, R576, RM77, RB77, RU76, RKO77, ROe75, RL79, RS79, RK77, Ros78b, Rout79, San72, SM73a, SD78, SN79, Sas79, Sha77a, Sha78a, Sim72, SJ79, SDB74, SC78b, 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].


carcinogenic [HK79, KPP78]. Carcinogenicity [SR78, SS78]. carcinogens [HK79, KPP78a, NKK79, Nee75]. carcinoma [WLS77]. career [An076a]. Carlo [Cas78b, Col77a, CL78, Col79, RC78]. Cartesian [BM71a, GM73a, KOW77, SC78b]. case [AP77, BS78b, Dmi75a, Dmi75b, Kib75b, MK75b, NRS79, PAC77, ST79a, DRCT78]. casino [Fox75].
catalysis [DS76a, Gol70, Sal79]. catalysts [KGB76]. catalytic [JM76a, BCR+78]. catalyzed [LDP79, PDEB78, WEH74]. catastrophic [KKP77]. catechol [SS78a]. catechols [SS78a]. Cation [PBG76, Hin77, LB79b, MEW70, NIT0b, PGDM77, SLOKP79, W077, LB79b]. Cation-ligand [PBG76, LB79b, PGDM77]. Cation-water [LB79b]. cations [KR73b, PPB78, Urr77]. CC [BVO72]. Center [Eng72, Thu75, AM74, AT75, BA78, CM76, HR79, HNT78, Jet73, LPT+74, Mag79, MH72, PAM75, SR72b, Sha76, ST70, SBM72, MM74]. centered [MVM75, ML75, Mi74, SDM74]. centers [MVM75, Fan70]. Centre [AM72a, AM77b, AM77a, KZ73]. CEPA [Bur77]. CEPA-PNO [Bur77]. certain [BL79]. CF [Cur77]. CH [Cur77, FJP70, JŽ79a, JR74, Cur77, FMZ70, FJP70, GG79a, GV77, HPK79, HE77, KC72, MHA70, RMB78, WK72]. chain [BBA73, DDH78, KKA78, KG77, LR77, MOV75, TGS70]. chaine [TGS70]. chains [KG76, KG77, Urr72]. chalcogenides [SKS77]. chalcone [BT79]. champ [Gou73]. change [Amo72, HY78]. changes [BZD79]. channel [MM72a]. channels [GRB74, SLOKP79, USK+79, VU79]. character [KG78, KE79, NT79]. Characteristics [ÖL78, ÖL79a, Sl79, WCK+76]. characterization [BT78b, Chr73, Har77b, Jan76, USK+79]. characters [TTS+79]. Charge [CM75b, KPP78b, SRE+79, Sin75, ZL78, BT71, BK75, BW73, Cho79, Csa77a, DC73, DTY76, DT75, HRBB76, JPM78, Kar70a, Kar70b, Kar70c, KFY71, Kau73, KKA78, KKKP79, Kib75b, Lad76, LH77, OMC76, OSL77, Psl73, PK75, PS75a, RM72, Sl73a, Sha77a, SL78, Van72]. charge-conserving [PK75]. charge-dependent [Kar70a, Kar70b, Kar70c, KFY71]. charge-transfer [Van72]. charged [Csa79a, NG73]. Charges [Hal75a, BT71]. Chemical [FL79, Gos78a, GJLL75, SLOKP79, BS79, BCL77, CSR79, Chr79c, CP71, Dau77, ES73a, Ema74, HG75, INY+71, Jan76, J78, KK72, Kau74a, KKK74, KK75, KK76a, Kau79a, Kau79b, LS78, Lar76, LPP78, LP79a, LJB75, MN79, Mos73, NKKY79, Pul79a, Sal79, SDD+77, ST73, SJ79, TP77a, TWC73, TPC77, Wei75]. chemicophysical [Kau76]. chemin [Lei74]. Chemisorption [DS76a, Sl77c]. Chemistry [Cal73b, Lar78c, Ost79, Pul78b, St79, And79, BP70, Cal79a, Cas78b, Csl77, DAC+79, GM73a, GM73b, Gos78b, Hal75a, Hal79a, D79, K76, KG77, KB77, Mat72a, MF73, MSP73, MCP73, MP75, MW75a, Mat76a, Mat76b, MW77, MW77, MK78, Par77, PHL+76, PS75a, Ran79, SP75c, Sin73c, Sl79, Wil77a, Wtb73a, MN79, Cal75c, Lar78c]. chimique [JJ78]. chloramphenicol [BS77]. chloranil [DT75]. chloranil/para [DT75]. chloranil/para-phenylenediamine [DT75]. chloro [BS70]. chloro-substituted [BS70]. chlorofluoromethanes [PK77b]. chlorophyll [Mag79]. chlorophyllide [OMC76]. Chlorophylls [SCY77]. chlorpromazine [PPK78, PK76a]. choice [SP79]. choosing [HC72]. chromophores [KIl79]. Chrysene [BS79]. CI
[Hil79, APČ77, BNLS72, BS78b, KT77, KSP78, KPÖ76, KMLB77, KL79, Lar78a, MW74a, MLB76, ML79, Mey71, NRS79, PAČ77, PCMS77, SH75a, SHR76, Sin73b, WJ79, WMB75]. CIBS [Med79]. Circular [Tin79, BCL79, Dub72, MSSF79]. circumvent [LAV72]. cis} [TS78, WMB75]. cis-butadiene [TS78]. Cl [Cur78, FM78a, MMR74, FM78a, PK76b]. Classical [FM78a, Dub72, Sch71c, Sch76b, WO74]. classification [KR76, MCM73, MLM75]. Clebsch [KG76, KG77]. Cliffs [Cal76a]. cis [TS78, WMB75]. cis-butadiene [TS78]. Cl [Cur78, FM78a, MMR74, FM78a, PK76b]. CNDO [CS74, DMS 78, Duk79, Kau70b, KPKC73, SL73, SSH78]. 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, VG78, KTO 78]. co-ordination [FM72]. Co-porphine [KTO 78]. Coarse [MF73]. cobalt [KTO 78]. code [Coo78a, FM79]. coefficients [Ahl74, Bar79, DH73, JW78]. coefficient [DH73, JW78]. coefficients [Ahl74, Bar79, DH78, GK76, KK77, L77, 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, Mie74, Nis75, R74, Tru76]. Colloquium [Sim79]. combination [Com77c]. combinations [Sol71]. Combined [SH75a, SHR76, ZF76, Nis75, RCE79]. Comment [Coo78a, Nov73, Pos70, WRS70, Amo71, HMC71, Sab71]. Comments [Bar77, KSL76, Kle74a, CR72, LB79a]. commonality [Kau74a]. comorosan [Bas75]. compact [BW76b, But76, BW76c, KE79, SH75a]. Company [Ahl77a, Lar78c, Sti79, Ano78c]. Comparative [Lec76a, PLYM78, TGG79, Ada78, KL78, Muk74, PD77, TWC73, ABM78, BB74]. Comparison [KPKC73, Kib75b, Lun79, MCST72, SRP76, SS70, SL75, 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, Jun76, MCW78, Bar70, BFH78, CG78, DT75, FHB77, Hen74, Hen77, Hil79, Joh73, JG72, KTO 78, Kib75a, MH74, NI70a, NI70b, NB78, Nut78, PLYM78, Rei76, RRS75, Sim78a, SP71, Sun74b, Sun75b]. Complex-coordinate [MCW78]. complexes [AMC73, BR78, BV73, BV76, ...
CSFM72, ENRM78, HČZ79, INY+71, JW72, LL72, Lew78, LH77, Loc77c, Loc77d, LH79, MCM73, MLM75, Pet78, SC78a, Van72, WO77, Wel77a. complicated [PP71]. component [LD71]. components [Boy70a, GC77, Har79a, Pul74, SMB+79]. Composition [RK79]. compound [LK77]. compounds [BS77a, BP70, FM72, Gin78, KKK70, KPP78b, KJ75, Kot76, MYTC77, PN71, PKK75]. Compton [BY76, Dec70, Kai77, MBM73a]. Computational [ADFL71, ADDLG76, Ano79o, BDT77, Duf77]. Computations [SK73, BP74, BP75a, Ber76, BCR+78, Bur77, GCP79, Pul77, TK78, TG76, YD75]. Computed [Bor74]. computers [Ost79]. computing [SB78]. Concentration [Fog71, BF75]. concept [KK77b, SW79]. Concepts [LH74, Atk74, Atk91, Sha77b, Gos78b]. concerned [Sch78]. concerning [Jeh73, Mem77, Sab71]. concerted [TC70]. condensation [MBMM79, MPMK79]. condensed [Chr79c, Sti78]. condensed-phase [Sti78]. condition [CM72b, Kij72]. Conditional [Hun74, Hun75a, Hun75b]. Conditions [Khe79, Erd78a, Kum77, Lai77, RT77, WO75, WZ70, Fan70]. Condon [Sla73b, Lon73, Nis77]. conductance [VU79]. Conduct [Lew78, Lad74b, Pet78, SKS77]. conductivity [BK75b, FB72]. Conference [Cal76b, Ano78d]. Configuration [CS76, Fro70, HPK72, LD74, PW79, Sas74, Spe72b, TS71, TTS+79, WP79, YW73, BS77b, BS78a, BS78c, CPH74, Cof74b, DD72, FTP77, GHS79, Har74, HY78, HT75, JC72, JKS75a, JKS75b, KR73a, Kau74b, Kau79b, KKM70, LED73, MM70, N70a, N70b, PPK77, Roe75, SD79a, Sas77, SRP76, SRP77, SDJ79, SDB76, SBD+70, Tat73, Tru73b, Wei76, WY74]. Configuration-Interaction [TTS+79, BS78c, SD79a, SDJ79, Tru73b]. Configurations [ENRM78, Cha77, Csa77b, DN75, Dav74, KZ73, MST71a, Muk75, PH77, SM71a, SM71c, YW73]. confined [Wei76]. Confirmation [Ram78]. Conformation [AMC73, Kan74, CC79, DS79, FS79, KD79b, LL72, LCPP79, MGT79, PPC72, PGPP79, PS79b, Pul70, PS75b, PS75b, PC76, RRNS75, BP73, RRNS75, SMP77]. conformation-energy [KD79b]. Conformational [AJ79, AMJS79, BZSD79, BWRD79, IZZ+79, KK77a, KP79a, KVSG79, ME78, MDA78, RRS75, RU76, RSK+78, Rou73, Rou74, SD77, Set77, VU79, WTB+76, Wei77, WN78, HPW79, IE79, KM72, PPC72, PBC74b, RKOU77, Sm74a, VGS79a, KL77a]. conformations [DSMM79, Har75, Kar78, Pop79, Pul76, SY77, ULM76, SM77]. conformer [Bur77]. congeners [WOEG78]. conjugate [RE70, RP7K78]. Conjugated [LL73, BV072, DM72, ICS74, MCST72, MUK74, NMS77, NS78, SN79, SG77a, TTN76, TSE76]. conjugation [MOV75]. Connection [SF76, LP74a, Tic79]. conservation [BBT71]. conserving [PK75]. considerations [HBB77]. considering [HPW79, ST79a]. consistence [KS75]. consistency [BS77b, BS78a]. Consistent [OL78, Sla70a, Abs72, BKS79, BBP71, Bor70, BK75c, CWE71, DS74, GOU73, HAC74, HAL78, JLT4, KAR70b, KAR70c, KFY71,
coupled-pair [BP78, ČP71]. Coupling
[GO68, HL79, BOP76, BAA73, GPP73, Hal75b, IMN79, JE79, KK74b, KK77c, Laz79, LRD+77, LRD+78, Mak71, Men71, Shu77c, TGLSL70, TB74, GÖJ+73].

courte [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, Sl7a70a, BF71, Cal75a, DS70a, Dav72, DF76, GMG75, HKM71, JMP78, Kho79, Kun78a, KOW78, Kun78b, Lip72, Loc77b, MCM73, Sch71d, Spe73, SLM70, TW77, Wój76, Fan70, Cal79a]. Csizmadia
[KD77, RRS75]. Cubic [KOW77, Kun78a, KOW78, Kun78b, SS77b]. CuCl
[FJW+79, KWC79]. cumulene [Ukr72]. current [Löw77]. curve
[Liu71a, MVN75]. Curves
[HL79, Gub79, GBK77b, Jor75, May78, NS73, PK71, Wil77b]. cusp [CM72b].
[Bur77, Kar78, LV71b, LV72, ME78, Ra76a, Sun74b, Sun75b, ST78, ST79b].
Cyclo [RSK+78]. cyclobutane [K79]. cyclohexapeptide [RSK+78].
cyclopropane [LG77]. cysteinyl [PPC72]. cyt [Han79]. cytochrome
[Har77a, LHK77, PL79, RL79]. cytosine [CLP79b, KD77, PZP79, ZR78].

D [AS78, Cal73a, Cal73b, Sti79, AC70, AK78, MS71b, Rit76, Ros78a, TP77b, Wei76]. D- [AJK78]. Dancoff [HU74, Lar78a]. dans
[DQ77, TGLSL70, TBB70]. Darboux [BG72]. data
[CFMO73, FKS76, SW72, WEH74, Ahl77a]. dC [PPP79]. decade [Van71].
decay [BYB79, HLMV77, HF72]. decaying [HMV77, HMV78].
decomposition [Jor77, KM76]. Decoupled [NS72, NS73]. Decoupling
[WZ70]. defects [FCL79, Lar75, PB78, 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 [BH75, BW73, CG79b, Hen78, HY78, Lim75a, NN2, Pail73, Pau78, RR72, Sch73a, Sha77a, Sh78a, Sin75, SMB70]. Density
[Ave79b, AB79, Ave79a, Gar78, HS79, Har71b, K75, LS71, LL70, MW75b, SLM70, SJH79, Spe72a, Spe72b, S77a, Ada72a, Ada79, AM72b, Ano78d, Ave79c, BG75, Bun77, CM72b, Cij73, CFMO73, Col78, CH77, CES70, Csa77a, CM75b, DC73, Del74, DD77a, DR75, FM78b, GF76, GH78, Gás71,
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].

**dépendance** [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, Har77b, 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** [KL79].

**detected** [MSSF79].

**Determination** [BS77b, BS78a, BCL79, Boy70a, HE77, JW72, JMP78, KZ73, OJB77, Ben72, LP74b, Pal73, RK77, WB73, BJ73, BJ73].

**determining** [CD74, CSFM72, MCF70, MCM73, Sol73].

**deux** [TBB70].

**Development** [SC78b].

**developments** [Mes73b, Mic74, Mic76b, Pai73, PHL76, Pol79a, 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, SS71b, SB7+10, WO76, YG77, vDR79].

**Diatomics** [NS79b, Dun78, Moh77, Pul78a].

**Diatomics-in-molecules** [NS79b].

**diatoms** [CB72].

**dibenzo** [CT79].

**dibenzop-dioxins** [CT79].

**dibenzo-fulurans** [CT79].

**dichroism** [BCL79, Dub72, MSSF79, Tin79].

**dielectric** [Bre75, Bre75, Csa76, Csa78b].

**diene** [Par72].

**Difference** [Fro79, FW75, FU76, HPK79, TTS71, WK72].

**differences** [Hal71, JS70, Sim77a].

**different** [CL73, HMV77, Kuf78, MK76a, May78, SRP76, SRP77, TB74].

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

**Differentiation** [AJK78].

**Difficulties** [ML79, BK71, LAV72].

**diffraction** [CFM73, FM78b, MP75].

**diffusion** [Ta77, WR73].

**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, We77a].

**dimethyl** [LCPP79].

**dimethylphosphate**
E. [Sla73b]. earth [PBG76, RW74, LB73a]. easier [Col77a]. Easy [Gia73]. Eckart [Jør78]. economic [Bil72]. ecosystem [BCL77]. Ed [Lar78c, Sla79, Dun78]. ediﬁces [RS78c]. Edited [Cal73b, Cal75c, Cal76b, Shu77a]. Editorial [Sab75b]. Edward [Lon73]. Effect [JMM71, KGP79, LRJ73, MK72, NMS77, Nor75, San71, SM75, SS77a, SH75b, Tat73, Ave75, Bas75, BN74, BMM75, CHH+78, CPH74, DH76, Han71, HT75, JVM78, KN79, KBKCD78, LCPP79, MSSF79, MG77, PK72, Rei76, SHO71, VH75, Vol79, YR76, GZ72b, Sch71e]. Effective [BW76a, Bra75, GJ73, MW75c, ST79a, TP78, TOED79, Wes79, Bra79a, CW77, Jor77, KK74a, Sla79, Wes73, WJC70]. Effectiveness [Sas77, Jak76c]. Effects [ST73, BBB73, BS79, BL77d, CPH74, CPP75, CJC73, DN75, DBJ74, Han79, HPW79, KC73, KC77, KLe74b, LC77, Lun77, Mat73a, Mat76c, MIV75, 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, GTC70, MS75, RB75a]. Eigenproblem [Kun78a]. Eigenspace [ACH72, Car74]. eigenstates [Bri73, Gol79]. eigenvalue [Kar70b, Kar70c, FK71, KA76, LA70, LWA74, Nor75, RE70, WAL71, Woo72, KBA76]. Eigenvalues [LL70, Cas78a, Gra77, Koe74, LC77, Ste74, Wel70, Wel71]. eigenvectors [Koe74]. Eigenwertberechnung [KA76, KBA76]. Eikonal [CL76, GLS79]. Einﬂuß [BK75]. einsamen [BK75]. Einstein [MBMM79, Wil79a]. Elaboration [RCE75]. elastic [BG78, SS75]. elastin [RU76, RS78+]. Electric [Als73, LG75, BS72, CE73, Gra77, HU77, Kob78, Lar78a, LCP76, Loc72, MCST72, PP73, TSE76]. électrique [Loc72]. electrolyte [Tal77]. Electron [BL77b, BH71, Bra75, Com77b, ES73b, ED79, Gal72a, GN77, GOK79, GLS79, Goo76, GP79, Hur76a, JMP79, KM74a, LS72, LRD+77, LRD+78, Mic76b, Mil71, PKS78, Spe70, Spe72a, VGS79a, WES73, Aha72, AC76, Abs78, Ada72a, AB73, AM76b, AM77a, AM72b, AT75, Ano79a, ACK+75, BFS73, BB70, BP78, BTD79, BN74, BL77a, BM74, BBP71, BDP73, BG78, Ben72, BL70, Bil72, BK75a, BK76, BW73, Bra79a, BY76, BB73, BB78, Cal72a, Cal73c, CM72a, CHD71, CB72, CSY+74, CP71, CP77, CJC73, CM72b, CFM073, CH77, CESW70, Coo78a, CS72, CSa77b, Dah8, DL75, DSC+77, DT72, Dec70, Des72, Feu77, FU76, Gal74, Gás71, GT79, GCh77, Gru70, GL74, HR79, HLG73, Hen79, Hos72, HP77b, Hur76b, HY78, HR76, Jak76a, Jak76b, Jak76c]. electron [Jak76d, JMM71, JZ79a, JPTM78, JM73, Jun78, KL75, Kle74b, KP78, Kun78a, KOW78, Kun78b, KS72, KK77d, KKK79, KPÖ76, Lad74a, LH74, LP74a, LG77, Lim76b, LE72, LS74a, LÖ77, LBÄF78, LB73a, LG75, LPT+74, Lun77, LAM71, MMB70, MW74a, MS71a, Man77, Mar79, MM74, Mat76b, Mat9a, May74a, May74b, MK75b, MK75a, May78, MLB72, Moh77, NN74, Ne77, NB78, PCL78, Pau78, Pet77, Pet79, PN76, PBS76, PK77c, PÖ77, RL77, Rat78, RC70, RC71, RC72, Rob71, Rob72b, RJ73, RB75b, RK76]
electron [TOED79, WMB75, WRS70, WV74, YL74, ZV79, SL79, SDS76, Com77a].
electron-atom [CM72a]. Electron-conformational [VGS79a].
electron-density [CFMO73]. Electron-intramolecular [LRD77, LRD78].
electron-lattice [CS72].
electron-density [Joh77, MR72].

Electronic [AFL78, BT78a, CT79, CSR79, Chr79a, Duk79, EP71, Fau71, Fau76, FWJ79, GPC71, GML77, GL74, KMO77, KWC79, LSS78, LF77, LGM77, LM72, LG75, LV71c, MW74a, MHW78, MHW78, MOV75, Nes70, Nes71, Pet78, Pop71, Rit76, RL79, SM71b, SP72c, SCYB75, SM79, Sto71, Ukr72, AeAs78, AN75, Ada75a, AM77, BF71, Boy72a, BS78c, Bu77, Car75, CSFM72, CS76, CPP75, CR72, CL78, CK74, CS78, D78, DD77a, DM72, Fin73, FBL79, GP79, GK75, Har78, HS70a, Hin77, Hop78, HT75, HR76, JR74, Joh75, JW72, JG72, Kau74, KR71, Kj75, KL77a, KC74, KD79a, KU70, KS79, Lad75b, LL76, LDVC74, LP79a, LFF79, LKK79, LE72, LOS73, LK78, LS79, Lud71, Lud75, MP79, MS72a, MS74, MCF70, MCM73, Mic76b, ME78].
electronic [MR72, NS75, NT79, Pai71, Pal75, PH77, Pet77, PNC78, RM79, SHO71, SP74, SP75b, SLB77, SLC78, Spe73, SWP77, SG76a, TB74, Tho76, Tru73b, Tru73a, VG78, WS79, ZF76, LL72, PLS78].

Electronic-structure [KMO77]. Electronically [FMRG75, BS75c].

electronique [LL72]. Electrons [JBC70, TW77, AL71, BKW75, Col77b, GG77, Hil79, KMLB77, Lin71, MK76a, SIM75, SK77, SM73b, Tat76, TL71, Wan79].

Electrophic [Mem75, Mem79, HG75].

Electrostatic [CM75a, CFH77, HKP79, NS79a, SS73c, DRCT78, GPP79, Kib75b, OMC76, PPP79, PT75, PPK78, PD77, PZP79, SBB79, GJP79].

Elektronenpaars [BK75], elektrophilen [HG75], element [Sha78b], elementary [Bra79b, CZ79, Lan74, Rei70].

Elements [Gal72b, HL79, Sas74, DD72, Dav74, HBB77, HLGC73, KR73a, LS74a, Nis77, Oda73, PW79, PN76, Pos78, RCE75, Sur71, Tru72, WG74, Wit76, WP79].

Eleventh [Pul78b, St79]. elliptical [LGR73].

Elsevier [Ahl77a, Ano78c, Lar78c]. elucidation [Pul77]. embedded [Dmi75b].

embedding [BHL78], emergence [Pea74a], emission [GK75]. emitted [Hea71]. empirical [BBL77, CAMC71, HLYC77, LOS73, NMS77, San71, San72, SM77, SG77a, WJC70]. End [RBD77]. End-on [RBD77].

endowed [KMT77]. energetic [KC77]. energetics [VU79], énergie [BJ73, BPTLYM73, eAJ76].

Energies [OJB77, Abd71b, Abd71b, BM74, BJ73, BP75b, Cal72, Cal73c, Cal74, CM72a, Cas79, CJS77, CP72, CR72, CAMC71, CV73, DGC77, DCM74, DMR74, Dau74, GJP79, GBT79, GLS79, Gln78, Hal75a, Har77c, HE77, Jak76d, JMP79, JSC78, KZ73, Kau70a, KPK7C3, Med79, Mey71, MS75,
Muk74, MMM75, Nir75, PT78, PNC78, Rit76, SHO71, SBM72, SP75d, SO77, Tal77, TNB79, Tru73b, Tyu75, Tyu78, WJ79, ZR78, ZBH78. **Energy** [BG75, CD76, DL75, Dav72, DF76, FY79, HF72, Jai70, KKA78, Lad70, Lad76, LL70, LB73b, OK75, Sch71a, SW71, TC70, Wan79, AF73, BFT73, BA78, BS74a, BS76a, BNL72, BZD79, Bor70, Bor74, BP77, BF78, BH74, BWRD79, CZNL70, CB72, CJ73a, CJ73b, Cha71, CL76, Col74a, CESW70, CEK72, CH74, CH75, CZ75, DMS78, DEC78, EL73, EH73, Eng71, Euw71, FN73, Gar74, GTBB77, Gra77, GBK77b, HS76, Han77a, HST75, Hen79, Höll77, JTR77, JZ79a, Jing75, KS73a, KP71a, KP76, KM76, KD79b, KBK72, KP78, KKK79, KMLB77, Lad74b, Lar78a, LV71b, LV72, LW77, Lin77, LG70, Lip72, MP71b, Moh78, MDA78, Muf76, NY76, PT78, PPC72, Pet78, FK71, PD78b, Pop71, RU76, RKOU77, RE70, Rue79]. **energy** [San71, SP75a, Sco71, SDD72, SW70, SB78, Spe73, Sri77, SP77, SK79, SL73, TB78, TTS71, TDB77, Vog79, WK72, WS75, Wei77, WN78, Wel76, 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** [Av75]. **enhancements** [BC76]. **enol** [ZR78, ZBH78]. **ensemble** [BHLM78]. **enthalpy** [BCR78]. **entropy** [HČZ79, Pri75, Sch76a]. **environment** [ST73]. **Environmental** [TP77a, PP77]. **environments** [Boy70a]. **enzymatic** [BCR78]. **enzymatically** [LHK77]. **enzyme** [Gol70, LP79b, VGS79a, WEH74, Ano76e]. **enzyme-catalyzed** [WEH74]. **enzymes** [AMSS79, LKK79]. **epihaptic** [Wal77]. **Epoxide** [PDEB78, LP77, LP79c]. **epoxides** [LP79a, PDE79]. **Equation** [Lib76, TN73, Ada73, Amo71, Bie75, Csa79a, ESG79, Fro79, Hen77, Koe74, LA70, LWA74, NS75, Not75, PW74b, PW74a, RL77, SH73, SI71, VB72, WA71, Wel70, We71, WZ70, WAL71, Woo72, YL74]. **Equations** [FG79, HY78, Ada78, BEH77b, Cal79c, CIL73, DSY74, DR75, FW75, HS78, HBE78, JM73, Kar70a, Kar70b, Kar70c, KFY71, 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** [GÖ68, GÖJ73, Sch77b, BS74b, DN75, PW74b]. **Erich** [Ano771, Par77]. **Errata** [GZMM73, GÖJ73]. **Erratum** [May75, 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** [DBBJ76, GBS70, GB70]. **ethidium** [PL77, RKE79]. **ethyl** [MEW70, OMC76]. **ethylating** [HPK79]. **ethylcarbonium** [TWC73]. **ethylene** [CSR79, FWFM77, FJP70, HMC71, MMD78, PDEB78, Rat71, Rou74, TS78, WC75b, Wes79]. **etiology** [Kau74a]. **Etude** [DQ77]. **étudié** [TGSL70]. **europium** [Fog71, Liu71b, SK77].
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].

Exact [BS71, CJD73a, HKM71, LC77, Nis77, HL78a]. Examination [Dub72, Jak76c].

examples [BG72]. Exchange

[GMZ73, SW71, AM77b, BYB79, CJ73a, CJ73b, CESW70, CEK72, Csa75, Dan72, ES70, Hir70, IVE74, Kle70a, Lin71, LPT74, Ove73, Pie71, Sco71, Si17, SW70, Sl77a, SC78a, Suz77, Tat73, SJH79]. exchange-correlation [CEK72]. excimer [AZ72, Fla79, MHWC78]. Excitation

[CK74, OJB77, Abd71a, BS78a, BK76, BZSD79, Bow79, CW77, CS76, CP72, DC75, Gos75, Har77c, NM77, Oni79, Tru73b]. excitations [BP78, Bra79, CKI75, Gre71, Mi71, MOV75, MMS70, Ner76]. Excited [LS79, SCYB77, WMB75, Abd71b, AS78, Bar77, BN76, BJ73, BS75c, Cha77, CD74, CPH74, CKD73, DS76b, DY73, DC75, GB75, GL74, HNT78, Hea71, HT75, Hos72, KKW73, KSP78, Lin77, LG75, LAM71, MW74a, MCST72, MMS70, MM72b, MG77, MMS70, MB71, Muk74, Mult71b, PCH74, PLMB73, RB77, Ros78a, SMB79, SC76a, Tan74, TTS79, TSE76, You72, YD75, SP72]. excited-state [BN76]. excités [BJ73]. exciton [Par72].

Excitons [MBMM79]. Exclusion [Lim76a]. Existence [Ziv77, RT77, TK78]. expanded [Ber73]. Expansion [Dal79, ADA72a, Ada79, Csa77a, Ema74, FB76, GPP79, Gra77, HNT78, Lin70, Man77, MHPS70, Mat71a, Mcd79, MW75c, Rob71, Rob72b, RK79, SR72a, Sfl73, Sr72b, SP79, WS79, You75]. expansions [BG72, CJS77, GbK77a, Gor71, Gor72, JSC78, KL75, Kle77, KGB77, MCST72, Meh73b, NY75, PAM75, SP76, SF75, Wes73]. expectation [BSG77, BL77d, SK71]. experiment [BP72, Ber75, Gin78, IZZ79].

Experimental [WBKL70]. explicitly [Sim72]. exploration [PBC74b]. explore [SDD77]. exponent [LS74b]. exponential [CM76, HÖ79a, HÖ79b, Sch72]. exponential-type [HÖ79a, HÖ79b]. exponentials [Sol71]. exposants [BPTLVM73, Vla70].

exposants [BPTLVM73]. expression [Gar74, KD79a]. expressions [KP71a, LG70]. Extended [BRS75, BEF78, EB74, FME70, JLT74, K77, AM72b, Als73, BFH78, Bur72, CFHS77, Chi77, FHB77, JS70, JNZ72, KPKC73, MLB73, May74b, Mes73b, Pel77, Han79]. Extension

[KP72, MDS75, TB75]. extensions [Lun75]. external [Sim78b]. extrapolations [BG70].
Fehlerminimierung [KA76]. Fermi
[Csa79a, GY75, Goo76, YG77, Bie75, Csa77b, Csa79b, DH76, GJ75, Han70a, Han7a, HB79, KW76, Lm75, PN71, SKW72, SC73, WC75a]. Fermi-like [GJ75]. Fermion [Col71, Col70, GH78, Per78]. fermions
[Lei74, ST72]. Fibrous [GK78]. Field
[GÖ68, GOJ+73, Sl70a, AD77, Bal71, BKS79, BM73, Bow71, CE73, DS74, DL79, El73, Gou73, Gra77, GL74, Hac74, Hal78, Har71c, HP77a, HD71, Hor71, JL74, KKW73, KK74b, KK77c, LG75, LG77, LG75, NL78, Ni75, PS75a, RW74, SF76, Sch71a, Sch71b, Sol73, TGL70, WN71, Wan79, Wól71]. fields [DL75, Gás71, LL73, MGM78, NL78]. Fifth
[Ano78d, Boy70b, BM71a]. Fifth-rank [Boy70b, BM71a]. Filled [Bee76]. filling [Kau79b]. final [Rou73, Tru76]. Fine [BK77]. Finite
[HB79, BF70, Bl72, Bl73, ES79, Fae79, FW75, FU76, KE79]. finite-difference [FW75, FU76]. First
[CH74, JBP76, Lip72, NRS79, Bu77, Cal74, Coo79, CH75, DGC77, G70, GL74, HS76, LN73, LF77, LA78, LZ79, MCST72, Moc74, NG73, RB77, ST72, SC73, Van71, W77b, Raf75]. 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, RM78, TL71, AF73, AM72a, ADDL76, RR77]. fluctuation [Bra79b]. fluorescence [AZ72]. fluoride
[AD77, Le74, ST78, VG78]. fluorides [PK77c]. fluorinated [KR73b]. fluorine
[SDD72, WR73]. fluorine-containing [WR73]. fluoro [BL77c]. fluoro-
[BL77c]. fluorocatic [BL75]. fluoronium [Le74]. fluorosulphate
[HS70b]. fluorouracil [GJP79]. fluorur [Le74]. fluxional [TB73]. FNO
[HR79, MG77]. Fock [BR78, Bre73, Cli73, MBM73a, SS71a, SDS73, BM72, BM73, BMM75, BEH77b, BK71, Bu72, Bur73, DSG74, FW75, Fr70, Fr74, GH79, GM75, GBM74, GRM75, HKM71, IRE74, Jam70, Jor73, JL70, JLG4, Kar70a, KKA78, KM76, KT76, KBK72, KMO77, La73, LS70, LS71, LL75, LZ78, MHP70, MN79, MLB73, May74b, MC79, M73b, MW74b, Mes78, Mes79, NM72, NN74, NS72, NS73, OKM74, PCL78, PS73, PS70, PK79, RS79, RGM77, SA77, SH73, SL77, SD77, SJ79, SB74, SBD76, SB78, Sp75d, SE73, TTT76, Tru73a, Van70, V79]. fold [Lét74]. folding [PF79]. follow [BCR78]. fonction [BPTLM73]. fonctions [eAJ76]. fundamental
[BJ73]. forbidden [TH78]. Force [MGM78, CJCM73, KP71a, NL78]. forces
[Abd71a, AM77b, Br70, CL71, FY71, G78, J73, KKW73, ML71a, Mal71b, Pie71, RM72, RM73, RMP71, WB76]. forcing [JSC78]. form
Formaldehyde [DRCT78, LED73, Tan74]. formaldehyde [Bra75, Bra79a]. formalism [ADDLG76, ACD74, Car74, CDEO76, Con77c, CE73, Feu77, GP74, GJLL75, GJ76, KP72, Min79, Mor75, Sac72, TC70, ZF76, ZF77]. formalisms [Mic76a]. formally [NG73]. Formamide [PK76b, LB˚AF78, OSL77, OSL77]. formation [BB70, HČZ79, Kho79]. forming [Mor75]. forms [GPC71, Kob78, KL79, LH76]. formula [CA78, JW78, MRR76, Tu75, Tu78, WW71]. formulae [Har71a]. Formulas [BSG77, BSZ78, CM78, Gor71, Gor72, Har77a, Hos72, KE79, Spe71a]. formulation [Cli73, HST71, KPJM70, Lar79, Mat74a, Mat76b, Mat79a, MW74b, Nel79]. formulations [KC74]. formycin [SMP77]. found [ZBH78]. foundation [CD71]. Four [NY75, HR79, HP77b, LH74, LPT74, May74a, PK72, SR72b, Sey76, SHR76, SDS73]. four-atomic [PK72]. Four-body [NY75]. four-center [SR72b]. four-electron [HR79, HP77b, LH74, LPT74, May74a, SDS73]. Fourier [AFD78, GMZ73, GMG75, MH72, Sha71, Thu75, ZF76]. Fourth [WS79, KP78]. Fourth-Order [WS79, KP78]. fractional [KK77b]. Fraga [Ahl77a]. fragment [GG79c, GG79b]. fragments [CSM71, Chr73, Kau70a, OMC76, PCMS77]. frame [Jor78]. framework [ABM78, LW76, Loc77a, Loc77b, Loc77d, PD78a, WJ79]. Franck [Nis77]. Free [BTD79, Mat76b, MW77, MN79, SD79a, AB73, BL70, DMS78, GPC71, KPJM70, KC74, Lim74b, Lim75a, Lim76b, Lim77b, LB73a, MW74a, Mat72a, MF73, BSP73, MCP73, MPW75, MW75a, Mat76a, MWY77, MK78, S73a, S73b, SM73b]. Free-electron [BTD79]. French [BJ73, BPTLVM73, Gou73, JM76b, eAJ76, JJ78, LL72, Lei74, Loc72, Mar73a, TGL70, TBB70]. Frequency [Hea71, RGM75, Ahl74, Bow71, BR72, Bre73]. Frequency-dependent [RGM75, Ahl74, Bre73]. Friedlich [Ano77m, Par77]. frozen [Lar75, Lar78a]. frozen-K-shell [Lar75]. Fues [SS71b]. Fukui [Cal77b]. Full [KKM70, Lar78a]. Function [LV71b, Ada73, BSS79, BS79, BS75b, BPTLVM73, Bre75, CB72, ČP72, CSH74, CS72, DRC78, De76, Duf71, FMZ70, HSBD78, Jo79, KM74a, Ku78, LD71, LV72, LA76, Meh73b, Meh78, NS75, NR79, PPPL78, Pau78, PGPP79, Rat71, Sch72, SB75, SD70, SDB76, SL70, WFS77, Sim77a]. Function-Level [Sim77a]. functional [BG75, Fin73, Gia73, GJLL75, GJ76, HS79, KS73a, PS75a, RS75, SP75c, SJH79, SM71, TB78]. functionals [HS79]. functioning [AMSS79, VGS79a]. Functions [Gal72b, Ja70, Ada73, ANR75, Ada75a, AB73, Als73, ADFL71, Ban74, BA76, BND76, BD73, BS71, Ben72, BSG77, BC79, BBA73, BG72, Bre73, Bu77, Cas78a, Cha77, CL78, CI79, DS74, DMM75, Eng72, Gal74, GN77, GM73a, GM73b, Grel71, GH72a, Gru70, GB72, GC73, HO73, HHR70, HK79, Ho79a, Hjo79a, Hur77, HR76, Jak76a, Jak76b, Jak76c, Jak76d, JTR77, JW78, Jo73, eAJ76, KC72, KC77, KK76c, LF77, Lau79, Lec76a, LTR74, Li76,
functions [SW78, SWP77, SSH78, Tan74, Tru72, Tru73a, Urr78, VB72, VF76, Wel76, Wel77b, Wit76, WV74, Mos73, Pos77]. fundamental [HPK79, Kauf79, Ful74]. fundus [JG74]. Future [Sla73a, Ost79].

G [Ano78c, Cal76a, Cal79b, Lár78c, Már78, Sab75a, IMN79, Nam75].

Galerkin [Jan76]. gallium [Fog71]. gap [Bor74, Cal79c]. garnet [Fog71, Liu71b].

gas [BM74, BY76, ČZ79, Chr77, Csa77b, FBL79, Fla79, GOK79, LW77, LRJ73, LPT+74, MHW78, MS76b, NY75, RJ73, Sti78, TW77]. gas- [Sti78]. gas-phase [ČZ79]. gas-solid [FBL79, LW77].

Gaussian [AF73, ADDLG76, BBP71, BP74, BSG77, DPGC79, Euro71, GM73a, GM73b, Hal73, 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, SBM72, SC78b, TB74, TL71, Van74, Van70]. Gaussian-Lobe [RS78a, RS78b, RS78c]. Gaussian-type [Lec76b, Mat73a, Mat76c, NY76].

Gaussians [FHP70]. Geminal [SP72]. geminals [Lya78, LB73b].

genealogical [GTG76]. General [ADDLG76, KSP78, Gar74, Hac74, Jak76a, JG72, JN72, KR73a, Kau74b, Klb75b, PW74a, Rob72b, SP75a, ACD+74, BSZ78, BS78c, Car74, Kle77, Lar79, NI70a, Rob72b]. Generalization [GHS79, KS73b, SL79, DSG74, Ste77]. Generalized [CGRC74, Car72, Hal78, Hal79b, Joh70, LG70, RT77, RK76, Sch76a, Suz77, Ahl77b, CW76, FM79, LA70, LWA74, Lev78b, MW47b, Pet77, PNC+78, RC70, RC71, RC72, SB75, SL70, Tu75, Tu78, Van74, AVL71, Wuo72, 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, Láz79, Har77b, HTG77a]. géométrie [TBB70].

geometries [ZR78, ZBH+78]. Geometry [Har79a, JZ79b, AF73, AMSS79, BSZ78, CD71, CLP79a, CLP79b, FWFM77, JR74, KL78, TBB70].

gerichteter [BKW75]. German [Ahl70, BKW75, FJP70, HG75, KBA76, KA76, PTUK69, Sch73b]. giant [Cal79a, Jul78]. Given [GO68, GOJ+73, KMLB77, May78]. Gly [SU79].

Glauber [GLS79]. globular [MME79]. Gly [BWRD79, CBV79, RSK+78].

Gly-Pro-Pro [CBV79]. glycine [DEC78, RRNS75, RR78, RC78].

Glycosyl [SY77]. glyoxal [DEC78, DAP79, ED79, LP79, OL77].

glyoxalase [SWF79]. glyoxals [Abd76]. glyoxylase [LP79b]. Goldstone [LH76].

Gordan [KG76, KG77]. Goscinski [Shu77b]. Gradient [Gar74, CE73, LGP75]. gradients [RP78]. Graph [Ran78, RW79, Sha77b, Ran79]. Graph-theoretical [Ran78]. graphical
graphs [Ran79].

Ground-state [Ive74, Sin73b, WB73]. Group-function [Meh73b]. Group-theoretical [CSFM72, MCF+70].

Groups [Gal72a, Blo72, Blo73, BW76b, But76, BW76c, Flu72, Gal74, GP72, KG76, KG77, KE79, KK77b, LP79c, Lén74, Lén77b, Ros78a, SAM79, Sin73c, SS73c, SLOKP79]. growing [Lak76]. growth [BC75, MDA78].

Gruppentheorie [Cal73a, PTUK69]. guanine [PNC+78].

Gy"orgyi [Lak76]. Gyrotropique [DQ77].

H [Bur77, DY73, GG79a, HG75, HLJC77, JŽ79a, KP71a, Koc74, Lar76, LB79a, RR77, RW75, RKOU77, Sab75a, Sl71b, TG76, SY77, ŠAW77, Abd71a, Ada78, Ada73, Ada77, AM72a, AM74, AM77b, And79, BB74, BC79, BDT77, CJ73a, CJ73b, Doo78, EH73, FMZ70, GG77, HNT78, HG75, HP77b, JTR77, JE79, KP71, Kat72, KSP78, Koc74, Kut78, Lec76a, Lec76b, LTR74, LG77, Liu71a, LG73, MM71b, 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 [Lak76]. Half [SD73, SDB74, SB78, SDB76].

Half-Projected [SD73, SDB74, SB78, SDB76]. halide [PL75, Moh79]. halides [BB72c, CK73, JM76b, LVDC74, LR73, LPT+74]. Halkjaer [OL79b]. Hall [Cal76a]. halogenated [DBBJ6]. halogens [Hal75b].

Halogénures [JM76]. HAM [AF78, LBAF78]. Hameka [Lar76].

Hamilton [TL72]. Hamiltonian [AC76, Abs78, CK74, DD72, Fe77, HL78a, Jor77, KS72, KK77d, MLM75, MMM75, WJC70]. Hamiltonians [BW76a, 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].

hardcover [Gos78]. harmonic [Bas78, DR77, Hun74, RB75a, WO75, ST79a]. harmonics [KOW77, Sch77b, SR72c, SF75]. Hartree [BR78, Har78, Jam70, Jor73, KKA78, KMO77, PS70, SD73, BBK76, BSM72,
Hartree-like [Har78]. having [Lé74, SP75b]. HBeCH [RMB78].

HBF [TB74]. HCl [PK76b]. HBF [TB74]. He* [RM79]. He-like [BS71].

He-sequence [MMS70]. Heinesberg [GB72, SHI73, SK73, SL70]. Heitler [Ada72, Ada77, Ano77-28, LP74a, LP74b, Wil77a]. Heitler-London [Ada77, LP74a, LP74b, Wil77a]. held

[B70, BP71, BP72, BP73, Pul78b, Sti79]. helical

[IZZ79, KP79a, SY77, Urr78, VU79]. helices [VBC78]. Helium

[B70, LP74c, AC70, BK74, CL78, DD71, HG78, LA70, MCW78, SK71, SK72, SE79, Spe70, Tat76, WAL71, YD75, Pel77]. heliumlike [Lin70]. helix [CC79, DS79, MHH74]. HKS [Har79b].

H嘴唇 [Har75, WLS77]. Humanities [Cal73b]. Hund [Ano77a, Com77b]. Hurley [Com77a, Com77b]. HY [SH75a, SHR76]. Hybrid

[Lec76b, Loh76, DF76, Eng72, MI78, Pol70, Sil71]. Hybridization

[Ran74, AAC76]. hydration [LCP79, LDP79, PP74, PA74]. hydrazines

BM73, BMM75, BEH77b, BK71, Bre73, Bur72, Bur73, Cli73, DSG74, FW75, Fro70, Fro74, GHS79, GMG75, GBM74, GRM75, HKM71, IVE74, J70, J74, Kar70a, KM76, KT76, KBK72, Lai73, LS70, LS71, LL75, Laz78, Lim74b, Lim75a, Lim75b, Lin76b, Lin77b, MHP70, MN79, MLB73, May74b, MCd79, MBM73a, 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].
[GPC+71]. hydrazyl [GPC+71]. hydride [Bur72, DCS77, MVN75, SDB74].
hydrides [DGC77, DSC+77, KC77, NG73, PK77a, PK77c, Swi71].
hydrocarbon [GBTB78, Her74, KT76, NN72, GG79c]. hydrocarbons
[BOP76, BK71, ČPH74, DBBJ76, DEE+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, BRSp+75, Bas78,
BS75c, BFH74, Cho79, Coo79, CSH74, Cur77, DBBJ76, DMS+78, Dea72,
GZ72a, GZ72b, GGCK79, HKM71, Kol74, Kol75, KMO77, KGB76, Lei74,
Lib76, LS72, Loc77c, LS79, Mal71a, Meh79, MO77, MS76b, Nis75, OKM74,
OK75, Pie71, PDE79, PGPP79, Rei76, Rit76, Sab71, Sch77c, SLC78, St78,
SH74, TP77a, Woll77a, Wil77a, Wój76, Woj78, Woo72, Zer74, CP70, GGCK79].
hydrogen-bond [DMS+78]. hydrogen-bonded [BS75c, Cho79].
Hydrogen-like [PPI73]. hydrogen-molecule [BRSp+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, BSM72, LS70]. Hyper-Hartree [LS71, LS70].
hyper-polarizabilities [BSM72]. hypercycle [Eig78]. hyperfine
[BNLS72, IMN79, 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
[DSMM79]. identity [Lat77]. IETS [Feu77, Feu77]. II
[Har77a, KD77, MSSF79, RRS75, Abs78, APČ77, AM77a, AB79, Bar79,
Blo73, But76, CW78, CD78, CSFM72, CSR79, Coo78b, CH75, DSC+77,
DMR74, Dmi75b, DDD77, Fun76, GZ72b, GL74, HH77, HS79, HR79, Höj79b,
Jik76b, KC73, KG77, KBA76, KOW78, LZ79, LP74b, MBB70, Mal71b,
MM74, May74b, MK75b, MHR76, MVN75, NI70b, NS73, PCH74, PW79,
PHL+76, Pet77, Pos79, PS75a, Ran79, RC71, Rob72b, Röe73, RS78b, Sch71c,
SG77a, SPČ72, SDM74, SS73b, SH75a, SDB74, SCYB77, Spe71b, SC73,
ST78, Tuq78, Woll77b, Woll71]. III [AM72b, Ave79c, Ave79a, BB72c,
BW76c, CP71, Dau74, DH78, FBT2, Gás71, Har70a, Har79a, Jak76c, Kun78b,
LBAF78, LG75, MW74a, MK75a, MHR75, MCM73, MLB72,
MDS75, PP74, RC72, RS78c, SP75c, Sch71d, Spe72a, Spe73, ST79b].
imaginary [BR72]. imidazole [KRKŠ78]. imidazolium [WO77]. imino
[ZR78, ZBH+78]. imino-enol [ZBH+78]. immunity [Ram78]. Impact
[Wil77a, BK76, PS79b]. impacting [HG78]. Implications
[KKK70, Kau74b]. Improved
improvements [ESR74, SLA74].
improves [Ram78].
impurities [JVM78].
Impurity [Fan70, Ada72a, AD77, BHLM78, CD78, Csa76, Csa77a, Csa78b, DT72, KGP79, MCM73, SLC78].
imadequacy [Cla71, Feu77].
imcluant [JVM78].
imcomplete [ESR74, Sla74].
imcomplete [Meh73a, Coo74, GG77, GM76, Luc75, Man77, Sol73, TGG79].
imcomplete [Meh73a, Coo74, GG77, GM76, Luc75, Man77, Sol73, TGG79].
Inter-level [JS70]. interacting
[CS72, DT72, DDD70, GHS79, Mal71a, Meh78]. Interaction
[BB74, Bas78, CC79, DEC78, Höl77, RM74, Sas74, SO77, TTS+79, TL79, 
Abd77, AMJS79, ACK+75, BS77b, BS78a, BP74, BK75c, BR72, BS78c, 
CJS77, Cha71, ČPH74, CoL74b, Dah78, DD72, DAV77, DMS+78, Dea72, 
DY3, DAP79, ED79, FY79, Fro70, GHS79, HB79, HSBD78, HPK72, 
JMM71, JSC78, JSK75b, Kap79, Kau74b, Kau79b, KL77b, Kob78, Kol74, 
Kol75, Kol76, KD77, KKK70, KKK79, LED73, LD74, LL75, LB79b, LSB+79, 
MCP73, MCF+70, MSS79, Moh79, NY76, OK75, PW79, PSK77, RSR72, 
Roy75, 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, BRI+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, MRH76, MHR77, MP75, 
MS76b, OCR71, PLY78, PD78a, PDE78b, Pol79, PB76, PGM77, 
Pol78a, RKF79, RM73, SRE+79, SC78a, SM70, Sun74b, Sun75b, ST78, 
ST79b, VGS79a, VGS79b, Wei75, WO77, Ves73, WM77, Ano76e].
Interative [HR76]. Interatomic [RMP71, DY76, FY71, GKT78, Kle70a].
intercalation [PL77]. interest [KG76, KG77, Mos73, Ran79]. interface 
[FBL79]. interfaces [Jo77, BP73]. interference [HL77].

Interfragment [VGS79b]. interhalogen [SM73a]. Intermediate [Rei72a, 
Ste74, BL79, BKW75, CL76, GL79, Kol74, Kol75, Kol76, KK74b, Sac72].

intermediate-energy [CL76]. intermediate-field [KK74b].
intermediate-range [Kol74, Kol75, Kol76]. intermediates [Tho76, TPC77].
intermetallic [Gin78, PN71]. Intermolecular
[aro78, BB72a, Cho79, GCP79, MME79, MS76b, Psys78a, AM77b, BB72b, 
Brä70, Cla71, DCM74, DMR74, Dan74, FL79, HSBD78, JEH73, Kap79, 
Kle70a, KR78, LW76, Loc77a, Loc77d, MGT79, Pol79, PGDM77, RKF79, 
RM72, RM73, SC78a, WB76, Dun78]. Internal
[Bor71, GP72, MEW70, TBB70, WC75b]. International
[Cal76b, BP70, BP71, BP72, BP73, Pys78b, Ede70]. internuclear [TBB70].

Interneuronal [COD77, GZ72b, Mui74, Zer74]. Interpolation
[Thu75, Sha71]. Interpretation
[LB75, DB74, Feu77, INY+71, JJ78, Kot76, Woi78, JJ77, BEF78].
Interpretative [SL70]. Interrelations [AMSS79, HYL78]. Interscience
[Cal75c, Gos78a]. intramolecular [Bri73, LRD+77, LRD+78, Pol79, Rat78].
intrinsically [BMD70]. Introduction [Ano78e, Chr79b, Hur76b, Löw71b, 
Löw78, Slm71b, Slm73b, Bar78, JW76, Com77b]. Introductory
[Nau77, Nau78, Wij78]. Invariance [SP79, FG77, Kob78, NN77]. Invariant 
[CA72, Hal73]. invariants [BM71a]. inverse [Ste77]. inverses [Ra76a].
inversion [SK72, SMA73]. Investigation
[Csa77a, AFW77, Coo78a, Ema74, KJ75, LÖS73, LAM71, MP71a, MP79, 
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, MBM73b, PK71, RR77, Sun74b, Sun75b,
Tal77, TWC73, Urr75, Woo72, Zer74, CJ73b, DT75, ST78]. ion-molecule
[GRB74, CJ73a, CSH74, GZ72a, GZ72b, GGCK79, Goo76, HS70a, INI71,
JS71, KKK70, KP71a, KSP78, Kol76, KD77, KD79b, LH74, Lar75, Lar78a,
Lar78b, Lei74, LS79, MFRE76, MBM73b, PK71, RR77, Sun74b, Sun75b,
Tal77, TWC73, Urr75, Woo72, Zer74, CJ73b, DT75, ST78]. ionic
[Cal75a, GPC71, H¨ol77, RKE79, SM76b, SM76a]. Ionization
[Hun75b, Mey71, ˚ASW77, CSDV78, Con72, Gos75, Hal79b, HLGC73, HYL78,
MVN75, MK72, Ner75, PT78, PK77c, PÖ77, RM79, SMH77, SG77a, TS79,
DH78, Jak76d, MDS78, TWC73, Urr75, Woo72, Zer74, CJ73b, DT75, ST78]. ionizations
[Ner76]. ionized
[KTO78, PLMB73]. ions
[AMJS79, BFS73, BT78a, Bar79, BS71, BM73,
Cal73c, Cal74, Col79, CS74, Csa75, Csa76, Csa77a, Csa77b, Csa78b, Csa79a,
Fro79, GGJ75, Joh75, KR71, Lin70, MHW78, MSS70, MM72b, PA74,
PBC76, RW74, RGM77, Sim77b, ST78].
Irreducible
[KK74b, KK77c, BF70, Blo72, Blo73, BO73, BS74b, Sol73]. irregular
[SR72c].  isethionic
[CS74]. isocyanate
[Mof79]. Isocyanide
[Mo79]. isoelectronic
[CLP79b]. isoelectronic
[BG70, AC70, AS78, BK74,
BG72, Mar73a, PD78b, SK71, SK72, SA77, TTS71, Tat73, Jak76b].
isoelectronique
[Mar73a]. isomeric
[JE79]. isomerism
[Sl79]. isomerization
[BB79, GP78, Mat78, Mof79]. isomers
[Mof79, PLMB73]. isopotential
[NS79a]. isotopic
[Hal71]. isotropic
[BM71a, Mal71b, TB74]. isovalent
[AC76]. Israel
[Put78b, Sti79]. iteration
[BEH77b, Gia73]. iterations
[KÖ71]. Iterative
[Cas78a, JW76, AM72b, Als73, BEH77a, Gol79, TRPB77]. IUCHF
[Vog79]. IV
[BL77c, CP70, CT77, Hir70, Hos72, Jak76d, LCPP79,
May78, PK77a, RTM77, Sch71e, SHR76]. IX
[KPPH78, TS78].
J
[Cal73a, Cal79b, Cal75c, Gos78a, RKO77, Shu77b, Sla71b, Mak71]. J.-L
[Shu77b]. Jacobi
[TL72]. Jahn
[MSSF79, Ham71, INI71]. Jansen
[Suz77]. January
[Sl71b, Sl73b]. Jeremy
[Ano76a, Cus75]. Jersey
[Cal76a]. Jerusalem
[BP70, BP71, BP72, BP73, Cal73a, Pul78b, Sti79]. John
[Cal79b, Cal75c, Dun78, Lin73, Shu77a]. Johnson
[LB79a]. Julg
[Cal79a].
June
[Cal76b, Mar73b]. justification
[Nov73].
K-shell
[CV73, Lar78a]. K.
[LB79a]. Karger
[Cal76b]. Karwowski
[Ahl77a]. Kashiwagi
[Ste77]. Kenichi
[Cal77b]. ket
[Mor75]. kets
[Kle74a]. keV
[BW73]. kind
[Lau79]. kinetic
[Han77a, Na78, TB78]. Kinked
[VBC78]. KNIF
[WN71]. Knight
[DV79]. Kondo
[JVM78]. Konvergenz
[Ahl70]. Koopmans
[Cui77, CT77, MD75]. Kr
[ES70]. Kramers
[BMD70, Bow71]. KrF
[SD78]. Kronecker
[Lét74]. Kronig
[RT77, WO76]. krypton
[Bo74].
L
[Cal75c, Sab75a, Shu77b, RRS75, AJK78, BP75a, Fae79, Mem77]. l-alanine
[RRS75]. L-region
[Mem77]. L-shell
[Fae79]. L-Thyroxine
LaB  [ACK+75].  Lactam  [Boy77].  ladder  [HBB77].
Ladungsverteilungen  [BKW75].  Laguerre  [Mos73].  Landau  [Csa78a].
lantanide  [NTN+79].  lanthanide-substituted  [NTN+79].  Laplace
[MKF77, SF75].  Laplace-type  [SF75].  Large  [ACK+75, CSM71, Chr73,
DM72, DEE+75, Duk79, Hat75, KPP77, NS79a, OMC67, PLYM78,
PCMS77, PK75, Ra76a, RSR72, Rob72a, Sas77, Tim79, WKC+76].  laser
[DLG79, WS75, WLS77].  laser-Raman  [WS75, WLS77].  laserlike  [ESG79].
laser  [Fla79, MHWC78].  Latin  [BP79].  Lattice  [Enz73, MHRS76, MHRS77, OCRMLR+71, CJCM73, CS72, KOW78, Kun78b, SP75c, Sch71c, SP75d, SEW73, TTN76].  LCAO  [Abs72, Kau70b, LS74b, ADFL71, BR78, BDP73, BBL72, Bil72, Del73, Del74, DC77, FTT77, KS73a, Kar70a, KT77, KTO+78, LSOC77, LAVT2, Min79, NI70a, NI70b, PK78, PD78a, PK78a, PK78b, SL78, Spe72a, Spe73, SW78, VLC70].
least  [Ada73, BT71, HS75].  least-squares  [HS75].  Lebenslauf  [Ano77m].
Lecture  [Cal79a].  left  [SY77].  left-and  [SY77].  length  [Kob78, Sin73a, TTN76].  lente  [BP79].  Lenz  [Loh76].  leur  [Mar73a, TBB70].  Level  [BF78, 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, Fro75, GS70a, Jak76b, KP71a, LL75, LE72, MM72b, MDS75, RM74, RS79, SP75d, SBD+70, ZL78].  Li-like  [Bar79].  liason  [JJ78].  Liapunov  [SB75].  LiCH  [RMB78].  Lie  [Wiy73a].  LiF  [Pai71, SBD+70, ZF77].  life  [Con73, SG76b].  lifetimes  [BNLS72, BOP76, HE77, Naz72].  ligand  [Bal71, Han79, LB79b, PBG76, PGDM77, SF76, Sch71a, Van72, WN71, LK78, PD79].  ligands  [AMSS79].
Light  [Sch76b, Sch71c, TS71].  LiH  [BS74a, BS76a, BS76b, HH77, LG77, MM70].  like  [AM72a, AM74, Bar79, BS71, GG75, Har78, PPI73, YD75].  limit  [Kat72, OKM74, Ria76a].  Limitations  [CAA+75].  limited  [APC77, CPH74, KMLB77, NRS79, PAC77, WJ79].  limits  [Wei71].  Linda  [OL79b].  Lindenberg  [Shi77b, KSS73].  line  [BMD70, Fog71, HMV77, HMV78, Kot76, WEH74].  linéaire  [TGS70].  Linear  [Han77a, BBA73, BBT71, Com77c, DN75, GbK77a, Hur77, KB77, KL73, LR77, Liu71a, Nor75, Sol71, TK78, TGS70, KA76].  Lineare  [KA76].  linearly  [Sol73].  linkage  [Boy74, Har77a].  linked  [HL76, Man77, SMP77].  linked-cluster  [HL76].  linked-diagram  [Man77].  LiNO  [HR79].  Linus  [Ano78f, Ano78u, Eyr78].  LiOH  [NS79b].  LiON  [HR79].  lipophility  [Tic79].  lipoprotein  [Har75].  liquid  [Col79, HK74, DV79, Kho79, Nir75].  liquid-  [DV79].  lithium  [AS78, Bur72, Rei72a, SA77, SC73, Spe73, SDB74].  little
living [MBMM79, SGM78]. Lobe
[Pos77, RS78, Rou78, SC78b, RS78a, RS78b, RS78c]. Local
[CKI75, IVE74, SMW71, ZF77, EH73, GSE78, HS75, HK74, JTR77, MR73, Sco71, TW77, ZF76, LB73b, PS75a]. local-mode [GSE78]. Localization
[SPC72, BO79, Eng71, LB77, LuD71, RC72, Wen79]. Localized
[De 78, GHT2b, SS77b, Car75, Cof74b, DGC77, DSC77, DD72, DS70b, Del73, DC75, GbK77a, GC77, Kau74b, Kle77, KGB77, LAV72, Lin71, LuD77, 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, Aba72, Ada77, LP74a, LP74b, Mal71a, Mal71b, Moh78, Wil77a]. lone
[BKW75, DSC77, Kau74b]. Long
[AFD78, DY73, Kle79, Kol74, Kol75, Kol76, SMB72, Abd71a, Cha71, Dea72, FY71, GPP73, KP71a, KL73, MOV75, PD78a, SZ76, Utk72, WMV77]. Long-range
[Kol74, Kol75, Kol76]. Longitudinal [HDG71]. look [Tho75a]. Low
[Hen79, AMJS79, ACK75, Boy70a, CH74, DM72, GLS79, Han75, KTO78, KGP79, MSSF79, PCH74, PCMS77, Tan74]. Low-energy-electron [Hen79]. low-lying [PCH74, PCMS77, Tan74]. low-molecular [KGP79]. low-order [Han75]. low-spin [KTO78]. 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, SSB79, TTS79, Wei71, Gra77]. lower-bound [LTR74]. lowest
[FG79, JZ79b, Kol76, Mul71b, Pie71, SHR76, TTS79]. LSD
[JG74, WCK76, WOE78]. LSD/serotonin [WCK76]. luminescence
[BYB79]. lying [CH74, PCH74, PCMS77, Tan74].

M [Al77a, Cal73a, Cal73b, Cal76b, SS78a]. m- [SS78a]. macromolecules [BVO72, BL79, KGP79, NGR77]. macroscopic [Fog71]. Magee [Cal75c]. magic [CA78]. Magnesium [LB79b]. magnetic
[Da79]. manipulation [ACH72, Car74, NGR77]. Many
[BP78, CJCM73, DDD70, Feu77, Gás71, Lev78a, Lim76b, MVM75, AC76, ABS78, BS74a, BS76a, BWS77, BFH78, BB73, CHD71, CP71, Dav72, DF76, FP77, Gru70, JMM71, JBP76, KL75, Lim74a, LR77, LÓ77, Lin78, LR73, Lun77, MR73, Man77, Mat76b, Mat79a, MK75b, MMM75, Ner75, NB78,
Many-body [BP78, DDD70, Feu77, Lev78a, BS74a, BS76a, BWS77, BFH78, CJCJM73, LR77, Lin78, LRJ73, MMM75, Ner75]. Many-centered [MVM75].

Many-electron [CJCJM73, Gás71, Lim76b, AC76, Abs78, BP78, BB73, CHD71, ČP71, JMM71, KL75, ŁÒ77, Lun77, Man77, Mat76b, Mat79a, MK75b, NB78, RK76, Sha77b, SS73a, SS73b, Slå70b, WV74].

many-neighbor [Dav72, DP76]. many-particle [Lim74a]. many-points [MR73]. many-shell [FP77]. map [Sri77]. mapping [TC70]. maps [HKP79, Kau73, NS79a, PPC72, SBB79]. March [BP70, BP71]. Markoffian [SM77]. Masthead [Ano79n]. Mathematical [CA78, SW78, KN79]. Matrices [Gal72a, LL70, SLM70, Spe72a, Ano78d, DR75, GH78, GP79, Han70a, Han75, Har77b, Har79a, ICS74, KP71b, Kry77, Lar73, Lar78a, Lar78b, Ra76a, Spe71a, Spe71b, Wel70]. Matrix [Dav74, Gal72b, HBB77, HL79, Har71b, KR73a, LS71, LS74a, MW74b, PN76, Sas74, Sha78b, Spe72b, Ada72a, Ada79, BG75, Bun77, CM72b, Cil73, CFMO73, DDD72, Del74, Fox75, FM78b, GF76, Gar78, Gol79, Har70b, JW78, KL75, Kij72, Kry78, LS70, MST71b, MHR77, MW75b, SML73, Ni77, PW79, Pea74b, Pos78, Ros78b, Sco73, SDB76, SCT7, Sur71, Tru72, WG74, Wit76, WP79].


MCSCF [BS76b, Gal78, RD79, RCE79]. mean [TL72]. means [ET79, Fin73, LG71, MI78, Ni77, Nor79, Pol79]. Measurement [BW73, Con74]. measurements [KKK70]. mechanical [CBV79, Che71, Coo74, DAP79, FJP70, N79, HS79, HSBD78, H78, KKK79, M77a, M77b, MP74, PG77, PS75b, 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, SLOKP79, TPC77, UP71].
[KKKP79, Pet79, BDT77, LSS78, TB75, Urr75, WO77, WOEG78]. Meianismus [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, BBT71, Chr79c]. metallic [KMO77, OKM74]. metal-ferroelectric [CHHS74]. Metal-to-nonmetal [Ber73]. metalloporphyrins [DAC79]. metals [CJCM73, CM75b, De 78, FMRG75, KW76, LB73a, MGM78, PK77c, Sch77c, SKW72]. metastable [DD71]. metastables [KSP78]. Methadone [LJBN75]. Methane [Dan72, DPGC79, HSBD78]. methionyl [PPC72]. Method [Hen74, LS71, Rei76, Aba72, AFD78, BR78, BB75, BBL72, Bil72, BK75c, BFH74, Bur72, CS73, CK75, Cas78a, Cas78b, CD74, CODM77, CSY74, Cla71, CSH74, DCT73, DRC78, Eps77, FFCH79, FG79, FRM74, FHB77, GH79, GB75, GML77, GL74, GJ76, GH77, Hal78, HS77, Har77c, HC72, Hen76, Hen77, HC78, Jan76, Jet73, JW72, Joh73, JM76a, Joh77, JM73, JS70, JNZ72, KKW73, Kau73, KSP78, KA76, KR78, KU70, KK77d, LS70, LVDC74, LV71a, LV78, LP74a, LP74b, LF77, LG77, Lim74b, Lin75a, Lin75b, Lim76b, Lim77b, LG75,Loc76, MK77, Mak71, Mat71a, May74a, MK75b, MK75a, May78, MCF70, MS76a, Mes73b, Mes78, MW75c, Mon77, Mor78, MMR74, MS75, Nam75, NI74, Pa71, P78a, Ran74, Rob71, Rob72b, RD79, RK77]. method [Rue79, RP78, Sac72, Sam75, SF76, SM76a, SH73, SC76a, SM75, SK79, Shu77b, SM72a, Sla73a, Sla74, SC76b, SC73, Spec73, Sri77, TGS70, Tru73b, Van70, VK74, WEH74, WK73, WA71, Wei74, Wei76, YJ76, Z78, ZBH78, ZF76, DCM74, K72, LB73b, Wel76]. method [TGS70]. Methodology [BW76b]. Methods [Chi77, CFMO73, GMZ73, Shu77b, SBD78b, T74, AP77, Ano79a, BG76, Bar70, BNLS72, BBL77, BS78b, BL77c, BS78c, CGL76, CSFM72, CP71, Co74a, DS76b, DCS77, Eil73, Em74, Fan71, Gar78, GV77, Har77b, Har78, Kar70b, Kar70c, KFY71, Kau70b, KK74b, KK77c, KVS79, Lar78a, Lev78a, Lun79, MK76a, May78, MCM73, MW74b, Min79, ML76, NS72, NS73, PLYM78, PAC77, PCL78, PBPL78, PS77, Pos79, RW77, Sin73b, SS70, SL73b, Vog79, WFS77, Cal76a]. methyl [BS79, Kla78, MLB72, MK72, RRNS75, Sha77a]. methylated [Sha77a]. methylacetamide [DEC78]. methylamine [Ab77]. methylation [HPK79]. methylation [SS78a]. Methylbenz [SS78b]. methylene [LED73, LD73, TRS73]. methylglyoxal [Ab77]. methylglyoxal-protein [Lew78]. methylinidazole [KRS78]. methyltransferase [SS78a]. Metric [Mor78]. Metric-constrained [Mor78]. Mg [PPB78]. MgH [BL70]. MgO
[KGB76]. microelectronics [Ost79]. microscopic [Coo78a]. microwave [Web74, WLS77]. migration [FY79]. Milne [YL74]. MINDO [Boy77, SL73, ZR78, ZBH'78]. MINDO/2 [SL73, ZBH'78]. MINDO/3 [Boy77]. minicomputer [Spa78]. minimal [Cur78, KP76, Mal71a, RPK78].

minimisation [BJ73, Muk75]. minimization [BJ73, HS75, Jol79, KS73a, KA76, KBK72, Wel76, Wel77b]. Minimum [GY75, HHR70, JZ'79a, M178, You72]. mixed [ACG74, Euw71]. mixing [LV71a]. mixtures [GH72a]. MO [Ano78c, BBLL72, Csi77, KPT77, Kau70, KL79, Lar78c, LAV72, MH74a, NN77, PCMS77, PPK78, PK76a, PK77b, Vla70, WMB75, MM77b, Abs72, Bil72, CA78, CF7M2, Cof74a, Csi76, Del73, Fm72, Hi79, KHI79, KS73a, Kar70a, Kar70b, Kar70c, KFY71, KTO'78, LS74b, MSKM77, MR72, Moh77, N70a, N70b, Sam75, SD78, SM77, SG77a, SS74, SL7C8, SW78, WRF73, ZR78, ZBH'78, BF74].

mode [DBBJ76, GSE78]. Model [KL77b, LPP78, LP79a, PD79, SP7C2, AF73, ADDLG76, ABD'79, BS77b, BS78a, BL70, BFR78, BK71, Bra79b, CB72, CD78, Cho79, CPP75, CE73, Coo74, Coo78a, Coo78b, Coo79, CZ75, Dav77b, Dec70, Doo78, Duk79, ERW75, ED79, FCL79, FM78b, Gbk77a, GOK79, Goo76, GJ75, Hal75b, Han77a, HB79, HC78, ICS74, J7T1, JVM78, JL70, JM76b, Kib75b, Kl79, KBK72, Lar75, Lar78a, LP79c, LP79b, LW77, LB73a, LK78, LPT'74, Lud75, Mal71a, MCP73, May74a, Mic76b, PCL78, Par72, Per78, Pet77, PNC'78, PP74, Por77, PGP79, RSS75, RR77, RMB78, RC70, RC71, RC72, RL79, SM76b, SP7C9, Sc71a, SP75a, Sha77a, Sha78a, SB78, SL70, St78, Tal77, TP77a, WN78, WO76, We76, YJ76, Sch71d, SP7C2, YD75]. mod`ele [JM67b]. Modeling [SKL79]. modelling [FHP70]. Models [LHK77, Pau78, AM77a, CPH74, GK76, Höl77, JPTM78, Lad74a, LS74a, Löw77, Mag79, PL79, PCH74, PBS76, TW77, Urr77, WOE78, SK73].

Modern [Kap79]. modes [BDT77, Hor71, SLOK79]. Modification [Bee79]. Modified [GM73a, GM73b, KK77d, KL79, Rue79, BSG77, Csa77b, JW78, PS73].

MODPOT [HK79, HP79, KPP78a, KPP78b, KPP78b, PK76b, PK77a, PK77b]. MODPOT/VRDDO [HP79, KPP78a, KPP78b, PK77b]. MODPOT/VRDDO/MERGE [HK79]. MODPOT/VRDO [PK76b]. modulus [SEW73]. moiety [RKOU77]. MOLE [PHL'76]. moléculaire [LL72]. moléculaires [BB70, BL77a, BH71, CD78, Cur78, DH73, DL79, DK77, Eis76, Eld73, FWF77b, FB72, FHP70, GPP73, GMZ73, GH77, JG74, KC73, Kau76, KPP78, KPP78b, KL77a, Kot76, KD77, LV78, Lev70, LGR73, MS72a, MST2b, Mat73a, Mat76c, MHA70, Mid74, MHH74, NPL'79, PPC72, PPP79, PK76b, PK77a, PK77b, Pul70, PZP79, SMP77, SS78a, SJ79, SR72c, TPM70, Urr75, Van72, Van74, AF73, AM74, Ano79o, BTD79, BNLS72, BL77a, BJ73, BPP71, BV73, BVS76, BT71, BT78b, BV78, Boy70b, BS78c, BS77, Cal76a, CM75a, CW76, Cas79, CSDV78, CJS77, CSM71, Chr73, CP71, CR72,
CDEO76, CM76, Con77c, Con72, CAMC71, CSH74, CD71, C75, CA72, DCG77, DSC+77, DRCT78, DT75, DEE+75, Ell73, Eng71, F7N77, FCL79.

molecular
[Fla79, Flu72, GGCK79, GG79a, GG79c, GC79, GG79b, Gia73, GC77, GPP79, HO73, Hac74, HH77, Hal78, Hal97, HLMV77, HK79, HLGC73, Hen74, Hen76, Hen77, HLYC77, HL78a, Ho72, HTG77a, HTG77b, IS75, JSC78, Joh70, JS71, JP77, KR76, KTO+78, Kau70a, Kel75, KM76, KK77b, KGP79, KP77, LL72, Lau77, LGAM77, LP74a, LP74b, LFF79, Lev78a, Lib76, Lo75, Loc77b, Loc72, MMB70, MEW70, MS74, Mat71a, MLB76, MDC79, Mic74, Mic76a, MHWC78, Mil74, Na78, NBT2, Nee75, Ner75, OMC76, PH77, PCMS77, PT75, PK75, PPG79, PT75a, PBC74b, Pul76, Pul78b, Pul79b, PÖ77, RR72, RWFS71, RK77, Rou78, Sab75a, SM73a, SD79a, SP79, Sch2, SLB77, SLJ78, Sel75, SMMA73, SDM74, SBB79, Shn77a, Sil71, Sim72].

molecular
[Fla79, Flu72, GGCK79, GG79a, GG79b, Gia73, GC77, GPP79, HO73, Hac74, HH77, Hal78, Hal97, HLMV77, HK79, HLGC73, Hen74, Hen76, Hen77, HLYC77, HL78a, Ho72, HTG77a, HTG77b, IS75, JSC78, Joh70, JS71, JP77, KR76, KTO+78, Kau70a, Kel75, KM76, KK77b, KGP79, KP77, LL72, Lau77, LGAM77, LP74a, LP74b, LFF79, Lev78a, Lib76, Lo75, Loc77b, Loc72, MMB70, MEW70, MS74, Mat71a, MLB76, MDC79, Mic74, Mic76a, MHWC78, Mil74, Na78, NBT2, Nee75, Ner75, OMC76, PH77, PCMS77, PT75, PK75, PPG79, PT75a, PBC74b, Pul76, Pul78b, Pul79b, PÖ77, RR72, RWFS71, RK77, Rou78, Sab75a, SM73a, SD79a, SP79, Sch2, SLB77, SLJ78, Sel75, SMMA73, SDM74, SBB79, Shn77a, Sil71, Sim72].

Molecular-orbital
[Van72, BTD79, CSD78, Joh70, JS71, KPD78, KD79b].

Molecule
[OJB77, Ada78, AF73, BRS+75, BWS77, B78, DN75, ES73a, FSV79, GZ72a, GZ72b, GGCK9, GLS79, GS70a, HH77, Hen79, HK74, IM73, JZ79b, Jør78, KPT7a, KSP78, KD79a, KL73, LD74, Laz79, LE72, MO77, MS76a, Min79, Pie71, PK71, R76, SH74, TDB77, TOED79, WO76, Wil77b, Wil77a, Zen74, xDR79].

Molecules
[Fla79, Flu72, GGCK79, GG79a, GG79b, Gia73, GC77, GPP79, HO73, Hac74, HH77, Hal78, Hal97, HLMV77, HK79, HLGC73, Hen74, Hen76, Hen77, HLYC77, HL78a, Ho72, HTG77a, HTG77b, IS75, JSC78, Joh70, JS71, JP77, KR76, KTO+78, Kau70a, Kel75, KM76, KK77b, KGP79, KP77, LL72, Lau77, LGAM77, LP74a, LP74b, LFF79, Lev78a, Lib76, Lo75, Loc77b, Loc72, MMB70, MEW70, MS74, Mat71a, MLB76, MDC79, Mic74, Mic76a, MHWC78, Mil74, Na78, NBT2, Nee75, Ner75, OMC76, PH77, PCMS77, PT75, PK75, PPG79, PT75a, PBC74b, Pul76, Pul78b, Pul79b, PÖ77, RR72, RWFS71, RK77, Rou78, Sab75a, SM73a, SD79a, SP79, Sch2, SLB77, SLJ78, Sel75, SMMA73, SDM74, SBB79, Shn77a, Sil71, Sim72].

Molecules-in-molecules
[Fla79, Flu72, GGCK79, GG79a, GG79b, Gia73, GC77, GPP79, HO73, Hac74, HH77, Hal78, Hal97, HLMV77, HK79, HLGC73, Hen74, Hen76, Hen77, HLYC77, HL78a, Ho72, HTG77a, HTG77b, IS75, JSC78, Joh70, JS71, JP77, KR76, KTO+78, Kau70a, Kel75, KM76, KK77b, KGP79, KP77, LL72, Lau77, LGAM77, LP74a, LP74b, LFF79, Lev78a, Lib76, Lo75, Loc77b, Loc72, MMB70, MEW70, MS74, Mat71a, MLB76, MDC79, Mic74, Mic76a, MHWC78, Mil74, Na78, NBT2, Nee75, Ner75, OMC76, PH77, PCMS77, PT75, PK75, PPG79, PT75a, PBC74b, Pul76, Pul78b, Pul79b, PÖ77, RR72, RWFS71, RK77, Rou78, Sab75a, SM73a, SD79a, SP79, Sch2, SLB77, SLJ78, Sel75, SMMA73, SDM74, SBB79, Shn77a, Sil71, Sim72].

Moment-polarized
[Ell77, AAC76, Als73, CA72, DSC+77, Fae79, KP71a, MMD78, Tru72].
Monday [Sla71b]. mono [Har77a, INI71]. mono-negative [INI71]. Monocyclic [Boy77]. monoelectric [BSG77]. Monographs [Gos78a]. monolayers [VI75]. monomer [AZ72]. monomolecular [Chr77]. monopole [KP71a]. monopole-transition [KP71a]. monosubstituierter [FJP70]. monosubstituted [FJP70]. Monosubstitutions [MR72]. monoxide [BWS77, SD70, Wil77b, WFS77]. Monte [Cas78b, Col77a, CL78, Col79, RC78]. more-electron [Sin73b]. Mössbauer [GML77, Kot76]. motion [DR75, FG79, GP79, LG71, SHI73, SIM75, SD74, SLOKP79, 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, GHJ77, Pai73, Sl74, Wil74]. muffin-tin [FFCB79, GHJ77, Sla74, Wil74]. Mulliken [CM75a, CA78, Kau70b]. Multi [MM70, Has74, NI70a, NI70b]. Multi-configuration [MM70, Has74, NI70a, NI70b]. multibody [NY75]. Multichannel [RM79]. Multiconfiguration [Har71b, SC76a, BG76, BSS78, BKS79, Fro74, GB76, Hal78, Har70b, JS77, KK73, PNC+78]. Multiconfigurational [GBV77, Gre71, KK76c]. multidimensional [BF78, LG71]. Multimolecular [Sla79]. Multiple [AD77, Dav77a, WI74, BL77c, CW76, CW78, Dan72, DC73, FFCB79, GC79, Gin78, KL78, Kil75, LVDC74, Li76, MMR74, RK77, W73]. multiple-scattering [Dan72, FFCB79, Li76]. multiple-scattering-X [DC73]. multiplet [BF73]. multiplets [LP74b]. Multipole [CJ73b, DH76, GG79, MM72a, SP79]. muons [Fri72]. muscarinic [Kan74]. muscle [Dav79, NTN+79]. Musher [Ano76m, Cus75]. mutation [GRE+77]. mutations [Coo74, Coo78b, RCE75]. Mutually [Abs72]. my [SG6b]. myosin [BZD79].

N [PK71, RKO4U77, SY77, AAC76, Bur77, DEC78, Har70a, HLYC77, KP70, ML76, PL79, PK71, RRS75, RC71, SBD+70, Tru72, WK73]. N-acetyl [RRS75]. n-h [SY77]. N-hydroxylation [PL79]. N-methyl [RRS75]. N-methylacetamide [DEC78]. N3 [ME78]. Nakajima [HLMV77]. nalorphine [KK77a]. Nanosecond [GC75]. naphtalene [BOP76]. napthalene [KT77]. narcotic [KK72, KKK74, KK75]. narcotics [KM72, KKK74, KK75, LBB75]. native [FSV79]. Natural [BS70, BC79, KÔ71, SD74, EIG78, RCE79, SDB76, TRP77, ICS74]. Nature [KBKCD78, Sim78c, BVO72, BM71b, MPS70]. Naturel [DQ77]. Nb [MM77b]. Near [De 78]. nearest [SS77a, SS77b]. nearly [BL70, BEF78, LB73a, SM73b]. necessary [Kum77]. necessity [Kau79b]. need [Del74]. negative [BT78a, Csa77b, Csa79a, INI71, KSP78, Sim77b]. neighbor [Dav72, DF76, MHR76, MHR77, OCRMRL71, S77b, WJC70]. neighborhood [KL73]. neighbour [SS77a]. Neon [Fae79, NY76]. nerve [BK75b, NM77]. nested [MHPS70]. networks [KHI79]. neuroleptics
CHS77, DD72, GJ76, RS79, Sur71, WA71, BBL77, DD72, ES79, TW77].

**Nutrition** [Web74].

O [BMD70, FM78a, Har70a, Har77a, LGP75, LGM77, Shu77b, ASW77, BZSD79, Bur77, CV73, DMS78, FM78a, FMZ70, Gub79, HL79, Han79, HNT78, HPK72, LG77, LE72, LK78, MS71b, MG77, PK71, Ros78a, ST72, SS78a, TTS79, Tru73b, WK73]. **O-methyltransferase** [SS78a].

**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].

**odor** [LC77, Mil71, ST79a]. **off** [LC77, Mil71, ST79a]. **off-diagonal** [ST79a]. **OH** [Cur77, LV71c]. Öhrn [Shu77b].

**old** [Tho75a]. **Ole** [ÖL79b]. Olov [CGLÖ76]. **on-line** [WEH74]. One [BSS78, BDP73, BH71, Eng72, SMB70, 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, KS72, KK77d, May78, ST70, SR72c].

One-particle [BSS78, DSG74]. **only** [Lé74, MPW75]. onto [MHPS70].

Open [CRGC74, APCT77, BS78c, GH79, GBM74, GRM73, HP77b, JD74, KBK72, Lin78, MMB70, MW75b, MB72, MM72b, MDS75, MMM71, Muk75, Nel79, Nes77, PT78, RGM75, RGM77, SP79, SM77, CDO76, Hen76].

open-shell [BS78c, GH79, HP77b, JD74, Lin78, MMB70, MB72, MDS75, Muk75, Nel79, Nes77, PT78, RGM75, RGM77, SP79, CDO76, Hen76].

Opening [Ede70, Lon74, Lon75, Lon73]. **Operator** [BL72, Mic76a, Mor75, BB76, CE73, Dal79, DC75, HBB77, KK74b, KK77c, Ner76, P75a, Sur71, WG74, Sim77a]. **Operator-Level** [Sim77a].

Operatoren [KA76]. **operators** [Bal78, BS77, BHH77, CS78, CEK72, Cro77, GOS75, KA76, LAR75, LAR79, Lin75b, MK78, MW75c, SL79, Sch71a, Sol73]. opiate [LBJN75].

**Oppenheimer** [CL78, CS79, Ess77]. Optical [PS79a, BBT71, DRT77, GML77, INY71, IM73, LSP72, Mes73a, Sch71e, SH74, SH75b]. optically [Cha71]. **Optimal** [Raf75, Ra76b, Abs78]. optimization [Muk75].

Optimization [BT71, G173, ABM78, BS78, Bur77, CLP79a, CLP79b, Gar78, Jak76a, Jak76c, LS74b, MK75b, RCE79, Sun75a, Wel75, BPTLYM73]. Optimized [Sol71, Jak76a, Jak76b, Jak76c, Jak76d, JP73, LTR74, SBB79, SBD70].

optimizing [KK76c]. **Optimum** [Cas78b, Pol70, ZR78, ZBH78, CH71].
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, GM73, HRBB76, MVEN75, Muk75, Abs78, AeAs78, AF73, Ald75, ADDLG76, Ave79c, BTD79, BBP71, BT71, BC79, BVR78, BS77, Cal76a, Cas79, CSDV78, CR72, Co74b, CDEO76, CM76, Com77c, CAMC71, Cur78, DHT3, DEE + 75, FB72, Gar78, GPP73, GC77, GH72b, GHJ77, HO73, Hal78, Hal79b, HLC73, Hen76, HLYC77, HLC76b, HP77b, Joh70, JS71, JC74, Joh77, KC73, KTO + 78, KPKC73, Kau79b, KSL76, KL77a, Kot76, KD77, KPD78, KD79b, KO71, LV71a, LB77, LGR73, LS74b, Mar73a, MEW70, MHA70, MHT2, MG77, MHH74, NPL + 79, Ne75, NG73, PPC72, PK75, Pop71, 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, BS78, Bur72, CW77, Coh74b, CM76, CA72, CA73, DGC77, DSC + 77, DD72, Des72, DT75, Eng71, FGV77, Gia73, GB72, Hal73, HLC73, Hen74, Hen77, Hos72, HTG77a, ICS74, JP73, JP77, JG72, JSK75a, JSK75b, KR73a, KT77, KP72, Kau74b, Lec76b, LAV72, LGR73, LO75, Loh76, MM70, Mar73a, MS72b, Mat73a, Mat76c, MK75b, Mcd79, Mi78, Mul74, NN72, NN74, NS72, Pal73, PS73, Pol70, PAM75, Ra76b, Rob72a, Ros78a, RS78a, RS78b, RS78c, Rou78, RCE79, RPK78, SR72b, SD79a, SBD79, ST70, SC76b, SDB76, SD74, SR72c, SW77, SW78, Tat73, TP77b, Tu75, Tyu78, Van72, Wyb73a, JBG70]. Orbitalstruktur [Sch73b]. orbiting [SM75]. Order [JBP76, OJB77, SL70, WS79, Abd71b, BBB73, BWS77, Bun77, Coo79, HS76, Han75, HBE78, KD74, Kle79, KP78, Lan73, LF77, Laz78, L79, Mec74, Mos73, NRS79, PLMB73, RM73, SK71, SKL79, SC73, TTN76, Vog79, You75]. ordered [PN71]. ordering [AS78]. orders [KHI79, Mal71a, Mal71b].

ordination [FM72]. organic [Ano78c, Csi76, Csi77, DT75, Lar78c, RD79]. Organization [GH79, Eig78, Pea74a]. organo [MYTC77]. organo-silicon [MYTC77]. organometallic [RMB78]. orientatiion [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]. Orthonormalization [Jør77, Jør78, Sch77a]. Oscillator [WG74, AC70, BHL78, CM78, GBV77, Lar78a, RB75a, ST79a, Sin73a, WO75, Wit76, WM79]. oscillators [Bas78, BBA73, BHL78, HVM77, HVM78, Hun74]. other [Boy74, Har77b, Jan77, KKK74, KK75, LDP79, RU76, SM71a, SM71b].

outer [Des72, GB79]. Overlap [Thu75, BB72a, BKW75, DL75, DY76, GPP79, KP76, Kib75b, LV71b, LV72, Mak71, MI78, PNC + 78, PK75, Ra76a,
RR72, Ran74, RM72, Sch71a, Van70, WW71. overlapping [CG79b, Ra76b, SC76b, YJ76]. overlapping-sphere [SC76b, YJ76].

overlaps [Nis77]. overview [Sim78a]. Oxford [Ahl77a, Ano78c, Gos78b, Sab75a]. oxide [KÖ71, PDEB78]. oxocomplexes [BL77a]. oxopyridine [KPP78c]. oxopyridine-water [KPP78c]. oxopyridines [CLP79a]. oxopyrimidines [CLP79a]. oxy [RL79]. oxycumulenes [LÖS73]. oxygen [˚ASW77, DAC79, Har71a, HK74, IM73, KC77, LGAM79, Sal72, TH78]. oxygenases [Har77a]. oxyhemoglobin [Har77a]. ozone [Bur77]. ozonides [Rou73, Rou74].

P [Gos78b, LL72, Sab75a, Sim78c, AMSS79, CT79, LHK77, MK72, NT79, SS78a, AC70, GL74, Har77a, LL75, LG75, MSM70, MBM71, SHR76, TTS71, Tat73]. p-450 [LHK77]. P-450-dependent [Har77a]. p-benzoquinone [MK72]. p-methylation [SS78a]. p-quinones [NT79]. P. [Jan77]. P.-O. [Jan77].

P450 [Han79, PL79, RL79]. Padé [GBL73, CPP75, CM78, GB71, PW74a, Ro73, Ro75]. Padé-type [PW74a]. Pages [Sab75a, Cal73a, Cal76a, Cal77b, Lin73, Shu79, Shu77a]. Pair [GH72a, Nes71, Ada78, BP78, BKW75, CP71, ENRM78, JMP79, KP76, Lan73, LET7, Mag79, Meh73a, MSL73, MMM75, NS75, Nes70, PNC+78, PZ79, RC70, RC71, RC72, SE79, Sin73b, Sri77, WV74, SP72].

pair-correlated [WV74]. pair-correlation [Lan73, MMM75].


photoreceptor [Eno76]. photosynthesis [Chr79a, CD76, KKP79].
phthalocyanine [MS72b]. phthalocyanines [MS72a, MS74]. Physical
[GB71, GBL73, HL78a, ML97, Pea74a, Pet77, Coo78b]. Physicochemical
[KK75, KKK74, Kau79a]. Physics
[Gos78a, Cal76b, Ess77, Fri72, DV79, Mar73b, Sin73c]. photochrome
[SCYB77]. pi [NN72], picoline [BKW75]. Picolines [BKW75]. picture
[CSDV78]. pigment [Kli79]. pigments [MP71a]. pilocarpine [Kan74].
Pioneers [Par77]. planar [Tan74, CSR79]. plane
[CWE71, Euw71, KMO77, ML76, OKM74, WFS77]. plane-wave
[CWE71, KMO77]. plane-wave-Gaussian [Euw71]. plasma
[AJK78, Har75, Hor71]. plasmon [HDG71]. Plenum [Shu77b]. Plesset
[BP75b, PKSB79]. plethysm [MCM73]. plethysms [MVM75, MLM75]. plots
[SY77]. PNC [Tho76]. PNO [Bur77, Mey71]. PNO-CI [Mey71].
Point [BG70, FCL79, MM77b, SC79, ACD74, CB72, ˇCPP75, Flu72, Kib75b,
KK77b, L´et74, PBPL78, RCE75]. point-charge [Kib75b]. Point-group
[MM77b]. points [BF78, MR73]. Pointwise [Lev78b].
Poison [Sii71]. polar [Jor77]. polarisability [Sri77]. polarity [PS79b]. polarizabilities
[HTG77b]. polarizabilities [ANR75, Ahi74, Ahi77b, Bar77,
BSM72, BM73, CG79a, ETF79, GBM74, HH77, HS77, HT77a, KKW73,
LC76, LG70, Ml71b, MM72b, MM71, RB77, RB75b, SSH78, TSE76].
Polarizability [LP74c, BR72, MCST72, NART2, RGM75, Zet74].
Polarization [BKS79, DM72, Ha71, HCE75, OJB77, Sti78, Boy70b, CJ73a,
CJ73b, KC77, Kc47b, KBKCD78, LW77, ML72, SSH78, YD75].
polarizations [RGM77]. polarized [Bor70, Ell77, Fro70]. pole [CG78].
Poly [PPP79, VUY79]. poly- [VU79]. polyamino [NJF77]. polyatomic
[Als73, BBP71, BP75a, CSFM72, HFT72, Jor78, Klc70b, LCP76, LZ77,
MM70, MCF70, ML72, Mu76, Pl79, RR72]. polycyclic
[Mem77, Mem79, PD77, SR78, UP71]. polycytosine [LSOC77].
polyelectronic [KP7M70]. Polyene [AL71]. polycenes
[KH79, LV71b, LV72]. polyglycine [KL77a]. polyhedral [PK75].
Polyhedral [RS78c]. polyions [RKE79]. polymals [Pos78, Pos79]. polymer
[DDH78]. polymers [ADFL71, ADDLG76, AFD78, ABD79, BP73, Del74,
DD77a, Par72, PTD78a, SKL79]. polymethines [FTN77]. polynomials
[Ra76b, Ra76b]. polynuclear [DEE77, NT79]. polynucleotide [SY77].
polynucleotides [KP79a]. Polypeptide [Urr77, ULM76]. polypeptides
[Kar78, KL77a, PCC72, Urr78]. polypolar [SF75]. Pople [JL70].
population [Kau70b, KP7C73]. populations [KP76]. porphin [Alm74].
porphine [KTO78]. porphins [MW74a]. porphyryns [Han79, MW74a].
portée [TBB70]. Position [Csa75]. positive [BT78a, Csa77b, Sco73].
possibilities [IZZ79]. Possible
[Tic79, WLS77, Coo78a, Gol70, HPK79, HK74, Kau74a, LSS78, SY77, Wei74].
potassium [CD74, Sun75b, Sun74b]. Potential
[BR75b, Coo74a, Gab79, GBBK77b, HL79, HG75, Jai70, Liu71a, ASW77,
ABD79, BA78, BNLS72, CL77, CL78, Col79, CG79b, CH74, Csa76, Csa77b,
potential-energy [BA78, Moh78, PD78b, SB78].

Potentialhyperfläche [HG75]. potentials [Ban74, CM75a, CK73, Con72, DMS + 78, DH78, Ell77, FRM74, GPP79, Hal79b, HLGC73, Hun75b, HYL78, KL77b, Naf78, Ner75, Nis77, Ove73, Pau73, PT78, PD77, PK77c, PÖ77, RM74, Sab73, SMH77, SG77a, SJH79, SB78, TGG79, TS78, TS79, Wei74, WO75].

Pour [Mar73a]. Pouvoir [DQ77].

Power [Lau79, BG72]. powers [Boy72c, RB75a].

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].

predissoociating [HE77]. predissociation [BFR78, BEF78].

Preface [CG77, Lów79]. Preliminary [BCR78, BS75c, BSB77, LDP79, BCL77, Meh79]. Prentice [Cal76a].

Prentice-Hall [Cal76a]. presence [Abd71a]. Present [DS70a, Ost79].

Press [Com77a, Com77b, Lar76, Sab75a, Shu77b]. pressure [Bor71, Lib76].

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, RSK78, BWDRD79].

Pro-Leu-Gly-NH [BWDRD79]. probabilities [BR75a]. probability [Ada75b, AC70, Ave75, Hun74, Hun75a].

Probing [SY77]. Problem [Gal72a, LL70, Aba72, AC76, Abs78, Ada72a, AFD + 78, AMJS79, BP78, Col78, Con74, DMR74, ES73a, FU76, Gop76, KPJM70, KBA76, KK70b, LR77, Lud71, Mal71a, MHP70, Mat74a, Mat76b, Med79, MVM75, MLB76, MFRE76, Nor75, Pal75, Per78, RS76, RE70, Sha77b, Sha78b, SMMA73, Shu77c, Sla70b, Ste77, Wes79, ZF76].

Problems [Loc77d, AM74, ČP71, Com78, DL75, DSY74, FBL79, Gási71, Kau79b, SPČ79, Ste74]. procedure [ADDLG76, BB71, BK71, But76, CM72a, Fro75, GCP79, HS70b, Jak76a, Kau74b, Koc74, Lan77, PD78a, PK75].

Procedures [PK76b, BB74, KPP78, KPP78b, KS75, LB77, MR73, PK77a, PK77b, TRPB77, Wei75].

Proceedings [Cal76b, Sti79, BP70, BP71, BP72, BP73, Csi77, Mar73b, Pul78b]. processes [CSDV78, Chr79c, Fla79, GP78, Kle74b, Plo79, Rat78, Rei70].

processing [Bi72]. prodines [LJBN75]. produce [KKK70].

Product [Meh73b, Ada73, Bri73, Lya78]. Production [BS77a]. products
[Létt74, MH72]. Professor [Sla71b]. profile [KK77a]. profiles

[Kai77, MBM73a]. program

[BF71, CAMC71, HC72, Jeh73, KSP78, Lin77, SP75c]. Progress

[Lar78c, Dau77]. project [Nes75]. Projected

[May74b, SDB74, MLB73, May74a, MK75b, MK75a, May78, PCL78, SLB77, SDB74, SDB76, SB78, Van70, SD73].

projected-unrestricted [SLB77]. Projection

[BL72, Fin73, CHD71, Cro77, LKH77, CE73, KGB77]. Projections

[GB71, Löw71a, Ahl77b, BÖ78, GBL73, Löw70, Sar75]. promazine

[PPK78, PK76a]. proof [Rei72b, You72]. propagation [LW77]. Propagator

[OJB77, KPO76, PO77]. propagators [LO77]. Properties

[BH71, GB71, HO73, Löw71a, Ahl77b, AMJS79, BBB73, BN74, BN76, BDP73, BL79, Boy74, Cal75a, CJS77, Chr79a, CS78, DR77, DBBJ76, DMS78, Del73, DDD70, DD71, GZ72a, GZ72b, GC77, GBL73, Hin77, JSC78, KMT77, KWC79, Lad74b, Lip72, Löw70, LG71, Mat71a, ME78, Moc74, Mon77, NRS79, Ove73, Pau77, Pet78, PBC74b, PBG76, PD79, Ra76a, Ran79, RL79, SD77, Sch76a, SP79, SZ76, Wei71, WV74, WB73, ZF77].

property [Boy70a, De 76, Ran78]. Proposed [Kau73]. propranolol

[KVSG79]. prospects [Ost79, Sl77a]. prostaglandins [KD79b]. Protein


proteins [Abd76, AMJS79, BCL79, Boy74, DAC79, Eis76, Eis77, GC75, LK78, MME79, PPC72, Pet79, Pop79, PP74]. protobiological [Fox75].

Proton

[Coo79, Coo78a, DBBJ76, DMS78, GPP73, GPP73, GPP73, GPP73, GPP73, NN72, NN74].

proton-acceptor [DMS78]. proton-proton [GP73]. protonated [KJ75].

protonation [FJP70, Kap73, Lei74]. Protonisierung [FJP70]. protons

[Gia76, HG78, Sal72, TL71]. prototype [FTN77]. proximate [LP78].

pseudo [BP71, CH74, Kar70b, Kar70c, KFY71, Mil74, SD74].

pseudo-aromaticity [BP71]. pseudo-eigenvalue [Kar70b, Kar70c, KFY71].

pseudonatural [Pal73]. Pseudopotential

[RTM77, Sch73a, CH75, LB79b, PP74]. pseudopotentials

[GG79a, GG79c, GG79b, PGDM77]. pseudorotation [BDT77].

pseudospectra [Fae79]. psoralens [SCYB75]. psychoactivities [DH78].

psychotropic [DH78, KK74a, KK75, Pur75]. PCl [BB77, Mes73a].

pteridines [Kap73]. Publications [Ano78u]. Published

[Cal73a, Cal76a, Cal76b, Cal75c, Cal76b, Cal77b, Lar76, Lin73, Sab75a].

Publishing [Ahl77a, Lar78c, Sti79, Ano78c]. puff [AM74]. Pullman

[Cal73b, D878, Shu77a, Sti79, Mem75, Mem79]. pure [Lim74a, WRF73].

Purine [GRE77, GJP79, GPP73, KP79b, ME78, SMB79]. Purine-purine

[GRE77]. Purines [BP72]. pyrazine [HO73, Hin77, PCMS77]. pyrazole

[KPK73, PK73]. pyrene [AZ72, HK79, KPPH78, LPP78, LP79c].

pyrene-7 [LPP78]. Pyridine [PK76b, AM72b, HO73, JL70]. pyridoxal

[AMSS79, WTB76]. pyridoxal-p-dependent [AMSS79]. pyrimidine
quadrupe [BP78]. quadrupolar [MMS70, SR72a]. Quadrupole
[ETF79, BM73, Boy72b, Kot76, LK78, RR72, Tru72]. Qualitative [ČPH74].
quality [DPGC79, GG79a, GG79c, MYTC77, MDC79]. Quanta
[Atk74, Atk91, Gos78b]. quantal [Ber76]. Quantenchemische [HG75].
Quantenmechanik [PTUK69, Cal73a]. quantique [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, Kan79a, LH75, LW77, LJBN75, MPN79,
PP74, PS75b, Pul76, PC76, Pul78b, Ric77, Sti79, SLOKP79, TPC77, Wal77,
WMV77, Awe72, Cas78b, Cle71, CP71, Col77a, Con73, Fox75, Gol73, GM73a,
GM73b, GCJ73, GJ76, Hal75a, Hal79a, HS79, HSBD78, Hat75, DV79, INY+71,
Jan76, KK75, KG76, KG77, KB77, KKK79, LLP78, LP79a, Lin73, MP71a,
Mat72a, MF73, MSP73, MCP73, MPW75, MW75a, Mat76a, Mat76b, MWY77,
MW77, MK78, MKT77, Mos73, NB72, Par77, PHL+76, PQ77, PTUK69,
PT75, PGPP79, PS75a, PP71, Pul77, Pul79b, RW75, Red79, Rei70, Ros74,
SP75c, Sch71b, Sch71c, Sch71d, Sch71e, Sch76b, SE79, SJ79, Sla79, Sre75].
quantum [TP77a, TL72, TW73, Tho75a, Van71, Wei71, Wei75, WOT4,
WO76, W179b, W179a, Wyb73a, BP70, HG75, Loc72, MN79, Sch71c, Lar76,
Mär78, Shu77b, Shu77a]. Quantum-Chemical
[FL79, SLOKP79, MPN79, LP78, SJ79]. Quantum-mechanical
[DAP79, Hos78, PP74, PS75b, PC76, TPC77, HSBD78, KKK79, MKT77,
PGPP79, PS75a, PP71, Pul77, Pul79b, RW75, Red79, Rei70, Ros74,
quartets [GHS79]. Quasi
[BBL72, BBL77, MMB70]. quasi-localized [MMB70]. Quasi-relativistic
[BBL72, BBL77]. Quasiclassical [Tru76, Ber76]. quasidegeneracy [Wes79].
quasidegenerate [Dmi75a]. quasimolecular [MFRE76]. quenching
[AZ72]. quinone [SP71]. quinones [NT79].
[Fla79, LRJ73, LPT+74, MS76b, RW74, TW77]. rare-earth [RW74].


Rayleigh [Amo72, Car72, CJS77, Cla71, Snc75, WB76].

[Dec70, MFRE76]. Re [MMR74]. reaction [BC76, BCR+78, BDT77, GTBB77, GBT79, JZ79a, LPP78, Mag79, Na78, PK71, PDEB78, PKSB78, Sa79, TB75, TH78]. reactions [ČZ79, CS79, Chr77, Chr79c, FM78a, GBTB78, RW75, TC70, WEH74].

reactive [Ber75, Ber76, Hii79, Mic74, Mic76a, Nes75, RW77, Red79, Tru76].

Reactivity [WCK+76, CW78, ES73a, Joh77, LP79a, Sa72, SS78b].

deck [Bar79, CF76, BCR+78, BDT77, GTBB77, GBT79, JZ79a, LPP78, Mag79, Na78, PK71, PDEB78, PKSB78, Sa79, TB75, TH78].

Reactions [ˇCZ79, CSR79, Chr77, Chr79c, FM78a, GBTB78, RW75, TC70, WEH74].

reactions [ˇCZ79, CSR79, Chr77, Chr79c, FM78a, GBTB78, RW75, TC70, WEH74].

reactive [Ber75, Ber76, Hii79, Mic74, Mic76a, Nes75, RW77, Red79, Tru76].

Reactivity [WCK+76, CW78, ES73a, Joh77, LP79a, Sa72, SS78b].

realistic [FRM74]. reality [ˇZiv77].

realization [SP75c]. Rearrangement [RB75b, BMM75].

rearrangements [BVR78, BDT77, CSR79, TG76].

reflected [Ano76c, CT79, Dav77b, Höi77, JG74, Wei75, WCK+76, WO77, WOEG78].


Rederivation [ˇCP71]. redox [LKK+79, DAC+79].

Reduced [AC76, Ab78, Bu77, Col78, JTR77, Kry78, LL70, SLM70, Spe72a, SW78, Ano78d, BB71, KP71b, Kry77, Lar79, MW74a, NS75, Spe71a, Spe71b, SW77].

Reduced-density-matrix [Kry78]. reduction [Per78]. reference [BSS78, BK79, Lar73, Lar78b].

region [BB72a, Mem77, PZP79]. regions [ZL78].

Regularity [CS78]. regulations [BC75]. regulations [SG77b]. related [BW73, NN74, OMC76, Woi71]. relation [Ab76, CBV79, Cas79, DEC78, KSS73, KCT4, LD71, Lin71b, ST79a, WV74, Rob71].

Relations [BH75, JW78, Kau79a, Lan74, ST79a].

Relationship [LB77, ZG79, BCL77, DGC77, Kum77, PCL78, PW79, WB76, WP79].

relationships [PD78b, Pur75, SJ79].

Relative [AS78, BKW75, CS74, JM76b, WJ79, ZR78, ZBH+78]. Relativistic [CW76, DS70b, Des72, ES70, MBB73a, RW74, Ros78a, TP77b, WC75a, BBL72, BBL77, BK75c, Cha71, CWT71, E77, Koe74, Mat73a, Mat76c, PIP73].

relaxation [MG77, SM77, Sch71d, Sch71e, Wen79].

relate [TP77a].

relevance [Urr77]. relevant [TP77c].

Remark [INY+71, Bie75, Bra70, BF75].

Remarks [Cos75, Rei70, Sin73c, Sis74, SC76b, Wei71, AT75, BVS76, Bry74, Han77b, KSS73, Kau74a, Mr76, Nau77, Nau78, San72, Sch78, SG77c, Eze74, Wij78].

Reminiscences [Con73, Pul79c, Tho75b, Van71, SG76b]. Removal [CH77, HT75, SHO71].

Remmer [PK72]. repeat [RU76, RKO77].

repetitive [CBV79]. replacement [Mil74, SDM74]. replication [Coo74].

report [BS75c, BS77].

Representability [Col71, Erd78b, LL70, Col70, Kum77, LD71].

Representable [Lar73, Lar78b].

representation [Spe72a, BS76b, BT71, Bow72, LH74].
NM77, Nis77, PGQ77, PS75a, SP75c, Spe71a, Spe71b, SL70, Sti78. representations
[BF70, Blo72, Blo73, Boy72c, Cor72, HS79, Lét74, Rei72b, RM72, SS73c]. Representing [Gal72a, Lar79]. Reproduction [GCP79]. repulsion
[AT75, HLGC73, JBP76, MM74, Sti78]. repulsive [Csa77b, GBTB78]. repulsive-dominant [GBTB78]. requirements [NN77]. research [Nes75]. residues [PPC72]. Resolvent [Res75, BÖ78]. resonance
[BMD70, Bow71, Boy72b, DL75, EL73, FY79, FB76, GBV77, HE77, HM74b, NTN77, Pul77b, RKOU77, San72, SS73c, Sti79]. Resonances
[Sim78a, BFH78, Doo78, FB77, JBP76, KSP78, LKH77, MCW78, NB78]. resonant [CG78]. respect [KMLB77, SP79]. response [Han77a]. responsible [BL79]. Restricted [Mes78, CDEO76, JD74, Spe71b]. restriction [HT75, Kij72]. restrictions [HT75, Kij72]. Results
[Col71, Fau76, SK72, BCL77, CS73, Col70, Doo78, GCP79, HKM71, JL74, Min79, PT75, RM77, Red79, Sch77b, SBD70, Wei76]. retarded [MP71b]. retention [BKW75, PK75]. retinal [WMB75]. retinol [GC75]. reunification [Bu11]. reversal [VF76]. Review
[Ahl77a, Ano78c, Cal73a, Cal76a, Cal76b, Cal78a, Cal78b, Cal73a, Com77a, Com77b, Dun78, Gos78a, Gos78b, Gos78a, Lar76, Lar78c, Lin73, Mär78, Sab77a, Shu77a, Shu77b, Sti79, DS70b, CS73]. Reviews [Ano74c]. revisited [Kle77]. RHF [SP79]. rhodium [AMC73]. ribonucleic [Sun77]. Riccati [PW74b]. Richards [Már78, Sab75a]. Riedel [Sti79]. 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
[HCZ79, KD79b, KKK79, GKS88, Har79b, KBKCD78, Lar79, Lim77a, Mem77, Per78, PDE79, Ros74, LW77]. roles [ULM76]. root [Sco73]. rotamers [BL75]. rotating [DLG79]. rotating-wave [DLG79]. rotation
[CK75, Cor72, IM73, KD79a, MEW70, WC75]. 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 [CPF74, CD71, HBB77, Hur77, Mat76a, Res78, TB75]. Runge [Loh76]. Rydberg [FWFM77, Hos72, Mil71, Rob72a, TTS79].

S [Ahl77a, AS78, Cal76b, OSL77, RS79, BS70, BM73, BK74, DD71, LG75, LM71, SH76, Spe70]. S-state [BM73]. S [Par73]. S3 [Duk79]. Sagamore
[Smi79]. 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, JS71, JW72, Joh73, JM76a, Wei74, YJ76]. scattered-wave
[Joh70, JS71, JW72, Joh73, JM76a, Wei74, YJ76]. Scattering
[Ada72b, Bal78, Nut78, AD77, Ano79o, BG78, Ber76, BW73, BL77c, BY76,
CMT2a, CW76, Com78, DH73, Dan72, DC73, Dav77a, Dec70, FFCB79,
GGCK79, Gia76, GLS79, Hen79, HYL78, KL78, Ke75, KL77b, LVDC74,
Lev78a, Li76, LKH77, Mic76a, Mil71, MMR74, Nes77, PBPL78, RW77,
Red79, RK77, SK72, SMM73, 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, EId73, FP77, GML77, HIl79, HS70b, JD74, JW76, JS77, JS71, JW72,
Joh73, JM76a, Kau70b, KPKC73, Kau73, KSP78, KS72, KS75, KK77d,
LSC77, LAV72, Lev70, Lim74a, Lud77, MW74a, MS76a, MR72, Moh77,
MG77, MM70, NN77, PCMS77, PPK78, PS70, PK76a, PK77b, PK73, PBG76,
PPB78, Sam75, Vla70, WRF73, WMB75, YJ76, ZR78]. SCF-MO [MR72].
SCF-MO-CI [PCMS77, WMB75]. SCF-MO-LCAO [BB72b]. SCF/CI
[KSP78]. scheme [Aro78, BEH77a, Gof79, HR76, JG72, KT77, KM76,
KK76c, MG77, Nov73, RK79]. schemes
[CSFM72, Kau74b, Kut78, MSL73, RC72]. Schi ff [WTB+76]. Schrödinger
[Ada73, Amo72, Bal78, BFH78, Car72, CJS77, Cla71, KA76, VB72, WA71,
Wel70, Well, WB76]. Schrödinger-Operatoren [KA76]. science
[CGLÔ76, 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, SLC78, YW73].
screening-charge [Csa77a]. SCRPA [Lar78a]. Se [Sch73a]. search
[Mar73a]. Second [KL77c, OJB77, SLM70, Abd71b, BBD73, CP70, HS76,
HE78, KPT2, Lau79, MHR76, MHR77, Moc74, OCRMLR+71, PLMB73,
RM73, SK71, SL79, Vog79, Wel77a, You75, KD74]. second-neighbor
[MHR77]. Second-Order [SLM70, Abd71b, BBD73, HS76, HEB78, Moc74,
PLMB73, Vog79, You75, KD74]. second-row [KP72]. secondary
[BCL79, MP75, Meh79, RU76]. section [BG78]. sections
[Ba79, Ch77, Fae79, ML76, SSM75]. secular [Amo71, Hen77, Koe74, Nor75].
Selected [Hat75, Moh77, SM73a, SD78, DGC77, SM76b, SM76a]. selection
[DLG79, HBB77]. selective [Tal77]. sel enide [YR76]. selenium
[Ald75, VK74]. Self [BBP71, Bor70, CWE71, Kar70b, Kar70c, KFY71,
Kle70b, Meh78, MM72b, MS70, MM71, Sla70a, BK79, BK75c, DS74,
Eig78, Gou73, Hac74, Hal78, JL74, KKW73, KS75, LG77, MM71, Sco73,
Sco74, Sel75, SLC78, Tal77, TGL70, Vla70, VK74, ZF76, GL74, LG75].
self-adjoint [Sco73]. self-consistence [KS75]. Self-Consistent
[Sla70a, Bor70, CWE71, Kar70b, Kar70c, KFY71, Kle70b, Meh78, MS70,
MM71, BK75c, DS74, Hac74, JL74, KKW73, MM71, Sco74, Sel75, SLC78,
TGL70, Vla70, VK74, ZF76]. self-consistent-field [BK79, Hal78, LG77].
Self-correlated [GL74, LG75]. self-diffusion [Tal77]. self-organization
Semi [Eig78]. Semi [BBL77, WJC70, CAMC71, Dub72, LÖS73, NMS77, PK75, RT77, San71, San72, Sch76b, SMH77, SG77a]. semi-ab [PK75]. semi-classical [Dub72, Sch76b]. Semi-empirical
[WJC70, BBL77, CAMC71, LÖS73, NMS77, San71, San72, SMH77, SG77a]. semi-infinite [RT77]. Semi-empirical [BBL77].
Semiclassical [Ada75b, FL79]. semiconductors
[CD78, CJCM73, Csa76, Csa77a, Csa78b, DT75, FCL79, RD79].
Semiempirical [HLGC73, JPTM78, KHI79, PL79, PT78, ABM78, AT75, BOP76, CoI74a, NS78, PLYM78, RL79, SN79]. Semiorthogonalized
[Kas76, KT77]. semiquantitative [Hal75b]. seniority [MLM75].
sensitizing [SCYB75]. separating [Kas76, KT77]. semiquantitative
[Hal75b]. separation
[Lan73, GZ72a, GP79, KKKP79, Ra76a, Zer74]. separations [RMP71].
Sequence
[BG70, Ell73, AC70, AS78, BSM72, BK74, MP75, MMS70, MM72b, PL77, SK71, SK72, SA77, TTS71, Tat73, Van72].
Sequence-adapted
[Ell73]. sequences
[BG72, RSK+78]. sequential
[Muk75, Urr78]. Serber
[Pau77]. Serber-type
[Pau77]. série
[Mar73a]. series
[BG72, ČZ79, DDH78, Gos78b, Jak76b, Mar73a, PD78b, ZG79, Cal75b].
Serotonin
[WOT77, WOEG78, WCK+76]. session
[KKK70, Pos70]. set
[ASW77, Aba72, Bur77, CHS77, CG79b, Cur78, DK77, FS77, HD78, HS70a, Mal71a, Mcd79, RPK78, Sol73, SSH78, RS77b]. sets
[Ab78, Dah78, DPGC79, ES79, Fin73, KB77, LCK76, MYTC77, Pel77, SWN78, SMH72, SC78b, TBB74, Van74]. Several
[Bar70, Kau79b, MCST72].
Sexena
[Ahl77a]. SH
[KPD78]. shape
[BMD70, CA73, HMV77, HMV78, RR77, SC73]. shaped
[WOT75]. shapes
[Fox75, ST72]. Sharma
[HW78]. Shell
[CGRC74, AP77, BV76a, BS78e, CP72, CDEO76, CV73, DK77, Fae79, FP77, GBT79, GHS79, GM174, GRM75, Hen76, HIL79, HP77b, JD74, JBP76, KC77, KKB72, Lai73, Lar73, Lar78a, Lin78, MMB70, MWT75b, MB72, MM72b, MDS75, MUM71, MUK75, MUM75, NN74, NEL79, Nes77, PA77, PT78, PAM75, RGM75, RGM77, SM73a, SM76b, SM76a, SD78, SH73, SP79, SS73a, SS73b, Sin75, Spe73b, SO77]. Shells
[Bee76, JGB70].
shielding
[BM73, GM74, GRM75, LZ77, MUM71, PGPP79]. shift
[DV79, MP71a, SKW72]. shifted
[CT77]. Shifting
[SH73]. shifts
[BK77, Emm74, GML77, Kot76, Sab73]. short
[HK74, JBP76, J76b, LS72, SKL79, TBB70]. Short-distance
[TBB70]. short-range
[JBP76, SKL79]. showdomyacin
[SMP77]. SHS
[Sab71]. side
[RBDV77]. side-on
[RBDV77]. sigma
[CP70, Kol76]. sigma-bonded
[CP70]. 

sigmatropic [BVR78]. SIH
[BT78a]. silane
[DPGC79]. Silbey
[CS77]. silicon
[DPGC79, MYTC77]. similarities
[KM72]. Similarity
[KP76, RW79, Sch78]. Simple
[PS73, Pel77, PP71, Spe72a, TS72, AP77, CP77, FTN77, GLS79, GMM75,
Han77a, KM74a, Lad74a, LDP79, NMS77, PČL78, PGQ77, Pet77, PKSB78, RTS74, SPC79, Sch72, Sol71, SS77b, TW77, Hal78. simplest [HPK79, VB72]. Simplification [L´et74]. Simplifications [BL77a, BL77b]. Simplified [CP70, GV77, BFR78, Rei72b]. simulate [CEK72]. Simulated [DEE75, CDEO76]. Simulation [Bai74, Pol79, NGR77, RC78]. simultaneous [Goł79, Vla70, Wel76, Wel77b]. sine [WO75]. sine-shaped [WO75]. Singer [Pos78, Pos79]. Single [Rat71, Ada72a, Ada79, BS77b, BS78a, BM74, CC79, CM76, Gre71, Mill74, Muk75, PAM75, SD79a, SDM74, SLC78, SC79]. single-center [PAM75]. single-centered [Mill74, SDM74]. single-electron [Ada72a, BM74]. single-parameter [SD79a]. single-particle [Ada79]. Singlet [BB75, TSE76, BP75a, MW74a, MCST72, NT79, PCMS77, SMB79, SDB74, TH78, SDB73]. singlets [GH79]. singly [Ca79a, LAM71]. Singularities [BG70, CH77, CB72]. Site [Flu72, AMSS79, CW78, Gbk77a, Höll77, Kap73, Kle77, KGB77, PD79, SS79]. sites [LK78]. six [AMC73, Jol79]. six-coordinate [AMC73]. six-parameter [Jol79]. sixtieth [Cal75b]. size [BS77b, BS78a]. size-consistency [BS77b, BS78a]. sizes [DGC77, Kau73, MDC79]. Skillman [HC72]. skin [SCY75]. skin-sensitizing [SCY75]. Slater [BR78, BS74a, BS76a, BPTLVM73, Bre73, Cha77, ERW75, GMZ73, LS70, Lc76b, MH72, SR72b, Sam75, ST70, SS71a, SR72c]. Slater-type [BS74a, BS76a, SR72b, ST70, SR72c]. slow [Gia76]. Small [Com77a, Com77b, Vla70, BB72a, CODM77, GJLL75, HS70a, Hu76a, Hu76b, KPF77, LGR73, Mu74, Pos70, Sim79]. Smooth [Thu75, Sha71]. SN [KKA78]. SOCL [GH72b]. sodium [Ber73, Bor70, BK75b, CD74, Col79, HCI75]. software [WH75]. solid [FBL79, DV79, LW77, Mu76, Nam75, Sla71a, SR72c, SP75d]. solid-state [DV79, Sla71a]. solides [KMO77]. solids [ADFL71, Bor71, Bre75, Car75, Dec70, Fau76, Joh73, JMP78, PBPL78, Sco74, Sla75, Wen79, ZF77]. Solitons [Dav79]. Solution [MHP570, Ada73, BEH77b, Csa79a, DSY74, FW75, HS75, JM73, Koe74, KK76b, KUN78a, Ner76, Nor75, Pul77, RRNS75, SD77, WA71, ZF76]. solutions [Ca79c, ENRM78, FG79, Fro79, KKA78, Kho79, Lai73, Mes79, Ta77, TNT76, Živ77]. Solvation [SAM79, WN78]. Solvent [AZ72, FSV79, HPW79, LCPP79, RC78]. Somatostatin [MDA78]. Some [AT75, BS75a, BVS76, ESR74, GSE78, GK76, HC78, Jai70, KSS73, LKK79, Lów70, Lów71a, Lów77, Mes73b, Na78, Oda73, PD78b, San72, Sch78, Spe72a, SG76b, Vol79, We75, AMSS79, BG76, BY79, BM74, BS75c, CK75, Cha77, CL73, DDH78, Doo78, DT75, JL74, KMT77, KR73b, Kum77, Lai73, LM72, MS76a, MR72, Mor75, Muk74, NN72, Nis77, PGQ77, PS70, PD77, PDE79, PK77c, RMB78, Ros78b, RD79, Sha77a, Sha78a, SKW72, Sim77b, Sto71, SL73, SBD70, Tho75a, TP78, WN78, DEC78, ED79, RTM77, SW78]. Sons [Ca79b, Cal75c, Dun78, Shu77a]. Space [GGCK79, Spe72b, Bee72, BS70, BS76b, Cll73, GHS79, HY78, KC74, Lan77, NM77, SP75c, Sla70b].
space-dependent [Cli73]. space-spin [KC74]. spanning [Bee72]. spatial [AMSS79, Gal74, MPN79, Rou79, ZG79]. spatially [Csa76, Csa78b]. special [Mag79, Pau77, WV74]. special-pair [Mag79]. Specific [Gol70, AMSS79, BL79, Jeh73, KMT77, Lar79]. specificity [PL77]. spectra [AeAs78, BCL79, BL77c, BEF78, CW77, DH78, GGJ77, GPC71, GK75, Hal75b, Kib75a, KJ75, KS79, LV78, LGM77, LBAF78, Lun77, MS71b, MR72, MK72, NT79, PNJB78, SLB77, Sch71e, SM79, SK79, Van72, WK73, Wój76, Wój78, LBAF78]. Spectral [BHM75, Boy74, BS72, Ra76b, BFH78].

Spectroscopic [Kli79, TPM70, KKK70, WB73]. spectroscopy [Bas78, Feu77, GC75, KKK70, Kla78, KRKS78, MF77, Mich6b, Pul78b, Rab77, Sti79, WS75, Gos78a]. spectrum [BHL78, BS72, FHB77, GML77, HG78, HDG71, On79, VG78, WJ79, Wan79, WFS77]. Speed [DMS78]. sphere [GH72a, Kau73, SC76b, Wei76, YJ76]. spherically [Csa77b]. spheroidal [SP74]. sphingomyelins [PC76]. Spin [BP74, BOP76, BK75a, Joh77, Kau79b, Kle74b, KT76, KR73b, Lim75a, MS71a, MF73, MSP73, MCP73, MP75, MW75a, Mat76a, Mat76b, MW77, MN79, MLB73, May74a, May74b, MK75b, MK75a, May78, MK78, Sar75, SD79a, SM71a, SM71b, SM71c, SK73, SS73a, SS73b, TH78, AP77, BP75a, Bor70, BK75c, CL73, CDEO76, DL75, Dav74, Fro70, GT76, GJLL75, GJ76, Hal75b, JMM71, JSDK75b, KR73a, KTO78, KPJ70, KC74, KGB77, Kle79, LED73, LD73, Laz79, Lim74a, Lim74b, Lim75b, Lim77b, MM74, Mat72a, MCF70, MML75, Mes73b, MLB72, MS75, NN72, PAC77, Pau77, Sh77a, Sha78a, SL70, TB73, VF76, Har79a, MSP73, MP75, 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, MP75, MW75a, Mat76a, MW77, SS73a, SS73b, KPJM70, KC74, Lim74b, Lim75a, Lim75b, Lim77b, Mat72a, MK78]. Spin-only [MP75]. Spin-Orbit [BOP76, BP74, BK75a, Hel75b, JSK75b, MM74, MCF70, SM71a]. Spin-orbital [Joh77]. Spin-other-orbit [SM71a, SM71b]. spin-polarized [Bor70, Fro70]. Spin-Projected [May74b, MK75b, MK75a, May78]. Spin-spin [MS71a, SM71c, MM74]. spin-wave [CL73]. spinfree [Lim75b]. spinless [DR77]. spinors [CW76]. spins [HLMV77]. 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 [RSS75, And79, Sco73]. squares [BT71, HS75]. stabilité [JM76b]. Stability [Lai73, MK76b, Bur77, Coo78b, JM76b, ŁOS73, LR73, LPT74, MHA70, Lai73]. stabilization [HK74, KSP78]. stabilized [MS71b]. stable [Hat75, RS79]. staggered [Hub71]. standard [RS78a]. Stanton [TB75]. Stark
starting [ACD+74]. State

[BK77, CHH+78, Rei76].

[LO77, NM77, OL78, Abd77, Bar77, BWS77, BN76, BJ73, BS70, BM73, BP75b, BCL77, Bow72, BK74, Bra79b, Bun77, Cal72, Cal74, CR72, CKD73, Dav77b, DD77, FWFM77, Fro75, GBV77, GL74, Hal79b, HE77, DV79, HMC71, Ive74, JZ79b, KR73a, Kap79, Kar78, Kol74, Kol75, KO71, Kut78, LH74, Lar75, Lar78a, Lar78b, Lec76a, Lec76b, Lib76, LKH77, Lin77, LG75, LHK77, MME79, Man77, Mat79b, MM72b, MSM70, MBM71, Mul71a, Nis77, OL79a, RS79, Ros78b, SK71, SK72, SA77, SH75a, Sin73b, SD70, Sl71a, SGM78, Tan74, Tat76, TSE76, Tru73a, Tru76, WR70, Wil77b, WB73, PCH74].

States [AFD+78, Lon75].

[Spe72a, Abd71b, AM77a, AS78, ADFL71, BSS78, BKS79, BP75a, Ber73, BL79, BF71, BS75c, Boy72a, BS78c, CSFM72, CP87, CPS77, CESW70, DC77, DS76b, DS70a, DS70b, DT72, De78, DD77a, DC75, Dmi75b, DMM75, ES73b, Fan71, Fan67, GV77, GB57, GL74, Hal75b, HNT78, Hai75, HS70b, HT75, Hos72, IS75, KR71, KR76, KKW73, KTO+78, KSP78, Kol76, Kun78a, KOW78, Kun78b, LD71, Lim74a, LV71c, LS79, LAM71, MW74a, MCST72, MCF+70, MCM73, MLM75, Mill71, MMS70, MG77, Muf76, Mul71b, PCH74, PC77, PS70, Pie71, Pop71, PLMB73, RB77, Rlt76, Ros78b, RT77, SMB+79, SP75a, SC76a, Sim78c, SH75a, SHR76, Sin75, SD74, SCYB75, SCYB77, Spe70, SS77a, SS77b, Sk79, Sto71, Tan74, TTS71, Tat73, TTS+79, TN79, TS72, Urr78, WS75, WMB75].

states [WK73, You72, YD75, SP72, CB72, SD73].

Static [WK73, You72, WD75, SP72, CB72, SD73].

Stationarity [CG78].

stationary [Com78].

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

statistics [TB73].

status [DS70a].

steady [BCL77, Dav77b].

steady-state [Dav77b].

steering [KSL76].

stentorin [SCYB77].

Stephen [Cha71].

stereoselection [FF70, Fuk75, Cal77b].

steric [Tic79].

Stickstoff [BKW75].

Stieljes [Lan74, Lan77].

Stieljes-integral [Lan74].

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

STO-3G [ZSR79].

stochastic [ESG79].

storage [Bil72, MHH74].

Störungsrechnung [Ahl70].

STOS [Wel77b].

STP [Eng72].

strain [BMD70].

strength [AC70].

strengths [CM78, GBV77, Lar78a, Sin73a, WM79].

stretch [SS71b].

strip [JG74].

Strong [Lun77, KK77c, LL73, Loc77d, SRE+79, Shu77c, Pet78].

strong-field [KK77c].

strongly [Kle74a].

Structural

[Boy74, Chr79a, Enz73, Mot79, RW79, RU76].

Structure

[BC75, LL72, Le74, AFL78, AF73, AMS79, AL71, BT78a, BK77, BCL77, Bur77, CB79, CGL076, Car75, CJ73b, CR72, Col77b, Duk79, EP71, Erd78a, Fin73, FBL79, FWJ+79, FS79, FR74, Fro74, GSE78, GK75, GML77, Har78, HS70a, Hin77, HK74, Hop78, HT75, JR74, Joh75, eAJ76, KK74a, Kau79a, Kel75, KKA78, KJ75, KL77a, KC74, KU70, KVSG79, KMO77, Lad74b, Lad75a, Lad75b, Lad76, LOSC77, LSS78, LVDC74, LP79a, Lay77, LFF79, Lev78a, LE72, LM72, LOS73, LK78, Lud75, Lun79, MW74a, MP79, MS72a, MS74, MF73, Meh79, MHWC78, MHW78, MR72, MOV75, Ove73, Pai71, Pai73, PN71, Pea74a, Pet77, PNC+78, Pul77, Pur75, Ran78, RL79, SMB+79, SP74,
symmetrical \[ \text{symmetrischer} \] [Sch73b].

symmetrized \[ \text{symmetrischer} \] [Sch73b].

symmetry \[ \text{Symmetry} \] [Bee76, BBT71, BH71, BB73, De 76, Eld73, GP78, GO68, 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, Lim6a, LG71, MK76b, MM77b, Ros78a, Rou78, Rou79, GOJ +73].

symmetry-adapted \[ \text{symmetry-adapted} \] [Kut78].

symmetry-lobe \[ \text{symmetry-lobe} \] [Rou78].

symposia \[ \text{Symposium} \] [Cal73b].

symposium \[ \text{Symposium} \] [Pul78b, Sla71b, Sla73b, Sti79, BP70, BP71, BP72, BP73, Lon73, Ede70].

synaptic \[ \text{synaptic} \] [Wal77].

synthesis \[ \text{synthesis} \] [Gab76].

system \[ \text{system} \] [Spe72a, AM72b, BZSD79, BS75c, Bra79b, BS78c, CS72, HL79, HBE78, HG75, HP77b, JBP76, KR76, KP71a, Lad75a, Man77, May74a, PCL78, PHL + 76, Res78, Sre75, SP79, TBB70, WH75].

systematibus \[ \text{systematibus} \] [BP79].

système \[ \text{système} \] [TBB70].

systèmes \[ \text{systèmes} \] [ACG74, AM72b, Bai74, BA78, Bar70, BB72c, BEH77a, BEH77b, BFH78, BL77d, CP70, Cho79, CP71, CP72, CP73, CP75, CP77, CK74, CI79, ESG79, GOK79, GP74, GBS70, GL74, GBM74, GRM75, HHR70, HS79, Hat75, Hea71, HG75, HR76, IS75, JMM71, JM76a, JPTM78, JS70, JL74, KL75, KPP77, KKP77, KMT77, KL77c, Lai73, Lar79, Lat77, Lin78, LRD + 77, LRD + 78, LG75, May74a, MK75a, MS76a, Mic76b, Mil74, MBMM79, MPMK79, MMM71, MMM75, NS75, NB78, Oni79, OSL77, PT78, Pea74a, Per78, PGQ77, RMB78, RGM75, RB75b, SN79, Sar75, SP79, SM77, SMD74, SS73a, ST72, Sol71, SO77, TS71, TP77a, TL71, VB72, WOE78, YG77, SS73b, SD73].

Szent \[ \text{Szent} \] [Lak76].

Szent-Györgyi \[ \text{Szent-Györgyi} \] [Lak76].

T \[ T \] [Sab75a].

table \[ \text{table} \] [Oda73].

Tableau \[ \text{Tableau} \] [Gal72b].

taking \[ \text{taking} \] [MCF +70].

Tamm \[ \text{Tamm} \] [DS70a, HU74, Lar78a].

targets \[ \text{targets} \] [Gia76, GLS79].

taurine \[ \text{taurine} \] [CS74].

tautomer \[ \text{tautomer} \] [ZR78, ZBH +78].

Tautomerism \[ \text{Tautomerism} \] [CLP79a, CLP79b, ZSR79].

tautomers \[ \text{tautomers} \] [HLYC77].

Te \[ \text{Te} \] [MM77b].

Tchebycheff \[ \text{Tchebycheff} \] [Lau77].

TCNQ \[ \text{TCNQ} \] [DT75, AF78, CHHS74, HRBB76, Joh75, Lad75a, LRD + 77, LRD + 78].

TCNQ-TTF \[ \text{TCNQ-TTF} \] [Lad75a].

Te \[ \text{Te} \] [Sch73a].

Technique \[ \text{Technique} \] [BL72, BPTLVM73, AFD + 78, ABD + 79, BF78, CHD71, ČP72, CDEO76, Dan72, GS70b, HLMV77, HPK79, KPP78, LS74b, MSKM77, Mil74, Muk75, Ner76, PW74a, Rsc73, Rsc75, SD74, SMD74, Sun75a].

techniques \[ \text{techniques} \] [ABM78, Che71, DD72, FB76, GGCK79, JS77, PBC74b, Pul77].

Teller \[ \text{Teller} \] [Ham73, INI +71, MSSF79].

Temperature \[ \text{Temperature} \] [Tul77, ACK +75, MSSF79, PBC74a].

temperatures \[ \text{temperatures} \] [AMJS79].

tempered \[ \text{tempered} \] [Raf75].

Tempering \[ \text{Tempering} \] [Pos79].

template \[ \text{template} \] [Gab76].

ten \[ \text{ten} \] [DSC +77].

ten-electron \[ \text{ten-electron} \] [DSC +77].

tensor \[ \text{tensor} \] [KK74b, KK77c].

tensors \[ \text{tensors} \] [Boy70a, Boy70b, BM71a, BM71b, BO73, BS74b, El173, IMN79].

teratogens \[ \text{teratogens} \] [KPP78a].

term \[ \text{term} \] [Cha71, Koc74, WJC70].

terms \[ \text{terms} \] [Ada73, AF73, CSFM72, CD71, FTN77, GC77, JPTM78, MCF +70, MCM73]
ternary [Mat77]. Test [KT77, Kij72, PK75, BS78b, CZ79, NJF+77, PS73, GJ76]. tests [MMD78, Sin75]. tetracyanoquinodimethane [DT75]. Tetrahedral [Pos77, SC78b]. tetrahedrally [JMP78]. TFD [Sla75]. their tests [MMD78, Sin75]. tetracyanoquinodimethane [DT75]. Tetrahedral [Pos77, SC78b]. tetrahedrally [JMP78]. TFD [Sla75]. their tests [MMD78, Sin75]. tetracyanoquinodimethane [DT75]. Tetrahedral [Pos77, SC78b]. tetrahedrally [JMP78]. TFD [Sla75]. their theorems [Dal79, Lev78b]. Theorems [BB72c, GZ72a, GZ72b, GBS70, HPW79, IMN79, Kau77, KN79, KJ75, KS79, KJ78, Lar78c, LP79c, PBS76, Rat78, RRNS75, SS79, SP71, VG78, WOEQ78, Wój78, WB73, BB75, Boy72b, Cal76b, CSFM72, Con70, CD71, GS70a, JVM78, KR76, KKK74, KK74a, KK75, Kau76, LDP79, LP79b, LAN71, Mar73b, MCF+70, MCM73, Nes75, Nov73, Ran78, RW79, Sha77b, Sin77b, SS78b, SR77, UP71, WMV77, CLP79a, CLP79b]. theoretically [JŻ79b]. Theorie [Mar73a, Loc72]. theories [ANR75, BB73, CA78, Feu77, FGV77, PKSB78, PKSB79, PS75a, WB76].

Theory [BN76, BMD70, BHF78, Bra75, Bra76, CGRC74, Chr79c, Cla71, Con77b, Coo74, Coo78b, CSI76, DCS+77, Fuk70, Fuk75, JBGO70, ON79, RKE79, Sch77c, Wój76, ZV79, AC70, An70, AFD+78, ACH72, ACD+74, Ave72, BFS73, Bal71, Bal78, Bar70, BRS+75, BS74a, BS75a, BS76a, BWS77, BP78, BB72b, BV73, BP72, BV74, BMM75, BP75b, Blo72, Blo73, BDT77, Bov79, Bra70, BO79, Bra79a, Bur73, Car72, CFH77, Car74, CZ76, CW76, CT77, CL73, Chr77, CP71, Csa79b, Csi77, Dav77a, DT72, DH76, DY76, Dmi75a, Dmi75b, Dub72, ES73a, Elf73, Eps77, ES79, ETF79, Fac79, FP77, FY71, Goo76, GS70b, Hal78, Hal79b, Han70a, Han77a, HS79, Har78, Har79b, HBE78, Hen76, Her74, Hir70, Hos78, Hur76b, IS75, JD74, Jam70, JS77, Jol70].

theory [JNZ72, KL75, Kap79, Kib75a, Kle70a, kle77, KLE79, KR78, KP78, Kry78, KS72, KS75, KKK77d, LL76, LH75, Lar73, Lar76, Lar78c, LWA74, Laz78, LZ79, Lev78a, Lim6b, LÖ77, Lin78, Lin73, Loc72, LPT+74, LG71, Lim75, MKF77, Mar73a, MF73, Mat76a, Mat78, MN79, Mat79a, MCST72, Mem75, Mem79, MW75b, Mic74, MMM71, NI70a, Naz72, PP79, PGQ77, PTUK69, PN76, PSS77, RRT2, RSR2, Ram78, Red79, RCE79, Rob75, Rob72b, Ros74, RK76, Sam75, SF76, SLB77, Sch71b, Sch71c, Sch71d, Sch71e, Sch76b, Sel75, SMH77, SG77a, SM74, SS73a, SS73b, Sin75, Sl71a, SJH79, SMW71, Su77, SG76a, Tho75a, Tri77, TB75, TOED79, Tur74, Vla70, Vog79, Vol79, WN71, Wil74, Wil77b, Wol71, Ber75, IZZ+79, JMP78, NN77, Cal76a].

Theory [Ano78c, Cal77b]. there [Sey76]. thermal [Mat78, NJF+77, SWF79]. Thermodynamic [CI79]. Thermodynamics [Por78, Van75]. Theta [LV71b, LV72]. Theta-Function [LV71b, LV72]. thioridazine [KK76a]. thiouracils [GJP79]. Third [BWS77, Cal76b].
Third-order [BWS77]. Thomas [Bie75, Csa77b, Csa79a, Csa79b, DH76, GY75, Goo76, GG75, Han70a, Han77a, Lun75, WC75a, YG77]. **Three** [RW75, Bal78, CK73, HR79, Kol76, LG75, LPT+74, PCLL78, 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]. **Time** [Gol73, JL70, Moc73, NB78, Sch71b, Sch71c, Sch71d, SF76, BF75, Han70b, Man77, SB75, WA71, Jan70]. **Time-Dependent** [Sch71e, Gol73, JL70, Moc73, Sch71b, Sch71c, Sch71d, Han70b, WA71, Jam70]. **time-independent** [Man77]. tin [DC73, FFCB79, FRM74, GHJ77, Kot76, Pai73, Sla74, Wilt74, GK75]. TiNi [PN71]. TiO [GK75]. **tissue** [Jeh73]. **tissue-specific** [Jeh73]. titanium [ES73b]. Tm [DS74]. today [Wyby73]. Toivo [Cal75b]. tomorrow [Wyby73b]. top [DM75]. **Topological** [KM72, BT77]. **topology** [Sch73b]. Torsional [BBG79, SY77]. Total [BG78, SW71, BM74, Cas79, KP76, SW70, Spe73]. traditional [CP71]. **trajectories** [CG78, CH77]. trans [TS78, WMB75]. trans-[TS78]. transfer [BZSD79, Cho79, CD76, DT75, Feu77, Lad76, LKK+79, LW77, LH77, OSL77, Pet79, Rat78, SRE+79, Van72, ZV79]. Transferability [CSM71, SDD+77, SWN78]. **Transferable** [Ave79c, Ave79b, AB79, Ave79a]. **Transform** [GMZ73, Ban74, BS75b, GMG75, GB72, GCJ73, MFK77, MH72, ZF76]. **Transformation** [Thu75, VW74, AFD+78, BL77a, Cof74b, FHB77, Jer77, Sch78, Sha71, Shu77c]. **transformed** [Wes73]. **Transition** [AC70, MMD78, OJB77, BR78, BFS73, BR75a, Cal77a, CHHS74, De 78, DR75, DC77, FN73, GBV77, Gos75, Joh77, KP71a, KGB76, LH75, Lar78a, Lar79, LVDC74, MM77b, Por77, Por87, San71, Sch77c, SKW72, Sin75, SD74, SR77, Sto71, Van72]. **transition-metal** [BR78, BFS73, Joh77, KGB76]. **transitions** [BP75a, Ber73, Coo79, DM72, DD77b, Enz73, FWM77, GML77, KD74, Lar78a, Mes73a, NT79, SIM75]. **translation** [BBA73, FM72]. **Transmembrane** [USK+79, VU79]. **Transmission** [DS79, Wal77]. **transport** [Fro79, Hos78, KWC79, Mar79]. **transversion** [GRE+77]. **transversion-type** [GRE+77]. trapped [BBA73]. treated [BK75c]. treating [FHB77, Pai73]. **Treatment** [Sla71a, AM72a, BBB73, BTD79, CW78, Chr77, Cla71, CSH74, Csa78b, DS70b, Des72, FJP70, GS70a, Hil79, JBP76, Kau76, KMO77, MM74, MLB72, RTS74, RM79, SA77, SDJ79, Shu77c, SS71a, SW78, WRS70, LG71, SIM75]. treatments [AM74, AM77b, AM77a, CHD71, TS72]. tri [IN71]. **tri-phenylene** [INI71]. **tribute** [CGLÔ76, Cus75]. **Tridiagonal** [Wel70]. **tridiagonalization** [Wel71]. **trifluoromethyluracil**
[PLSL78]. **Trifonow** [Cal73a]. trigonal [Sch73a]. trigonometric [DDH78]. trimers [Moh78]. trimolecular [CW78]. triple [Kle70b, MPS70, Wei76]. triple-dipole [Wei76]. Triplet [SN79, Abd77, BB75, BP75a, IMN79, JZ79b, NS78, PCMS77, PS70, San71, SMB+79, SCYB75, TH78, TSE76]. tRNA [Pul77]. tropoeastin [RKOU77]. 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, Gal72b, H¨oj79a, H¨oj79b, MSKM77, Thu75, Aba72, BA78, BB74, Bas78, BL77a, BBP71, Bil72, Cal72, Cal73c, CPP75, CL78, Col79, Dea72, Eng72, GL74, HMV77, HLMV77, HMV78, Har75, Jet73, KM47a, Kij72, KBA76, Koc74, Kol74, LAM71, MKF77, Mal71b, MM74, Me78, MH72, OK75, Pie71, Rat71, Ros78b, RB75b, Sha76, SJH79, SS70, SJH79, SL70, TBB70, TTS+79, WR70, JBG70, Mal71a]. two-body [KBA76, Ros78b]. Two-Center [Thu75, BA78, Eng72, MH72, Sha76]. Two-Electron [BL77b, BH71, DT72, Aba72, BL77a, BBP71, Bil72, Cal72, Cal73c, GL74, KM47a, LAM71, MM74, RB75b, SJH79, WR70]. two-matrix [Kij72]. Two-parameter [H¨oj79a, H¨oj79b, MSK77]. two-particle [Rat71]. two-photon [MKF77]. two-point [CPP75]. two-spin [SL70]. Type [Spe72a, BS74a, BS76a, BS71, Cha77, CL78, FTM77, GRE+77, H¨oj79a, H¨oj79b, KGP79, LS72, LM72, LGR73, Mat73a, Mat76c, NY76, OK75, Pan77, PF74, PAM75, PW74a, RL77, Ros73, Sab71, SR72b, ST70, SLC78, SR72c, SF75, Lec67b].

**U** [Lon73, Sla73b]. **U.** [LB79a]. **UHF** [Cla70, Lum79, Sha77a, Sha78a]. ultimate [HPK79]. ultrasonic [PP71]. Ultraviolet [Gos78a, PLSL78, Ros75, Rab77]. unbounded [BFH78]. unconstrained [Muk75]. unconventional [Lec76a]. uncoupled [Vog79]. understand [KK74]. Understanding [HP77a, Kau76]. uniaxial [Hub71]. Unified [MM74, CL73, LO77]. Uniform [MYTC77, BM73]. unit [CB79]. Unitary [PH77, Mat74a, Mat76b, Mat79a, Ne79, Pal75, PW79, Sha77b, Sha78b, WP79]. unitary-group [Mat79a, Ne79]. united [CSH74]. units [HR79, SRI77]. Universal [SWN78]. universe [Lay77]. Universitatis [Cal75b]. University [Sab75a]. unperturbed [AM74]. Unrestricted [NN72, NN74, PCL78, SLB77, Jor73, KKA78, PS70]. unsaturated [NI70a, NI70b]. unstable [Tho76, TPC77]. Untersuchungen [HG75]. upon [DRTC78, LCPP79, Sc71]. 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, HHR70, Kau73, Laz78, LZ79, MCM73, Nee75, NER76, PT75, PAM75, PGDM77, RK77, Rou79, RCE79, Sch72, Sim72, Sol73, Sti78, Wei74, Wol71]. used [BC75, KB77, San72]. useful [LH74]. Using
V [FTN77, HMC71, IM73, Kla78, Kle70b, KMO77, LGP75, LGM77, PPP79, PNC+78, PK77b]. 

Vacin [FTN77, HMC71, IM73, Kla78, Kle70b, KMO77, LGP75, LGM77, PPP79, PNC+78, PK77b]. 

Vak [FTN77, HMC71, IM73, Kla78, Kle70b, KMO77, LGP75, LGM77, PPP79, PNC+78, PK77b]. vacancy [SC79]. Väää [Cal75b]. Valence [CESW70, Gal72b, Gin78, Goo76, Har70a, Har77a, HR79, WJ79, AM72b, BW76a, Bra79b, GN77, GV77, Har71a, HLYC77, Kle79, Lad74a, LS74a, MW74a, MiI71, Moh77, NN74, NG73, OK75, Pet77, PNC+78, RTS74, RS76, SM73a, SM76b, SM76a, SD78, SBD+70, TRS73, TS77, TS78, TS79, WMB75, TTS+79]. Valence-Bond [Gal72b, HR79, GN77, OK75]. Valence-Electron [Goo76, SD78, WMB75]. valence-fluctuation [Bra79b]. Valence-shell [BW76a, NN74]. Valency [CR72]. Validity [LPT+74, CD78, TL72]. Valinomycin [Sun75b, ST78, ST79b, Sun74b]. Valinomycin-potassium [Sun75b]. Values [Spe72b, BBK76, BS71, BSG77, BL77d, RK77, SK71, SG77a, SP77]. Vanadium [WFS77, PNJB78]. Variable [ES79, MR72, SeI75, Amo72, Csa76, Csa78b, PK75]. variance [HS75]. Variation [BL72, BEH77b, Zer74, Eps77, GZ72a, Mor78, MI78, MMM71, NI74, PGPP79, SY77, TS72, Wel76, Wel77b]. variation-perturbation [GZ72b, MMM71]. Variational [BR75a, BR72, Bri73, Csa78a, GbK77a, Kle77, KGB77, LFF79, Lud75, PSK77, ACD+74, CK75, CSH74, Csa76, Csa78b, Csa79a, CZ75, DR75, GF76, HS77, Moc73, Moc74, MK76b, NS75, Pal71, PBC74a, TK78, WW71, Wei76, ZF76]. variationally [Csa77b, LTR74]. various [BB74, Gal74, JM76b, eAJ76]. varying [GZ72b]. vascular [ULM76]. vector [Bre73, Loh76]. vectors [LÖ77, Mor75]. velocity [Kob78, Sin73a]. verdazyl [MPN79]. Verdet [IM73]. Verfahren [KA76]. Verlag [Cal73a, Cal79a, Cal77b]. Vers [JF78]. Versailles [Cal76b, Mar73b]. versions [BBL77]. versus [AM77b, Ber75, ES79, HPK79, Ige74, Kob78, PPB78, RBDV77]. Vertebrate [Eno76]. vertical [VG78, SG77a, TS79]. VI [CDEO76, Kle77, Sni79, Tho76]. Via [GB71, Als73, FB76, GBL+73, SS77b, YL74]. vibrantibus [BP79]. Vibration [CK75, BBA73, KD79a, LRD+77, LRD+78]. vibration-translation [BBA73]. Vibrational [Tru72, BS77a, Bow79, GSE78, SchH1d, SR77, Ste77, Tru76]. vibrationally [MM72a]. vibronic [CI179, WZ70, TGL70]. vibronique [TGL70]. vibrotors [SI71b]. VII [GbK77a, LaI73, SP7C79, TS77]. VIII [Com77a, FWFM77, KPP78b, KGB77]. violin [Cl70, MMB70, MB72]. viral [WLS77]. virial [BEF78, BFH78, FSB77, Lev78b, Nai78, WO74, WO75, WO76]. Virtual [Bee79, CoF74b, Med79]. visual [Kli79, MP71a]. vitamin [ED79, Ram78]. vivo [Dav77b, Web74, WS75]. Vleck [Sla71b, Gor71, Gor72]. Vol
years [Lak76]. yesterday [Wyb73b]. Yield [HG78, GGJ77]. York [Ahl77a, Ano78c, Cal79b, Cal75c, Cal77b, Dun77, Gos78a, Lar76, Lar78c, Shu77b]. Young [Lim75b].

Zero [Col77a, Boy70a, Har71c, Nan78c]. zeta [GG79a, GG79c]. zinc [MS72b, MHH74, RTM77]. zinc-histamine [MHH74]. ZN [JMP79, KPD78]. ZnSe [CESW70, CWE71]. zum [BKW75, HG75]. zur [KA76, HG75]. Zwanzig [HLMV77]. zwitterion [RC78].

References


[Abd71a] Suheil F. Abdulnur. Bounds to excitation energies of H in the presence of long range dispersion forces. *International Journal
REFERENCES


Abdulnur:1971:BSO


Abdulnur:1976:IGP


Abdulnur:1977:IMM


Andre:1979:NMP


Absar:1972:MCI


Absar:1978:RHO


Ali:1970:TPO


Absar:1976:RHO


Aslangul:1974:LTS


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


Adamowicz:1978:CAP


Adawi:1979:PES


Andre:1976:FSG


Andre:1971:CLW


Abu-eittah:1978:MOS

Afzal:1973:FSG


Andre:1978:LRC


AAsbrink:1978:EST


Ahlrichs:1970:KBW


Ahlberg:1974:DCF


Ahlberg:1977:BRB

References


REFERENCES


[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,

**Ali:1977:COCa**


**Aldrich:1973:CBF**


**Andronikashvili:1979:CPB**


**Amos:1971:CSS**


**Amos:1972:CVP**

REFERENCES


REFERENCES

Anonymous:1970:Ma


Anonymous:1970:Mb


Anonymous:1970:Mc


Anonymous:1970:Md


Anonymous:1970:Me


Anonymous:1970:Mf


Anonymous:1970:M


Anonymous:1971:Aa

REFERENCES

Anonymous:1971:Ab

Anonymous:1971:Ma

Anonymous:1971:Mb

Anonymous:1971:Mc

Anonymous:1971:Md

Anonymous:1971:Me

Anonymous:1971:Mf

Anonymous:1971:M
Anonymous:1972:Aa


Anonymous:1972:Ab


Anonymous:1972:Ma


Anonymous:1972:Mb


Anonymous:1972:Mc


Anonymous:1972:Md


Anonymous:1972:Me


Anonymous:1972:M

Anonymous:1973:Aa


Anonymous:1973:Ab


Anonymous:1973:Ac


Anonymous:1973:Ma


Anonymous:1973:Mb


Anonymous:1973:Mc


Anonymous:1973:Md


Anonymous:1973:Me

Anonymous:1973:Mf

Anonymous:1973:M

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

Anonymous:1975:Mb


Anonymous:1975:Mc


Anonymous:1975:Md


Anonymous:1975:Me


Anonymous:1975:Mf


Anonymous:1975:Mg


Anonymous:1975:Mh

Anonymous:1976:Aa


Anonymous:1976:Ab


Anonymous:1976:Ac


Anonymous:1976:Ad


Anonymous:1976:DRD


Anonymous:1976:Ma


Anonymous:1976:Mb


Anonymous:1976:Mc

Anonymous:1976:Md

Anonymous:1976:Me

Anonymous:1976:Mf

Anonymous:1976:Mg

Anonymous:1976:Mh

Anonymous:1976:RSC

Anonymous:1977:Ab
Anonymous:1977:Af

Anonymous:1977:Ag

Anonymous:1977:Ak

Anonymous:1977:Aa

Anonymous:1977:Ac

Anonymous:1977:Ad

Anonymous:1977:Ae

Anonymous:1977:Ah
REFERENCES


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


REFERENCES


REFERENCES


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:Mnm

Anonymous:1979:Mn

Anonymous:1979:SES

Adams:1975:PTW

Adams:1977:AGM

Aronowitz:1978:ICN
Ali:1978:ROD


AAgren:1977:BSI


Anno:1975:SRS


Atkins:1974:QHC


Atkins:1991:QHC


Avery:1972:QTA


REFERENCES


REFERENCES

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


[B] Basilevsky:1972:IIR


[B] Bhattacharyya:1972:TCS


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


REFERENCES


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

[Blakemore:1977:NIS]

[Blakemore:1977:VIS]

[Benesch:1972:DRE]

[Berggren:1973:MNT]

[Bernstein:1975:BRR]
REFERENCES


REFERENCES


REFERENCES


REFERENCES


Blum:1975:SAE


Born:1975:HBS


Boyer:1975:SCR


Blum:1976:CIE


Beyer:1977:FSS


[Bak:1975:HBF]


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES

Boyle:1972:ESI


Boyle:1972:GTA


Boyle:1972:SPG


Boyd:1974:SSP


Boyd:1977:MSS


Bergmann:1970:QAH

REFERENCES


REFERENCES


REFERENCES


REFERENCES

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


### REFERENCES


<table>
<thead>
<tr>
<th>Reference</th>
<th>Title</th>
</tr>
</thead>
</table>
REFERENCES


Bartlett:1975:SAD


Bishop:1975:NIT


Born:1975:ICS


Bartlett:1976:CEL


Besson:1976:ASC


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


Butler:1976:CSAa


Butler:1976:CSAc


Buttt:1979:CEC


Bartlett:1977:TOM


Buchler:1976:CSD

Bazhin:1979:ESP


Bogach:1979:CCE


Cusachs:1972:IAO


Cusachs:1973:SAO


Carbo:1978:MBA


Cusachs:1975:LRT

REFERENCES


REFERENCES


Caldwell:1975:BRB


REFERENCES


[Carbo:1972:GRS]


[Carbo:1974:EMS]


[Cartling:1975:ULD]


[Castro:1978:IHS]


[Castro:1978:OSM]


[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


[CG79a] Sylvio Canuto and Osvaldo Goscinski. Continuum contribution to polarizabilities and scaling. *International Journal of

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

Collins:1973:ESA


Collins:1975:LEC


Chow:1973:UAS


Chen:1976:EAI


Chojnacki:1977:DPB


Coldwell:1978:MCC


**Claxton:1970:IUC**


**Claverie:1971:TIF**


**Clinton:1973:DMF**


**Czerminski:1979:TOO**


**Czerminski:1979:TPB**

REFERENCES


REFERENCES


Chao:1977:AMS

Coffey:1974:PEI

Coffey:1974:VOT

Coleman:1970:RRF

Coleman:1971:RRF

Coldwell:1977:ZMC
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


ČPH74

REFERENCES


the International Symposium on Quantum Biology and Quantum Pharmacology.


REFERENCES


REFERENCES


REFERENCES


REFERENCES

Collins:1971:SCR


Cullen:1975:AVP


Carsky:1979:ICA


Callaway:1970:TBC


Dolphin:1979:HPM

<table>
<thead>
<tr>
<th>REFERENCE</th>
<th>Title</th>
<th>Journal</th>
<th>Volume</th>
<th>Issue</th>
<th>Pages</th>
<th>Year</th>
<th>DOI</th>
</tr>
</thead>
</table>
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-

[Dutta:1971:DPM]


[Daudey:1972:PPC]


[Delhalle:1977:CED]


[Dugay:1977:AIM]


[Dutta:1970:MBA]

REFERENCES


REFERENCES

DELCONDE:1978:IGG


DUKE:1975:SIM


DELRE:1973:BPL


DELHALLE:1974:NPC


DESLAUX:1972:RTO

REFERENCES


REFERENCES


Doktorov:1975:CSA


Daudey:1974:PICb


Davies:1978:SAA


Dalton:1975:NME


Doolen:1978:CSA


Daudel:1979:SQG

REFERENCES


REFERENCES


REFERENCES

Deal:1973:LRD


Deal:1976:PTA


Julg:1976:ISD


Engelke:1974:EHP


Elbert:1974:ICU


Estrada:1979:EAG

REFERENCES


Edmiston:1973:DBA


Elder:1973:UMS


Ellzey:1973:SAM


Ellis:1977:MPR


Emanuel:1974:IUE


England:1971:CDE

REFERENCES


REFERENCES


[Erdahl:1978:SDC]


[Erdahl:1978:R]


[Ellis:1975:ADS]


[Euwema:1970:REA]


[Ellinger:1973:ANM]

REFERENCES


REFERENCES


REFERENCES


Fazzio:1979:PDC


Feuchtwang:1977:MBT


Ferreira:1979:SMT


Flament:1979:EMM


Figeys:1977:RII

Froelich:1977:NCT


Ford:1970:MMS


Fink:1973:PBB


Fratev:1970:WBP


Fraga:1976:HAD


Frischleder:1979:QCS

REFERENCES

203–213, August 1979. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Flannery:1979:AMC


Flurry:1972:SSM


Farberov:1972:TBM


Farantos:1978:CDC


Frishberg:1978:NDM


Findley:1979:GGC

March 4–10, 1979. CODEN IJQCB2. ISSN 0020-7608 (print),
1097-461X (electronic). Supplement: Proceedings of the Inter-
national Symposium on Quantum Biology and Quantum Phar-
macology.

tronically driven instabilities in metals. *International Journal of
Quantum Chemistry*, 9(S9):535–550, January 19–25, 1975. CO-
DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (elec-
tronic). Supplement: Proceedings of the International Sympo-
sium on Atomic, Molecular, and Solid-State Theory and Quan-
tum Statistics.

[FMZ70] P. F. Franchini, R. Moccia, and M. Zandomeneghi. Extended
group function calculations for H$_2$O, NH$_3$ and CH$_4$. *International Journal of Quantum Chemistry*, 4(5):487–501, Septem-
ber 1970. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (elec-
tronic).

energy bands on Hubbard parameters. *International Journal of
Quantum Chemistry*, 7(S7):619–627, January 21–27, 1973. CO-
DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).
Supplement: Proceedings of the International Symposium on
Atomic, Molecular and Solid-State Theory and Quantum Biol-
ogy.

[Fog71] Mario E. Foglio. Concentration dependence of the macroscopic
magnetic anisotropy and of the ferrimagnetic line width in
the gallium substituted europium iron garnet. *International Journal of Quantum Chemistry*, 5(S5):653–659, January 18–
23, 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-
461X (electronic). Supplement: Proceedings of the Interna-
tional Symposium on Atomic, Molecular and Solid-State The-
ory and Quantum Biology.

[Fox75] Sidney W. Fox. The matrix for the protobiological quantum:
Cosmic casino or shapes of molecules? *International Journal of
REFERENCES


**Firsht:1977:CMS**


**Fricke:1972:WCO**


**Fritsche:1974:BSC**


**FroeseFischer:1970:CIS**


**FroeseFischer:1974:MHF**

REFERENCES

FroeseFischer:1975:CSL

Fromhold:1979:DES

Frisman:1979:ISS

Fabian:1977:MLC

Fimple:1976:FDA

Fukui:1970:OST
Ken’ichi Fukui. *Orientation and stereoselection: Theory of orientation and stereoselection*, volume 1 of *Topics in current...


Fedyanin:1979:EMO

Gabbay:1976:RAS

Gallup:1972:EPM

Gallup:1972:VBC

Gallup:1974:SEW

Garton:1974:GGE
REFERENCES


REFERENCES


REFERENCES


REFERENCES


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

Green:1977:AYS


Grundke:1972:PDF


Guest:1972:LOC


Garrod:1978:IFD


Govil:1979:OPB


Gunnarsson:1977:MCU

REFERENCES

186


**Gunnarsson:1975:CBS**


**Geller:1979:ADA**


**Gubanov:1975:XRE**


**Green:1976:SOA**


**Gilardi:1978:FST**

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


Guerillot:1974:ECS


Gianturco:1979:EMS


Golebiewski:1973:MCG


Golebiewski:1973:MGF


Graovac:1975:CFT

REFERENCES


José Luis Gázquez, Elba Ortíz, and Jaime Keller. Electron gas model for inhomogeneous systems. International Journal

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


REFERENCES

194

tronic). Supplement: Proceedings of the International Symposi-

um on Quantum Biology and Quantum Pharmacology.


the International Symposium on Quantum Biology and Quantum Pharmacology.


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


REFERENCES


REFERENCES

Hanson:1979:ALE


Harcourt:1970:VSI


Harriman:1970:DMA


Harcourt:1971:IVF


Harriman:1971:DMA


Harrison:1971:CZF

REFERENCES


[Harc77a] R. D. Harcourt. Valence formulas for the Fe(II)O


REFERENCES

[Harriman:1979:GDM]

[Harris:1979:RON]

[Hatch:1975:SSS]

[Hannesson:1979:FNMI]

[Hadinger:1977:MET]

[Hehenberger:1978:WTS]
REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


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


[Holtje:1977] Hans-Dieter Hölte. Interaction energy calculations on interactions between pharmacon models and ionic receptor site mod-
REFERENCES


state Theory, Collision Phenomena, and Computational Methods.

Huang:1977:FSG

Heaton:1972:CIC

Hariharan:1979:NIM

Hofmann:1979:TCA

Hyslop:1976:ISE
[HR76] J. Hyslop and D. Rees. An interactive scheme for electronic systems using one-electron Green’s functions. *International Jour-


REFERENCES


Yasuyo Horino and Hiroshi Tatewaki. The electronic structure of the excited states for B, C+, and C arising from the config-

**Howat:1977:DSO**


**Howat:1977:GAM**


**Henkel:1974:LDN**


**Huber:1971:CDS**


**Hudson:1972:A**


**Hunter:1974:CPA**

REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES

Jette:1973:CME

Jucys:1972:GSU

Johnson:1974:MOS

Julg:1978:VNI

Jorgensen:1970:TDH

Jucys:1974:EHF
Josefson:1973:AMS

Johnson:1976:RAS

Julg:1976:HAM

Jankowski:1971:EEC

Julg:1978:DCD
REFERENCES

Jankowski:1979:EPC


Jucys:1972:GTE


Johnson:1970:GSW


Johnson:1973:RAS


Johansen:1975:ICE


Johnson:1977:SOE

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


References


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


REFERENCES

Julg:1978:CGM


Junker:1978:CCC


Johnson:1978:NTM


Johnson:1972:DES


Jafri:1976:III


Jones:1978:MFS


Jeziorek:1979:ICI

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

Jeziorek:1979:GAM


Kleindienst:1976:LFV


Kajjser:1977:DCP


Kang:1974:CES


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-


[Kau79b] Joyce J. Kaufman. Spin, symmetry, and orbital filling restrictions indicate the necessity for ab-initio configuration interac-
REFERENCES


**Klahn:1977:CLI**


**Kleindienst:1976:IEB**


**Koutecky:1972:DMH**


**Koutecky:1978:NSP**

REFERENCES


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


Kibler:1976:CGC


Kibler:1977:CGC

Kibler:1976:CGC


Kunz:1976:AHS

Kunz:1976:AHS


Klein:1977:VLSb

Klein:1977:VLSb


Kosevich:1979:ELM

Kosevich:1979:ELM


REFERENCES


REFERENCES


REFERENCES

Kuprievich:1970:FCI


Kaufman:1977:SCT


Karo:1973:RAM


Krizan:1973:IBM


Kamel:1975:DME


Kleier:1977:MOS

REFERENCES


Knirk:1977:MIP


Koutecky:1977:SQS


Kai:1978:CSM


Kwiatkowski:1979:MSM


Klasic:1978:APS


Kochanski:1974:DDT


Koelling:1974:ESR


Kolos:1974:LIR


Kolos:1975:LIR

Kothekar:1976:MOI


Kwiatkowski:1977:CHC


Kunert:1978:ISNb


Kaufman:1971:NAL


Kijewski:1971:NCC


Kaufman:1972:EIF

REFERENCES


REFERENCES


REFERENCES

\begin{itemize}


\end{itemize}


REFERENCES


REFERENCES


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


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


Laki:1975:AAN


Laki:1976:TYG


Lyslo:1971:TIS


Langhoff:1973:STF


Langhoff:1974:SIA


Langhoff:1977:AST

P. W. Langhoff. Applications of the Stieltjes–Tchebycheff procedure for atomic and molecular photoionization calculations in
REFERENCES


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


Letcher:1972:ULO


Layzer:1977:SMS


Lazzeretti:1978:USF


Lazzeretti:1979:GAN


Lindner:1973:NFE


Lyast:1973:ALE

Levy:1977:RBO


Larsson:1979:BDN


Les:1979:MCC


Lindholm:1978:IES


Linz:1977:EEC


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**

**[Lec76a]** Jean-Claude Leclerc. Comparative study of unconventional 1s basis functions for the $^1\Sigma$ ground state of H$_2$ and He. *International Journal of Quantum Chemistry*, 10(3):439–454, May 1976. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Leclerc:1976:HSG**

**[Lec76b]** Jean-Claude Leclerc. Hybrid Slater–Gaussian-type 1s orbitals for the $^1\Sigma$ ground state of H$_2$ and He. *International Journal of Quantum Chemistry*, 10(5):781–789, September 1976. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**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


REFERENCES


REFERENCES


REFERENCES

Lim:1977:RDA


Lim:1977:SGW


Lindner:1970:LBE


Lindgren:1971:SEA


Lindner:1973:BRB


Linderberg:1977:PCG

Lindgren:1978:CCA


Lipari:1972:FPE


Liu:1971:PCL


Liu:1971:MDR


Loew:1975:QCC

Loew:1978:BNC


Liedtke:1977:FPC


Likhtenstein:1979:SPE


Lowdin:1970:CLB


Labarre:1972:SEC

REFERENCES


Labzowsky:1973:CMS


Laskowski:1975:APH


Laki:1976:NET


Lindner:1972:ESS


Lo:1975:OOM


[Loc77d] R. Lochmann. Problems of the calculation of intermolecular interactions on complexes with strong delocalized π-bonds within


REFERENCES


REFERENCES

Lavery:1979:TMSa

Lavery:1978:MQC

Lombardi:1974:VTC

Linder:1977:ABL

Lipari:1977:EIV


REFERENCES


REFERENCES


REFERENCES


Lunell:1979:CUP


Laskowski:1971:POM


Laskowski:1971:TFO


Liu:1971:ESN


Laskowski:1972:TFO

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>Reference</th>
<th>Title</th>
<th>Journal</th>
<th>Volume</th>
<th>Issue</th>
<th>Pages</th>
<th>Month</th>
<th>Year</th>
<th>Supplement</th>
</tr>
</thead>
</table>
REFERENCES

Lyast:1978:APW


Lazzeretti:1977:CMS


Lazzeretti:1979:USF


Maggiora:1979:ARC


Maksic:1971:CJJ


Malrieu:1971:HOCa

REFERENCES


REFERENCES


REFERENCES


Matthias:1979:SSP

Mayer:1974:SPEa

Mayer:1974:SPEb

Mayer:1975:E

Mayer:1978:SPE

Mukherjee:1971:SCC


REFERENCES


REFERENCES


[Meh78] Ernest L. Mehler. Self-consistent, nonorthogonal group function approximation: Application to two interacting, rigid HF

[**Mehler:1979:ICP**]


[**Memory:1975:ESP**]


[**Memory:1977:SCR**]


[**Memory:1979:ESC**]


[**Menne:1971:PCH**]

REFERENCES


REFERENCES


REFERENCES

Michels:1970:MOS

Murphy:1974:MOS

Marron:1970:SHF

McIntosh:1976:LDS

McIntosh:1977:LDS
REFERENCES


REFERENCES

Miller:1971:ESA

Miller:1974:PMS

Mintmire:1979:LMX

Mitra:1972:EMH

Mayer:1975:SPEb


Mohraz:1976:COP


Meunier:1979:DCP


Millie:1972:AEC


Mayer:1973:SPE


Meunier:1976:PMC


Men:1975:SCS

Mukherjee:1970:MCS


Mcguire:1972:CCI


Moitra:1972:SCC


Matcha:1974:UTT


Mayer:1977:SM


Mueller:1977:PGS


Mortola:1974:AMS


Moitra:1970:SDQ


Matsen:1979:SFQ


Merrifield:1977:RRP


Moccia:1973:TDV


Moccia:1974:SDF

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

Moskalenko:1979:BCP


Markovsky:1979:QCI


Millie:1970:NTB


Matsen:1975:SFQa


Mishra:1972:VES


Majorino:1973:AMP

REFERENCES


Murty:1975:MCO


Messmer:1976:RAS


Mintmire:1976:IPS


Mathur:1977:TPT


Morrison:1973:PSM


Mukherjee:1970:SCC

REFERENCES

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


REFERENCES


REFERENCES


Nerbrant:1975:AMB


Nerbrant:1976:UPT


Nesbet:1970:EPC


Nesbet:1971:EPC


Nesbet:1975:AMR


Nesbet:1977:CEE


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


REFERENCES


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


Öhrn:1978:CCG


Öhrn:1979:CCG


Öhrn:1979:LOH


Oie:1976:ICL

REFERENCES


REFERENCES


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


Pokrant:1974:NTV


Pullman:1974:ECP


Pullman:1976:CLI


Pantelides:1978:GFS


**Politzer:1977:CAE**


**Piela:1978:EPE**


**Politzer:1978:SPE**


**Pullman:1979:MSA**


**Politzer:1979:RHB**

REFERENCES

(Politzer:1978:ENI)


(Peat:1974:ESO)


(Peat:1974:SAD)


(Pellegatti:1977:SES)


(Percus:1978:RMS)


(Petersson:1977:PCG)

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


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


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

**Plotnikov:1979:**


**Peng:1978:**


**Pack:1978:**


**Papaconstantopoulos:1971:**

REFERENCES


REFERENCES


REFERENCES

Poshusta:1977:TGL


Poshusta:1978:SPE


Poshusta:1979:SPI


Prohofsky:1971:SQM


Port:1974:QMS


Paine:1979:DTD

REFERENCES


REFERENCES


[i] Prigogine:1975:DSD


[PS73] Palting:1973:STU


[PS75a] Primas:1975:DFR


[PS75b] Pullman:1975:QMS

REFERENCES

Philippot:1979:OAN


Prasad:1979:PAG


Pople:1977:VCI


Petrongolo:1975:UEM


Pamuk:1978:SEC

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
<table>
<thead>
<tr>
<th><strong>REFERENCES</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>[Pullman:1978:NMR]</strong></td>
</tr>
<tr>
<td><strong>[Pullman:1979:RDM]</strong></td>
</tr>
<tr>
<td><strong>[Pullman:1979:MIA]</strong></td>
</tr>
<tr>
<td><strong>[Pullman:1979:R]</strong></td>
</tr>
<tr>
<td><strong>[Purcell:1975:QSA]</strong></td>
</tr>
<tr>
<td><strong>[Pulfer:1974:HIEb]</strong></td>
</tr>
<tr>
<td>J. D. Pulfer and M. A. Whitehead. The Hammerstein integral equation: a general technique for constructing a rapidly con-</td>
</tr>
</tbody>
</table>


REFERENCES


REFERENCES


Roustan:1979:RAS


Roothaan:1979:IMM


Robinson:1970:EBD


Redmon:1979:RRT


Rein:1970:REP


Reid:1972:IHL

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


REFERENCES


Renugopalakrishnan:1977:NMR


Rai:1977:BTT


Rohmer:1979:ESP


Riera:1972:GRC


Riera:1973:NSO


Redmon:1974:IPD

Michael J. Redmon and David A. Micha. Interaction potentials and dynamics for Li + F collisions. *International Journal
REFERENCES

Relyea: 1979: MTP


Ray: 1978: FSG


Robinson: 1971: IFW


Roby: 1971: TEC


Robin: 1972: ESR

Roby:1972:TEC


Røeggen:1973:APA


Roeggen:1975:RTP


Rosen:1974:RQT


Rosen:1975:UC


Rosen:1978:RSO

REFERENCES


REFERENCES


REFERENCES


REFERENCES


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


REFERENCES


REFERENCES

Schieve:1975:HTD


Smeyers:1978:HPH


Shillady:1979:DOG


Sutton:1970:MCM


Stoddart:1970:OBP

REFERENCES


Singhal:1979:PDA


Schaffer:1971:EOI


Schurr:1971:TDQa


Schurr:1971:TDQb


Schurr:1971:TDQc

Schurr:1971:TDQd


Scherr:1972:SNE


Schluter:1973:PCD


Schmidtke:1973:TOS


Schieve:1976:GEP


Schurr:1976:LAH

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

Scharfenberg:1977:NAS


Schmelzer:1977:ESH


Schönhammer:1977:THC


Scharfenberg:1978:SRT


Scofield:1971:ASE


REFERENCES


[Sarma:1979:SCS] C. R. Sarma and K. V. Dinesha. Subduction coefficients for $\langle 2^{N/2-S_1} \uparrow \rangle < 2^{N_1/2-S_1} 1^{2S_1} > \otimes < 2^{N_2/2-S_2} 1^{2S_2} >$ 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).


Yves G. Smeyers and L. Doreste-Suarez. Half-projected and Projected Hartree–Fock Calculations for Singlet Ground
REFERENCES


Shukla:1979:DIB


Selby:1975:VCS


Surratt:1973:HFL


Seybold:1976:WTF


Steinborn:1975:LTB

REFERENCES


REFERENCES

[Szent-Gyorgyi:1977:WR]

[Szent-Gyorgyi:1978:LS]

[Saunders:1973:LSM]

[Svendsen:1974:CMO]

[Sims:1975:CCH]

[Svendsen:1975:ERM]
REFERENCES


REFERENCES


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

Sinkkonen:1977:IBC


Shaw:1972:PSI


Stanley:1970:DRT


Suhai:1973:CME


Saute:1979:GSQ

REFERENCES


REFERENCES


*Srivastava:1979:ESS*


[Savin:1979:ESP]


*Selsby:1977:SEMa*


[Smith:1979:SV]


*Sheen:1973:PIP*

REFERENCES


REFERENCES


REFERENCES


Saute:1979:CPA


Sperber:1970:ECS


Sperber:1971:ARDa


Sperber:1971:ARDb


Sperber:1972:ARD


Sperber:1972:CDM


[Sperber:1973:AMb]

[Salmon:1972:QER]

[Salmons:1972:EFC]

[Steinborn:1972:MOE]

[So:1977:TSV]

[Slater:1978:CPH]
REFERENCES


REFERENCES

[S Singh:1970:CTP]

[S Singh:1971:PTH]

[S Stettler:1971:BSD]

[S Shibuya:1973:SFWa]

[S Shibuya:1973:SFWb]

[S Stigter:1973:ERM]
Dirk Stigter and John A. Schellman. Electrostatic representations of molecular groups. *International Journal of Quantum
Shinagawa:1974:HMS

Steslicka:1977:DLS

Steslicka:1977:LSS

Shinagawa:1978:MOS

Smith:1978:MCB
REFERENCES

the International Symposium on Quantum Biology and Quantum Pharmacology.


REFERENCES


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


REFERENCES


REFERENCES


REFERENCES


Thomson:1974:ISE


Trindle:1975:GTR


Tal:1978:SED


Tapia:1970:IMC

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


**REFERENCES**


REFERENCES


Thomson:1977:QMI


Thompson:1970:MSS


Trinajstic:1977:NDH


Thunemann:1977:SCI


Tantardini:1973:IVB

REFERENCES

401


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


Tantardini:1977:IVB


Tantardini:1978:IVB


Tantardini:1979:IVB


Trsic:1976:STE


Toyota:1976:IHF


REFERENCES


REFERENCES


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


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**
  
Weltin:1971:BES


Weltin:1975:DON


Weltin:1976:DME


Weller:1977:PCH


Weltin:1977:DME


Wendin:1979:CER

REFERENCES


**Westhaus:1973:CEC**


**Westhaus:1979:EHQ**


**Wepfer:1973:EMD**


**Wolf:1977:VME**

REFERENCES

Witschel:1974:OHM


Weintraub:1975:CSS


Wijkman:1978:IR


Williams:1974:MST


Wilson:1977:IHL


Wilson:1977:DPT

REFERENCES


REFERENCES


Weimann:1975:ESA


Wormer:1977:QTC


Wachters:1971:CFS


Weintraub:1978:CEC


Weislinger:1974:CQM


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

White:1970:CPT


Webb:1975:DVE


Wilson:1979:FOT


Weintraub:1976:CAP


Wormer:1974:TPM

REFERENCES


REFERENCES


Zielinski:1978:OGRb


Zeroka:1974:VPH


Zunger:1976:CFT


Zunger:1977:LDF


Zhorov:1979:RBS

REFERENCES


Zivkovic:1977:ERS


Zuvia:1978:CDA


Zielinski:1978:OGRa


Zielinski:1979:ISE


Zasukha:1979:TET