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## Title word cross-reference

+ [GL69]. **\$15** [Sey69]. **\$18.50** [Jør68a].  $1s$  [Kol67, WP67].  $1s2s$  [Brä68a].  
 $1s^22s^n2p^m$  [SÖS68].  $1s\sigma2p\sigma^1\Sigma_u^+$  [Brä68c]. **\$27** [Löw69a].  $2p$  [Kol67].  $2s$   
[Kol67]. **\$6.50** [Brä69b].  $^+$   
[Ali69, DP67c, HJ69, Pie69, Sha69, SJP69b, VDP67].  $^-$   
[JPD67a, PD67g, PD67e].  $^1$  [PL69].  $^{1,3}$  [AC69].  $^1\Sigma_u^+$  [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].  $\beta'$   
[JC69].  $\cdot$  [Sha69].  $d$  [CWS67].  $f^2$  [SM69].  $f^3$  [SM69].  $k \cdot p$  [PP67].  $l^2$  [Bow68].  
 $\leftrightarrow$  [GL69].  $^N$  [Sch68d].  $\pi$   
[FHK67, FK68, Sab68a, Sab68b, SB68b, SB69a, Son68a].  $r$  [CR69b].  $r_{12}$



[CR69b].  $r_{<}$  [RHC<sup>+</sup>68].  $r_{>}$  [RHC<sup>+</sup>68].  $s$  [Rot67a].  $\sigma$  [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]. **Announcements** [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, Kol67, 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<sup>+</sup>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<sup>+</sup>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<sup>+</sup>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, Kol67, Lan69, PBWFN69, RCP68, Sch69a, Sch69b]. **beyond** [WBDG67]. **binding** [CS68, PD67f]. **Bindungsbeteiligung** [PD67f]. **binomial** [Hak67b]. **biological** [BGPP67, FHGR<sup>+</sup>67, Frö68, Pul68]. **biology** [Bra69a, Els69, Pul69, Seg69a]. **Biorbital** [BMB67]. **biorbitales** [BMB67]. **biorbitals** [BEB69]. **biphenylene** [PDFA69]. **Bison** [WBKL69]. **BN** [SBD<sup>+</sup>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<sup>+</sup>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, Co69, 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** [HK67]. **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<sup>+</sup>69, Seg69a, Brä69b]. **chloride** [JC69]. **chloropurine** [SM67, Son68a]. **Choice** [LL67, Del67, RD69]. **chromium** [YA67a]. **CI** [CPD68, Kup67]. **Circular** [MIR<sup>+</sup>69, PO69]. **Clar** [PD67a]. **Clar'schen** [PD67a]. **Classification** [SK68]. **Clebsch** [Cal68a]. **CIO** [GH69]. **closed** [KS68, SK68]. **closed-shell** [KS68, SK68]. **Cluster** [ČPŠ69, SBŽ67]. **CM** [KP69]. **Co** [Cal69, AGL67b, GLM67, JS68, SBD<sup>+</sup>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<sup>+</sup>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<sup>+</sup>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].  
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**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].  
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**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<sup>+</sup>67, BN67, BD67, DC68b, FHK67, FK68, Fos69, Gás67, GS68b, HLL67, Hoo68, IK67, Jør68b, JK69, Kol68, 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<sup>+</sup>69, Sch68b, SB69b, SBL69, Son69, Suc69, PDFA69, Son68a, Son68b]. **électronique** [Suc69]. **electrons** [BBDB69, 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]. **Energiehyperflächen** [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]. **entraîne** [Suc69]. **Equation** [Löw67b, Wil67, GD69].



**equilibrium** [Suc69]. **Equivalence** [CW67]. **Equivalent** [GÖ68, GÖJ<sup>+</sup>73, JRS69]. **Errata** [GÖJ<sup>+</sup>73, JH68]. **Error** [Gor68, Wan69].  
**especialy** [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<sup>+</sup>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<sup>+</sup>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<sup>+</sup>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]. **FORTTRAN** [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]. **uran** [Her68].

**G** [Cal69]. **gas** [Bas67, BD67, HLL67]. **gases** [Zuc68]. **Gaussian** [FRV68]. **Gaussians** [Les68, MB68]. **Gebiete** [PD67a]. **geminal** [LC69, PB67]. **geminals** [Lar68a, MK68]. **General** [RKS<sup>+</sup>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<sup>+</sup>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<sup>+</sup>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<sup>+</sup>68, AC69, CMR69, ES68, RW68, SS68]. **Hellmann** [Coo69, Hur67]. **Helmholz** [JHHT67, LRBG69]. **HeNe** [SBD<sup>+</sup>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, Kol67, 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<sup>+</sup>68, RD69,  
 Sab68b, Sch68a, Sme69b, SK68, Son68a]. **III**  
 [PD67d, Brä68a, CD68, PD67d, Son68b]. **imidazole** [VFC68]. **imidazoles**  
 [VFC68]. **imino** [Son68c]. **importance** [FHGR<sup>+</sup>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<sup>+</sup>67, BS68, Ell68, GS67,  
 GMRS69, HR69, HM67, HM69, KSH68, Kol67, 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<sup>+</sup>69]. **LiC** [JDP67b]. **LiF** [SBD<sup>+</sup>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, Kol67, Lan69, Pie69, Sch69b, CR69a, FY68, Ste69a]. **Long-range** [DMP67, Frö68, Kol67, 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<sup>+</sup>67]. **magnon-electron** [BFR<sup>+</sup>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<sup>+</sup>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<sup>+</sup>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<sup>+</sup>69, WL67, CPD68, DD68, HM69, Juc67b, Mar67, PS67, SS68].

**methyl** [Jan68, MB68, Son69, VFC68, VDP67]. **methyl-** [Jan68].

**methyl-substituted** [VFC68]. **Methylation** [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<sup>+</sup>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, Kol68, MM67a, McW67, MB68,

Mul67, Nie67, PD67b, PD67c, PD67d, PD67f, PD67g, PD67e, SG67, SS67a,

SF69, Sch68a, Sch68b, Sme69a, Sme69b, Suc69, SBD<sup>+</sup>69, VDP67, WBDG67,

WP67, WS69a, YM67, Sme69b]. **Moleküle** [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<sup>+</sup>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<sup>+</sup>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, Kol68, SR67]. **one-** [Kol68]. **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<sup>+</sup>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<sup>+</sup>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<sup>+</sup>68].



**perturbations** [Wel69]. **perturbed** [WB67b]. **phase**  
 [Har67, JRS69, Ric68, WB67a]. **phenomena** [Boy67]. **Phenomenon** [LG69].  
**Phenyl** [OB69]. **philosophy** [Seg69a]. **phonon**  
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**prediction** [HJ69]. **préliminaire** [BMB67]. **preliminary**  
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**pressure** [PS69]. **Price** [Brä69b, Cal69, Jør68a, Löw69a, Sey69]. **principal**  
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**pyrimidine** [RCP68]. **pyrimidines** [BGPP67, Pul68, Son68a, Son68b].  
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[Flo67, II68, JC69, Juc67a, Juc67b, Pep69, Son68a, Son68b].  
**strukturuntersuchung** [JPD67b]. **strukturuntersuchungen** [JDP67b].  
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**two-center** [Lau69]. **two-centre** [CJ67]. **Two-electron**

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**valued** [CG68]. **vapor** [Ric68]. **Varianten** [Pre68]. **Variation**

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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].

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**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].

## References

**Andre:1969:TSI**

- [AALW69] J.-M. André, M. Cl. André, G. Leroy, and J. Weiler. Theoretical study of isoelectronic systems: Diazomethane, ketene and allene. *International Journal of Quantum Chemistry*, 3(6):1013–1025, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Adamov:1969:AVC**

- [ABR69] M. N. Adamov, M. D. Balmakov, and T. K. Rebane. Accurate variational calculation of upper and lower bounds of dispersion interaction constant of two hydrogen atoms. *International Journal of Quantum Chemistry*, 3(1):13–15, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Ali:1969:TPO**

- [AC69] M. Asgar Ali and Richard J. S. Crossley. Transition probability and oscillator strength by perturbation theory:  $1s\ 3p\ ^1P - 1s\ 3d\ ^1D$  transition in helium isoelectronic sequence. *International Journal of Quantum Chemistry*, 3(1):17–24, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Andre:1967:LTSa**

- [AGL67a] Jean-Marie André, Louis Gouverneur, and Et. Georges Leroy. L'Étude théorique des systèmes périodiques. I. La méthode LCAO HCO. (French) [Theoretical study of periodic systems. I. The



LCAO HCO method]. *International Journal of Quantum Chemistry*, 1(4):427–450, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Andre:1967:LTSb**

- [AGL67b] Jean-Marie André, Louis Gouverneur, and Et. Georges Leroy. L'Étude théorique des systèmes périodiques. II. La méthode LCAO SCF CO. (French) [Theoretical study of periodic systems. II. The LCAO SCF CO method]. *International Journal of Quantum Chemistry*, 1(4):451–461, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Andre:1969:ESG**

- [AL69] J.-M. André and G. Leroy. Electronic structure of graphite. *International Journal of Quantum Chemistry*, 3(6):983–999, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Ali:1969:THF**

- [Ali69] M. A. Ali. Theoretical Hartree–Fock multiplet strength for transitions between excited quartet states of  $\text{Ne}^+$  isoelectronic sequence. *International Journal of Quantum Chemistry*, 4(S3b):359–366, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Anonymous:1963:PSS**

- [Ano63] Anonymous. Participants in the Sanibel Symposium 14–19 January 1963. *Reviews of Modern Physics*, 35(3):416–420, July 1963. CODEN RMPHAT. ISSN 0034-6861 (print), 1538-4527 (electronic), 1539-0756. URL <http://link.aps.org/doi/10.1103/RevModPhys.35.416>; [http://rmp.aps.org/abstract/RMP/v35/i3/p416\\_1](http://rmp.aps.org/abstract/RMP/v35/i3/p416_1).

**Anonymous:1967:Ma**

- [Ano67a] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 1(1):fmi–fmii, January 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Anonymous:1967:Mb**

- [Ano67b] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 1(2):fmi–fmii, March 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1967:Mc**

- [Ano67c] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 1(3):fmi–fmii, May 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1967:Md**

- [Ano67d] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 1(4):fmi–fmii, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1967:Me**

- [Ano67e] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 1(5):fmi–fmii, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1967:Mf**

- [Ano67f] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 1(S1):fmi, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Anonymous:1967:RPO**

- [Ano67g] Anonymous, editor. *Reactivity of the photoexcited organic molecule; proceedings*. Interscience Publishers, New York, NY, USA, 1967. LCCN QD601.A1 C57 1965.

**Anonymous:1968:Aa**

- [Ano68a] Anonymous. Announcement. *International Journal of Quantum Chemistry*, 2(1):181, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1968:Ab**

- [Ano68b] Anonymous. Announcement. *International Journal of Quantum Chemistry*, 2(2):321, March 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Anonymous:1968:Ac**

- [Ano68c] Anonymous. Announcements. *International Journal of Quantum Chemistry*, 2(6):933, November 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1968:BRa**

- [Ano68d] Anonymous. Books received. *International Journal of Quantum Chemistry*, 2(2):323, March 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1968:BRb**

- [Ano68e] Anonymous. Books received. *International Journal of Quantum Chemistry*, 2(3):431, May 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1968:BRc**

- [Ano68f] Anonymous. Books received. *International Journal of Quantum Chemistry*, 2(5):739, September 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1968:Ma**

- [Ano68g] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 2(1):fmi, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1968:Mb**

- [Ano68h] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 2(2):fmi, March 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1968:Mc**

- [Ano68i] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 2(3):fmi, May 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1968:Md**

- [Ano68j] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 2(4):fmi, July 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Anonymous:1968:Me**

- [Ano68k] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 2(5):fmi, September 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1968:Mf**

- [Ano68l] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 2(6):fmi, November 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1968:M**

- [Ano68m] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 2(S2):fmi, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Anonymous:1969:Ab**

- [Ano69a] Anonymous. Announcement. *International Journal of Quantum Chemistry*, 3(4):535, July 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1969:Ac**

- [Ano69b] Anonymous. Announcement. *International Journal of Quantum Chemistry*, 3(5):749, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1969:Ad**

- [Ano69c] Anonymous. Announcement. *International Journal of Quantum Chemistry*, 3(5):750, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1969:Aa**

- [Ano69d] Anonymous. Announcements. *International Journal of Quantum Chemistry*, 3(1):145, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1969:Ma**

- [Ano69e] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 3(1):fmi–fmii, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Anonymous:1969:Mb**

- [Ano69f] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 3(2):fmi–fmii, March 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1969:Mc**

- [Ano69g] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 3(3):fmi–fmii, May 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1969:Md**

- [Ano69h] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 3(4):fmi–fmii, July 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1969:Me**

- [Ano69i] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 3(5):fmi–fmii, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1969:Mf**

- [Ano69j] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 3(6):fmi–fmii, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Anonymous:1969:Mg**

- [Ano69k] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 3(S3a):fmi, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Anonymous:1969:Mh**

- [Ano69l] Anonymous. Masthead. *International Journal of Quantum Chemistry*, 4(S3b):fmi, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Argyres:1967:VTS**

- [Arg67] Petros N. Argyres. The virial theorem for a system of interacting particles under external forces and constraints. *International*



*Journal of Quantum Chemistry*, 1(S1):669–675, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Arlinghaus:1967:EBO**

- [Arl67] Frank J. Arlinghaus. Energy bands in ordered beta-brass. *International Journal of Quantum Chemistry*, 1(S1):605–609, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Bingel:1969:BLB**

- [BA69] W. A. Bingel and R. Ahlrichs. Best lower bounds for the convergence radius of RS-perturbation theory. *International Journal of Quantum Chemistry*, 3(1):141–143, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Bak:1969:SVF**

- [Bak69] Børge Bak. Structure and vibrational frequencies of lithium cyanide from calculations of Hartree–Fock energies. *International Journal of Quantum Chemistry*, 4(S3b):527–528, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Basu:1967:TGM**

- [Bas67] Sadhan Basu. A Tomonaga gas model for aromatic hydrocarbons. *International Journal of Quantum Chemistry*, 1(2):187–190, March 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Barbier:1967:SCA**

- [BB67] Claudette Barbier and Gaston Berthier. Symmetry components analysis of nuclear spin-spin coupling constants. *International Journal of Quantum Chemistry*, 1(5):657–673, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Broyles:1969:MCD**

- [BBDP69] A. A. Broyles, A. A. Barker, Tucson Dunn, and M. A. Pokrant. Methods for computing distribution functions for electrons and nuclei in fluids. *International Journal of Quantum Chemistry*, 3 (S3a):293–305, January 13–18, 1969. CODEN IJQCB2. ISSN



0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Burstein:1967:DIC**

- [BBL67] E. Burstein, M. H. Brodsky, and G. Lucovsky. The dynamic ionic charge of zincblende type crystals. *International Journal of Quantum Chemistry*, 1(S1):759–765, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Broyles:1967:PCF**

- [BD67] A. A. Broyles and Tucson Dunn. Pair-correlation functions and correlation energies of a quantum electron gas. *International Journal of Quantum Chemistry*, 1(S1):803–809, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Bessis:1969:TBS**

- [BEB69] G. Bessis, P. Espagnet, and S. Bratož. Theory of biorbitals. Study of conjugated systems in their ground and excited electronic states. *International Journal of Quantum Chemistry*, 3(2):205–218, March 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Berezin:1969:SAP**

- [Ber69a] A. A. Berezin. Semiempirical approach to the problem of the radiative lifetime of the excited F-color center. *International Journal of Quantum Chemistry*, 3(4):485–487, July 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Bernstein:1969:NEC**

- [Ber69b] R. B. Bernstein. New experimental challenges for the theorist in reaction kinetics. *International Journal of Quantum Chemistry*, 3(S3a):41–45, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.



**Bazley:1969:LBE**

- [BF69a] Norman Bazley and David W. Fox. Lower bounds to eigenvalues of quantum mechanical systems. *International Journal of Quantum Chemistry*, 3(5):587–592, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Bazley:1969:BEO**

- [BF69b] Norman W. Bazley and David W. Fox. Bounds for eigenfunctions of one-electron molecular systems. *International Journal of Quantum Chemistry*, 3(5):581–586, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Bonham:1969:MCD**

- [BFKP69] R. A. Bonham, M. Fink, D. A. Kohl, and E. M. A. Peixoto. The measurement of charge densities by diffraction techniques. *International Journal of Quantum Chemistry*, 4(S3b):447–459, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Blatt:1967:EME**

- [BFR<sup>+</sup>67] F. J. Blatt, D. J. Flood, V. Rowe, P. A. Schroeder, and J. E. Cox. Evidence of magnon-electron interaction from transport measurements. *International Journal of Quantum Chemistry*, 1(S1):647, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Brandas:1969:SOP**

- [BG69] E. Brändas and O. Goscinski. Is second-order perturbation theory sufficient to treat second-order properties? *International Journal of Quantum Chemistry*, 4(S3b):383–390, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Berthod:1967:TSE**

- [BGPP67] Hélène Berthod, Claude Giessner-Prettre, and Alberte Pullman. Theoretical study of the electronic properties of biological purines and pyrimidines. II. The effect of configuration mixing. *International Journal of Quantum Chemistry*, 1(2):123–137, March 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Bradley:1967:KHR**

- [BH67] C. J. Bradley and D. E. Hughes. The application of hypervirial relations to periodic potentials. *International Journal of Quantum Chemistry*, 1(S1):687–701, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Bradley:1969:DHR**

- [BH69] C. J. Bradley and D. E. Hughes. Off-diagonal hypervirial relations. *International Journal of Quantum Chemistry*, 3(5):699–710, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Bingel:1968:ILB**

- [Bin68] W. A. Bingel. Improved lower bounds for the convergence radius of RS-perturbation theory. *International Journal of Quantum Chemistry*, 2(1):101–107, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Berggren:1968:FTD**

- [BJ68] K.-F. Berggren and B. Johansson. A field theoretical description of states with different orbitals for different spins. *International Journal of Quantum Chemistry*, 2(4):483–508, July 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Berrondo:1969:POS**

- [BL69] Manuel Berrondo and Per-Olov Löwdin. The projection operator for a space spanned by a linearly dependent set. *International Journal of Quantum Chemistry*, 3(6):767–780, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Blinder:1967:EES**

- [Bli67a] S. M. Blinder. Energy eigenvalue spectroscopy. *International Journal of Quantum Chemistry*, 1(3):271–283, May 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Blinder:1967:SAG**

- [Bli67b] S. M. Blinder. Spectral analysis of the Green’s function. *International Journal of Quantum Chemistry*, 1(3):285–291, May 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Blokker:1969:HAC**

- [Blo69] Esko Blokker. The hydrogen atom in a cubic field of electric dipoles. *International Journal of Quantum Chemistry*, 3(5):663–681, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Benesch:1968:XRE**

- [BM68] Robert Benesch and Gulzari Malli. X-ray and electron scattering factors for many-electron atomic system. *International Journal of Quantum Chemistry*, 2(3):371–389, May 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Bessis:1967:MBA**

- [BMB67] G. Bessis, C. Murez, and S. Bratož. Méthode des biorbitales: application préliminaire au calcul de l'énergie de l'état fondamental de l'atome de beryllium. (French) [Biorbital method: preliminary application to the calculation of the ground-state energy of the beryllium atom]. *International Journal of Quantum Chemistry*, 1(4):327–335, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Bowden:1969:SFT**

- [BMD69] C. M. Bowden, H. C. Meyer, and P. L. Donoho. Spin-1 formalism for transitions within a non-Kramers doublet. *International Journal of Quantum Chemistry*, 4(S3b):617–624, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Brown:1967:PTE**

- [BN67] W. Byers Brown and G. V. Nazarov. The perturbation theory of the extended Hartree–Fock approximation for two-electron atoms. *International Journal of Quantum Chemistry*, 1(4):463–491, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Boring:1968:SPE**

- [Bor68] A. M. Boring. Spin-polarized energy bands in sodium. *International Journal of Quantum Chemistry*, 2(S2):265–268, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International



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

**Bowden:1968:BLO**

- [Bow68] Charles M. Bowden. Boundedness of linear operators in the space  $l^2$ . *International Journal of Quantum Chemistry*, 2(S2):363–371, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Boyle:1967:PPS**

- [Boy67] L. L. Boyle. The polarization phenomena of spherical molecules. *International Journal of Quantum Chemistry*, 1(5):595–604, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Boyle:1969:SMP**

- [Boy69] L. L. Boyle. The symmetry of molecular polarization tensors. *International Journal of Quantum Chemistry*, 3(2):231–243, March 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Bader:1969:KEM**

- [BP69] R. F. W. Bader and H. J. T. Preston. The kinetic energy of molecular charge distributions and molecular stability. *International Journal of Quantum Chemistry*, 3(3):327–347, May 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Braun:1969:IVB**

- [BR69] P. A. Braun and T. K. Rebane. Improved variational bound for the overlap. *International Journal of Quantum Chemistry*, 3(6):1058–1061, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Brandas:1968:SACb**

- [Brä68a] Erkki Brändas. Scaled AMO calculations on the hydrogen molecule. III. The  $1s2s\ ^3\Sigma$  state. *International Journal of Quantum Chemistry*, 2(3):391–396, May 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Brandas:1968:SACc**

- [Brä68b] Erkki Brändas. Scaled AMO calculations on the hydrogen molecule IV. General remarks. *International Journal of Quantum Chemistry*, 2(6):793–799, November 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Brandas:1968:SACa**

- [Brä68c] Erkki J. Brändas. Scaled AMO calculations on the hydrogen molecule. II. the  $1s\sigma 2p\sigma^1\Sigma_u^+$  state. *International Journal of Quantum Chemistry*, 2(1):37–47, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Bradley:1969:QBS**

- [Bra69a] D. F. Bradley. Quantum biology: Solution effects. *International Journal of Quantum Chemistry*, 3(S3a):169–178, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Brandas:1969:BRB**

- [Brä69b] Erkki Brändas. Book review: *Foundations of quantum chemistry*. Author: T. E. Peacock. Published by: John Wiley & Sons Ltd., London, New York, Sydney, Toronto, 1968. Price: \$6.50. No. of pages: 162. *International Journal of Quantum Chemistry*, 3(6):1069–1070, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Pea68].

**Brown:1968:CIS**

- [BS68] Richard E. Brown and Harrison Shull. A configuration interaction study of the four lowest  $^1\Sigma^+$  states of the LiH molecule. *International Journal of Quantum Chemistry*, 2(5):663–685, September 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Benesch:1969:CEX**

- [BS69] Robert Benesch and Vedene H. Smith, Jr. Correlation effects in X-ray and electron scattering. *International Journal of Quantum Chemistry*, 4(S3b):413–421, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.



**Calais:1967:SSC**

- [Cal67] Jean-Louis Calais. Solid-state calculations in Uppsala. *International Journal of Quantum Chemistry*, 1(S1):661–668, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Calais:1968:DCG**

- [Cal68a] Jean-Louis Calais. Derivation of the Clebsch–Gordan coefficients by means of projection operators. *International Journal of Quantum Chemistry*, 2(5):715–727, September 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Callaway:1968:SWM**

- [Cal68b] Joseph Callaway. Spin waves in metals. *International Journal of Quantum Chemistry*, 2(S2):277–283, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Calais:1969:BRB**

- [Cal69] Jean-Louis Calais. Book review: *Applied group theory*. Author: G. G. Hall. Published by: Longmans, Green and Co, London, 1967. Price: 25 s. (paperback). No. of pages: 135. *International Journal of Quantum Chemistry*, 3(2):246–247, March 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Hal67].

**Corrington:1969:CSH**

- [CC69] Joyce H. Corrington and Louis Chopin Cusachs. Charge separation in a heteronuclear molecule: II, effects on calculated molecular properties. *International Journal of Quantum Chemistry*, 3(S3a):207–222, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Coulson:1968:EST**

- [CD68] C. A. Coulson and G. Doggett. The electronic structure of tetrahedral III–V compounds: The ground state of boron nitride. *International Journal of Quantum Chemistry*, 2(6):825–843, November



1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Chalvet:1968:MPI**

- [CDPR68] O. Chalvet, R. Daudel, C. Ponce, and J. Rigaudy. Mechanism of photooxidation: Interpretation of the substituent effects in the photooxidation of acenic derivatives. *International Journal of Quantum Chemistry*, 2(4):521–530, July 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Coulson:1968:ECV**

- [CG68] C. A. Coulson and R. B. Gerber. Effects of complex-valued electronic wave functions on nuclear motions. *International Journal of Quantum Chemistry*, 2(5):607–640, September 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Callaway:1967:LDS**

- [CH67] Joseph Callaway and A. James Hughes. Localized defects in semiconductors. *International Journal of Quantum Chemistry*, 1(S1):769–771, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Coulson:1967:CMT**

- [CJ67] C. A. Coulson and A. Joseph. A constant of the motion for the two-centre Kepler problem. *International Journal of Quantum Chemistry*, 1(4):337–347, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Cusachs:1969:CMO**

- [CKM69] L. C. Cusachs, M. Krieger, and C. W. Mccurdy. Conservation of molecular orbital configuration in chemical reactions. *International Journal of Quantum Chemistry*, 3(S3a):67–74, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Claverie:1969:SCR**

- [Cla69] Pierre Claverie. Study of the convergence radius of the Rayleigh–Schrödinger perturbation series for the delta-function model of H. *International Journal of Quantum Chemistry*, 3(3):349–370,



May 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Clementi:1967:CC**

- [Cle67] Enrico Clementi. Chemistry and computers. *International Journal of Quantum Chemistry*, 1(S1):307–312, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Clementi:1969:SES**

- [Cle69] E. Clementi. Study of the electronic structure of molecules. XI. Comments on some present aspects and tentative extrapolations. *International Journal of Quantum Chemistry*, 3(S3a):179–205, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Crosswhite:1967:OPI**

- [CM67] H. M. (Henry Milton) Crosswhite and H. Warren (Henry Warren) Moos, editors. *Optical properties of ions in crystals*. Interscience Publishers, New York, NY, USA, 1967. LCCN QD941 .C65 1966aa.

**Cressy:1969:CNO**

- [CMR69] Norman Cressy, K. R. Miller, and Klaus Ruedenberg. Compact natural orbital expansions for the helium ground state. *International Journal of Quantum Chemistry*, 3(1):107–113, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Coleman:1967:DMQ**

- [Col67] A. J. Coleman. Density matrices in the quantum theory of matter: Energy, intracules and extracules. *International Journal of Quantum Chemistry*, 1(S1):457–464, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Connolly:1967:SCC**

- [Con67] John W. D. Connolly. A self-consistent calculation of the energy bands in ferromagnetic nickel. *International Journal of Quantum Chemistry*, 1(S1):615–618, January 16–21, 1967. CODEN



IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Connolly:1968:EBS**

- [Con68] John W. D. Connolly. The energy band structure of magnetic transition metals. *International Journal of Quantum Chemistry*, 2 (S2):257–263, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Connolly:1969:ESM**

- [Con69] John W. D. Connolly. Excited states in metallic Al. *International Journal of Quantum Chemistry*, 4(S3b):807–812, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Cooney:1969:NCC**

- [Coo69] William A. Cooney. Note concerning conclusions from integral Hellmann–Feynman theorem calculations. *International Journal of Quantum Chemistry*, 4(S3b):381–382, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Cizek:1967:CLC**

- [ČP67] Jíří Čížek and Alain Pellégatti. Calcul de l'énergie de corrélation pour l'état fondamental de la molécule d'acétylène. (French) [Calculation of the correlation energy for the ground state of the acetylene molecule]. *International Journal of Quantum Chemistry*, 1 (5):653–655, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Craig:1969:ACP**

- [CP69] D. P. Craig and E. A. Power. The asymptotic Casimir–Polder potential from second-order perturbation theory and its generalization for anisotropic polarizabilities. *International Journal of Quantum Chemistry*, 3(6):903–911, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Carpentieri:1968:NST**

- [CPD68] M. Carpentieri, L. Porro, and G. Del Re. Numerical studies for a theoretical analysis of semiempirical LCAO–CI methods. *International Journal of Quantum Chemistry*, 2(6):807–824, November 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Cizek:1969:CEA**

- [ČPŠ69] J. Čížek, J. Paldus, and L. Šroubková. Cluster expansion analysis for delocalized systems. *International Journal of Quantum Chemistry*, 3(2):149–167, March 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Claverie:1969:TII**

- [CR69a] Pierre Claverie and Robert Rein. Theory of intermolecular interactions: The long range terms in the dipole–dipole, monopoles–dipole, and monopoles–bond polarizabilities approximations. *International Journal of Quantum Chemistry*, 3(5):537–551, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Cressy:1969:ETA**

- [CR69b] Norman Cressy and Klaus Ruedenberg. Expansion of  $r_{12}$  and  $r$  in terms of analytical functions. *International Journal of Quantum Chemistry*, 3(4):493–501, July 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Craft:1969:SER**

- [Cra69] Lawrence N. Craft. Symmetry effects in the radiation damping of degenerate states. *International Journal of Quantum Chemistry*, 3(6):781–793, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Cusachs:1967:SOM**

- [CS67] Louis Chopin Cusachs and Richard H. Steele. Singlet oxygen molecules and carcinogenic aromatic hydrocarbons. *International Journal of Quantum Chemistry*, 1(S1):175–178, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.



**Conklin:1968:EBS**

- [CS68] James B. Conklin, Jr. and Donald J. Silversmith. Energy-band structure and binding mechanism of TiC. *International Journal of Quantum Chemistry*, 2(S2):243–255, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Cusachs:1967:OMA**

- [CTCM67] Louis Chopin Cusachs, Benes Louis Trus, Daniel G. Carroll, and Sean P. McGlynn. Overlap-matched atomic orbitals. *International Journal of Quantum Chemistry*, 1(S1):423–430, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Cusachs:1967:BSR**

- [Cus67] Louis Chopin Cusachs. Bounds for semiempirical resonance integral approximations. *International Journal of Quantum Chemistry*, 1(S1):419–421, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Carlson:1967:ERB**

- [CW67] K. Douglas Carlson and Donald R. Whitman. Equivalence restrictions and the Brillouin condition for Hartree–Fock wave functions. *International Journal of Quantum Chemistry*, 1(S1):81–87, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Cruickshank:1967:OSR**

- [CWS67] D. W. J. Cruickshank, B. C. Webster, and M. A. Spinnler. The *d* orbitals of second-row elements. *International Journal of Quantum Chemistry*, 1(S1):225–231, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.



**Dash:1969:QTP**

- [Das69] Harriman H. Dash. A quantum table of the periodic system of elements. *International Journal of Quantum Chemistry*, 3(S3a): 335–340, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Daudel:1968:A**

- [Dau68] Raymond Daudel. Announcement. *International Journal of Quantum Chemistry*, 2(1):179, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Davison:1968:RWM**

- [Dav68] Sydney G. Davison. Recent work in the molecular-orbital theory of surface states. *International Journal of Quantum Chemistry*, 2 (S2):291–301, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Davison:1968:SIS**

- [DC68a] S. G. Davison and Y. C. Cheng. Surface and interface states of composite crystals. *International Journal of Quantum Chemistry*, 2(S2):303–311, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Davison:1968:TET**

- [DC68b] S. G. Davison and Y. C. Cheng. Two-electron theory of surface and impurity states. *International Journal of Quantum Chemistry*, 2 (S2):313–322, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Dresselhaus:1967:EHO**

- [DD67] G. Dresselhaus and M. S. Dresselhaus. An effective Hamiltonian for the optical properties of silicon and germanium. *International Journal of Quantum Chemistry*, 1(S1):595–603, January 16–21,



1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Dresselhaus:1968:IMP**

- [DD68] G. Dresselhaus and M. S. Dresselhaus. Interpolation methods for phonon spectra in crystals. *International Journal of Quantum Chemistry*, 2(S2):333–345, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Deepak:1969:SAF**

- [DDTM69] Adarsh Deepak, Victor Dulock, Billy S. Thomas, and Harold V. McIntosh. Symmetry adapted functions belonging to the Dirac groups. *International Journal of Quantum Chemistry*, 3(4):445–483, July 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**DelRe:1967:CDA**

- [Del67] Giuseppe Del Re. On the choice and definition of atomic-orbital bases. I. General considerations; promotion and hybridization; electric dipole moments. *International Journal of Quantum Chemistry*, 1(3):293–310, May 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**DeLaVega:1969:RBC**

- [DFH69] Jose R. De La Vega, Yeong Fang, and Edward F. Hayes. Rotational barriers: Comparison of semiempirical and ab initio quantum mechanical calculations. *International Journal of Quantum Chemistry*, 3(S3a):113–117, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Diercksen:1968:NLS**

- [Die68] G. Diercksen. Über eine Näherung zur Lösung des “Self-consistent-field”; Verfahrens für Systeme mit ungepaarten Elektronen. I. Die Methode. (German) [On an approximation for the solution of the “self-consistent field”: Procedure for systems with unpaired electrons. I. The method]. *International Journal of Quantum Chemistry*, 2(1):55–67, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Dutta:1969:MBA**

- [DIMD69] N. C. Dutta, T. Ishihara, C. Matsubara, and T. P. Das. Many-body approach to the properties of interacting atoms. *International Journal of Quantum Chemistry*, 4(S3b):367–380, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Dalgarno:1967:LRI**

- [DMP67] A. Dalgarno, I. H. Morrison, and R. M. Pengelly. Long-range interactions between atoms and molecules. *International Journal of Quantum Chemistry*, 1(2):161–167, March 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Doggett:1969:DEC**

- [Dog69] G. Doggett. The distribution of electronic charge in the ground state of cubic boron nitride. *International Journal of Quantum Chemistry*, 3(6):753–762, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Diercksen:1967:WAMa**

- [DP67a] G. Diercksen and H. Preuss. Wellenmechanische Absolutrechnungen an Molekülen und Atomsystemen mit der SCF MO LC (LCGO) Methode. II. Das Benzol ( $C_6H_6$ ). (German) [Wave-mechanical ab initio calculation for molecules and atomic systems with the SCF MO LC (LCGO) method. II. Benzene ( $C_6H_6$ )]. *International Journal of Quantum Chemistry*, 1(4):357–359, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Diercksen:1967:WAMb**

- [DP67b] G. Diercksen and H. Preuss. Wellenmechanische Absolutrechnungen an Molekülen und Atomsystemen mit der SCF MO LC (LCGO) Methode. IV. Das Äthylen ( $C_2H_4$ ). (German) [Wave-mechanical ab initio calculation for molecules and atomic systems with the SCF MO LC (LCGO) method. IV. Ethylene ( $C_2H_4$ )]. *International Journal of Quantum Chemistry*, 1(4):365–368, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Diercksen:1967:WAMc**

- [DP67c] G. Diercksen and H. Preuss. Wellenmechanische Absolutrechnungen an Molekülen und Atomsystemen mit der SCF MO LC



(LCGO) Methode. VIII. Das System  $(\text{Li}_2\text{H})^+$ . (German) [Wave-mechanical ab initio calculation for molecules and atomic systems with the SCF MO LC (LCGO) method. VIII. The  $(\text{Li}_2\text{H})^+$  system]. *International Journal of Quantum Chemistry*, 1(5):637–640, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Dmitriev:1967:VPI**

- [DY67] Y. Y. Dmitriev and M. S. Yuriev. Variational principle for the intensity of forbidden transitions. *International Journal of Quantum Chemistry*, 1(4):321–325, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Ellis:1968:ADI**

- [Ell68] D. E. Ellis. Application of Diophantine integration to Hartree–Fock and configuration interaction calculations. *International Journal of Quantum Chemistry*, 2(S2):35–42, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Elsasser:1969:CBR**

- [Els69] Walter M. Elsasser. Can biology be reduced into chemistry and physics, and vice versa? *International Journal of Quantum Chemistry*, 3(S3a):347–348, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Empedocles:1969:RRD**

- [Emp69] Philip Empedocles. Range relaxation 2. Determination of a reaction coordinate over an energy surface of several dimensions. *International Journal of Quantum Chemistry*, 3(S3a):47–62, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Ermolaev:1968:SH**

- [ES68] A. M. Ermolaev and G. B. Sochilin.  $2^3\text{S}$  state of helium. *International Journal of Quantum Chemistry*, 2(3):333–339, May 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Eyring:1969:MR**

- [Eyr69] Henry Eyring. Models in research. *International Journal of Quantum Chemistry*, 3(S3a):5–15, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Fankhauser:1969:DCM**

- [Fan69] Hans R. Fankhauser. On the dynamics of crystals with molecular impurity centers. I. Compatibility conditions. *International Journal of Quantum Chemistry*, 4(S3b):881–901, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Farmer:1969:LTW**

- [Far69a] Christine M. Farmer. Laplace transform wave functions. *International Journal of Quantum Chemistry*, 3(6):1027–1043, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Farmer:1969:CTR**

- [Far69b] Gerald Farmer. Comment on time-resolved spectra of organic dye lasers. *International Journal of Quantum Chemistry*, 3(S3a):327, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Flodmark:1967:CPC**

- [FB67] Stig Flodmark and Esko Blokker. A computer program for calculation of irreducible representations of finite groups. *International Journal of Quantum Chemistry*, 1(S1):703–711, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Fischer-Hjalmar:1967:SSM**

- [FHGR<sup>+</sup>67] I. Fischer-Hjalmar, B. Grabe, B. Roos, P. N. Skancke, and M. Sundbom. Semiempirical studies of metal complexes of biological importance. *International Journal of Quantum Chemistry*, 1(S1):233–246, January 16–21, 1967. CODEN IJQCB2. ISSN



0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Forsterling:1967:PED**

- [FHK67] H. D. Försterling, W. Huber, and H. Kuhn. Projected electron density method of  $\pi$ -electron systems. I. Electron distribution in the ground state. *International Journal of Quantum Chemistry*, 1(3):225–241, May 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Fischer:1967:CEH**

- [Fis67] Sighart F. Fischer. Collective excitation of hydrogen-bonded ferroelectrics. *International Journal of Quantum Chemistry*, 1(S1):745–753, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Fischer:1969:SPS**

- [Fis69] Sighart Fischer. On the sigma-pi separability problem. *International Journal of Quantum Chemistry*, 4(S3b):651–657, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Fratev:1969:WBP**

- [FJP69] F. Fratev, R. Janoschek, and H. Preuss. Wellenmechanische Behandlung der Protonisierung des Äthylens unter Berücksichtigung aller Elektronen. (German) [Wave-mechanical treatment of protonation of ethylene considering all electrons]. *International Journal of Quantum Chemistry*, 3(6):873–879, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Forsterling:1968:PED**

- [FK68] H. D. Försterling and H. Kuhn. Projected electron density method of  $\pi$ -electron systems II. Excited states. *International Journal of Quantum Chemistry*, 2(3):413–430, May 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Flodmark:1967:DPP**

- [Flo67] Stig Flodmark. A data programme for population analysis of crystal-band structures. *International Journal of Quantum Chem-*



*istry*, 1(2):147–159, March 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Foster:1969:FSE**

- [Fos69] Howard J. Foster. Fermi surfaces and electron–impurity interactions in simple metals. *International Journal of Quantum Chemistry*, 3(6):969–981, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Frohlich:1968:LRC**

- [Frö68] H. Fröhlich. Long-range coherence and energy storage in biological systems. *International Journal of Quantum Chemistry*, 2(5):641–649, September 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Frost:1968:FSG**

- [FRV68] Arthur A. Frost, Robert A. Rouse, and Lee Vescelius. A floating spherical Gaussian orbital model of molecular structure V. computer programs. *International Journal of Quantum Chemistry*, 2(S2):43–66, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Fukui:1968:NTI**

- [FY68] Kenichi Fukui and Tokio Yamabe. A note on the theory of interatomic long-range forces. *International Journal of Quantum Chemistry*, 2(3):359–369, May 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Gallup:1968:FSD**

- [Gal68] G. A. Gallup. Factorization of the secular determinant by constants of the motion. *International Journal of Quantum Chemistry*, 2(5):695–706, September 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Gaspar:1967:MEP**

- [Gás67] R. Gáspár. Many-electron problems. I. Energy relations in the theory of neutral atoms. *International Journal of Quantum Chemistry*, 1(2):139–145, March 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Gaspar:1969:MEP**

- [Gás69] R. Gáspár. Many-electron problems. II. Energy expansions and internal fields. *International Journal of Quantum Chemistry*, 3 (5):723–730, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Glasser:1969:ASD**

- [GD69] M. L. Glasser and S. G. Davison. Analytic solution of the Dirac equation for the Kronig–Penney potential. *International Journal of Quantum Chemistry*, 4(S3b):867–877, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**George:1968:NUP**

- [Geo68] C. George. Note on the usual perturbation theory. *International Journal of Quantum Chemistry*, 2(4):445–451, July 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Gershgorn:1968:PLI**

- [Ger68] Z. Gershgorn. Proof of the linear independence of properly selected projected spin eigenfunctions. *International Journal of Quantum Chemistry*, 2(3):341–347, May 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Gole:1969:MBF**

- [GH69] James L. Gole and Edward F. Hayes. Molecular bonding in FO<sub>2</sub> and ClO<sub>2</sub>. *International Journal of Quantum Chemistry*, 4(S3b):519–525, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Girifalco:1969:SCW**

- [Gir69] L. A. Girifalco. Some comments on Wannier functions in metallic cohesion. *International Journal of Quantum Chemistry*, 4 (S3b):879, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.



**Goddard:1969:OOH**

- [GL69] William A. Goddard III and Robert C. Ladner. The optimum orbitals for the  $\text{H}_2 + \text{D} \leftrightarrow \text{H} + \text{HD}$  exchange reaction. *International Journal of Quantum Chemistry*, 3(S3a):63–66, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Grimaldi:1967:CED**

- [GLM67] F. Grimaldi, A. Lecourt, and C. Moser. The calculation of the electric dipole moment of CO. *International Journal of Quantum Chemistry*, 1(S1):153–161, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Gianinetti:1969:CIS**

- [GMRS69] E. Gianinetti, G. F. Majorino, E. Rusconi, and M. Simonetta. Configuration interaction study of  $\text{H}_2$  and  $\text{H}_3$  systems. *International Journal of Quantum Chemistry*, 3(1):45–56, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Goscinski:1968:CEP**

- [GÖ68] Osvaldo Goscinski and Yngve Öhrn. Coupling of equivalent particles in a field of given symmetry. *International Journal of Quantum Chemistry*, 2(6):845–856, November 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See errata [GÖJ<sup>+</sup>73].

**Goddard:1969:SGS**

- [God69] William A. Goddard III. The symmetric group and the spin generalized SCF method. *International Journal of Quantum Chemistry*, 4(S3b):593–600, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Goscinski:1973:ECE**

- [GÖJ<sup>+</sup>73] O. Goscinski, Y. Öhrn, A. Norman Jette, E. Lombardi, R. Ritter, and L. Jansen. Errata: Coupling of Equivalent Particles in a Field of Given Symmetry. *International Journal of Quantum Chemistry*,



7(5):1039–1043, September 1973. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [GÖ68].

**Gordon:1968:EBQ**

- [Gor68] Roy G. Gordon. Error bounds for quantum-mechanical perturbation theory. *International Journal of Quantum Chemistry*, 2(S2):151–159, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Goscinski:1968:ULBb**

- [Gos68] Osvaldo Goscinski. Upper and lower bounds to polarizabilities and van der Waals forces I. General theory. *International Journal of Quantum Chemistry*, 2(6):761–784, November 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Goscinski:1969:BO**

- [Gos69] Osvaldo Goscinski. Bounds to the overlap. *International Journal of Quantum Chemistry*, 3(6):1064–1066, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Gershgorn:1967:CSA**

- [GS67] Z. Gershgorn and I. Shavitt. The construction of symmetry-adapted functions in configuration interaction calculations for molecules with one principal axis of symmetry. *International Journal of Quantum Chemistry*, 1(S1):403–417, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Gershgorn:1968:APT**

- [GS68a] Z. Gershgorn and I. Shavitt. An application of perturbation theory ideas in configuration interaction calculations. *International Journal of Quantum Chemistry*, 2(6):751–759, November 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Goscinski:1968:ULBa**

- [GS68b] Osvaldo Goscinski and Oktay Sinanoğlu. Upper and lower bounds and the generalized variation-perturbation approach of many-electron theory. *International Journal of Quantum Chemistry*, 2(3):397–403, May 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Ha:1967:ICS**

- [HA67] Tae-Kyu Ha and Leland C. Allen. The influence of chemical substitution on inner shells. *International Journal of Quantum Chemistry*, 1(S1):199–203, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Hakala:1967:SWC**

- [Hak67a] Reino W. Hakala. Simple ways to calculate the empirical resonance energies of benzenoid hydrocarbons, their derivatives, and graphite. *International Journal of Quantum Chemistry*, 1(S1):187–196, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Hakala:1967:UNB**

- [Hak67b] Reino W. Hakala. The use of normalized binomial coefficients as weights to accelerate convergence of oscillatory first-order iterations. *International Journal of Quantum Chemistry*, 1(S1):277–284, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Hall:1967:AGT**

- [Hal67] George G. Hall. *Applied group theory*. Longmans, London, UK, 1967. vii + 128 pp. LCCN ????

**Hall:1969:OPG**

- [Hal69] G. G. Hall. The one-particle Green's function and the evaluation of ionization potentials. *International Journal of Quantum Chemistry*, 4(S3b):659–660, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Hansen:1967:SVT**

- [Han67] Karl Heinz Hansen. Spin valence theory is a directional theory of valence. *International Journal of Quantum Chemistry*, 1(S1):217–223, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608



(print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Handler:1969:ETF**

- [Han69] George S. Handler. On the energy of a Thomas–Fermi system. *International Journal of Quantum Chemistry*, 4(S3b):703–706, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Harrison:1967:SLP**

- [Har67] Ralph J. Harrison. On the solid–liquid phase transition. *International Journal of Quantum Chemistry*, 1(S1):839–843, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Harris:1968:EPI**

- [Har68] A. Brooks Harris. The effect of phonon interactions on the orientational state of  $\text{H}_2$ . *International Journal of Quantum Chemistry*, 2(S2):347–357, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Henderson:1969:TLS**

- [HBK69] D. Henderson, J. A. Barker, and S. Kim. Theory of the liquid state. *International Journal of Quantum Chemistry*, 3(S3a):265–292, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Hirschfelder:1968:SEP**

- [HC68] Joseph O. Hirschfelder and Phillip R. Certain. Summary of exchange perturbation calculations for  $\text{H}_2$  at large separations. *International Journal of Quantum Chemistry*, 2(S2):125–135, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.



**Heitler:1967:QCE**

- [Hei67] W. Heitler. Quantum chemistry: The early period. *International Journal of Quantum Chemistry*, 1(1):13–36, January 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Heldmann:1968:FSF**

- [Hel68] G. Heldmann. On the formulation of spin-free quantum chemistry. *International Journal of Quantum Chemistry*, 2(6):785–792, November 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Hermann:1968:MOC**

- [Her68] Robert B. Hermann. Molecular-orbital calculations on electrophilic substitution and relative basicities in pyrrole, indole, furan, and benzofuran. *International Journal of Quantum Chemistry*, 2(1):165–177, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Hakala:1967:ECI**

- [HF67] Reino W. Hakala and Alfred E. Fields. Electrostatic contribution to the internal rotational barrier in ethane. *International Journal of Quantum Chemistry*, 1(S1):197–198, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Ha:1967:MDM**

- [HFA67] Tae-Kyu Ha, William H. Fink, and Leland C. Allen. Multicenter distribution of molecular integrals and energy components. *International Journal of Quantum Chemistry*, 1(S1):431–443, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Hall:1969:MPA**

- [HHR69] G. G. Hall, J. Hyslop, and D. Rees. A minimum principle for atomic systems allowing the use of discontinuous wave functions. *International Journal of Quantum Chemistry*, 3(2):195–204, March 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Hirschfelder:1969:CWD**

- [Hir69a] Joseph O. Hirschfelder. Coordinates which diagonalize the kinetic energy of relative motion. *International Journal of Quantum Chemistry*, 3(S3a):17–31, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Hirschfelder:1969:FRS**

- [Hir69b] Joseph O. Hirschfelder. Formal Rayleigh–Schrödinger perturbation theory for both degenerate and non-degenerate energy states. *International Journal of Quantum Chemistry*, 3(5):731–748, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Handler:1969:PMG**

- [HJ69] George S. Handler and Hubert W. Joy. The prediction of molecular geometry.  $\text{CH}_4^+$ . *International Journal of Quantum Chemistry*, 4(S3b):529–531, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Herman:1967:EBS**

- [HKK67] Frank Herman, Richard L. Kortum, and Charles D. Kuglin. Energy band structure of diamond, cubic silicon carbide, silicon, and germanium. *International Journal of Quantum Chemistry*, 1(S1):533–566, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Hill:1969:QPP**

- [HL69] C. O. Hill and S. H. Lin. Quenching of phosphorescence by paramagnetic molecules in rigid media. I. *International Journal of Quantum Chemistry*, 3(S3a):307–314, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Hedin:1967:SPS**

- [HLL67] L. Hedin, B. I. Lundqvist, and S. Lundqvist. On the single-particle spectrum of an interacting electron gas. *International*



*Journal of Quantum Chemistry*, 1(S1):791–801, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Harris:1967:OSV**

- [HM67] F. E. Harris and H. H. Michels. Open-shell valence configuration-interaction studies of diatomic and polyatomic molecules. *International Journal of Quantum Chemistry*, 1(S1):329–338, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Harris:1969:CCI**

- [HM69] Frank E. Harris and H. H. Michels. Comparison of configuration-interaction methods for  $F_2$ . *International Journal of Quantum Chemistry*, 4(S3b):461–467, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Hofacker:1969:LDE**

- [Hof69] G. Ludwig Hofacker. Later developments of Eyring’s ideas of the activated complex. *International Journal of Quantum Chemistry*, 3(S3a):33–37, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Hoor:1968:GSA**

- [Hoo68] Marten J. Ten Hoor. The ground state of atomic two-electron systems in the independent particle model. *International Journal of Quantum Chemistry*, 2(1):109–128, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Herman:1969:MIP**

- [HOV69] F. Herman, I. B. Ortenburger, and J. P. Van Dyke. A method for improving the physical realism of first-principles band structure calculations. *International Journal of Quantum Chemistry*, 4(S3b):827–846, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.



**Hall:1969:EIB**

- [HR69] G. G. Hall and W. Rodwell. The electrostatic interaction between TCQ and DNA. *International Journal of Quantum Chemistry*, 3(S3a):237–240, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Hurley:1967:IIH**

- [Hur67] A. C. Hurley. Integrated and integral Hellmann–Feynman formulae II. Construction of super-floating functions. *International Journal of Quantum Chemistry*, 1(S1):677–685, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Hillier:1969:POC**

- [HW69] Ian H. Hillier and John F. Wyatt. On partitioning the overlap charge density in self-consistent charge molecular-orbital calculations. *International Journal of Quantum Chemistry*, 3(1):67–71, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**I'Haya:1967:MOR**

- [I'H67] Y. I'Haya. Magneto-optical rotation in molecules. IV. The Verdet constant for the nitrogen molecule. *International Journal of Quantum Chemistry*, 1(5):693–698, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Ito:1968:ESS**

- [II68] Hirotoshi Ito and Y. J. I'Haya. The electronic structures and spectra of proflavine, acridine orange, and their DNA complexes. *International Journal of Quantum Chemistry*, 2(1):5–21, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Izuyama:1967:MSN**

- [IK67] Takeo Izuyama and Yasunari Kurihara. Magnetic scattering of neutrons by the itinerant electron ferromagnets at high temperatures. *International Journal of Quantum Chemistry*, 1(S1):651–660, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the



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

**Janoschek:1968:WAI**

- [Jan68] R. Janoschek. Wellenmechanische Absolutrechnung an einer intramolekularen Radikalreaktion an einem methyl- und hydroxyl-substituierten ungesättigten Kohlenwasserstoff. (German) [Wave-mechanical ab initio calculation in an intramolecular reaction on a methyl- and hydroxyl-unsaturated hydrocarbon]. *International Journal of Quantum Chemistry*, 2(5):707–713, September 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Johansson:1969:IAI**

- [JB69] B. Johansson and K.-F. Berggren. Itinerant antiferromagnetism in an infinite linear chain. *International Journal of Quantum Chemistry*, 4(S3b):865, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Jucys:1969:TTS**

- [JBG69] A. P. Jucys, A. A. Bandzaitis, and J. J. Grudzinskas. Theory of two shells of atomic electrons using non-orthogonal radial orbitals. *International Journal of Quantum Chemistry*, 3(6):913–930, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Johnson:1969:ESC**

- [JC69] K. H. Johnson and J. W. D. Connolly. The electronic structures of cesium chloride type intermetallic compounds I. Preliminary energy bands of  $\beta'$ AuZn and  $\beta'$ NiAl. *International Journal of Quantum Chemistry*, 4(S3b):813–825, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Janoschek:1967:WAMa**

- [JDP67a] R. Janoschek, G. Diercksen, and H. Preuss. Wellenmechanische Absolutrechnungen an Molekülen und Atomsystemen mit der SCF MO LC (LCGO) Methode. VI. Das Methan ( $\text{CH}_4$ ). (German) [Wave-mechanical ab initio calculation for molecules and atomic systems with the SCF MO LC (LCGO) method. VI. Methane



(CH<sub>4</sub>)]. *International Journal of Quantum Chemistry*, 1(4):373–378, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Janoschek:1967:WSL**

- [JDP67b] R. Janoschek, G. Diercksen, and H. Preuss. Wellenmechanische strukturuntersuchungen am lithiumcyclopentadienyl (LiC<sub>5</sub>H<sub>5</sub>). (German) [Wave-mechanical structure investigation of lithiumcyclopentadienyl (LiC<sub>5</sub>H<sub>5</sub>)]. *International Journal of Quantum Chemistry*, 1(S1):205–208, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Janoschek:1968:WUW**

- [JDP68] R. Janoschek, G. Diercksen, and H. Preuss. Wellenmechanische Untersuchungen an der Wasserstoffbrücke zwischen zwei Berylliumatomen. (German) [Wave-mechanical investigation of the hydrogen bond between two beryllium atoms]. *International Journal of Quantum Chemistry*, 2(1):159–163, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Jehle:1968:RFQ**

- [Jeh68] Herbert Jehle. The relationship of flux quantization to charge quantization and the fine structure constant. *International Journal of Quantum Chemistry*, 2(S2):373–375, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Jehle:1969:CRD**

- [Jeh69a] Herbert Jehle. Comments in relation to the discussion on transition rates. *International Journal of Quantum Chemistry*, 3(S3a):39, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Jehle:1969:RFQ**

- [Jeh69b] Herbert Jehle. The relationship of flux quantization to charge quantization and the fine structure constant. *International Jour-*



*nal of Quantum Chemistry*, 3(3):269–287, May 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Jehle:1969:RPM**

- [Jeh69c] Herbert Jehle. Remarks on the problem of morphogenetic movements in the development of embryos. *International Journal of Quantum Chemistry*, 3(S3a):75–82, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Johnson:1968:E**

- [JH68] Keith H. Johnson and Marten J. Ten Hoor. Errata. *International Journal of Quantum Chemistry*, 2(4):563, July 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Jorgensen:1967:IMI**

- [JHHT67] Chr. Klixbüll Jørgensen, Sally M. Horner, William E. Hatfield, and S. Y. Tyree, Jr. Influence of Madelung (interatomic Coulomb) energy on Wolfsberg–Helmholz calculations. *International Journal of Quantum Chemistry*, 1(2):191–215, March 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Joshi:1969:MCI**

- [JK69] Bhairav D. Joshi and K. L. Kapoor. Molecular correlation integrals. Two center one electron integrals containing a function of interparticle distance in one center expansion approximation. *International Journal of Quantum Chemistry*, 3(4):397–415, July 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Jucys:1968:AEM**

- [JKK68] A. P. Jucys, V. A. Kaminskas, and V. J. Kaveckis. Application of the extended method of calculation for atoms and ions having the electronic configurations  $1s^2 2s^2 2p^N$ . *International Journal of Quantum Chemistry*, 2(3):405–411, May 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Jucys:1969:EMC**

- [JN69] A. P. Jucys and E. P. Našlenas. Extended method of calculation for two shells of atomic electrons having the same orbital quantum



number. *International Journal of Quantum Chemistry*, 3(6):931–943, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Johnson:1967:MSG**

- [Joh67] Keith H. Johnson. Multiple scattering (Green’s function) model for polyatomic molecules II. theory. *International Journal of Quantum Chemistry*, 1(S1):361–367, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Johnson:1968:SMB**

- [Joh68] K. H. Johnson. Scattering model for the bound electronic states of an impurity complex in a crystal. *International Journal of Quantum Chemistry*, 2(S2):233–242, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Jorgensen:1968:BRB**

- [Jør68a] Chr. Klixbüll Jørgensen. Book review: *Optical properties of ions in crystals*. Edited by: H. M. Crosswhite and H. W. Moos. Published by: Interscience Publishers, New York, 1967. Price: \$18.50. No. of pages: 552. *International Journal of Quantum Chemistry*, 2(6):935, November 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [CM67].

**Jorgensen:1968:MDB**

- [Jør68b] Chr. Klixbüll Jørgensen. Might the difference between Schrödinger and Ruedenberg’s local contributions to the kinetic energy represent elastic deformations of the electron? *International Journal of Quantum Chemistry*, 2(1):49–54, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Joseph:1967:DEN**

- [Jos67a] A. Joseph. On the determination of the exact number of bound states of a given potential. I. General method. *International Journal of Quantum Chemistry*, 1(5):615–629, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Joseph:1967:TLD**

- [Jos67b] A. Joseph. The theory of local degeneracy. *International Journal of Quantum Chemistry*, 1(5):535–559, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Janoschek:1969:WUB**

- [JP69] R. Janoschek and H. Preuss. Wellenmechanische untersuchungen am 2-Buten unter Berücksichtigung aller Elektronen. (German) [Wave-mechanical investigations of 2-butene including all electrons]. *International Journal of Quantum Chemistry*, 3(6):889–891, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Janoschek:1967:WAMb**

- [JPD67a] R. Janoschek, H. Preuss, and G. Dierksen. Wellenmechanische Absolutrechnungen an Molekülen und Atomsystemen mit der SCF MO LC (LCGO) Methode. XI. Das Hydroxylanion  $(\text{OH})^-$ . (German) [Wave-mechanical ab initio calculation for molecules and atomic systems with the SCF MO LC (LCGO) method. XI. the hydroxyl anion  $(\text{OH})^-$ ]. *International Journal of Quantum Chemistry*, 1(5):649–652, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Janoschek:1967:WSB**

- [JPD67b] R. Janoschek, H. Preuss, and G. Dierksen. Wellenmechanische strukturuntersuchung am benzol (German) [Wave-mechanical structure investigation of benzol]. *International Journal of Quantum Chemistry*, 1(S1):209–216, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Jucys:1969:MRS**

- [JRS69] A. P. Jucys, Z. B. Rudzikas, and A. J. Savukynas. Mirror reflection symmetry and the phase relations for partially and almost filled shells of equivalent atomic electrons. *International Journal of Quantum Chemistry*, 3(6):1001–1012, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Jain:1968:TPI**

- [JS68] D. C. Jain and R. C. Sahni. Transition probabilities for the ionization of  $\text{N}_2$ ,  $\text{O}_2$ ,  $\text{NO}$  and  $\text{CO}$  molecules. *International Journal of*



*Quantum Chemistry*, 2(3):325–332, May 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Jucys:1967:EMC**

- [Juc67a] Adolfas Pranaitis Jucys. On the extended method of calculation of atomic structures. *International Journal of Quantum Chemistry*, 1(4):311–319, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Jucys:1967:SAD**

- [Juc67b] Adolfas Pranaitis Jucys. Some aspects of the development of the methods of calculation of atomic structures. *International Journal of Quantum Chemistry*, 1(S1):37–43, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Jug:1969:IPA**

- [Jug69] Karl Jug. On invariant procedures in approximate SCF MO theories. *International Journal of Quantum Chemistry*, 3(S3a):241–249, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Kaplan:1969:SAT**

- [KA69] T. A. Kaplan and Petros N. Argyres. Some applications of the thermal single-determinant approximation. *International Journal of Quantum Chemistry*, 4(S3b):851–855, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Kaufman:1967:PCW**

- [Kau67] Joyce J. Kaufman. A probable condition which a density matrix representing a real molecule should satisfy. *International Journal of Quantum Chemistry*, 1(S1):485–486, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.



**Koutecky:1968:ESG**

- [KD68] Jaroslav Koutecký and Sydney G. Davison. Electronic states of general mixed crystals. *International Journal of Quantum Chemistry*, 2(1):73–88, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Kelly:1967:MBP**

- [Kel67] Hugh P. Kelly. Many-body perturbation theory for atoms. *International Journal of Quantum Chemistry*, 1(S1):25–35, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Kelly:1969:APC**

- [Kel69] Hugh P. Kelly. Atomic properties calculated by many-body theory. *International Journal of Quantum Chemistry*, 4(S3b):349–358, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Kaufman:1967:TTH**

- [KHK67] Joyce J. Kaufman, Jerome J. Harkins, and Walter S. Koski. Theoretical treatment of hydrogen abstraction by hot tritium atoms. *International Journal of Quantum Chemistry*, 1(S1):261–276, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Kibler:1969:ELP**

- [Kib69] Maurice Kibler. Energy levels of paramagnetic ions: Algebra. II. *International Journal of Quantum Chemistry*, 3(6):795–822, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Kimball:1967:R**

- [Kim67] George E. Kimball. Reminiscences of 1933–1935. *International Journal of Quantum Chemistry*, 1(S1):845–847, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.



**Klein:1969:SRDa**

- [KK69] D. J. Klein and R. W. Kramling. The symmetry of reduced density matrices. I. General algebraic approach and permutational symmetry. *International Journal of Quantum Chemistry*, 4(S3b):661–674, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Klein:1969:SRDb**

- [Kle69] D. J. Klein. The symmetry of reduced density matrices. II. Spin-free quantum chemistry and point group symmetry. *International Journal of Quantum Chemistry*, 4(S3b):675–688, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Kouba:1969:PME**

- [KÖ69] Joseph Kouba and Yngve Öhrn. On the projection of many-electron spin eigenstates. *International Journal of Quantum Chemistry*, 3(4):513–521, July 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Kolos:1967:LRI**

- [Kol67] W. Kolos. Long-range interaction between  $1s$  and  $2s$  or  $2p$  hydrogen atoms. *International Journal of Quantum Chemistry*, 1(2):169–186, March 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Kolos:1968:RDT**

- [Kol68] W. Kolos. Recent developments in the theory of one- and two-electron molecules. *International Journal of Quantum Chemistry*, 2(4):471–481, July 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Kochanski:1969:ZFS**

- [KP69] E. Kochanski and A. Pullman. Zero-field splitting parameters in heterocyclic molecules II. Calculations using SCF, SCF CM and UHF wave functions. *International Journal of Quantum Chemistry*, 3(6):1055–1058, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Kutzelnigg:1968:OCS**

- [KS68] Werner Kutzelnigg and Vedene H. Smith, Jr. Open- and closed-shell states in few-particle quantum mechanics. I. Definitions. *International Journal of Quantum Chemistry*, 2(4):531–552, July 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Kubarev:1969:MCP**

- [KS69] S. I. Kubarev and M. I. Shedrin. A model calculation of protonic mobility in ice. *International Journal of Quantum Chemistry*, 3(6):893–901, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Kaldor:1968:SEC**

- [KSH68] Uzi Kaldor, Henry F. Schaefer, and Frank E. Harris. Spin-extended and configuration-interaction studies of first-row atoms. *International Journal of Quantum Chemistry*, 2(S2):13–20, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Kay:1967:SOC**

- [KT67] K. Kay and A. G. Turner. Some one-center calculations for He<sub>2</sub> at small internuclear distances. *International Journal of Quantum Chemistry*, 1(S1):167–169, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Kuprievich:1967:SCS**

- [Kup67] V. A. Kuprievich. SCF CI and SCF open-shell studies of the base components of the nucleic acids. *International Journal of Quantum Chemistry*, 1(5):561–575, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Landman:1969:LRI**

- [Lan69] U. Landman. Long-range interactions between atoms and charges by double-perturbation treatment. *International Journal of Quantum Chemistry*, 3(3):317–325, May 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Larson:1968:AWF**

- [Lar68a] Everett G. Larson. An approximate wave function involving geminals of mixed spin. *International Journal of Quantum Chemistry*, 2(S2):75–81, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Larson:1968:SRH**

- [Lar68b] Everett G. Larson. Stability of a restricted Hartree–Fock-like wave function under the removal of a symmetry restriction. *International Journal of Quantum Chemistry*, 2(S2):83–87, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Larson:1969:SOH**

- [Lar69] Everett G. Larson. Specification of an orbital Hilbert space using a minimal number of parameters. *International Journal of Quantum Chemistry*, 4(S3b):707–714, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Laurenzi:1969:NTC**

- [Lau69] Bernard J. Laurenzi. Note on two-center Fourier transforms. *International Journal of Quantum Chemistry*, 3(4):489–492, July 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Layzer:1967:ECE**

- [Lay67] David Layzer.  $Z$ -expansion calculations of energy levels and transition probabilities in many-electron atoms. *International Journal of Quantum Chemistry*, 1(S1):45–59, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Levy:1968:GBT**

- [LB68] Bernard Levy and Gaston Berthier. Generalized Brillouin theorem for multiconfigurational SCF theories. *International Journal of Quantum Chemistry*, 2(2):307–319, March 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Levy:1969:GBT**

- [LB69] Bernard Levy and Gaston Berthier. Generalized Brillouin theorem for multiconfigurational SCF theories. *International Journal of Quantum Chemistry*, 3(2):247, March 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Loter:1969:QCI**

- [LC69] Joe Loter and Ralph E. Christoffersen. Quadratically convergent iteration procedure for geminal determinations. *International Journal of Quantum Chemistry*, 3(5):651–661, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Lloyd:1969:LSP**

- [LD69] M. H. Lloyd and L. M. Delves. On the least squares procedure for atomic calculations. *International Journal of Quantum Chemistry*, 3(2):169–184, March 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Leclercq:1969:EMD**

- [Lec69] J.-M. Leclercq. Exposé d’une méthode de détermination des orbitales virtuelles pour les interactions de configurations. Application à l’état fondamental de l’atome de béryllium. (French) [Description of a method for determining virtual orbitals for configuration interaction]. *International Journal of Quantum Chemistry*, 3(1):3–11, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Lesk:1968:CDP**

- [Les68] Arthur M. Lesk. Computation of derivatives for parameter optimization in least-squares fitting of linear combinations of Slater-type orbitals by Gaussians. *International Journal of Quantum Chemistry*, 2(6):801–805, November 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Lesk:1969:ELC**

- [Les69] Arthur M. Lesk. Expansion of linear combinations of Slater-type orbitals in eigenfunctions of the three-dimensional isotropic harmonic oscillator. *International Journal of Quantum Chemistry*, 3(3):289–295, May 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Levine:1967:DRI**

- [Lev67] Raphael D. Levine. On the dynamic response of impure molecular crystals. *International Journal of Quantum Chemistry*, 1(S1):727–744, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Levy:1969:TAR**

- [Lev69] Joseph Levy. Une théorie adiabatique de la relaxation spin-réseau. (French) [An adiabatic theory of spin-lattice relaxation]. *International Journal of Quantum Chemistry*, 3(1):73–78, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Lowdin:1969:EPS**

- [LG69] Per-Olov Löwdin and Osvaldo Goscinski. The exchange phenomenon, the symmetric group, and the spin degeneracy problem. *International Journal of Quantum Chemistry*, 4(S3b):533–591, January 13–18, 1969. CODEN IJQSAF. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Lax:1967:IBT**

- [LH67] M. Lax and B. I. Halperin. Impurity band tails in degenerate semiconductors. *International Journal of Quantum Chemistry*, 1(S1):767, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Linderberg:1967:LFA**

- [Lin67] Jan Linderberg. London forces as an aspect of the correlation problem in molecular solids. *International Journal of Quantum Chemistry*, 1(S1):719–726, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Lindner:1967:CSF**

- [LL67] P. Lindner and S. Lunell. On the choice of spin functions in the AMO method. *International Journal of Quantum Chemistry*, 1



(?):841–??, ?? 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Lindner:1968:ULB**

- [LL68] Peter Lindner and Per-Olov Löwdin. Upper and lower bounds in second-order perturbation theory and the Unsöld approximation. *International Journal of Quantum Chemistry*, 2(S2):161–173, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Lowdin:1969:CLB**

- [LL69] Per-Olov Löwdin and Tiong-Koon Lim. Calculation of lower bounds to energy eigenvalues by reduced density matrices and the representability problem. *International Journal of Quantum Chemistry*, 4(S3b):697–702, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Loucks:1968:FSP**

- [Lou68] T. L. Loucks. Fermi surfaces and periodic moment arrangements. *International Journal of Quantum Chemistry*, 2(S2):285–290, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Lowdin:1963:ISAb**

- [Löw63] Per-Olov Löwdin. International Symposium on Atomic and Molecular Quantum Mechanics: Proceedings in Honor of Professor Egil A. Hylleraas and arranged by the University of Florida at Sanibel Island, 14–19 January 1963: Introduction. *Reviews of Modern Physics*, 35(3):415, July 1963. CODEN RM-PHAT. ISSN 0034-6861 (print), 1538-4527 (electronic), 1539-0756. URL <http://link.aps.org/doi/10.1103/RevModPhys.35.415>; [http://rmp.aps.org/abstract/RMP/v35/i3/p415\\_1](http://rmp.aps.org/abstract/RMP/v35/i3/p415_1).

**Lowdin:1967:P**

- [Löw67a] Per-Olov Löwdin. Program. *International Journal of Quantum Chemistry*, 1(1):1–6, January 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Lowdin:1967:EPL**

- [Löw67b] Per-Olov O. Löwdin. Eigenvalue problem in a linearly dependent basis and the super secular equation. *International Journal of Quantum Chemistry*, 1(S1):811–827, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Lowdin:1967:NQC**

- [Löw67c] Per-Olov O. Löwdin. Nature of quantum chemistry. *International Journal of Quantum Chemistry*, 1(1):7–12, January 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Lowdin:1968:SCT**

- [Löw68a] Per-Olov Löwdin. Some comments on the treatment of symmetry properties in perturbation theory. *International Journal of Quantum Chemistry*, 2(S2):137–150, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Lowdin:1968:SPT**

- [Löw68b] Per-Olov O. Löwdin. Studies in perturbation theory XIII. Treatment of constants of motion in resolvent method, partitioning technique, and perturbation theory. *International Journal of Quantum Chemistry*, 2(6):867–931, November 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Lowdin:1969:BRB**

- [Löw69a] Per-Olov Löwdin. Book review: *Selected scientific papers of Egil A. Hylleraas*. Edited by: John Midtdal, Harald Wergeland, and Knut Thalberg. Published by: NTH Press, Trondheim, Norway, 1968. Price: \$27 for both volumes. *International Journal of Quantum Chemistry*, 3(2):246, March 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [MTW68].

**Lowdin:1969:I**

- [Low69b] Per-Olov Lowdin. Introduction. *International Journal of Quantum Chemistry*, 3(S3a):iv–x, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.



**Lowdin:1969:SCP**

- [Löw69c] Per-Olov Löwdin. Some comments on the periodic system of the elements. *International Journal of Quantum Chemistry*, 3(S3a):331–334, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Loxsom:1969:ORH**

- [Lox69] F. M. Loxsom. Optical rotation of helical polymers: End effects. *International Journal of Quantum Chemistry*, 3(S3a):147–152, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Lefebvre:1969:EMH**

- [LP69] R. Lefebvre and R. F. Prat. Études en méthode de Hartree–Fock avec projection. I. Fonctions propres de  $S^2$ . Evaluation de l’énergie. (french) [Studies of the projective Hartree–Fock method. I. eigenfunctions of  $S^2$ . Energy evaluation]. *International Journal of Quantum Chemistry*, 3(1):93–105, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Litinskij:1969:EWH**

- [LRBG69] A. Litinskij, R. Rakauskas, J. Batarūas, and J. Glembockis. An extended Wolfsberg–Helmholz calculation on europium tetraacetylacetonate. *International Journal of Quantum Chemistry*, 3(3):373–376, May 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Lefebvre:1967:BOA**

- [LS67a] R. Lefebvre and M. Garcia Sucre. Born–Oppenheimer approach to the vibronic structure of molecular dimers. *International Journal of Quantum Chemistry*, 1(S1):339–350, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Lefebvre:1967:EHF**

- [LS67b] Roland Lefebvre and Yves G. Smeyers. Extended Hartree–Fock calculations for the helium ground state. *International Journal of*



*Quantum Chemistry*, 1(4):403–419, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Lin:1969:HAE**

- [LT69] S. H. Lin and D. Tweed. The heavy atom effect on the phosphorescence of aromatic hydrocarbons. I. *International Journal of Quantum Chemistry*, 3(S3a):315–324, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Malli:1967:MHS**

- [Mal67] Gulzari Malli. Magnetic hyperfine structure constants calculated from numerical Hartree–Fock wave functions. *International Journal of Quantum Chemistry*, 1(S1):115–122, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Malinowski:1969:UAA**

- [Mal69] S. Malinowski. On uncoupled approximation with approximate form of the Hartree–Fock operator. *International Journal of Quantum Chemistry*, 3(6):763–766, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Manne:1968:NKO**

- [Man68] Rolf Manne. A note on Kaufman’s overlap population criterion for molecular stability. *International Journal of Quantum Chemistry*, 2(1):69–71, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Mantione:1969:PCD**

- [Man69] Marie-José Mantione. Polarization contribution to the dipole moment and infrared spectrum intensity of the benzene–iodine complex. *International Journal of Quantum Chemistry*, 3(2):185–194, March 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Marcus:1967:VMC**

- [Mar67] Paul M. Marcus. Variational methods in the computation of energy bands. *International Journal of Quantum Chemistry*, 1(S1):567–588, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the



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

**Martino:1968:LISa**

- [Mar68a] F. Martino. Localized impurity states in the Hartree–Fock, LCAO approximation. I. *International Journal of Quantum Chemistry*, 2(2):217–232, March 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Martino:1968:LISb**

- [Mar68b] F. Martino. Localized impurity states in the Hartree–Fock, LCAO approximation II. The F Center in KCl. *International Journal of Quantum Chemistry*, 2(2):233–263, March 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Matthias:1967:TGS**

- [Mat67] B. T. Matthias. Three groups of superconductors. *International Journal of Quantum Chemistry*, 1(S1):773–774, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Matthias:1968:RDS**

- [Mat68] Bernd T. Matthias. Recent discoveries in superconductivity. *International Journal of Quantum Chemistry*, 2(S2):359–361, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Matthias:1969:RRN**

- [Mat69] Bernd T. Matthias. Recent results with new superconductors. *International Journal of Quantum Chemistry*, 4(S3b):903–904, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Millie:1968:AEC**

- [MB68] Philippe Millie and Gaston Berthier. All-electron calculations of open-shell polyatomic molecules I. SCF wave function in Gaussians for methyl and vinyl radicals. *International Journal of Quantum Chemistry*, 2(S2):67–73, January 15–20, 1968. CODEN IJQCB2.



ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Moody:1969:TDV**

- [MB69] Sandra Z. Moody and Charles L. Beckel. Theoretical determination of vibration-rotation properties for the  $B^1\Sigma_u^+$  state of  $H_2$ . *International Journal of Quantum Chemistry*, 4(S3b):469–478, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**McWeeny:1967:NEC**

- [McW67] R. McWeeny. The nature of electron correlation in molecules. *International Journal of Quantum Chemistry*, 1(S1):351–359, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Mestechkin:1967:DMT**

- [Mes67a] M. M. Mestechkin. The density matrix in the two-particle function method. *International Journal of Quantum Chemistry*, 1(5):675–692, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Mestechkin:1967:TPD**

- [Mes67b] M. M. Mestechkin. Two-particle density functions for a spin-projected single Slater determinant. *International Journal of Quantum Chemistry*, 1(4):421–425, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Malli:1967:DSC**

- [MF67a] Gulzari Malli and Charlotte Froese. Diamagnetic susceptibilities calculated from numerical Hartree–Fock wave functions. *International Journal of Quantum Chemistry*, 1(S1):99–101, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Malli:1967:EFG**

- [MF67b] Gulzari Malli and Charlotte Froese. Electric field gradients and quadrupole coupling constants calculated from numerical Hartree–Fock wave functions. *International Journal of Quantum Chem-*



*istry*, 1(S1):103–109, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Malli:1967:FCI**

- [MF67c] Gulzari Malli and Charlotte Froese. Fermi contact interaction constants calculated from numerical Hartree–Fock wave functions. *International Journal of Quantum Chemistry*, 1(S1):111–114, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Malli:1967:NMS**

- [MF67d] Gulzari Malli and Charlotte Froese. Nuclear magnetic shielding constants calculated from numerical Hartree–Fock wave functions. *International Journal of Quantum Chemistry*, 1(S1):95–98, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Michels:1968:VCIa**

- [MH68] H. H. Michels and F. E. Harris. Valence configuration interaction calculations for atomic scattering. *International Journal of Quantum Chemistry*, 2(S2):21–27, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Michels:1969:VCI**

- [MH69] H. H. Michels and F. E. Harris. Valence configuration interaction calculations for atomic scattering. *International Journal of Quantum Chemistry*, 3(5):751, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Miles:1969:CDN**

- [MIR<sup>+</sup>69] Daniel W. Miles, Warren H. Inskeep, Morris J. Robins, Michael W. Winkley, Roland K. Robins, and H. Eyring. Circular dichroism of nucleoside derivatives. VII. The electronic structure and spectra of some simple nucleoside derivatives. *International Journal of Quantum Chemistry*, 3(S3a):129–145, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Sup-



plement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**McWeeny:1968:SPN**

- [MK68] R. McWeeny and W. Kutzelnigg. Symmetry properties of natural orbitals and geminals I. Construction of spin- and symmetry-adapted functions. *International Journal of Quantum Chemistry*, 2(2):187–203, March 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Macintyre:1968:EED**

- [ML68] Walter M. Macintyre and Per-Olov Löwdin. Electronic energy of the DNA replication plane. *International Journal of Quantum Chemistry*, 2(S2):207–217, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Mathur:1967:OTL**

- [MM67a] S. C. Mathur and E. G. Mckannan. The omega technique LCAO–MO calculations for the hydrogen phthalocyanine molecules. *International Journal of Quantum Chemistry*, 1(S1):247–250, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Mead:1967:DLV**

- [MM67b] C. Alden Mead and Albert Moscovitz. Dipole length versus dipole velocity in the calculation of infrared intensities with Born–Oppenheimer wave functions. *International Journal of Quantum Chemistry*, 1(3):243–249, May 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Modrak:1968:SCF**

- [Mod68] P. Modrak. Self-consistent-field method including correlation effect for atomic systems. Three- and four-electron atomic systems. *International Journal of Quantum Chemistry*, 2(6):857–866, November 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Moffat:1968:PNC**

- [MP68] J. B. Moffat and H. E. Popkie. Physical nature of the chemical bond II. Valence atomic orbital and energy partitioning studies



of linear nitriles. *International Journal of Quantum Chemistry*, 2 (5):565–597, September 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Mcnaughton:1969:IKS**

- [MS69] David J. Mcnaughton and Vedene H. Smith, Jr. An investigation of the Kohn–Sham and Slater approximations to the Hartree–Fock exchange potential. *International Journal of Quantum Chemistry*, 4(S3b):775–788, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Midtdal:1968:SSPa**

- [MTW68] John Midtdal, Knut Thalberg, and Harald Wergeland, editors. *Selected Scientific Papers of Egil A. Hylleraas*, volume 1. NTH-Trykk, Trondheim, Norway, 1968. viii + 445 pp. LCCN Q143.H98 A25 1968.

**Mulliken:1967:AQN**

- [Mul67] Robert S. Mulliken. The assignment of quantum numbers for electrons in molecules. Extracts from Phys. Rev. 32, 186–222 (1928), plus currently written annotations. *International Journal of Quantum Chemistry*, 1(1):103–117, January 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Mulliken:1969:IHP**

- [Mul69] Robert S. Mulliken. Introduction of the Honorary President of the Symposium. *International Journal of Quantum Chemistry*, 3 (S3a):3, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Marron:1968:VPE**

- [MW68] Michael T. Marron and Johan H. Weare. A variation principle for energy differences between states of two different Hamiltonians. *International Journal of Quantum Chemistry*, 2(5):729–734, September 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Nesbet:1967:TMA**

- [Nes67] R. K. Nesbet. Transition metal atoms in cubic configurations. *International Journal of Quantum Chemistry*, 1(S1):633–643, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Newton:1969:SCM**

- [New69] Marshall D. Newton. Self-consistent molecular orbital calculations by least-squares projection of 2-center charge distributions. *International Journal of Quantum Chemistry*, 3(S3a):251–255, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Nielsen:1967:AID**

- [Nie67] Harald H. Nielsen. Anomalies in the intensity distributions of rotation-vibration lines in the spectra of polyatomic molecules. *International Journal of Quantum Chemistry*, 1(3):217–223, May 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Orloff:1969:ZFS**

- [OB69] M. K. Orloff and J. S. Brinen. Zero-field splitting in phosphorescent triplet states of aromatic hydrocarbons IV. Phenyl naphthalenes. *International Journal of Quantum Chemistry*, 3(2):225–230, March 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Packer:1969:FET**

- [PALB69] J. C. Packer, J. S. Avery, J. Ladik, and G. Biczó. The first excited triplet states of the nucleotide bases calculated with different semiempirical SCF schemes. *International Journal of Quantum Chemistry*, 3(1):79–92, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Peat:1967:AGW**

- [PB67] F. David Peat and R. J. C. Brown. The antisymmetrization of geminal wave functions. *International Journal of Quantum Chemistry*, 1(S1):464–474, January 16–21, 1967. CODEN IJQCB2.



ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Pople:1967:RPA**

- [PBO67] J. A. Pople, D. L. Beveridge, and N. S. Ostlund. Recent progress in approximate self-consistent-field theory. *International Journal of Quantum Chemistry*, 1(S1):293–305, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Pullman:1969:TFP**

- [PBWFN69] Bernard Pullman, Ernst D. Bergmann, Hannah Weiler-Feilchenfeld, and Zohar Neiman. Tautomeric forms of purines resulting from proton shifts between nitrogens N<sub>7</sub> and N<sub>9</sub>. *International Journal of Quantum Chemistry*, 3(S3a):103–111, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Polansky:1967:CTL**

- [PD67a] Oskar E. Polansky and Gerhard Derflinger. Zur Clar'schen Theorie Lokaler Benzoider Gebiete in Kondensierten Aromaten. (German) [On the Clar localization theory in condensed aromatic benzenoids]. *International Journal of Quantum Chemistry*, 1(4):379–401, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Preuss:1967:RPW**

- [PD67b] H. Preuss and G. Diercksen. Eine Rechenzeitsparende Programmierung des Wellenmechanischen Self-Consistent-Field Verfahrens für Moleküle (SCF MO LCGO-Verfahren). (German) [A computational time-saving programming of the wave-mechanical self-consistent field method for molecules (SCF MO LCGO method)]. *International Journal of Quantum Chemistry*, 1(5):605–613, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Preuss:1967:WAMa**

- [PD67c] H. Preuss and G. Diercksen. Wellenmechanische Absolutrechnungen an Molekülen und Atomsystemen mit der SCF MO LC



(LCGO) Methode. I. Das Cyclopentadienylanion ( $C_5H$ ). (German) [Wave-mechanical ab initio calculation for molecules and atomic systems with the SCF MO LC (LCGO) method. I. Cyclopentadienylanion ( $C_5H$ )]. *International Journal of Quantum Chemistry*, 1(4):349–355, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Preuss:1967:WAMb**

- [PD67d] H. Preuss and G. Dierksen. Wellenmechanische Absolutrechnungen an Molekülen und Atomsystemen mit der SCF MO LC (LCGO) Methode. III. Das Cyclopropan ( $C_3H_6$ ). (German) [Wave-mechanical ab initio calculation for molecules and atomic systems with the SCF MO LC (LCGO) method. III. Cyclopropane ( $C_3H_6$ )]. *International Journal of Quantum Chemistry*, 1(4):361–364, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Preuss:1967:WAMe**

- [PD67e] H. Preuss and G. Dierksen. Wellenmechanische Absolutrechnungen an Molekülen und Atomsystemen mit der SCF MO LC (LCGO) Methode. IX. Das System  $(Li_2H)^-$ . (German) [Wave-mechanical ab initio calculation for molecules and atomic systems with the SCF MO LC (LCGO) method. IX The  $(Li_2H)^-$  system]. *International Journal of Quantum Chemistry*, 1(5):641–644, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Preuss:1967:WAMc**

- [PD67f] H. Preuss and G. Dierksen. Wellenmechanische Absolutrechnungen an Molekülen und Atomsystemen mit der SCF MO LC (LCGO) Methode. V. Bindungsbeteiligung der Inneren Elektronen des C-Atoms. (German) [Wave-mechanical ab initio calculation for molecules and atomic systems with the SCF MO LC (LCGO) method. V. Binding of inner electrons of the C atom]. *International Journal of Quantum Chemistry*, 1(4):369–372, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Preuss:1967:WAMd**

- [PD67g] H. Preuss and G. Dierksen. Wellenmechanische Absolutrechnungen an Molekülen und Atomsystemen mit der SCF MO LC (LCGO) Methode. VII. Das System  $(LiH_2)^-$ . (German) [Wave-mechanical ab initio calculation for molecules and atomic systems



with the SCF MO LC (LCGO) method. VII. The  $(\text{LiH}_2)^-$  system]. *International Journal of Quantum Chemistry*, 1(5):631–635, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Pack:1969:AEW**

- [PD69] Russell T. Pack and John S. Dahler. Asymptotic evaluation of WKB matrix elements. *International Journal of Quantum Chemistry*, 3(S3a):329, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Peradejordi:1969:TSD**

- [PDFA69] F. Peradejordi, R. Domingo, and J. I. Fernández-Alonso. Theoretical study of the derivative hydrocarbons of biphenylene. I. Electronic spectrum of the biphenylene. *International Journal of Quantum Chemistry*, 3(5):683–698, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Painter:1969:DNM**

- [PE69] G. S. Painter and D. E. Ellis. A direct numerical method for the energy band problem: Preliminary results for Li. *International Journal of Quantum Chemistry*, 4(S3b):801–805, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Peacock:1968:FQC**

- [Pea68] T. E. (Thomas Edward) Peacock. *Foundations of quantum chemistry*. John Wiley, New York, NY, USA, 1968. ISBN 0-471-67454-0. ix + 162 pp. LCCN QD462 .P4.

**Pepinsky:1969:ESS**

- [Pep69] Ray Pepinsky. Exchange scattering of slow electrons by antiferromagnetic surface structures. *International Journal of Quantum Chemistry*, 4(S3b):423–445, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.



**Pao:1967:DQL**

- [PFB67] Yoh-Han Pao, H. L. Frisch, and R. Bersohn. Double quantum light scattering and orientational correlations in liquids. *International Journal of Quantum Chemistry*, 1(S1):829–837, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Prosser:1968:RCM**

- [PH68] Franklin Prosser and Stanley Hagstrom. On the rapid computation of matrix elements. *International Journal of Quantum Chemistry*, 2(1):89–99, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Piela:1969:LRI**

- [Pie69] Lucjan Piela. Long-range interactions in the ground and two excited states of the  $\text{HeH}^+$  molecule. *International Journal of Quantum Chemistry*, 3(6):945–968, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Pullman:1967:PSC**

- [PK67] A. Pullman and E. Kochanski. On the possibilities of semiempirical calculations of zero-field splitting parameters. *International Journal of Quantum Chemistry*, 1(S1):251–259, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Prat:1969:EMH**

- [PL69] R. F. Prat and R. Lefebvre. Etudes en méthode de Hartree–Fock avec projection ... II. La fonction d’onde exacte d’un système de deux électrons dans un état  $^1\text{S}$  comme projection d’un déterminant de Slater. (French) [Studies of the projective Hartree–Fock method. II. The exact wavefunction for a two-electron system in a  $^1\text{S}$  state as a projection of a Slater determinant]. *International Journal of Quantum Chemistry*, 3(4):503–511, July 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Pao:1969:RCD**

- [PO69] Yoh-Han Pao and J. R. Onstott. Reflection circular dichroism of naturally optically active substances. *International Journal of*



*Quantum Chemistry*, 3(S3a):119–128, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Pratt:1967:IMM**

- [PP67] G. W. Pratt, Jr. and N. J. Parada. Interband momentum matrix elements and a  $k \cdot p$  interpolation method applied to PbTe. *International Journal of Quantum Chemistry*, 1(S1):589–594, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Pohl:1967:SSC**

- [PR67] Herbert A. Pohl and L. M. Raff. Simplified SCF calculations for  $\sigma$ -bonded systems. II. The interhalogens. *International Journal of Quantum Chemistry*, 1(5):577–589, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Preuss:1968:SMP**

- [Pre68] H. Preuss. Das SCF–MO–P (LCGO)-Verfahren und seine Varianten. (German) [The SCF–MO–P (LCGO)-method and variations]. *International Journal of Quantum Chemistry*, 2(5):651–662, September 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Preuss:1969:EDE**

- [Pre69a] H. Preuss. Zur Eindeutigkeit der Darstellungen von Energiehyperflächen. (German) [On the uniqueness of the representations of energy surfaces]. *International Journal of Quantum Chemistry*, 3(1):123–130, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Preuss:1969:KEG**

- [Pre69b] H. Preuss. Zur konstruktion von energiehyperflächen. (German) [On the construction of energy surfaces]. *International Journal of Quantum Chemistry*, 3(1):131–139, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Primas:1967:DFR**

- [Pri67] H. Primas. A density functional representation of quantum chemistry. I. Motivation and general formalism. *International Jour-*



*nal of Quantum Chemistry*, 1(4):493–519, July 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Polansky:1967:ERF**

- [PS67] O. E. Polansky and P. Schuster. Estimation of relative free enthalpies of activation by HMO methods. *International Journal of Quantum Chemistry*, 1(S1):285–292, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Pipano:1968:CSC**

- [PS68] A. Pipano and I. Shavitt. Convergence studies in configuration interaction calculations. *International Journal of Quantum Chemistry*, 2(6):741–749, November 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Pollak:1969:NPD**

- [PS69] M. Pollak and A. Sagar. A note on the pressure dependence of the ionization energies of some donor states. *International Journal of Quantum Chemistry*, 4(S3b):857–864, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Pullman:1967:A**

- [Pul67] B. Pullman. Announcement. *International Journal of Quantum Chemistry*, 1(1):119, January 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Pullman:1968:CSD**

- [Pul68] Alberte Pullman. A comparative study of different all-valence-electrons calculations on biological purines and pyrimidines. *International Journal of Quantum Chemistry*, 2(S2):187–205, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Pullman:1969:CSB**

- [Pul69] Bernard Pullman. Conjugated systems in biology. *International Journal of Quantum Chemistry*, 3(S3a):83–102, January 13–18,



1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Rebane:1969:VLB**

- [RB69] T. K. Rebane and P. A. Braun. Variational lower bound for the polarizability of the ground state. *International Journal of Quantum Chemistry*, 3(6):1061–1064, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Rein:1968:CLV**

- [RCP68] Robert Rein, Pierre Claverie, and Michael Pollak. On the calculation of London–van der Waals interactions in a monopole-bond polarizability approximation with application to interaction between purine and pyrimidine bases. *International Journal of Quantum Chemistry*, 2(1):129–144, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Rastelli:1969:CDA**

- [RD69] Augusto Rastelli and Giuseppe Del Re. On the choice and definition of atomic orbital-bases. II. Promoted Slater orbitals and best-atom hydrogen-like orbitals. *International Journal of Quantum Chemistry*, 3(5):553–568, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Reid:1967:TPS**

- [Rei67] Charles E. Reid. Transformation of perturbation series into continued fractions, with application to an anharmonic oscillator. *International Journal of Quantum Chemistry*, 1(5):521–534, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Raccah:1969:ECH**

- [RH69] P. M. Raccah and V. E. Henrich. Experimental comparison of Hartree–Fock and Slater exchange potentials in aluminum from the charge density point of view. *International Journal of Quantum Chemistry*, 4(S3b):797–800, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.



**Ramaker:1968:HSI**

- [RHC<sup>+</sup>68] D. E. Ramaker, G. L. Hagnauer, R. E. Carlson, R. F. Gaetano, H. Crain, and David M. Schrader. Helium states II. Perturbation treatment of the ground state using the coordinates  $r_<$  and  $r_>$ . *International Journal of Quantum Chemistry*, 2(4):509–520, July 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Rice:1968:CTC**

- [Ric68] O. K. Rice. On charge-transfer complexes in the vapor phase. *International Journal of Quantum Chemistry*, 2(S2):219–224, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Rothenberg:1969:MSQ**

- [RKS<sup>+</sup>69] Stephen Rothenberg, With Peter Kollman, Maurice E. Schwartz, Edward F. Hayes, and Leland C. Allen. Mole. A system for quantum chemistry I. general description. *International Journal of Quantum Chemistry*, 4(S3b):715–725, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Roth:1967:SWS**

- [Rot67a] Laura M. Roth. Spin wave stability of the ferromagnetic state for a narrow  $s$  band. *International Journal of Quantum Chemistry*, 1(S1):649–650, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Rothenberg:1967:MEW**

- [Rot67b] Stephen Rothenberg. Many-electron wave functions represented as naturally correlated pairs: I. Method and application to  $H_2$  and  $LiH$ . *International Journal of Quantum Chemistry*, 1(S1):475–484, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.



**Raffenetti:1969:POM**

- [RR69] Richard C. Raffenetti and Klaus Ruedenberg. Parametrization of an orthogonal matrix in terms of generalized Eulerian angles. *International Journal of Quantum Chemistry*, 4(S3b):625–634, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Rein:1967:TPV**

- [RS67] Robert Rein and Saša Svetina. The two proton vibrational states in nucleic acid hydrogen bonds. *International Journal of Quantum Chemistry*, 1(S1):171–174, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Roby:1969:PPP**

- [RS69] Keith R. Roby and Oktay Sinanoğlu. On the performance and parameter problems of approximate molecular orbital theory, with comparative calculations on the carbon monoxide molecule. *International Journal of Quantum Chemistry*, 3(S3a):223–236, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Rosenthal:1968:CUL**

- [RW68] C. M. Rosenthal and E. Bright Wilson, Jr. Calculation of upper and lower bounds for eigenvalues by a boundary condition method: The quartic oscillator, hydrogen molecule ion, and helium atom. *International Journal of Quantum Chemistry*, 2(S2):175–185, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Sabin:1968:HBSa**

- [Sab68a] John R. Sabin. Hydrogen bonding in simple  $\pi$ -electron systems I. Pyridinium–pyridine. *International Journal of Quantum Chemistry*, 2(1):23–30, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Sabin:1968:HBSb**

- [Sab68b] John R. Sabin. Hydrogen bonding in simple  $\pi$ -electron systems II. Pyridine–pyrrol. *International Journal of Quantum Chemistry*, 2(1):31–36, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Sack:1967:AME**

- [Sac67a] R. A. Sack. An alternative method for expanding the product of two Slater wave functions. *International Journal of Quantum Chemistry*, 1(S1):369–373, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Sack:1967:ERR**

- [Sac67b] R. A. Sack. An extension of the Rayleigh–Ritz method for finding upper and lower bounds of eigenvalues. *International Journal of Quantum Chemistry*, 1(S1):517–522, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Sadlej:1969:VAS**

- [Sad69] Andrzej J. Sadlej. Vibronic absorption spectrum of the ethylene dimer. *International Journal of Quantum Chemistry*, 3(5):569–580, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Sen:1967:FEM**

- [SB67] Purnendra Nath Sen and Sadhan Basu. Free-electron model for the inelastic collision of fast electrons with benzene. *International Journal of Quantum Chemistry*, 1(5):591–594, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Sen:1968:FEMa**

- [SB68a] Purnendranath Sen and Sadhan Basu. Free-electron model and triplet-state lifetime of benzene. *International Journal of Quantum Chemistry*, 2(2):183–186, March 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Sen:1968:FEMb**

- [SB68b] Purnendranath Sen and Sadhan Basu. Free-electron model for hyperpolarizability of the  $\pi$ -electron system in benzene. *Interna-*



*tional Journal of Quantum Chemistry*, 2(5):687–694, September 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Sen:1969:FEMa**

- [SB69a] Purnendranath Sen and Sadhan Basu. Free-electron model for anisotropy of  $\pi$ -electron polarizability in benzene. *International Journal of Quantum Chemistry*, 3(1):1–2, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Sen:1969:FEMb**

- [SB69b] Purnendranath Sen and Sadhan Basu. Free-electron model for electronic spectra of benzene. *International Journal of Quantum Chemistry*, 3(5):611–619, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Sutton:1969:MCM**

- [SBD<sup>+</sup>69] P. Sutton, P. Bertoncini, G. Das, T. L. Gilbert, Arnold C. Wahl, and O. Sinanoğlu. Methods for correlating molecules and some optimized valence configuration results on the diatomic molecules Li<sub>2</sub>, Be<sub>2</sub>, B<sub>2</sub>, C<sub>2</sub>, N<sub>2</sub>, F<sub>2</sub>, BN, BeO, LiF, HeNe, CO, and BF. *International Journal of Quantum Chemistry*, 4(S3b):479–497, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Seprödi:1969:EEF**

- [SBL69] L. Seprödi, G. Biczó, and J. Ladik. The effect of electric field on the electronic structure of DNA. I. Calculation of the polarizability and of the permanent dipole moment for the nucleotide bases and base pairs. *International Journal of Quantum Chemistry*, 3(5):621–634, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Svetina:1967:CCF**

- [SBŽ67] S. Svetina, R. Blinc, and B. Žekš. Consistency criterion for ferroelectric free energy cluster expansion. *International Journal of Quantum Chemistry*, 1(S1):755–758, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.



**Shatas:1968:CMI**

- [SC68] Romas A. Shatas and C. Alton Coulter. Constants of motion in an interacting electron-lattice system. *International Journal of Quantum Chemistry*, 2(S2):323–332, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Schmidtke:1968:TAS**

- [Sch68a] Hans-Herbert Schmidtke. Topological aspects of symmetric molecules. II. *International Journal of Quantum Chemistry*, 2(S2):101–105, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Schneiderman:1968:AMC**

- [Sch68b] S. B. Schneiderman. Atom-molecule correlation tables for linear ( $D_{\infty h}$ ) and bent ( $C_{2v}$ ) molecular electronic states of symmetric triatomic molecules. *International Journal of Quantum Chemistry*, 2(S2):89–100, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Schnupp:1968:CAA**

- [Sch68c] P. Schnupp. The calculation of atomic associations using LISP. *International Journal of Quantum Chemistry*, 2(5):599–605, September 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Schnupp:1968:TNA**

- [Sch68d] Peter Schnupp. On the total number of atomic associations of an  $N$ -atomic molecule. *International Journal of Quantum Chemistry*, 2(3):349–357, May 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Schuster:1969:LMS**

- [Sch69a] Peter Schuster. LCAO–MO studies on hydrogen bonding: The interaction between carbonyl and hydroxyl groups. *International Journal of Quantum Chemistry*, 3(6):851–871, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Schweig:1969:LRI**

- [Sch69b] A. Schweig. Long range intermolecular forces between conjugated systems. *International Journal of Quantum Chemistry*, 3(6):823–849, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Steele:1967:CAS**

- [SCM67] Richard H. Steele, Louis Chopin Cusachs, and S. P. McGlynn. Carcinogenic activity and the spectra of aromatic hydrocarbons. *International Journal of Quantum Chemistry*, 1(S1):179–186, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Synek:1967:SAA**

- [SCRG67] M. Synek, L. Corsiglia, R. Repka, and P. Grossgut. Some applications of atomic analytical wave functions. *International Journal of Quantum Chemistry*, 1(S1):89–94, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Stukel:1969:CVE**

- [SEC69] D. J. Stukel, R. N. Euwema, and T. C. Collins. Comparison of various exchange potentials in self-consistent OPW energy band calculations for cubic ZnS and ZnSe. *International Journal of Quantum Chemistry*, 4(S3b):789–796, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Segerstедt:1969:CBC**

- [Seg69a] Torgny Segerstedt. Can biology, chemistry and physics be reduced into moral and social philosophy? or the duty of scholars to cooperate. *International Journal of Quantum Chemistry*, 3(S3a):341–345, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Segerstедt:1969:OAH**

- [Seg69b] Torgny Segerstedt. Opening Address at the Henry Eyring Symposium. *International Journal of Quantum Chemistry*, 3(S3a):1–2,



January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Seiler:1969:RBO**

- [Sei69] Rudolf Seiler. A remark on the Born–Oppenheimer approximation. *International Journal of Quantum Chemistry*, 3(1):25–32, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Serre:1967:SCN**

- [Ser67] Josiane Serre. On the subgroups contained in the nuclear magnetic resonance symmetry group. *International Journal of Quantum Chemistry*, 1(S1):713–717, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Serre:1968:CTS**

- [Ser68] Josiane Serre. Character tables of the Schrödinger supergroups. *International Journal of Quantum Chemistry*, 2(S2):107–123, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Seybold:1969:BRB**

- [Sey69] Paul G. Seybold. Book review: *Reactivity of the photoexcited organic molecule. Proceedings of the Thirteenth Conference on Chemistry at the University of Brussels, October 1965*. Published by: Interscience Publishers, London, New York, Sydney, 1967. Price: \$15. *International Journal of Quantum Chemistry*, 3(2):245–246, March 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Ano67g].

**Sallavanti:1969:SSL**

- [SF69] Robert A. Sallavanti and Donald D. Fitts. A semiempirical SCF–LCAO–MO treatment of some oxygen- and nitrogen-containing heterocyclic molecules. *International Journal of Quantum Chemistry*, 3(1):33–43, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Sabin:1969:SCP**

- [SFH69] John R. Sabin, Sighart Fischer, and G. L. Hofacker. SCF Calculation for proton-phonon coupling in a linear model of ice. *International Journal of Quantum Chemistry*, 3(S3a):257–263, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Sachs:1967:MFI**

- [SG67] Lester M. Sachs and Murraray Geller. MOSES, a FORTRAN IV system for polyatomic molecules. *International Journal of Quantum Chemistry*, 1(S1):445–455, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Szent-Gyorgyi:1969:ETI**

- [SG69] Albert Szent-Györgyi. Energy transport and DA interactions. *International Journal of Quantum Chemistry*, 3(S3a):157–168, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Silberman:1968:AAM**

- [SGP68] Z. Silberman, Z. Gershgorin, and R. Pauncz. Application of the AMO method to non-alternant systems. *International Journal of Quantum Chemistry*, 2(4):453–462, July 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Shaw:1969:SCH**

- [Sha69] G. Shaw. Some calculations on the hydrogen bond: The system  $\text{LiH} \cdot \text{Li}^+$ . *International Journal of Quantum Chemistry*, 3(2):219–224, March 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Shin:1968:IMC**

- [Shi68] Hyung Kyu Shin. Inelastic molecular collisions with an orientation-averaged interaction energy. *International Journal of Quantum Chemistry*, 2(2):265–279, March 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Shull:1969:CME**

- [Shu69] Harrison Shull. The calculation of matrix elements for valence bond functions. *International Journal of Quantum Chemistry*, 3(4):523–534, July 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Swanstrom:1969:WAS**

- [SJP69a] P. Swanstrøm, R. Janoschek, and H. Preuss. Wellenmechanische Absolutberechnung Schwingungsspektroskopischer Daten am Äthylen. (German) [Wave-mechanical ab initio calculation: Vibrational data for ethylene]. *International Journal of Quantum Chemistry*, 3(6):881–887, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Swanstrom:1969:WAH**

- [SJP69b] P. Swanstrøm, R. Janoschek, and H. Preuss. Wellenmechanische absolutrechnung am  $\text{HeHHe}^+$ . (German) [Wave-mechanical ab initio calculation of  $\text{HeHHe}^+$ ]. *International Journal of Quantum Chemistry*, 3(1):115–121, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Smith:1968:OCS**

- [SK68] Vedene H. Smith, Jr. and Werner Kutzelnigg. Open- and closed-shell states in few-particle quantum mechanics. II. Classification of atomic states. *International Journal of Quantum Chemistry*, 2(4):553–562, July 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Slater:1967:CPS**

- [Sla67a] J. C. Slater. Correlation problems in solids. *International Journal of Quantum Chemistry*, 1(S1):783–789, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Slater:1967:EBF**

- [Sla67b] J. C. Slater. Energy bands and Fermi surfaces. *International Journal of Quantum Chemistry*, 1(S1):523–531, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.



**Slater:1967:QPA**

- [Sla67c] J. C. Slater. Quantum physics in America between the wars. *International Journal of Quantum Chemistry*, 1(S1):1–23, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Slater:1967:CSS**

- [Sla67d] John C. Slater. The current state of solid-state and molecular theory. *International Journal of Quantum Chemistry*, 1(1):37–102, January 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Slater:1969:SCF**

- [Sla69] J. C. Slater. The self-consistent field for crystals. *International Journal of Quantum Chemistry*, 4(S3b):727–746, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Smith:1969:IAS**

- [SLM69] Darwin W. Smith, Everett G. Larson, and Robert C. Morrison. On the interpretative aspects of second-order reduced density matrices. *International Journal of Quantum Chemistry*, 4(S3b):689–696, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Song:1967:MOS**

- [SM67] Pill-Soon Song and Thomas A. Moore. Molecular-orbital studies of the mechanism of xanthine oxidase-catalyzed oxidation of purines, especially 2-chloropurine. *International Journal of Quantum Chemistry*, 1(5):699–719, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Saxena:1969:SOO**

- [SM69] K. M. S. Saxena and Gulzari Malli. Spin-other-orbit and spin-orbit interactions in  $f^2$  and  $f^3$  electron configurations. *International Journal of Quantum Chemistry*, 3(6):1045–1054, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Smet:1969:TQDa**

- [Sme69a] P. Smet. Théorie quantique du pouvoir rotatoire magnétique des molécules diamagnétiques. I. Formalisme general. (French) [Quantum theory of magnetic rotatory power of diamagnetic molecules. I. General formalism]. *International Journal of Quantum Chemistry*, 3(4):417–444, July 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Smet:1969:TQDb**

- [Sme69b] P. Smet. Théorie quantique du pouvoir rotatoire magnétique des molécules diamagnétiques. II. Applications. (French) [Quantum theory of magnetic rotatory power of diamagnetic molecules. II. Applications]. *International Journal of Quantum Chemistry*, 3(5):593–610, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Sochilin:1969:BWF**

- [Soc69] G. B. Sochilin. On the behaviour of the wave function for the  $2^3S$  state of the two-electron atom in the region where both electron–nuclear distances are small. *International Journal of Quantum Chemistry*, 3(3):297–301, May 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Song:1968:ESSa**

- [Son68a] Pill-Soon Song. Electronic structures and spectra of halogenated purines and pyrimidines II.  $\pi$ -Electronic structure of 2-chloropurine and its related derivatives. *International Journal of Quantum Chemistry*, 2(2):281–296, March 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Song:1968:ESSb**

- [Son68b] Pill-Soon Song. Electronic structures and spectra of halogenated purines and pyrimidines III.  $\sigma$ -Electronic structure and some comments on the mechanism of the xanthine oxidase reaction of 2-halopurines and related analogs. *International Journal of Quantum Chemistry*, 2(2):297–306, March 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Song:1968:TCS**

- [Son68c] Pill-Soon Song. A theoretical consideration of the spectral properties of flavin tautomers and imino flavins. *International Journal of*



*Quantum Chemistry*, 2(4):463–470, July 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Song:1969:TCE**

- [Son69] Pill-Soon Song. Theoretical considerations of the electronic spectra of methyl flavins. *International Journal of Quantum Chemistry*, 3(3):303–316, May 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Skutnik:1968:CEE**

- [SÖS68] B. Skutnik, I. Öksüz, and O. Sinanoğlu. Correlation effects in the excited states of atoms the  $1s^2 2s^n 2p^m$  configuration of carbon, nitrogen, and oxygen. *International Journal of Quantum Chemistry*, 2(S2):1–11, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Sundaram:1968:MOC**

- [SP68] K. Sundaram and William P. Purcell. Molecular-orbital calculations on some mesoionic compounds. *International Journal of Quantum Chemistry*, 2(1):145–157, January 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Saturno:1967:COC**

- [SR67] Antony F. Saturno and Ronald M. Rutledge. Correlation and the one-center method. *International Journal of Quantum Chemistry*, 1(S1):327, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Sahni:1967:QMT**

- [SS67a] R. C. Sahni and B. C. Sawhney. Quantum-mechanical treatment of molecules. I. Calculations of the potential energy curves and molecular constants of the ground and ionized states of  $N_2$ . *International Journal of Quantum Chemistry*, 1(3):251–270, May 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Stettler:1967:EPI**

- [SS67b] John D. Stettler and Romas A. Shatas. Electron-phonon interaction and piezospectroscopic shifts of sharp spectral lines in solids.



*International Journal of Quantum Chemistry*, 1(S1):775–782, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Scherr:1968:STM**

- [SS68] Charles W. Scherr and Frank C. Sanders. Some transition moments via perturbation methods for the helium isoelectronic series. *International Journal of Quantum Chemistry*, 2(S2):29–34, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Stettler:1969:BSD**

- [SS69] John D. Stettler and Romas A. Shatas. Bond stretch in diatomic vibrotors induced by rotational-vibrational interaction. *International Journal of Quantum Chemistry*, 4(S3b):635–640, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Sternheimer:1967:QAF**

- [Ste67] R. M. Sternheimer. Quadrupole antishielding factors for ions and atomic states. *International Journal of Quantum Chemistry*, 1(S1):67–80, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Steinfeld:1969:ALR**

- [Ste69a] J. I. Steinfeld. Appearance of long-range interatomic forces in molecular potential curves. *International Journal of Quantum Chemistry*, 4(S3b):615–616, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Steinfeld:1969:SVR**

- [Ste69b] J. I. Steinfeld. Slow vibrational relaxation in liquids. *International Journal of Quantum Chemistry*, 3(S3a):325, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium



on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Sucre:1969:DCM**

- [Suc69] M. García Sucre. Dimères composés de molécules dont l'excitation électronique entraîne un déplacement de la configuration nucléaire d'équilibre accompagné d'un changement de constante de force. (French) [dimers composed of molecules whose excitation electronic results in a shift of equilibrium nuclear configuration with a change of force constant]. *International Journal of Quantum Chemistry*, 3(4):377–396, July 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Sullivan:1969:SFC**

- [Sul69] John J. Sullivan. Some formal comments on spin projected Hartree–Fock theory. *International Journal of Quantum Chemistry*, 4(S3b):601–606, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Soda:1969:RLB**

- [SW69] Kunitsugu Soda and Akiyoshi Wada. Rayleigh-line broadening in the scattered light from chemically reacting media. *International Journal of Quantum Chemistry*, 3(S3a):153–156, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory and Quantum Biology.

**Taylor:1968:UPF**

- [Tay68] William J. Taylor. Uniqueness of Parseval's formula and Born's hypothesis on probability densities in quantum mechanics. *International Journal of Quantum Chemistry*, 2(5):735–737, September 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Thorson:1967:RDM**

- [TCH67] W. R. Thorson, J. H. Choi, and R. B. Hake. Reduced density matrices for valence-bond wave functions. *International Journal of Quantum Chemistry*, 1(S1):487–510, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Thompson:1967:SWD**

- [Tho67] Eric D. Thompson. Spin wave dispersion and energy bands in fcc metals. *International Journal of Quantum Chemistry*, 1(S1): 619–625, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Thulstrup:1969:ALE**

- [Thu69] Erik W. Thulstrup. Assignment of the lowest electronic transitions in benzene,  $C_6H_6$ . *International Journal of Quantum Chemistry*, 4(S3b):641–649, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Tomasek:1969:NCB**

- [TK69] M. Tomášek and J. Koutecký. Nature of the chemisorption bond on semiconductor surfaces. *International Journal of Quantum Chemistry*, 3(3):249–267, May 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Tomasek:1969:CBS**

- [Tom69a] Mojmir Tomášek. Complex band structure and localized states on solid surfaces. *International Journal of Quantum Chemistry*, 4(S3b):847–848, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Tomasek:1969:FTA**

- [Tom69b] Mojmir Tomášek. Field theoretical approach to a correlation model in solids. *International Journal of Quantum Chemistry*, 4(S3b):849–850, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.



**Tamir:1968:SDP**

- [TP68] Ilana Tamir and Ruben Pauncz. The spin degeneracy problem in the AMO method. *International Journal of Quantum Chemistry*, 2(4):433–444, July 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Thompson:1969:MSS**

- [TPM69] Jess Thompson, Michael Povich, and Boris Musulin. Molecular screening and spectroscopic constants. *International Journal of Quantum Chemistry*, 4(S3b):513–518, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**VonBunau:1967:WAM**

- [VDP67] G. Von Bünau, G. Dierksen, and H. Preuss. Wellenmechanische Absolutrechnungen an Molekülen und Atomsystemen mit der SCF MO LC (LCGO) Methode. X. Das Methylkation  $(\text{CH}_3)^+$ . (German) [Wave-mechanical ab initio calculation for molecules and atomic systems with the SCF MO LC (LCGO) method. X. The methyl cation  $(\text{CH}_3)^+$ ]. *International Journal of Quantum Chemistry*, 1(5):645–647, September 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Vaughan:1968:SMO**

- [VFC68] John D. Vaughan, David C. Fullerton, and Chin-An Chang. Semiempirical molecular-orbital calculations of the basicities of pyrazole, imidazole, and methyl-substituted pyrazoles and imidazoles: Inductive model of electron release. *International Journal of Quantum Chemistry*, 2(2):205–216, March 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Wang:1969:EBO**

- [Wan69] P. S. C. Wang. Error bounds for the overlap of approximate wave functions. *International Journal of Quantum Chemistry*, 3(1):57–66, January 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Watson:1967:CFS**

- [WB67a] R. E. Watson and M. Blume. Crystal field splittings and first-order magnetic phase transitions. *International Journal of Quantum Chemistry*, 1(S1):645, January 16–21, 1967. CODEN IJQCB2.



ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**White:1967:ASF**

- [WB67b] Ronald J. White and W. Byers Brown. On the analytic solution of the first-order perturbed wave function of the two-electron atom. *International Journal of Quantum Chemistry*, 1(S1):61–66, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Wahl:1967:RPB**

- [WBDG67] Arnold C. Wahl, Peter J. Bertoncini, G. Das, and T. L. Gilbert. Recent progress beyond the Hartree–Fock method for diatomic molecules: The method of optimized valence configurations. *International Journal of Quantum Chemistry*, 1(S1):123–152, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Wahl:1969:BNI**

- [WBKL69] Arnold C. Wahl, P. Bertoncini, K. Kaiser, and R. Land. Bison: A new instrument for the experimentalist. *International Journal of Quantum Chemistry*, 4(S3b):499–512, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Weinhold:1969:RLBa**

- [Wei69a] F. Weinhold. Remark on lower bounds to eigenvalues. *International Journal of Quantum Chemistry*, 3(3):371–373, May 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Weinhold:1969:RLBb**

- [Wei69b] F. Weinhold. Remark on lower bounds to eigenvalues. *International Journal of Quantum Chemistry*, 3(5):751, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Weltin:1969:CIS**

- [Wel69] E. Weltin. Convergent iterative solutions for the lowest state of a system with large perturbations. *International Journal of Quan-*



*tum Chemistry*, 3(5):635–650, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Wilson:1967:LBE**

- [Wil67] Timothy M. Wilson. Lower bounds to eigenvalues of the Schrödinger equation by the partitioning technique. *International Journal of Quantum Chemistry*, 1(S1):511–516, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Wilson:1968:SPE**

- [Wil68] Timothy M. Wilson. Spin-polarized energy bands in antiferromagnetic MnO. *International Journal of Quantum Chemistry*, 2(S2):269–276, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

**Wilson:1969:SES**

- [Wil69] Timothy M. Wilson. A study of the electronic structure of the first-row transition-metal compounds. *International Journal of Quantum Chemistry*, 4(S3b):757–774, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Wahl:1967:EMI**

- [WL67] Arnold C. Wahl and Robert H. Land. The evaluation of multicenter integrals by polished brute force techniques. I. analysis, numerical methods, and computational design of the potential-charge distribution scheme. *International Journal of Quantum Chemistry*, 1(S1):375–401, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Wallis:1969:VMA**

- [WMP69] A. Wallis, D. L. S. McElwain, and H. O. Pritchard. The variation method and the algebraic eigenvalue problem. *International Journal of Quantum Chemistry*, 3(5):711–722, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).



**Wood:1969:ASC**

- [Woo69] J. H. Wood. Atomic SCF calculations for the first transition series. *International Journal of Quantum Chemistry*, 4(S3b):747–755, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Weare:1967:RAF**

- [WP67] John H. Weare and Robert G. Parr. Remark on the analytical form of  $1s$  orbitals in atoms and molecules. *International Journal of Quantum Chemistry*, 1(S1):163–165, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Westhaus:1969:STP**

- [WS69a] P. Westhaus and O. Sinanoğlu. The structure and transformation properties of correlation functions for open shell states of molecules in non-orthogonal AO as well as in MO bases. *International Journal of Quantum Chemistry*, 4(S3b):391–411, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Wilson:1969:RFA**

- [WS69b] Gail Wilson and Harris J. Silverstone. Rational function approximation for atomic and molecular wave functions. *International Journal of Quantum Chemistry*, 3(6):1067–1068, November 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

**Yamashita:1967:BSA**

- [YA67a] Jiro Yamashita and Seturo Asano. Band structure of antiferromagnetic chromium. *International Journal of Quantum Chemistry*, 1(S1):627–632, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Yamashita:1967:BSK**

- [YA67b] Jiro Yamashita and Seturo Asano. Band structure of KCl by Green's function method. *International Journal of Quantum Chemistry*, 1(S1):611–614, January 16–21, 1967. CODEN



IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Yoshimine:1967:GSL**

- [YM67] M. Yoshimine and A. D. Mclean. Ground states of linear molecules: Dissociation energies and dipole moments in the Hartree–Fock approximation. *International Journal of Quantum Chemistry*, 1(S1):313–326, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

**Young:1969:NI**

- [You69] John H. Young. Nonadiabatic interactions. *International Journal of Quantum Chemistry*, 4(S3b):607–613, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

**Zucker:1968:IPI**

- [Zuc68] I. J. Zucker. Intermolecular potentials of the inert gases from their melting curves. *International Journal of Quantum Chemistry*, 2(S2):225–232, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.