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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/

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+ [GL69]. **$15** [Sey69]. **$18.50** [Jør68a]. $1s$ [Koł67, WP67]. $1s2s$ [Brä68a]. $1s^2 2s^n 2p^m$ [SÖS68]. $1s\sigma 2p\sigma\ ^1\Sigma_u^+$ [Brä68c]. **$27** [Löw69a]. $2p$ [Koł67]. $2s$ [Koł67]. **$6.50** [Brä69b]. $^+$ [Ali69, DP67c, HJ69, Pie69, Sha69, SJP69b, VDP67]. $^-$ [JPD67a, PD67g, PD67e]. ^{1} [PL69]. ^{1,3} [AC69]. $^1\Sigma^+$ [BS68]. $^1\Sigma_u^+$ [MB69]. ^{2} [JKK68, LP69]. ^{3} [ES68, Soc69]. $^3\Sigma$ [Brä68a]. ^{N} [JKK68]. $_2$ [DP67b, DP67c, GMRS69, GL69, GH69, Har68, HM69, HC68, JS68, KT67, MB69, PD67g, PD67e, Rot67b, SS67a, SBD$^+$69]. $_{2v}$ [Sch68b]. $_3$ [GMRS69, PD67d, VDP67]. $_4$ [DP67b, HJ69, JDP67a]. $_5$ [JDP67b, PD67c]. $_6$ [DP67a, PD67d, Thu69]. $_7$ [PBWFN69]. $_9$ [PBWFN69]. $_{\infty h}$ [Sch68b]. β' [JC69]. $\cdot$ [Sha69]. d [CWS67]. f^2 [SM69]. f^3 [SM69]. $k \cdot p$ [PP67]. l^2 [Bow68]. $\leftrightarrow$ [GL69]. N [Sch68d]. π [FHK67, FK68, Sab68a, Sab68b, SB68b, SB69a, Son68a]. r [CR69b]. r_{12}

[CR69b]. $r_<$ [RHC$^+$68]. $r_>$ [RHC$^+$68]. s [Rot67a]. σ [PR67, Son68b]. Z [Lay67].

-atomic [Sch68d]. **-bonded** [PR67]. **-electron** [FHK67, FK68, Sab68a, Sab68b, SB68b, SB69a]. **-Electronic** [Son68a, Son68b]. **-expansion** [Lay67]. **-method** [Pre68]. **-Verfahren** [Pre68].

135 [Cal69]. **162** [Brä69b]. **1963** [Ano63, Löw63]. **1965** [Sey69]. **1s** [AC69].

2 [ES68, Soc69]. **2-Buten** [JP69]. **2-butene** [JP69]. **2-center** [New69]. **2-chloropurine** [SM67, Son68a]. **2-halopurines** [Son68b].

3d [AC69]. **3p** [AC69].

552 [Jør68a].

Absolutberechnung [SJP69a]. **Absolutrechnung** [Jan68, SJP69b]. **Absolutrechnungen** [DP67a, DP67b, DP67c, JDP67a, JPD67a, PD67c, PD67d, PD67f, PD67g, PD67e, VDP67]. **absorption** [Sad69]. **abstraction** [KHK67]. **accelerate** [Hak67b]. **accompagné** [Suc69]. **Accurate** [ABR69]. **acenic** [CDPR68]. **acetylene** [ČP67]. **acid** [RS67]. **acids** [Kup67]. **acridine** [II68]. **activated** [Hof69]. **activation** [PS67]. **active** [PO69]. **activity** [SCM67]. **adapted** [DDTM69, GS67, MK68]. **Address** [Seg69b]. **adiabatic** [Lev69]. **adiabatique** [Lev69]. **Al** [Con69]. **Algebra** [Kib69]. **Algebraic** [WMP69, KK69]. **All-electron** [MB68]. **all-valence-electrons** [Pul68]. **allene** [AALW69]. **aller** [FJP69, JP69]. **allowing** [HHR69]. **almost** [JRS69]. **alternant** [SGP68]. **alternative** [Sac67a]. **aluminum** [RH69]. **am** [JPD67b, JDP67b, JP69, SJP69b, SJP69a]. **America** [Sla67c]. **AMO** [Brä68c, Brä68a, Brä68b, LL67, SGP68, TP68]. **analogs** [Son68b]. **Analysis** [WL67, BB67, Bli67b, CPD68, ČPŠ69, Flo67]. **Analytic** [GD69, WB67b]. **analytical** [CR69b, SCRG67, WP67]. **angles** [RR69]. **anharmonic** [Rei67]. **anion** [JPD67a]. **anisotropic** [CP69]. **anisotropy** [SB69a]. **annotations** [Mul67]. **Announcement** [Ano68a, Ano68b, Ano69a, Ano69b, Ano69c, Dau68, Pul67]. **Announcements** [Ano68c]. **Announcments** [Ano69d]. **Anomalies** [Nie67]. **antiferromagnetic** [Pep69, Wil68, YA67a]. **antiferromagnetism** [JB69]. **antishielding** [Ste67]. **antisymmetrization** [PB67]. **AO** [WS69a]. **Appearance** [Ste69a]. **Application** [Ell68, GS68a, JKK68, SGP68, BMB67, BH67, Rei67, RCP68, Rot67b, Lec69]. **applications** [KA69, SCRG67, Sme69b]. **Applied** [Hal67, PP67, Cal69]. **Approach** [Tom69b, Ber69a, DIMD69, GS68b, KK69, LS67a]. **approximate** [Jug69, Lar68a, Mal69, PBO67, RS69, Wan69]. **Approximation** [LL68, BN67, Die68, JK69, KA69, Mal69, Mar68a, Mar68b, RCP68, Sei69,

WS69b, YM67]. **approximations** [CR69a, Cus67, MS69]. **Aromaten** [PD67a]. **aromatic** [Bas67, CS67, LT69, OB69, PD67a, SCM67]. **arranged** [Löw63]. **arrangements** [Lou68]. **aspect** [Lin67]. **aspects** [Cle69, Juc67b, Sch68a, SLM69]. **Assignment** [Thu69, Mul67]. **associations** [Sch68c, Sch68d]. **Asymptotic** [PD69, CP69]. **Äthylen** [DP67b, SJP69a]. **Äthylens** [FJP69]. **Atom** [Sch68b, BMB67, Blo69, LT69, PD67f, RD69, RW68, Soc69, WB67b]. **Atom-molecule** [Sch68b]. **atome** [BMB67, Lec69]. **Atomic** [Kel69, Löw63, MH68, Woo69, BM68, CTCM67, Del67, DP67a, DP67b, DP67c, HHR69, Hoo68, JDP67a, JPD67a, Juc67a, Juc67b, JN69, JRS69, JBG69, LD69, MH69, Mod68, MP68, PD67c, PD67d, PD67f, PD67g, PD67e, RD69, Sch68c, Sch68d, SK68, Ste67, SCRG67, VDP67, WS69b]. **atomic-orbital** [Del67]. **atoms** [ABR69, BN67, DMP67, DIMD69, Gás67, JDP68, JKK68, KSH68, KHK67, Kel67, Koł67, Lan69, Lay67, Nes67, SÖS68, WP67, PD67f]. **Atomsystemen** [DP67a, DP67b, DP67c, JDP67a, JPD67a, PD67c, PD67d, PD67f, PD67g, PD67e, VDP67]. **Author** [Brä69b, Cal69]. **AuZn** [JC69]. **averaged** [Shi68]. **axis** [GS67].

B [MB69, SBD$^+$69]. **Band** [YA67a, YA67b, CS68, Con68, Flo67, HKK67, HOV69, LH67, PE69, Rot67a, SEC69, Tom69a]. **bands** [Arl67, Bor68, Con67, JC69, Mar67, Sla67b, Tho67, Wil68]. **barrier** [HF67]. **barriers** [DFH69]. **base** [Kup67, SBL69]. **bases** [Del67, PALB69, RD69, RCP68, SBL69, WS69a]. **basicities** [Her68, VFC68]. **Basis** [Löw67b]. **be** [Els69, Seg69a, SBD$^+$69]. **Behandlung** [FJP69]. **behaviour** [Soc69]. **belonging** [DDTM69]. **bent** [Sch68b]. **Benzene** [Thu69, Man69, SB67, SB68a, SB68b, SB69a, SB69b, DP67a]. **benzenoid** [Hak67a]. **benzenoids** [PD67a]. **benzofuran** [Her68]. **Benzoider** [PD67a]. **Benzol** [DP67a, JPD67b, JPD67b]. **BeO** [SBD$^+$69]. **Berücksichtigung** [FJP69, JP69]. **beryllium** [BMB67, JDP68, Lec69]. **Berylliumatomen** [JDP68]. **Best** [BA69, RD69]. **best-atom** [RD69]. **beta** [Arl67]. **beta-brass** [Arl67]. **Between** [MW68, Sla67c, Ali69, DMP67, HR69, JDP68, Jør68b, Koł67, Lan69, PBWFN69, RCP68, Sch69a, Sch69b]. **beyond** [WBDG67]. **binding** [CS68, PD67f]. **Bindungsbeteiligung** [PD67f]. **binomial** [Hak67b]. **biological** [BGPP67, FHGR$^+$67, Frö68, Pul68]. **biology** [Bra69a, Els69, Pul69, Seg69a]. **Biorbital** [BMB67]. **biorbitales** [BMB67]. **biorbitals** [BEB69]. **biphenylene** [PDFA69]. **Bison** [WBKL69]. **BN** [SBD$^+$69]. **body** [DIMD69, Kel67, Kel69]. **Bond** [SS69, CR69a, JDP68, MP68, RCP68, Sha69, Shu69, TCH67, TK69]. **bonded** [Fis67, PR67]. **bonding** [GH69, Sab68a, Sab68b, Sch69a]. **bonds** [RS67]. **Book** [Brä69b, Cal69, Jør68a, Löw69a, Sey69]. **Books** [Ano68d, Ano68e, Ano68f]. **Born** [LS67a, MM67b, Sei69, Tay68]. **boron** [CD68, Dog69]. **Both** [Hir69b, Löw69a, Soc69]. **bound** [BR69, Joh68, Jos67a, RB69]. **boundary** [RW68]. **Boundedness** [Bow68].

Bounds [BF69b, Cus67, Gos69, LL68, Wil67, ABR69, BF69a, Bin68, BA69, Gor68, GS68b, Gos68, LL69, RW68, Sac67b, Wan69, Wei69a, Wei69b]. **brass** [Arl67]. **Brillouin** [CW67, LB68, LB69]. **broadening** [SW69]. **Brussels** [Sey69]. **Brute** [WL67]. **Buten** [JP69]. **butene** [JP69].

C [DP67a, DP67b, PD67c, PD67d, PD67f, Sch68b, SBD$^+$69, Thu69]. **C-Atoms** [PD67f]. **Calcul** [ČP67, BMB67]. **calculate** [Hak67a]. **calculated** [CC69, Kel69, MF67a, MF67b, MF67c, Mal67, MF67d, PALB69]. **Calculation** [LL69, RW68, ABR69, BMB67, Con67, DP67a, DP67b, DP67c, FB67, GLM67, JDP67a, JPD67a, Jan68, Juc67a, Juc67b, JKK68, JN69, KS69, LRBG69, MM67b, PD67c, PD67d, PD67f, PD67g, PD67e, RCP68, Sch68c, Shu69, SJP69b, SJP69a, VDP67, ČP67, SFH69, SBL69]. **Calculations** [Brä68c, GS68a, LS67b, MH68, PS68, Bak69, Brä68a, Brä68b, Cal67, Coo69, DFH69, Ell68, GS67, HOV69, Her68, HW69, HC68, JHHT67, KT67, Lay67, LD69, MM67a, MH69, MB68, New69, PR67, PK67, Pul68, RS69, Sha69, SEC69, SP68, VFC68, Woo69, KP69, SS67a]. **Can** [Els69, Seg69a]. **carbide** [HKK67]. **carbon** [RS69, SÖS68]. **carbonyl** [Sch69a]. **Carcinogenic** [SCM67, CS67]. **Casimir** [CP69]. **catalyzed** [SM67]. **cation** [VDP67]. **center** [Ber69a, JK69, KT67, Lau69, New69, SR67, Mar68b]. **centers** [Fan69]. **centre** [CJ67]. **cesium** [JC69]. **CH** [JDP67a, VDP67, HJ69]. **chain** [JB69]. **challenges** [Ber69b]. **change** [Suc69]. **changement** [Suc69]. **Character** [Ser68]. **Charge** [CC69, WL67, BP69, BFKP69, BBL67, Dog69, HW69, Jeh68, Jeh69b, New69, RH69, Ric68]. **charge-transfer** [Ric68]. **charges** [Lan69]. **chemical** [CKM69, HA67, MP68]. **chemically** [SW69]. **chemisorption** [TK69]. **Chemistry** [Cle67, Löw67c, Sey69, Els69, Hei67, Hel68, Kle69, Pea68, Pri67, RKS$^+$69, Seg69a, Brä69b]. **chloride** [JC69]. **chloropurine** [SM67, Son68a]. **Choice** [LL67, Del67, RD69]. **chromium** [YA67a]. **CI** [CPD68, Kup67]. **Circular** [MIR$^+$69, PO69]. **Clar** [PD67a]. **Clar'schen** [PD67a]. **Classification** [SK68]. **Clebsch** [Cal68a]. **ClO** [GH69]. **closed** [KS68, SK68]. **closed-shell** [KS68, SK68]. **Cluster** [ČPŠ69, SBŽ67]. **CM** [KP69]. **Co** [Cal69, AGL67b, GLM67, JS68, SBD$^+$69]. **coefficients** [Cal68a, Hak67b]. **coherence** [Frö68]. **cohesion** [Gir69]. **Collective** [Fis67]. **collision** [SB67]. **collisions** [Shi68]. **color** [Ber69a]. **combinations** [Les68, Les69]. **comme** [PL69]. **Comment** [Far69b]. **Comments** [Jeh69a, Löw68a, Gir69, Löw69c, Son68b, Sul69, Cle69]. **Compact** [CMR69]. **comparative** [Pul68, RS69]. **Comparison** [HM69, SEC69, RH69, DFH69]. **Compatibility** [Fan69]. **Complex** [Tom69a, CG68, Hof69, Joh68, Man69]. **complex-valued** [CG68]. **complexes** [FHGR$^+$67, II68, Ric68]. **components** [BB67, HFA67, Kup67]. **composed** [Suc69]. **composés** [Suc69]. **composite** [DC68a]. **Compounds** [Wil69, CD68, JC69, SP68]. **Computation** [Les68, Mar67, PH68]. **Computational** [WL67, PD67b]. **computer** [FB67, FRV68]. **computers** [Cle67]. **computing** [BBDP69]. **concerning** [Coo69]. **conclusions** [Coo69]. **condensed** [PD67a]. **condition** [CW67, Kau67, RW68]. **conditions** [Fan69]. **Conference** [Sey69].

Configuration [GS68a, GMRS69, MH68, PS68, BGPP67, BS68, CKM69, Ell68, GS67, HM67, HM69, KSH68, Lec69, MH69, SÖS68, Suc69, SBD+69]. **configuration-interaction** [HM67, HM69, KSH68]. **configurations** [JKK68, Lec69, Nes67, SM69, WBDG67]. **Conjugated** [Pul69, BEB69, Sch69b]. **Conservation** [CKM69]. **consideration** [Son68c]. **considerations** [Del67, Son69]. **considering** [FJP69]. **Consistency** [SBŽ67]. **Consistent** [PD67b, Con67, Die68, HW69, Mod68, New69, PBO67, Sla69, SEC69]. **constant** [ABR69, CJ67, I'H67, Jeh68, Jeh69b, Suc69]. **constante** [Suc69]. **Constants** [SC68, BB67, Gal68, Löw68b, MF67b, MF67c, Mal67, MF67d, SS67a, TPM69]. **constraints** [Arg67]. **construction** [GS67, Pre69b, Hur67, MK68]. **contact** [MF67c]. **contained** [Ser67]. **containing** [JK69, SF69]. **continued** [Rei67]. **contribution** [HF67, Man69]. **contributions** [Jør68b]. **Convergence** [PS68, Bin68, BA69, Cla69, Hak67b]. **Convergent** [Wel69, LC69]. **cooperate** [Seg69a]. **coordinate** [Emp69]. **Coordinates** [Hir69a, RHC+68]. **correlated** [Rot67b]. **correlating** [SBD+69]. **Correlation** [BS69, SR67, SÖS68, Sla67a, Tom69b, BD67, ČP67, JK69, Lin67, McW67, Mod68, Sch68b, WS69a, ČP67]. **correlations** [PFB67]. **Coulomb** [JHHT67]. **Coupling** [GÖ68, BB67, MF67b, SFH69, GÖJ+73]. **criterion** [Man68, SBŽ67]. **Crosswhite** [Jør68a]. **Crystal** [WB67a, Flo67, Joh68]. **crystal-band** [Flo67]. **crystals** [BBL67, DC68a, DD68, Fan69, KD68, Lev67, Sla69, CM67, Jør68a]. **cubic** [Blo69, Dog69, HKK67, Nes67, SEC69]. **Current** [Sla67d]. **currently** [Mul67]. **curves** [SS67a, Ste69a, Zuc68]. **cyanide** [Bak69]. **Cyclopentadienylanion** [PD67c, PD67c]. **Cyclopropan** [PD67d]. **Cyclopropane** [PD67d].

D [GL69, AC69, Sch68b]. **d'acétylène** [ČP67]. **damping** [Cra69]. **dans** [PL69]. **Darstellungen** [Pre69a]. **data** [Flo67, SJP69a]. **Daten** [SJP69a]. **defects** [CH67]. **definition** [Del67, RD69]. **Definitions** [KS68]. **deformations** [Jør68b]. **Degeneracy** [LG69, Jos67b, TP68]. **Degenerate** [Hir69b, Cra69, LH67]. **delocalized** [ČPŠ69]. **delta** [Cla69]. **delta-function** [Cla69]. **densities** [BFKP69, Tay68]. **Density** [Col67, FHK67, FK68, HW69, Kau67, KK69, Kle69, LL69, Mes67a, Mes67b, Pri67, RH69, SLM69, TCH67]. **dependence** [PS69]. **Dependent** [Löw67b, BL69]. **déplacement** [Suc69]. **d'équilibre** [Suc69]. **Derivation** [Cal68a]. **derivative** [PDFA69]. **derivatives** [CDPR68, Hak67a, Les68, MIR+69, Son68a]. **description** [BJ68, RKS+69, Lec69]. **Design** [WL67]. **determinant** [Gal68, KA69, Mes67b, PL69, PL69]. **determination** [Jos67a, MB69, Lec69, Emp69]. **determinations** [LC69]. **determining** [Lec69]. **deux** [PL69]. **development** [Jeh69c, Juc67b]. **developments** [Hof69, Koł68]. **Diagonal** [BH69]. **Diagonalize** [Hir69a]. **Diamagnetic** [MF67a, Sme69a, Sme69b]. **diamagnétiques** [Sme69a, Sme69b]. **diamond** [HKK67]. **diatomic** [HM67, SS69, SBD+69, WBDG67]. **Diazomethane**

[AALW69]. **dichroism** [MIR$^+$69, PO69]. **difference** [Jør68b]. **Differences** [MW68]. **Different** [MW68, BJ68, PALB69, Pul68]. **diffraction** [BFKP69]. **dimensional** [Les69]. **dimensions** [Emp69]. **dimer** [Sad69]. **Dimères** [Suc69]. **Dimers** [Suc69, LS67a]. **Diophantine** [Ell68]. **Dipole** [MM67b, CR69a, Del67, GLM67, Man69, SBL69, YM67]. **dipoles** [Blo69]. **Dirac** [DDTM69, GD69]. **direct** [PE69]. **directional** [Han67]. **discontinuous** [HHR69]. **discoveries** [Mat68]. **discussion** [Jeh69a]. **dispersion** [ABR69, Tho67]. **Dissociation** [YM67]. **distance** [JK69]. **distances** [KT67, Soc69]. **Distribution** [WL67, BBDP69, Dog69, FHK67, HFA67]. **distributions** [BP69, New69, Nie67]. **DNA** [HR69, II68, ML68, SBL69]. **d'onde** [PL69]. **donor** [PS69]. **dont** [Suc69]. **Double** [PFB67, Lan69]. **double-perturbation** [Lan69]. **doublet** [BMD69]. **d'un** [PL69, Suc69]. **d'une** [Lec69]. **duty** [Seg69a]. **dye** [Far69b]. **dynamic** [BBL67, Lev67]. **dynamics** [Fan69].

early [Hei67]. **Edited** [Jør68a, Löw69a]. **effect** [BGPP67, Har68, LT69, Mod68, SBL69]. **effective** [DD67]. **Effects** [CG68, BS69, Bra69a, CDPR68, CC69, Cra69, Lox69, SÖS68]. **Egil** [Löw63, Löw69a, MTW68]. **Eigenfunctions** [LP69, BF69b, Ger68, Les69]. **Eigenstates** [KÖ69]. **Eigenvalue** [Löw67b, WMP69, Bli67a]. **Eigenvalues** [Wil67, BF69a, LL69, RW68, Sac67b, Wei69a, Wei69b]. **Eindeutigkeit** [Pre69a]. **einem** [Jan68]. **elastic** [Jør68b]. **Electric** [MF67b, Blo69, Del67, GLM67, SBL69]. **Electron** [Gás69, KÖ69, SS67b, BF69b, BM68, BS69, BFR$^+$67, BN67, BD67, DC68b, FHK67, FK68, Fos69, Gás67, GS68b, HLL67, Hoo68, IK67, Jør68b, JK69, Koł68, Lay67, McW67, MB68, Mod68, PL69, Rot67b, Sab68a, Sab68b, SM69, SB67, SB68a, SB68b, SB69a, SB69b, SC68, Soc69, VFC68, WB67b, FHK67]. **electron-lattice** [SC68]. **Electron-phonon** [SS67b]. **Electronic** [AL69, KD68, ML68, Son68a, Son68b, Thu69, Wil69, BGPP67, BEB69, Cle69, CG68, CD68, Dog69, II68, Joh68, JC69, JKK68, MIR$^+$69, Sch68b, SB69b, SBL69, Son69, Suc69, PDFA69, Son68a, Son68b]. **électronique** [Suc69]. **electrons** [BBDP69, Die68, FJP69, JP69, JN69, JRS69, JBG69, Mul67, Pep69, PD67f, Pul68, SB67, PL69]. **electrophilic** [Her68]. **Electrostatic** [HF67, HR69]. **Elektronen** [Die68, PD67f, FJP69, JP69]. **elements** [CWS67, Das69, Löw69c, PD69, PP67, PH68, Shu69]. **embryos** [Jeh69c]. **empirical** [Hak67a]. **End** [Lox69]. **énergie** [BMB67, LP69]. **Energiehyperflachen** [Pre69a, Pre69b]. **energies** [Bak69, BD67, Hak67a, PS69, YM67]. **Energy** [Arl67, Bli67a, CS68, HKK67, Hir69a, Hir69b, Kib69, MW68, Sla67b, SG69, BP69, BMB67, Bor68, ČP67, Con67, Con68, Emp69, Frö68, HFA67, Han69, JC69, JHHT67, Jør68b, Lay67, LL69, ML68, Mar67, MP68, PE69, Pre69a, Pre69b, SS67a, Shi68, SEC69, SBŽ67, Tho67, Wil68, Col67, Gás67, Gás69, LP69]. **Energy-band** [CS68]. **enthalpies** [PS67]. **entraine** [Suc69]. **Equation** [Löw67b, Wil67, GD69].

equilibrium [Suc69]. **Equivalence** [CW67]. **Equivalent** [GÖ68, GÖJ+73, JRS69]. **Errata** [GÖJ+73, JH68]. **Error** [Gor68, Wan69]. **especially** [SM67]. **Estimation** [PS67]. **etat** [Lec69, BMB67, PL69]. **ethane** [HF67]. **ethylene** [FJP69, Sad69, SJP69a, DP67b]. **Etudes** [PL69, LP69]. **Eulerian** [RR69]. **europium** [LRBG69]. **Evaluation** [WL67, Hal69, LP69, PD69, LP69]. **Evidence** [BFR+67]. **exact** [Jos67a, PL69]. **exacte** [PL69]. **Exchange** [LG69, Pep69, GL69, HC68, MS69, RH69, SEC69]. **excitation** [Fis67, Suc69]. **Excited** [Con69, Ali69, Ber69a, BEB69, PALB69, Pie69, SÖS68, FK68]. **expanding** [Sac67a]. **Expansion** [CR69b, Les69, ČPŠ69, JK69, Lay67, SBŽ67]. **expansions** [CMR69, Gás69]. **Experimental** [RH69, Ber69b]. **experimentalist** [WBKL69]. **Exposé** [Lec69]. **Extended** [JN69, LS67b, BN67, Juc67a, JKK68, KSH68, LRBG69]. **extension** [Sac67b]. **external** [Arg67]. **Extracts** [Mul67]. **extracules** [Col67]. **extrapolations** [Cle69]. **Eyring** [Seg69b, Hof69].

F [Mar68b, Ber69a, HM69, SBD+69]. **F-color** [Ber69a]. **Factorization** [Gal68]. **factors** [BM68, Ste67]. **fast** [SB67]. **fcc** [Tho67]. **Fermi** [Fos69, Han69, Lou68, MF67c, Sla67b]. **ferroelectric** [SBŽ67]. **ferroelectrics** [Fis67]. **ferromagnetic** [Con67, Rot67a]. **ferromagnets** [IK67]. **few** [KS68, SK68]. **few-particle** [KS68, SK68]. **Feynman** [Coo69, Hur67]. **Field** [GÖ68, GÖJ+73, PD67b, Tom69b, BJ68, Blo69, Die68, KP69, MF67b, Mod68, OB69, PBO67, PK67, SBL69, Sla69, WB67a]. **fields** [Gás69]. **filled** [JRS69]. **finding** [Sac67b]. **fine** [Jeh68, Jeh69b]. **finite** [FB67]. **First** [Wil69, Hak67b, HOV69, KSH68, PALB69, WB67a, WB67b, Woo69]. **first-order** [Hak67b, WB67a, WB67b]. **first-principles** [HOV69]. **First-Row** [Wil69, KSH68]. **fitting** [Les68]. **flavin** [Son68c]. **flavins** [Son68c, Son69]. **floating** [FRV68, Hur67]. **Florida** [Löw63]. **fluids** [BBDP69]. **flux** [Jeh68, Jeh69b]. **FO** [GH69]. **Fock** [Ali69, Bak69, BN67, CW67, Ell68, Lar68b, LS67b, LP69, Mal69, MF67a, MF67b, MF67c, Mal67, MF67d, Mar68a, Mar68b, MS69, PL69, RH69, Sul69, WBDG67, YM67]. **Fock-like** [Lar68b]. **fonction** [PL69]. **Fonctions** [LP69]. **fondamental** [BMB67, Lec69, ČP67]. **forbidden** [DY67]. **Force** [WL67, Suc69]. **forces** [Arg67, FY68, Gos68, Lin67, Sch69b, Ste69a]. **form** [Mal69, WP67]. **Formal** [Hir69b, Sul69]. **formalism** [BMD69, Pri67, Sme69a]. **Formalisme** [Sme69a]. **forms** [PBWFN69]. **formula** [Tay68]. **formulae** [Hur67]. **formulation** [Hel68]. **FORTRAN** [SG67]. **Foundations** [Pea68, Brä69b]. **four** [BS68, Mod68]. **four-electron** [Mod68]. **Fourier** [Lau69]. **fractions** [Rei67]. **Free** [SB67, SB68a, SB68b, SB69a, SB69b, Hel68, Kle69, PS67, SBŽ67]. **Free-electron** [SB67, SB68a, SB68b, SB69a, SB69b]. **French** [LP69, AGL67a, AGL67b, BMB67, ČP67, Lec69, Lev69, PL69, Sme69a, Sme69b, Suc69]. **frequencies** [Bak69]. **Function** [Joh67, Bli67b, Cla69, Hal69, JK69, Lar68a, Lar68b, Mes67a, MB68, Soc69, WB67b, WS69b, YA67b]. **functional** [Pri67]. **Functions** [LL67, BD67, BBDP69, CW67, CG68, CR69b,

DDTM69, Far69a, GS67, Gir69, HHR69, Hur67, KP69, MF67a, MF67b, MF67c, Mal67, MF67d, MK68, MM67b, Mes67b, PB67, Rot67b, Sac67a, Shu69, SCRG67, TCH67, Wan69, WS69a, WS69b]. **furan** [Her68].

G [Cal69]. **gas** [Bas67, BD67, HLL67]. **gases** [Zuc68]. **Gaussian** [FRV68]. **Gaussians** [Les68, MB68]. **Gebiete** [PD67a]. **geminal** [LC69, PB67]. **geminals** [Lar68a, MK68]. **General** [RKS$^+$69, KD68, Pri67, Sme69a, Brä68b, Del67, Gos68, Jos67a, KK69, Sme69a]. **generalization** [CP69]. **Generalized** [LB68, LB69, God69, GS68b, RR69]. **geometry** [HJ69]. **German** [DP67a, DP67b, DP67c, Die68, FJP69, JDP67a, JPD67a, JPD67b, JDP67b, Jan68, JDP68, JP69, PD67a, PD67b, PD67c, PD67d, PD67f, PD67g, PD67e, Pre68, Pre69a, Pre69b, SJP69b, SJP69a, VDP67]. **germanium** [DD67, HKK67]. **Given** [GÖ68, GÖJ$^+$73, Jos67a]. **Gordan** [Cal68a]. **gradients** [MF67b]. **graphite** [AL69, Hak67a]. **Green** [Cal69, Bli67b, Hal69, Joh67, YA67b]. **Ground** [LS67b, YM67, BMB67, BEB69, ČP67, CD68, CMR69, Dog69, FHK67, Hoo68, Pie69, RHC$^+$68, RB69, SS67a]. **ground-state** [BMB67]. **Group** [LG69, Cal69, God69, Hal67, Kle69, Ser67]. **groups** [DDTM69, FB67, Mat67, Sch69a].

H [DP67a, DP67b, DP67c, GL69, JDP67b, Jør68a, PD67c, PD67d, PD67e, Thu69, Cla69, GMRS69, GL69, Har68, HC68, MB69, Rot67b]. **Hall** [Cal69]. **halogenated** [Son68a, Son68b]. **halopurines** [Son68b]. **Hamiltonian** [DD67]. **Hamiltonians** [MW68]. **Harald** [Löw69a]. **harmonic** [Les69]. **Hartree** [Ali69, Bak69, BN67, CW67, Ell68, Lar68b, LS67b, LP69, Mal69, MF67a, MF67b, MF67c, Mal67, MF67d, Mar68a, Mar68b, MS69, PL69, RH69, Sul69, WBDG67, YM67]. **having** [JKK68, JN69]. **HCO** [AGL67a]. **HD** [GL69]. **heavy** [LT69]. **HeH** [Pie69]. **HeHHe** [SJP69b, SJP69b]. **helical** [Lox69]. **Helium** [LS67b, RHC$^+$68, AC69, CMR69, ES68, RW68, SS68]. **Hellmann** [Coo69, Hur67]. **Helmholz** [JHHT67, LRBG69]. **HeNe** [SBD$^+$69]. **Henry** [Seg69b]. **heterocyclic** [KP69, SF69]. **heteronuclear** [CC69]. **high** [IK67]. **Hilbert** [Lar69]. **HMO** [PS67]. **Honor** [Löw63]. **Honorary** [Mul69]. **hot** [KHK67]. **hybridization** [Del67]. **hydrocarbon** [Jan68]. **hydrocarbons** [Bas67, CS67, Hak67a, LT69, OB69, PDFA69, SCM67]. **Hydrogen** [Brä68c, Sab68a, Sab68b, ABR69, Blo69, Brä68a, Brä68b, Fis67, JDP68, KHK67, Koł67, MM67a, RD69, RS67, RW68, Sch69a, Sha69]. **hydrogen-bonded** [Fis67]. **hydrogen-like** [RD69]. **hydroxyl** [JPD67a, Jan68, Sch69a]. **hydroxyl-unsaturated** [Jan68]. **Hydroxylanion** [JPD67a]. **hydroxylsubstituierten** [Jan68]. **Hylleraas** [Löw63, MTW68, Löw69a]. **hyperfine** [Mal67]. **hyperpolarizability** [SB68b]. **hypervirial** [BH67, BH69]. **hypothesis** [Tay68].

ice [KS69, SFH69]. **Ideas** [GS68a, Hof69]. **II** [DP67a, AGL67b, BGPP67, Brä68c, CC69, DP67a, FK68, Gás69, Hur67, Joh67, Kib69, Kle69, KP69, Mar68b, MP68, PR67, PL69, RHC+68, RD69, Sab68b, Sch68a, Sme69b, SK68, Son68a]. **III** [PD67d, Brä68a, CD68, PD67d, Son68b]. **imidazole** [VFC68]. **imidazoles** [VFC68]. **imino** [Son68c]. **importance** [FHGR+67]. **Improved** [Bin68, BR69]. **improving** [HOV69]. **impure** [Lev67]. **Impurity** [LH67, DC68b, Fan69, Fos69, Joh68, Mar68a, Mar68b]. **including** [JP69, Mod68]. **independence** [Ger68]. **independent** [Hoo68]. **indole** [Her68]. **induced** [SS69]. **Inductive** [VFC68]. **Inelastic** [Shi68, SB67]. **inert** [Zuc68]. **infinite** [JB69]. **Influence** [JHHT67, HA67]. **infrared** [Man69, MM67b]. **initio** [DFH69, DP67a, DP67b, DP67c, JDP67a, JPD67a, Jan68, PD67c, PD67d, PD67f, PD67g, PD67e, SJP69b, SJP69a, VDP67]. **inner** [HA67, PD67f]. **Inneren** [PD67f]. **instrument** [WBKL69]. **integral** [Coo69, Cus67, Hur67]. **Integrals** [WL67, HFA67, JK69]. **Integrated** [Hur67]. **integration** [Ell68]. **intensities** [MM67b]. **intensity** [DY67, Man69, Nie67]. **interacting** [Arg67, DIMD69, HLL67, SC68]. **Interaction** [GS68a, MH68, PS68, ABR69, BFR+67, BS68, Ell68, GS67, GMRS69, HR69, HM67, HM69, KSH68, Koł67, Lec69, MF67c, MH69, RCP68, Sch69a, Shi68, SS67b, SS69]. **interactions** [CR69a, DMP67, Fos69, Har68, Lan69, Lec69, Pie69, RCP68, SM69, SG69, You69]. **interatomic** [FY68, JHHT67, Ste69a]. **Interband** [PP67]. **interface** [DC68a]. **interhalogens** [PR67]. **intermetallic** [JC69]. **Intermolecular** [Zuc68, CR69a, Sch69b]. **internal** [Gás69, HF67]. **International** [Löw63]. **internuclear** [KT67]. **interparticle** [JK69]. **Interpolation** [DD68, PP67]. **Interpretation** [CDPR68]. **interpretative** [SLM69]. **Interscience** [Jør68a, Sey69]. **intracules** [Col67]. **intramolecular** [Jan68]. **intramolekularen** [Jan68]. **Introduction** [Löw63, Low69b, Mul69]. **invariant** [Jug69]. **investigation** [JPD67b, JDP67b, JDP68, MS69]. **investigations** [JP69]. **involving** [Lar68a]. **iodine** [Man69]. **ion** [RW68]. **ionic** [BBL67]. **ionization** [Hal69, JS68, PS69]. **ionized** [SS67a]. **ions** [CM67, Jør68a, JKK68, Kib69, Ste67]. **irreducible** [FB67]. **Island** [Löw63]. **isoelectronic** [Ali69, AC69, AALW69, SS68]. **isotropic** [Les69]. **iteration** [LC69]. **iterations** [Hak67b]. **iterative** [Wel69]. **Itinerant** [JB69, IK67]. **IV** [DP67b, Brä68b, DP67b, I'H67, OB69, SG67]. **IX** [PD67e, PD67e].

January [Ano63, Löw63]. **John** [Brä69b, Löw69a].

Kaufman [Man68]. **KCI** [Mar68b]. **KCl** [YA67b]. **Kepler** [CJ67]. **ketene** [AALW69]. **Kinetic** [Hir69a, BP69, Jør68b]. **kinetics** [Ber69b]. **Knut** [Löw69a]. **Kohlenwasserstoff** [Jan68]. **Kohn** [MS69]. **Kondensierten** [PD67a]. **konstruktion** [Pre69b]. **Kramers** [BMD69]. **Kronig** [GD69].

Laplace [Far69a]. **large** [HC68, Wel69]. **lasers** [Far69b]. **Later** [Hof69].

lattice [Lev69, SC68]. **LC** [DP67a, DP67b, DP67c, JDP67a, JPD67a, PD67c, PD67d, PD67f, PD67g, PD67e, VDP67]. **LCAO** [SF69, AGL67a, AGL67b, CPD68, Mar68a, Mar68b, MM67a, Sch69a]. **LCGO** [DP67a, DP67b, DP67c, JDP67a, JPD67a, PD67b, PD67c, PD67d, PD67f, PD67g, PD67e, Pre68, VDP67, PD67b]. **least** [Les68, LD69, New69]. **least-squares** [Les68, New69]. **l'énergie** [ČP67]. **length** [MM67b]. **l'état** [ČP67]. **L'Étude** [AGL67a, AGL67b]. **levels** [Kib69, Lay67]. **Li** [DP67c, PD67e, PE69, Sha69, SBD$^+$69]. **LiC** [JDP67b]. **LiF** [SBD$^+$69]. **lifetime** [Ber69a, SB68a]. **light** [PFB67, SW69]. **LiH** [PD67g, PD67g, BS68, Rot67b, Sha69]. **like** [Lar68b, RD69]. **line** [SW69]. **linear** [Bow68, Ger68, JB69, Les68, Les69, MP68, SFH69, Sch68b, YM67]. **Linearly** [Löw67b, BL69]. **lines** [Nie67, SS67b]. **liquid** [Har67, HBK69]. **Liquids** [Ste69b, PFB67]. **LISP** [Sch68c]. **lithium** [Bak69]. **lithiumcyclopentadienyl** [JDP67b]. **local** [Jør68b, Jos67b]. **localization** [PD67a]. **Localized** [CH67, Mar68a, Mar68b, Tom69a]. **Lokaler** [PD67a]. **London** [Brä69b, Cal69, Sey69, Lin67, RCP68]. **Long** [DMP67, Frö68, Koł67, Lan69, Pie69, Sch69b, CR69a, FY68, Ste69a]. **Long-range** [DMP67, Frö68, Koł67, Lan69, Pie69, FY68, Ste69a]. **Longmans** [Cal69]. **Lösung** [Die68]. **Lower** [BF69a, LL68, Wil67, ABR69, Bin68, BA69, GS68b, Gos68, LL69, RB69, RW68, Sac67b, Wei69a, Wei69b]. **Lowest** [Thu69, BS68, Wel69]. **Ltd** [Brä69b].

M [Jør68a]. **Madelung** [JHHT67]. **Magnetic** [IK67, Mal67, Con68, MF67d, Ser67, Sme69a, Sme69b, WB67a]. **magnétique** [Sme69a, Sme69b]. **Magneto** [I'H67]. **Magneto-optical** [I'H67]. **magnon** [BFR$^+$67]. **magnon-electron** [BFR$^+$67]. **Many** [DIMD69, Gás67, Gás69, Kel67, KÖ69, Rot67b, BM68, GS68b, Kel69, Lay67]. **Many-body** [DIMD69, Kel67, Kel69]. **Many-Electron** [Gás69, KÖ69, Gás67, Rot67b, BM68, GS68b, Lay67]. **Masthead** [Ano67a, Ano67b, Ano67c, Ano67d, Ano67e, Ano67f, Ano68m, Ano68g, Ano68h, Ano68i, Ano68j, Ano68k, Ano68l, Ano69e, Ano69f, Ano69g, Ano69h, Ano69i, Ano69j, Ano69k, Ano69l]. **matched** [CTCM67]. **matrices** [Col67, KK69, Kle69, LL69, SLM69, TCH67]. **matrix** [Kau67, Mes67a, PD69, PP67, PH68, RR69, Shu69]. **matter** [Col67]. **means** [Cal68a]. **measurement** [BFKP69]. **measurements** [BFR$^+$67]. **mechanical** [BF69a, DFH69, DP67a, DP67b, DP67c, FJP69, Gor68, JDP67a, JPD67a, JPD67b, JDP67b, Jan68, JDP68, JP69, PD67b, PD67c, PD67d, PD67f, PD67g, PD67e, SS67a, SJP69b, SJP69a, VDP67]. **Mechanics** [Löw63, KS68, SK68, Tay68]. **Mechanism** [CDPR68, CS68, SM67, Son68b]. **media** [HL69, SW69]. **melting** [Zuc68]. **mesoionic** [SP68]. **Metal** [Wil69, FHGR$^+$67, Nes67]. **metallic** [Con69, Gir69]. **metals** [Cal68b, Con68, Fos69, Tho67]. **Methan** [JDP67a]. **Methane** [JDP67a]. **Method** [LL67, WMP69, AGL67a, AGL67b, BMB67, DP67a, DP67b, DP67c, Die68, FHK67, FK68, God69, HOV69, JDP67a, JPD67a, Jos67a, Juc67a,

JKK68, JN69, Lec69, LP69, Löw68b, Mes67a, Mod68, PE69, PL69, PP67, PD67b, PD67c, PD67d, PD67f, PD67g, PD67e, Pre68, RW68, Sac67a, Sac67b, SR67, SGP68, TP68, VDP67, WBDG67, YA67b, Rot67b]. **Methode** [DP67a, DP67b, DP67c, JDP67a, JPD67a, PD67c, PD67d, PD67f, PD67g, PD67e, VDP67, AGL67a, AGL67b, Lec69, LP69, PL69, Die68, BMB67]. **Methods** [BBDP69, SBD$^+$69, WL67, CPD68, DD68, HM69, Juc67b, Mar67, PS67, SS68]. **methyl** [Jan68, MB68, Son69, VFC68, VDP67]. **methyl-** [Jan68]. **methyl-substituted** [VFC68]. **Methylkation** [VDP67]. **Midtdal** [Löw69a]. **Might** [Jør68b]. **minimal** [Lar69]. **minimum** [HHR69]. **Mirror** [JRS69]. **mixed** [KD68, Lar68a]. **mixing** [BGPP67]. **MnO** [Wil68]. **MO** [DP67a, DP67b, DP67c, JDP67a, JPD67a, PD67b, PD67c, PD67d, PD67f, PD67g, PD67e, Pre68, VDP67, Jug69, MM67a, SF69, Sch69a, WS69a]. **mobility** [KS69]. **Model** [Joh67, Tom69b, Bas67, Cla69, FRV68, Hoo68, Joh68, KS69, SFH69, SB67, SB68a, SB68b, SB69a, SB69b, VFC68]. **Models** [Eyr69]. **Mole** [RKS$^+$69]. **Molecular** [GH69, Her68, JK69, Löw63, Sla67d, SM67, SP68, TPM69, BP69, BF69b, Boy69, CC69, CKM69, Dav68, Fan69, FRV68, HFA67, HJ69, HW69, LS67a, Lev67, Lin67, Man68, New69, RS69, SS67a, Sch68b, Shi68, Ste69a, VFC68, WS69b]. **Molecular-orbital** [Her68, SM67, SP68, Dav68, HW69, VFC68]. **Molecule** [Brä68c, Ano67g, Brä68a, Brä68b, BS68, ČP67, CC69, I'H67, Kau67, Pie69, RS69, RW68, Sch68b, Sch68d, Sey69, ČP67]. **Molecules** [Joh67, Boy67, Cle69, CS67, DMP67, DP67a, DP67b, DP67c, GS67, HM67, HL69, I'H67, JS68, JDP67a, JPD67a, KP69, Koł68, MM67a, McW67, MB68, Mul67, Nie67, PD67b, PD67c, PD67d, PD67f, PD67g, PD67e, SG67, SS67a, SF69, Sch68a, Sch68b, Sme69a, Sme69b, Suc69, SBD$^+$69, VDP67, WBDG67, WP67, WS69a, YM67, Sme69b]. **Molekül** [PD67b]. **Molekülen** [DP67a, DP67b, DP67c, JDP67a, JPD67a, PD67c, PD67d, PD67f, PD67g, PD67e, VDP67]. **moment** [GLM67, Lou68, Man69, SBL69]. **moments** [Del67, SS68, YM67]. **momentum** [PP67]. **monopole** [RCP68]. **monopole-bond** [RCP68]. **monopoles** [CR69a]. **monoxide** [RS69]. **Moos** [Jør68a]. **moral** [Seg69a]. **morphogenetic** [Jeh69c]. **MOSES** [SG67]. **Motion** [Hir69a, CJ67, Gal68, Löw68b, SC68]. **motions** [CG68]. **Motivation** [Pri67]. **movements** [Jeh69c]. **Multicenter** [HFA67, WL67]. **multiconfigurational** [LB68, LB69]. **Multiple** [Joh67]. **multiplet** [Ali69].

N [JS68, PBWFN69, SS67a, SBD$^+$69]. **Näherung** [Die68]. **naphthalenes** [OB69]. **narrow** [Rot67a]. **natural** [CMR69, MK68]. **naturally** [PO69, Rot67b]. **Nature** [Löw67c, TK69, McW67, MP68]. **neutral** [Gás67]. **neutrons** [IK67]. **NiAl** [JC69]. **nickel** [Con67]. **nitride** [CD68, Dog69]. **nitriles** [MP68]. **nitrogen** [I'H67, SF69, SÖS68]. **nitrogen-containing** [SF69]. **nitrogens** [PBWFN69]. **No** [Brä69b, Cal69, Jør68a, JS68]. **Non** [Hir69b, BMD69, JBG69, SGP68, WS69a]. **non-alternant** [SGP68]. **Non-Degenerate** [Hir69b]. **non-Kramers** [BMD69]. **non-orthogonal**

[JBG69, WS69a]. **Nonadiabatic** [You69]. **normalized** [Hak67b]. **Norway** [Löw69a]. **Note** [Coo69, Geo68, Lau69, FY68, Man68, PS69]. **NTH** [Löw69a]. **nucléaire** [Suc69]. **Nuclear** [MF67d, BB67, CG68, Ser67, Soc69, Suc69]. **nuclei** [BBDP69]. **nucleic** [Kup67, RS67]. **nucleoside** [MIR+69]. **nucleotide** [PALB69, SBL69]. **number** [Jos67a, JN69, Lar69, Sch68d]. **numbers** [Mul67]. **Numerical** [CPD68, WL67, MF67a, MF67b, MF67c, Mal67, MF67d, PE69].

O [JS68]. **October** [Sey69]. **Off** [BH69]. **Off-Diagonal** [BH69]. **OH** [JPD67a]. **omega** [MM67a]. **one** [BF69b, GS67, Hal69, JK69, KT67, Koł68, SR67]. **one-** [Koł68]. **one-center** [KT67, SR67]. **one-electron** [BF69b]. **one-particle** [Hal69]. **Open** [HM67, KS68, SK68, Kup67, MB68, WS69a]. **Open-** [KS68, SK68]. **Open-shell** [HM67, Kup67, MB68]. **Opening** [Seg69b]. **operator** [BL69, Mal69]. **operators** [Bow68, Cal68a]. **Oppenheimer** [LS67a, MM67b, Sei69]. **Optical** [Lox69, DD67, I'H67, CM67, Jør68a]. **optically** [PO69]. **optimization** [Les68]. **optimized** [SBD+69, WBDG67]. **optimum** [GL69]. **OPW** [SEC69]. **orange** [II68]. **orbit** [SM69]. **orbital** [CMR69, CKM69, Dav68, Del67, FRV68, Her68, HW69, JN69, Lar69, MP68, New69, RD69, RS69, SM67, SP68, VFC68]. **orbital-bases** [RD69]. **orbitales** [Lec69]. **orbitals** [BJ68, CWS67, CTCM67, GL69, JBG69, Lec69, Les68, Les69, MK68, RD69, WP67]. **Order** [LL68, BG69, CP69, Hak67b, SLM69, WB67a, WB67b]. **ordered** [Arl67]. **organic** [Ano67g, Far69b, Sey69]. **orientation** [Shi68]. **orientation-averaged** [Shi68]. **orientational** [Har68, PFB67]. **orthogonal** [JBG69, RR69, WS69a]. **oscillator** [AC69, Les69, Rei67, RW68]. **oscillatory** [Hak67b]. **other** [SM69]. **Overlap** [CTCM67, BR69, Gos69, HW69, Man68, Wan69]. **Overlap-matched** [CTCM67]. **oxidase** [SM67, Son68b]. **oxidase-catalyzed** [SM67]. **oxidation** [SM67]. **oxygen** [CS67, SF69, SÖS68]. **oxygen-** [SF69].

P [Pre68, AC69, JKK68]. **pages** [Brä69b, Cal69, Jør68a]. **Pair** [BD67]. **Pair-correlation** [BD67]. **pairs** [Rot67b, SBL69]. **paperback** [Cal69]. **Papers** [MTW68, Löw69a]. **paramagnetic** [HL69, Kib69]. **parameter** [Les68, RS69]. **parameters** [KP69, Lar69, PK67]. **Parametrization** [RR69]. **Parseval** [Tay68]. **partially** [JRS69]. **Participants** [Ano63]. **particle** [Hal69, HLL67, Hoo68, KS68, Mes67a, Mes67b, SK68]. **Particles** [GÖ68, GÖJ+73, Arg67]. **Partitioning** [Wil67, HW69, Löw68b, MP68]. **PbTe** [PP67]. **Peacock** [Brä69b]. **Penney** [GD69]. **performance** [RS69]. **period** [Hei67]. **periodic** [AGL67a, AGL67b, BH67, Das69, Lou68, Löw69c]. **périodiques** [AGL67a, AGL67b]. **permanent** [SBL69]. **permutational** [KK69]. **Perturbation** [GS68a, Hir69b, LL68, Löw68a, AC69, Bin68, BA69, BG69, BN67, Cla69, CP69, Geo68, Gor68, GS68b, HC68, Kel67, Lan69, Löw68b, Rei67, SS68, RHC+68].

perturbations [Wel69]. **perturbed** [WB67b]. **phase** [Har67, JRS69, Ric68, WB67a]. **phenomena** [Boy67]. **Phenomenon** [LG69]. **Phenyl** [OB69]. **philosophy** [Seg69a]. **phonon** [DD68, Har68, SFH69, SS67b]. **phosphorescence** [HL69, LT69]. **phosphorescent** [OB69]. **photoexcited** [Ano67g, Sey69]. **photooxidation** [CDPR68]. **phthalocyanine** [MM67a]. **Phys** [Mul67]. **Physical** [MP68, HOV69]. **Physics** [Sla67c, Els69, Seg69a]. **pi** [Fis69]. **piezospectroscopic** [SS67b]. **plane** [ML68]. **plus** [Mul67]. **point** [Kle69, RH69]. **polarizabilities** [CR69a, CP69, Gos68]. **polarizability** [RB69, RCP68, SB69a, SBL69]. **Polarization** [Man69, Boy67, Boy69]. **polarized** [Bor68, Wil68]. **Polder** [CP69]. **Polished** [WL67]. **Polyatomic** [Joh67, HM67, MB68, Nie67, SG67]. **polymers** [Lox69]. **population** [Flo67, Man68]. **possibilities** [PK67]. **Potential** [WL67, CP69, GD69, Jos67a, MS69, SS67a, Ste69a]. **Potential-Charge** [WL67]. **potentials** [BH67, Hal69, RH69, SEC69, Zuc68]. **pour** [ČP67, Lec69]. **pouvoir** [Sme69a, Sme69b]. **power** [Sme69a, Sme69b]. **prediction** [HJ69]. **préliminaire** [BMB67]. **preliminary** [BMB67, JC69, PE69]. **present** [Cle69]. **President** [Mul69]. **Press** [Löw69a]. **pressure** [PS69]. **Price** [Brä69b, Cal69, Jør68a, Löw69a, Sey69]. **principal** [GS67]. **Principle** [MW68, DY67, HHR69]. **principles** [HOV69]. **probabilities** [JS68, Lay67]. **probability** [AC69, Tay68]. **probable** [Kau67]. **Problem** [Löw67b, LG69, WMP69, Ber69a, CJ67, Fis69, Jeh69c, Lin67, LL69, PE69, TP68]. **problems** [Gás67, Gás69, RS69, Sla67a]. **Procedure** [Die68, LD69, LC69]. **procedures** [Jug69]. **Proceedings** [Löw63, Sey69, Ano67g]. **product** [Sac67a]. **Professor** [Löw63]. **proflavine** [II68]. **Program** [Löw67a, FB67]. **programme** [Flo67]. **Programmierung** [PD67b]. **programming** [PD67b]. **programs** [FRV68]. **progress** [PBO67, WBDG67]. **Projected** [FHK67, FK68, Ger68, Mes67b, Sul69]. **Projection** [KÖ69, BL69, Cal68a, LP69, New69, PL69]. **projective** [LP69, PL69]. **Promoted** [RD69]. **promotion** [Del67]. **Proof** [Ger68]. **properly** [Ger68]. **Properties** [Löw68a, BGPP67, BG69, CC69, CM67, DD67, DIMD69, Jør68a, Kel69, MK68, MB69, Son68c, WS69a]. **propres** [LP69]. **proton** [PBWFN69, RS67, SFH69]. **proton-phonon** [SFH69]. **protonation** [FJP69]. **protonic** [KS69]. **Protonisierung** [FJP69]. **Published** [Brä69b, Cal69, Jør68a, Löw69a, Sey69]. **Publishers** [Jør68a, Sey69]. **purine** [RCP68]. **purines** [BGPP67, Pul68, PBWFN69, SM67, Son68a, Son68b]. **pyrazole** [VFC68]. **pyrazoles** [VFC68]. **Pyridine** [Sab68b, Sab68a]. **Pyridinium** [Sab68a]. **pyrimidine** [RCP68]. **pyrimidines** [BGPP67, Pul68, Son68a, Son68b]. **pyrrol** [Sab68b]. **pyrrole** [Her68].

Quadratically [LC69]. **Quadrupole** [Ste67, MF67b]. **quantique** [Sme69a, Sme69b]. **quantization** [Jeh68, Jeh69b]. **Quantum** [Bra69a, Hei67, Löw63, Löw67c, SS67a, Sla67c, BF69a, Brä69b, BD67, Col67,

Das69, DFH69, Gor68, Hel68, JN69, Kle69, KS68, Mul67, PFB67, Pea68, Pri67, RKS+69, SK68, Tay68, Sme69a, Sme69b]. **Quantum-mechanical** [SS67a, Gor68]. **quartet** [Ali69]. **quartic** [RW68]. **Quenching** [HL69].

radial [JBG69]. **radiation** [Cra69]. **radiative** [Ber69a]. **radicals** [MB68]. **Radikalreaktion** [Jan68]. **radius** [Bin68, BA69, Cla69]. **Range** [Emp69, CR69a, DMP67, Frö68, FY68, Koł67, Lan69, Pie69, Sch69b, Ste69a]. **rapid** [PH68]. **rates** [Jeh69a]. **Rational** [WS69b]. **ray** [BM68, BS69]. **Rayleigh** [Cla69, Hir69b, Sac67b, SW69]. **Rayleigh-line** [SW69]. **reacting** [SW69]. **reaction** [Ber69b, Emp69, GL69, Jan68, Son68b]. **reactions** [CKM69]. **Reactivity** [Ano67g, Sey69]. **real** [Kau67]. **realism** [HOV69]. **received** [Ano68d, Ano68e, Ano68f]. **Rechenzeitsparende** [PD67b]. **Reduced** [TCH67, Els69, KK69, Kle69, LL69, Seg69a, SLM69]. **Reflection** [PO69, JRS69]. **region** [Soc69]. **related** [Son68a, Son68b]. **relation** [Jeh69a]. **relations** [BH67, BH69, Gás67, JRS69]. **relationship** [Jeh68, Jeh69b]. **Relative** [Hir69a, Her68, PS67]. **Relaxation** [Ste69b, Emp69, Lev69]. **release** [VFC68]. **Remark** [WP67, Wei69a, Wei69b, Sei69]. **Remarks** [Jeh69c, Brä68b]. **Reminiscences** [Kim67]. **removal** [Lar68b]. **replication** [ML68]. **represent** [Jør68b]. **representability** [LL69]. **representation** [Pri67]. **representations** [FB67, Pre69a]. **represented** [Rot67b]. **representing** [Kau67]. **research** [Eyr69]. **réseau** [Lev69]. **resolved** [Far69b]. **resolvent** [Löw68b]. **resonance** [Cus67, Hak67a, Ser67]. **response** [Lev67]. **restricted** [Lar68b]. **restriction** [Lar68b]. **restrictions** [CW67]. **resulting** [PBWFN69]. **results** [Mat69, PE69, Suc69, SBD+69]. **Rev** [Mul67]. **Review** [Brä69b, Cal69, Jør68a, Löw69a, Sey69]. **rigid** [HL69]. **Ritz** [Sac67b]. **rotation** [I'H67, Lox69, MB69, Nie67]. **rotation-vibration** [Nie67]. **Rotational** [DFH69, HF67, SS69]. **rotational-vibrational** [SS69]. **rotatoire** [Sme69a, Sme69b]. **rotatory** [Sme69a, Sme69b]. **Row** [Wil69, CWS67, KSH68]. **RS** [Bin68, BA69]. **RS-perturbation** [Bin68, BA69]. **Ruedenberg** [Jør68b].

s [Cal69, JKK68, ES68, LP69, PL69, Soc69]. **same** [JN69]. **Sanibel** [Löw63, Ano63]. **satisfy** [Kau67]. **saving** [PD67b]. **Scaled** [Brä68c, Brä68a, Brä68b]. **scattered** [SW69]. **Scattering** [Joh67, Joh68, MH68, BM68, BS69, IK67, MH69, PFB67, Pep69]. **SCF** [AGL67b, DP67a, DP67b, DP67c, JDP67a, JPD67a, PD67b, PD67c, PD67d, PD67f, PD67g, PD67e, Pre68, VDP67, DP67a, DP67b, DP67c, God69, JDP67a, JPD67a, Jug69, KP69, Kup67, LB68, LB69, MB68, PALB69, PR67, PD67b, PD67c, PD67d, PD67f, PD67g, PD67e, SFH69, SF69, VDP67, Woo69]. **Scheme** [WL67]. **schemes** [PALB69]. **scholars** [Seg69a]. **Schrödinger** [Cla69, Hir69b, Jør68b, Ser68, Wil67]. **Schwingungsspektroskopischer** [SJP69a]. **Scientific** [MTW68, Löw69a]. **screening** [TPM69]. **Second** [LL68, BG69, CP69, CWS67, SLM69]. **Second-Order** [LL68, BG69, CP69, SLM69]. **second-row** [CWS67]. **Secular**

[Löw67b, Gal68]. **seine** [Pre68]. **Selected** [MTW68, Ger68, Löw69a]. **Self** [Die68, Mod68, New69, PD67b, Con67, HW69, PBO67, Sla69, SEC69]. **Self-consistent** [New69, Con67, Die68, HW69, PD67b, Sla69, SEC69]. **Self-Consistent-Field** [PD67b, Die68, Mod68, PBO67]. **semiconductor** [TK69]. **semiconductors** [CH67, LH67]. **Semiempirical** [Ber69a, FHGR$^+$67, VFC68, CPD68, Cus67, DFH69, PALB69, PK67, SF69]. **separability** [Fis69]. **separation** [CC69]. **separations** [HC68]. **sequence** [Ali69, AC69]. **series** [Cla69, Rei67, SS68, Woo69]. **set** [BL69]. **several** [Emp69]. **Sham** [MS69]. **sharp** [SS67b]. **shell** [HM67, Kup67, KS68, MB68, SK68, WS69a]. **shells** [HA67, JN69, JRS69, JBG69]. **shielding** [MF67d]. **shift** [Suc69]. **shifts** [PBWFN69, SS67b]. **should** [Kau67]. **sigma** [Fis69]. **silicon** [DD67, HKK67]. **Simple** [Hak67a, Fos69, MIR$^+$69, Sab68a, Sab68b]. **Simplified** [PR67]. **single** [HLL67, KA69, Mes67b]. **single-determinant** [KA69]. **single-particle** [HLL67]. **Singlet** [CS67]. **Slater** [Les68, Les69, MS69, Mes67b, PL69, RH69, RD69, Sac67a]. **Slater-type** [Les68, Les69]. **Slow** [Ste69b, Pep69]. **small** [KT67, Soc69]. **social** [Seg69a]. **sodium** [Bor68]. **Solid** [Cal67, Sla67d, Har67, Tom69a]. **Solid-State** [Sla67d, Cal67]. **Solids** [Tom69b, Lin67, Sla67a, SS67b]. **solution** [Die68, GD69, WB67b, Bra69a]. **solutions** [Wel69]. **Some** [Gir69, Juc67b, KA69, KT67, Löw68a, Löw69c, SS68, Sha69, Sul69, SCRG67, Cle69, MIR$^+$69, PS69, SF69, Son68b, SP68, SBD$^+$69]. **Sons** [Brä69b]. **space** [BL69, Bow68, Lar69]. **spanned** [BL69]. **Specification** [Lar69]. **spectra** [DD68, Far69b, II68, MIR$^+$69, Nie67, SB69b, Son68a, Son68b, Son69, SCM67]. **Spectral** [Bli67b, Son68c, SS67b]. **spectroscopic** [TPM69]. **spectroscopy** [Bli67a]. **spectrum** [HLL67, Man69, PDFA69, Sad69]. **spherical** [Boy67, FRV68]. **Spin** [Bor68, BMD69, Cal68b, Han67, KSH68, KÖ69, LL67, LG69, Rot67a, SM69, Tho67, Wil68, BB67, Ger68, God69, Hel68, Lar68a, Lev69, MK68, Mes67b, Sul69, TP68, Kle69]. **spin-** [MK68]. **Spin-1** [BMD69]. **Spin-extended** [KSH68]. **spin-free** [Hel68, Kle69]. **spin-lattice** [Lev69]. **spin-orbit** [SM69]. **Spin-other-orbit** [SM69]. **Spin-polarized** [Bor68, Wil68]. **spin-projected** [Mes67b]. **spin-réseau** [Lev69]. **spin-spin** [BB67]. **spins** [BJ68]. **splitting** [KP69, OB69, PK67]. **splittings** [WB67a]. **squares** [Les68, LD69, New69]. **Stability** [Lar68b, BP69, Man68, Rot67a]. **State** [Brä68c, LS67b, Sla67d, BMB67, Brä68a, Cal67, ČP67, CD68, CMR69, Dog69, ES68, FHK67, Har68, HBK69, Hoo68, MB69, PL69, RHC$^+$68, RB69, Rot67a, SB68a, Soc69, Wel69]. **States** [Hir69b, MW68, Ali69, BJ68, BEB69, BS68, Con69, Cra69, Dav68, DC68a, DC68b, FK68, Joh68, Jos67a, KD68, KS68, Mar68a, Mar68b, OB69, PALB69, Pie69, PS69, RHC$^+$68, RS67, SS67a, Sch68b, SÖS68, SK68, Ste67, Tom69a, WS69a, YM67]. **storage** [Frö68]. **strength** [Ali69, AC69]. **stretch** [SS69]. **Structure** [Bak69, Wil69, AL69, Cle69, CS68, Con68, CD68, FRV68, HKK67, HOV69, JPD67b, JDP67b, Jeh68, Jeh69b, LS67a, Mal67, MIR$^+$69, SBL69, Son68a, Son68b, Tom69a, WS69a, YA67a, YA67b]. **structures**

[Flo67, II68, JC69, Juc67a, Juc67b, Pep69, Son68a, Son68b]. **strukturuntersuchung** [JPD67b]. **strukturuntersuchungen** [JDP67b]. **Studies** [Löw68b, PS68, CPD68, FHGR+67, HM67, KSH68, Kup67, MP68, Sch69a, SM67, LP69, PL69]. **Study** [Cla69, Cle69, Wil69, AGL67a, AGL67b, AALW69, BGPP67, BS68, GMRS69, PDFA69, Pul68, BEB69]. **subgroups** [Ser67]. **substances** [PO69]. **substituent** [CDPR68]. **substituted** [VFC68]. **substitution** [HA67, Her68]. **sufficient** [BG69]. **Summary** [HC68]. **Super** [Löw67b, Hur67]. **super-floating** [Hur67]. **superconductivity** [Mat68]. **superconductors** [Mat67, Mat69]. **supergroups** [Ser68]. **Surface** [DC68a, Dav68, DC68b, Emp69, Pep69]. **surfaces** [Fos69, Lou68, Pre69a, Pre69b, Sla67b, Tom69a, TK69]. **susceptibilities** [MF67a]. **Sydney** [Brä69b, Sey69]. **Symmetric** [LG69, God69, Sch68a, Sch68b]. **Symmetry** [BB67, Cra69, DDTM69, GÖ68, Löw68a, MK68, Boy69, GS67, JRS69, KK69, Kle69, Lar68b, Ser67, GÖJ+73]. **symmetry-adapted** [GS67, MK68]. **Symposium** [Ano63, Löw63, Mul69, Seg69b]. **System** [DP67c, PD67g, PD67e, Arg67, BM68, Das69, Han69, Löw69c, PL69, RKS+69, SG67, SB68b, SC68, Sha69, Wel69]. **Systeme** [Die68, PL69]. **systèmes** [AGL67a, AGL67b]. **systems** [AGL67a, AGL67b, AALW69, BF69b, BF69a, BEB69, ČPŠ69, DP67a, DP67b, DP67c, Die68, FHK67, FK68, Frö68, GMRS69, HHR69, Hoo68, JDP67a, JPD67a, Mod68, PR67, PD67c, PD67d, PD67f, PD67g, PD67e, Pul69, Sab68a, Sab68b, Sch69b, SGP68, VDP67].

T [Brä69b]. **table** [Das69]. **tables** [Sch68b, Ser68]. **tails** [LH67]. **Tautomeric** [PBWFN69]. **tautomers** [Son68c]. **TCQ** [HR69]. **Technique** [Wil67, Löw68b, MM67a]. **Techniques** [WL67, BFKP69]. **temperatures** [IK67]. **tensors** [Boy69]. **tentative** [Cle69]. **terms** [CR69a, CR69b, RR69]. **tetraacetylacetonate** [LRBG69]. **tetrahedral** [CD68]. **Thalberg** [Löw69a]. **their** [BEB69, Hak67a, II68, Zuc68]. **theorem** [Arg67, Coo69, LB68, LB69]. **Theoretical** [Ali69, AALW69, BGPP67, KHK67, MB69, PDFA69, Son69, Tom69b, BJ68, CPD68, Son68c, AGL67a, AGL67b]. **Theorie** [PD67a, Sme69a, Sme69b, Lev69]. **theories** [Jug69, LB68, LB69]. **théorique** [AGL67a, AGL67b]. **theorist** [Ber69b]. **Theory** [BEB69, CR69a, GS68a, HBK69, Hir69b, Joh67, JBG69, LL68, Löw68a, Sla67d, AC69, Bin68, BA69, BG69, BN67, Col67, CP69, Dav68, DC68b, FY68, Gás67, Geo68, Gor68, GS68b, Gos68, Hal67, Han67, Jos67b, Kel67, Kel69, Koł68, Lev69, Löw68b, PD67a, PBO67, RS69, Sme69a, Sme69b, Sul69, Cal69]. **thermal** [KA69]. **Thirteenth** [Sey69]. **Thomas** [Han69]. **Three** [Mat67, Les69, Mod68]. **Three-** [Mod68]. **three-dimensional** [Les69]. **TiC** [CS68]. **time** [Far69b, PD67b]. **time-resolved** [Far69b]. **time-saving** [PD67b]. **Tomonaga** [Bas67]. **Topological** [Sch68a]. **Toronto** [Brä69b]. **total** [Sch68d]. **transfer** [Ric68]. **transform** [Far69a]. **Transformation** [Rei67, WS69a]. **transforms** [Lau69]. **Transition** [AC69, JS68, Nes67, Wil69, Con68, Har67, Jeh69a, Lay67, SS68, Woo69].

Transition-Metal [Wil69]. **Transitions** [Thu69, Ali69, BMD69, DY67, WB67a]. **transport** [BFR+67, SG69]. **treat** [BG69]. **Treatment** [Löw68a, FJP69, KHK67, Lan69, RHC+68, SS67a, SF69, Löw68b]. **triatomic** [Sch68b]. **triplet** [OB69, PALB69, SB68a]. **triplet-state** [SB68a]. **tritium** [KHK67]. **Trondheim** [Löw69a]. **Two** [DC68b, MW68, Mes67b, ABR69, BN67, CJ67, Hoo68, JDP68, JN69, JBG69, Koł68, Lau69, Mes67a, Pie69, PL69, RS67, Sac67a, Soc69, WB67b, JK69]. **two-center** [Lau69]. **two-centre** [CJ67]. **Two-electron** [DC68b, BN67, Hoo68, Koł68, PL69, Soc69, WB67b]. **Two-particle** [Mes67b, Mes67a]. **type** [BBL67, JC69, Les68, Les69].

UHF [KP69]. **uncoupled** [Mal69]. **ungepaarten** [Die68]. **ungesättigten** [Jan68]. **Uniqueness** [Tay68, Pre69a]. **University** [Löw63, Sey69]. **unpaired** [Die68]. **unsaturated** [Jan68]. **Unsöld** [LL68]. **Untersuchungen** [JDP68, JP69]. **Upper** [GS68b, Gos68, LL68, ABR69, RW68, Sac67b]. **Uppsala** [Cal67]. **use** [Hak67b, HHR69]. **using** [JBG69, KP69, Lar69, RHC+68, Sch68c]. **usual** [Geo68].

V [PD67f, CD68, FRV68, PD67f]. **Valence** [MH68, MH69, Han67, HM67, Pul68, Shu69, SBD+69, TCH67, WBDG67, MP68]. **valence-bond** [TCH67]. **valued** [CG68]. **vapor** [Ric68]. **Varianten** [Pre68]. **Variation** [MW68, WMP69, GS68b]. **variation-perturbation** [GS68b]. **Variational** [DY67, Mar67, RB69, ABR69, BR69]. **variations** [Pre68]. **various** [SEC69]. **velocity** [MM67b]. **Verdet** [I'H67]. **Verfahren** [PD67b, Pre68]. **Verfahrens** [Die68, PD67b]. **versa** [Els69]. **versus** [MM67b]. **VI** [JDP67a, JDP67a]. **via** [SS68]. **vibration** [MB69, Nie67]. **vibration-rotation** [MB69]. **Vibrational** [Ste69b, SJP69a, Bak69, RS67, SS69]. **Vibronic** [Sad69, LS67a]. **vibrotors** [SS69]. **vice** [Els69]. **view** [RH69]. **VII** [PD67g, MIR+69, PD67g]. **VIII** [DP67c, DP67c]. **vinyl** [MB68]. **virial** [Arg67]. **virtual** [Lec69]. **virtuelles** [Lec69]. **volumes** [Löw69a].

W [Jør68a]. **Waals** [Gos68, RCP68]. **Wannier** [Gir69]. **Wars** [Sla67c]. **Wasserstoffbrücke** [JDP68]. **wave** [CW67, CG68, Far69a, HHR69, KP69, Lar68a, Lar68b, MF67a, MF67b, MF67c, Mal67, MF67d, MM67b, MB68, PB67, PD67b, Rot67a, Rot67b, Sac67a, Soc69, SCRG67, Tho67, TCH67, Wan69, WB67b, WS69b, DP67a, DP67b, DP67c, FJP69, JDP67a, JPD67a, JPD67b, JDP67b, Jan68, JDP68, JP69, PD67c, PD67d, PD67f, PD67g, PD67e, SJP69b, SJP69a, VDP67]. **wave-mechanical** [PD67b, DP67a, DP67b, DP67c, FJP69, JDP67a, JPD67a, JPD67b, JDP67b, Jan68, JDP68, JP69, PD67c, PD67d, PD67f, PD67g, PD67e, SJP69b, SJP69a, VDP67]. **wavefunction** [PL69]. **waves** [Cal68b]. **ways** [Hak67a]. **weights** [Hak67b]. **well** [WS69a]. **Wellenmechanische** [DP67a, DP67b, DP67c, FJP69, JDP67a, JPD67a, JPD67b, JDP67b, Jan68,

JDP68, JP69, PD67c, PD67d, PD67f, PD67g, PD67e, SJP69b, SJP69a, VDP67]. **Wellenmechanischen** [PD67b]. **Wergeland** [Löw69a]. **where** [Soc69]. **Which** [Hir69a, Kau67]. **whose** [Suc69]. **Wiley** [Brä69b]. **within** [BMD69]. **WKB** [PD69]. **Wolfsberg** [JHHT67, LRBG69]. **work** [Dav68]. **written** [Mul67].

X [VDP67, BM68, BS69, VDP67]. **X-ray** [BM68, BS69]. **xanthine** [SM67, Son68b]. **XI** [JPD67a, Cle69, JPD67a]. **XIII** [Löw68b].

York [Brä69b, Jør68a, Sey69].

Zero [KP69, OB69, PK67]. **Zero-field** [KP69, OB69, PK67]. **zincblende** [BBL67]. **ZnS** [SEC69]. **ZnSe** [SEC69]. **zur** [Die68, PD67a, Pre69a, Pre69b]. **zwei** [JDP68]. **zwischen** [JDP68].

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