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$^{+}$ [ANB94, BCMÖ97, BB95, CWZ98b, CLOFR98, Csa96, FV96, Gao93, HL79, JM93a, KKWT99, KGS93, KA95a, MMRSN92, NBS95, PS93, PHH94, Pro94, Pro95, SPS96b, SZ97b, STC96, TNSM99, WY99, WMD95, YD96, YSHD97]. $^{+(-)}$ [BCY95]. $_{2}^{+}$ [BK94b, ELMY96, SC95, ZTC97]. $_{3}^{+}$ [WSB94]. $^{-}$ [CLOFR98, Csa96, JPD67, KKWT99, KK93, KGS93, MTNF99, Oku98, Ort98a, SEKEB98, WYZ$^+$92]. $^{---}$ [Kal90]. $_{2}^{-}$ [ZTC97]. $_{I}^{-}$ [DM97b]. $_{II}^{-}$ [DM97b]. $_{II}^{-} \rightarrow$ [DM97b]. ^{0} [CBAM97]. ^{1} [BP93a, BYGA99, CBT93a, CRSP93, GAdAC97, HMK96a, HMK96c, HMK96b]. ^{119} [GAdAC97]. ^{13} [GS97b, GAdAC97, KH96a, RN96]. ^{131} [SCL96]. ^{17} [KH96a]. ^{19} [GAdAC97]. $^{1}A_{1}$ [CCS98]. $^{1}A\prime$ [KA96]. $^{1}B_{u}^{+}$ [NNH98]. $^{1}\mathrm{E}_{2g}^{-}$ [BČ95]. $^{1}\Sigma$ [CWJ$^+$99]. $^{1}\Sigma^{+}$ [BFV$^+$93, TGS99]. $^{1}\Sigma_{g}^{+}$ [BP93a]. $^{1}\Sigma_{g}^{+} - a^{1}\Delta_{g}$ [MLK94]. ^{2} [BKL97, BLK97, BP93a, ELMY96, Man99, PS93, Sel93, SZ97b, WY99]. $^{2+}$ [BL99, BB95, BDH$^+$97, CAJ95, CG97b, DWB98, EJ93, JM93a, KGS93, MMRSN92, OSS95, TJ97, Wil90]. $^{2+/3+}$ [ZBL99]. $_{1}^{2-}$ [LGT94]. $_{4}^{2-}$ [BADM97]. $_{II}^{2-}$ [DM97b]. ^{207} [GAdAC97]. ^{29} [GAdAC97]. $^{2}\Pi_{g}$ [MM94]. $^{2}\Sigma^{+}$ [LBG97]. ^{3} [BP93a, CBT93a, CRSP93]. $^{3+}$ [BDH$^+$97, DdJN95, MNC95]. $^{3-}$ [NG95]. ^{35} [GAdAC97]. $^{3}\Pi_{g}$ [TGS99]. $^{3}\Sigma^{-}$ [FV96]. ^{4} [HMLK98]. $^{4+}$ [ABCM93, SK99a]. $^{5+}$ [Cze99, SK99a]. ^{6} [Tew94, Tew97]. $^{6+}$ [SK99a]. $^{6-}$ [XYC98]. $^{7+}$ [SK99a]. $_{4}^{8+}$ [BB95]. ^{e} [BLK97]. $^{\infty}$ [KP97]. ^{M} [PAT93]. ^{N} [PAT93, KS95b]. $^{n+}$ [WMZ98]. ^{o} [BKL97]. $_{0.4}$ [Li97]. $_{0.6}$ [Li97]. $_{0.8}$ [Min96]. $_{1}$ [DM98, ELMY96, GJOV97, LGT94, MW92]. $_{1-x}$ [WZ99]. $_{1.2}$ [Min96]. $_{105}$ [RKPE95]. $_{111}$ [RKPE95]. $_{12}$ [Csa96, Eva97, TST$^+$99]. $_{123}$ [RKPE95]. $_{13}$ [LMC97a]. $_{1}^{2}$ [DM99]. $_{1A}$ [PW97]. $_{2}$ [AS93, ANB94, ACHT95, Ali99, ABCM93, ABDM94, ADM98, BA91, BILA95, BUZ94, BDNT97, BBC$^+$94, BP93b, BP93a, BHGC99, BML98, BB94, BYE$^+$97, BCY95, BDH$^+$97, CWX93, Cai93, Cai94, CPBC95, CR96b, CGG96, CB93b, CB94a, CF93, CPD$^+$98, CDP$^+$99, DSS90, DdJN95, DZ97, EBG95, FdCC92, FSBS$^+$95, FCVL98, FMD$^+$96, GKKM96, GJPZ97, Gin97, GS93, GJOV97, GZDZ97, GL96a, GL96b, HMGP93, HBL99, HP98, Hir92, IBS95, JMP99, JKK$^+$92, Jen94, JMD95, JJ97, Jur97e, KJ95, KA96, KP97, Li93, LF95, LV97, MSS95, Man95, MLT98, MHM95a, MECE97, MHY98, MK90, MLL99, MM94, MGNK95, MTD93, MTTS93, MCS98, MZ95, MDM94, MD91, NM95, NBS95, NL96b, OTS$^+$95, Oku98, Ort98b, PBS99, PSBL98, PPSK96, PPK97, PGS97, PK76, Pro94, RN96, RA91, RA97, RA96, RCWN94, RKH$^+$98]. $_{2}$ [Roz97, RP98b, RS97b, SE93b, SM96a, SCP$^+$95a, SAB$^+$97, SL93, SRP$^+$98, SX96, SZC97, SST93, STMR97, SCS94, SZCO99, SGGMGFS96, SES93, SG97, SGB98, Spe72a, Sta98b, SC95, STC96, SC99, SNH99, TJ97, TGS99, TMA97, TPR96, TFSZ95, TZCT97, TMD96a, TMD96c, VH96a, VJ95, VJ97, WY99, WI96a, WI96c, WI96b, WDS97, WL99, WMD95, YNMT98, YNST99, YD96, YSHD97, YK97, ZC96a, ZC96c, ZC96b, ZTC97, ZBL99, ZGPS97, vBN95]. $_{2}(A)$ [GL96c]. $_{20}$ [CXFP99]. $_{24}$ [WYW96]. $_{240}$ [CXFP99]. $_{26}$ [RG99]. $_{28}$ [LSC98]. $_{2}^{+}$ [Ata97a, BSHP97, CGG96, GSSD$^+$96, JEB92, LA97, LBG97, MUMH97, Pro95, RS97b, Sch97, SBOB97]. $_{2}^{-}$ [BMG95, CGG96, LBG97]. $_{2h}$

[BBC92]. $_{2n}$ [GFY$^+$99]. $_2 \rightarrow$ [XFF98]. $_3$ [AMC97, BUZ94, Boe91, BDD93, CCC$^+$95a, CLOFR98, CEM$^+$96, DZ97, DM98, DLF99, FCVL98, Fra99, Gao93, GWB97, GAdAC97, Hag99a, JMP99, Jen94, KP96, Kal90, KJ95, KLO$^+$98, KGS93, LJ95, LDGA96, Li93, LF95, MCL95, MLT98, MGNK95, Moc99, Nag96a, Nag96c, Nag96b, Oku98, PZTPMC99, PCF94, PPSK96, PPK97, RN96, RA91, SL93, SRP$^+$98, SBAD90, SP91, SZC97, SL97, SC99, VX99, WY99, WL99, WMZ98, WZ99, XFF98, YK97]. $_{3-\delta}$ [Li97]. $_{3-y}$ [Min98]. $_{32}$ [XYC98]. $^+_3$ [BMG95, Hag99a, KLT97, TMA97]. $^-_3$ [NG96]. $^2_3$ [DM99]. $_3 \cdots$ [PZTPMC99]. $_3 \rightarrow$ [YD96]. $_4$ [AS93, ABCM93, BL99, BILA95, BUZ94, BHGC99, BBC92, BB97a, BL98, DZ97, FCVL98, GS93, Gut99b, HP98, JKK$^+$92, JKJ94, JG95, Jen94, KP96, KGS93, KC97, LSC98, LCS98, MVS97, MHM95b, MNC95, PCF94, RKG96, SC99, WYW96, WY99, WI96a, WI96c, WI96b, vBN95]. $_{40}$ [LCS98]. $^{+1}_4$ [MVS97]. $^{2-}_4$ [CCWCF96]. $_{42}$ [BBC92]. $_4 \rightarrow$ [YSHD97]. $_5$ [CCC$^+$95a, DWB98, KJ95, KGS93, NM95, NG95, NG96, OSS95, RA91, SG96a, SG96c, SG96b, SC98b, SC99]. $_{5+\delta}$ [Min96]. $_6$ [BL99, BUZ94, BBC92, Bou96a, Bou96c, Bou96b, BDH$^+$97, Csa96, Cze99, DN96, DdJN95, JKK$^+$92, MLL99, RA91, RKG96, Spe72a, TJ97, Thu69, WG94, ZBL99]. $_{60}$ [BBZ91, BSS$^+$97b, CCC$^+$95a, DM98, DM99, HRRBL97, HL93b, LL99, SZCO99, TST$^+$99, TFSZ95, XY95, YZX96a, YZX96c]. $^{2-}_{60}$ [HOF$^+$97]. $^{3-}_{60}$ [HOF$^+$97]. $_7$ [Li93, SG97, WL99]. $_{70}$ [BBZ91, LFS94, TZCT97]. $_{78}$ [AS99, RG99]. $_8$ [BUZ94, CG97b, Csa96, Eva97, GSSD$^+$96, JG95, RA91]. $_{80}$ [CXFP99, SLA97]. $_{81}$ [REL$^+$90]. $_{86}$ [SLA97]. $_{87}$ [REL$^+$90]. $_{88}$ [SLA97]. $_9$ [KP97, XYC98]. $_{93}$ [RKPE95]. $_B$ [CMSF93]. $_c$ [DMB97, Fri93a, Fri93b, Li93]. $_I$ [DM97b]. $_{II} \rightarrow$ [DM97b]. $_\infty$ [FMD$^+$96]. $_J$ [Man99]. $_n$ [AS93, BDD93, Cas97, CCS99, GFY$^+$99, Ike99, IP93, IBS95, Kar90, LDP93, LCP$^+$91, MKRW99, NYKY98, ST97, SPR94, WMD95, XKB$^+$99]. ^-_n [KSN93]. $_s[\rho]$ [LBPL97]. $_X$ [YZX96c, BSS$^+$97b, GFRR94, LXWZ99, SZCO99, SL97, WZ99]. $_x[\rho]$ [LBPL97]. $_y$ [LF95, SZCO99]. $\mathrm{A}, \mathrm{A}' =$ [YZX96a]. a, a^* [GH96b]. A_1 [Min94a]. $\mathrm{A}_2\mathrm{B}_2 \leftarrow \mathrm{X}^2\mathrm{A}_1$ [BJ98]. $\mathrm{A}_x\mathrm{A}'_{3-x}\mathrm{C}_{60}$ [YZX96a]. AgCl^- [VABM94]. AgF^- [VABM94]. $\mathrm{Al}^+(^1S) + \mathrm{H}_2 \rightarrow \mathrm{AlH}^+(^2\Sigma^+) + \mathrm{H}$ [RNS93]. α [FMS$^+$99, HWB97a, JI95, KG98, NSS$^+$95, SWMB94, SST93, VABM94, Woo98]. $\alpha 2$ [VDD96]. α^2 [BSS97a]. α_N [ZLHZ94, ZLHZ94]. as [HHKM95]. Be [OJB77]. β [CFR96, FWZ97, HWB97b, HWB97a, NMSJ99, TCB99]. β_2 [GHB$^+$99]. C_2 [TMD96b]. C_{60} [LRM93, RRC94, YZX96b]. $C_{60}2n$ [LRM93]. $\mathrm{C}_{60}\mathrm{NH}_2^+$ [TFSZ95]. $\mathcal{L}_\mathcal{N}$ [FJR96]. $\mathcal{S}_N$ [FJRS97]. $\cdot$ [MTTS93]. $\cdots$ [CEM$^+$96, SST93, VH96a]. CH^+ [OJB77]. $\mathrm{CoAl}_2\mathrm{Cl}_8(g)$ [DDC97]. D [DBM99, Hos97, MK97a, Flo95, GFRR94, LTSL96a, Mor96a, TV92, BK95]. D_{2h} [Har97a]. δ [LTSL96b]. $\Delta^{-1/2}$ [NS95b]. e [Pai97, PL98, Pai99]. $e^- + \mathrm{N}_2$ [PGM95]. η [DMB97]. η^5 [SC98b, SC99]. f [Boe96a, Boe96c, Boe96b, MD94]. $f(r)$ [PZDM97, PZDM98]. g [LBG95, LG96b, LG96a, LG96c]. $GaAs_{1-x}P_x$ [SPFL93]. γ [Bla99, SRP$^+$98]. $h - b - 1$ [GT97, TG96]. H_2 [Cun92]. $\mathrm{H}_2\mathrm{N}$

SGB98, SL97, SC99, SNH99, TST+99, YZX96c, YZX96b].

A. [Kum93b]. **A/T** [LSGS91]. **A2** [ARdAB95]. **AA** [SST93]. **Ab-Initio** [FR92, FR93a, RK91, SKRK90]. **Abacus** [Sri97]. **Above** [CB96a, CB96c, CB96b]. **Above-Threshold** [CB96a, CB96c, CB96b]. **Absolute** [RPB+97, Sie93]. **Absolutrechnungen** [JPD67]. **Absorbed** [DP94]. **Absorption** [AEAO99, AHM97, BJ98, BFV92, BMG+98, Che96, CCZ97, GSSD+96, KLT97, SZ95, WDCA97, LA97, SZ97b]. **Abstraction** [BCS96, Jur97a, YNMT98]. **AC** [SST94, Moi97]. **Acceleration** [Sel93, TMR99]. **accelerator** [Kin99]. **Accelerators** [Hom93]. **Acceptor** [EE91, FKR92, Mor93a, Mor96b, AB99, GBS99, MCT99]. **Account** [MG93a, PTP95]. **Accounts** [PB97b]. **ACCs** [BG98c]. **Accuracy** [JKRW98, JGR98, JMR98, LDP93, LH94, MDM94, Nuñ95b, TNS96a, TNS96b, UWB94, TNS96c, Ber96b]. **Accurate** [Aqu95, BKL97, BLK97, BS95, DLV95, Dun96, Dun97, EJ93, FFD96c, FFD96b, FR93b, IYFI99, JM99, Jur97a, KKT93, KLLI97, MHL94, NB93, Nuñ94a, SGGC99, Sim98, SLD95, Tas93, Taş96a, BSS97a, FFD96a, New97, NL96b]. **ACE** [Ish96]. **ACES** [SGW+92]. **Acetaldehyde** [ADPS98]. **Acetaldehyde/Vinyl** [ADPS98]. **Acetaldimine** [ADPS98]. **Acetaldimine/Vinylamine** [ADPS98]. **Acetate** [STS95]. **Acetic** [FT95, FT96, FT97a, RTKP96a, RTKP96c, RTKP96b, RT99, RT98]. **Acetone** [MR92, PBB92, DV96]. **Acetonitrile** [MDD93]. **Acetyl** [RK95]. **Acetylene** [FF94a, Fou94, Jur99a]. **Acetyloxyl** [KVS98]. **acetylpropanamide** [ZH99a]. **ACh** [WJC+98]. **AChE** [WJC+98, WJC+99]. **AChE-catalyzed** [WJC+98, WJC+99]. **Achieving** [MVS97]. **Acid** [AP93, AP96, BKEMM94, BAK97, BHB+95, CLR+93, CFR96, DM95, FT95, FY95, FR92, Flo95, GJLA99, KE91, Les92, LX95, NSS+95, PHBB94, RFG99, Ram90, Ram94, RTKP95, RTKP96a, RTKP96b, RT98, SPG97, SHC+98, Tew94, YW92, FT96, FT97a, HWB97a, KK99b, LHNK99, RTKP96c, RT99, SSM+99, Tew97, TFR99, TBP99]. **Acid-Base** [SPG97]. **Acidic** [BKR97]. **Acidities** [BMP93, MBP91, RPB+97, SSN99]. **Acidity** [PLG95]. **Acids** [AHM97, BDG96, BKWL97, CLC90, MBP97, HWB97b, KKM99, MKBP97]. **ACPQ** [PTP95, PTP95]. **Acrylonitrile** [HDY+91, MMA+92]. **Action** [JGCJ96a, JGCJ96c, WD91, JGCJ96b]. **Activated** [NP96b]. **Activating** [DAF+96]. **Activation** [CBSR+98, Cun92, CC96, Jur97a, MÅ99b, MC94, PW97, PVU+93, RR94, RNS93, Sak98, ST96b, TWK+92, BYE+97, FMS+99, PBS99, SC98b, SC99]. **Activation/Cyclization** [MC94]. **Active** [EBG95, HM99, KM90, KN99b, KW98, KSK91, NK98, SBIP97b, TKK+90, VC92, GFGB99, KK99a, KN99a, MHY98, SZCO99, WWFR99]. **Active-site** [HM99, GFGB99]. **Active-Space** [EBG95]. **Activity** [BBE95, FT95, GJOV97, HB94, Khu92, Lev94, NHN97, NZA92, PW97, Pul90, RFM90, Reg92, SM94, SC96a, SC96c, TBBE98, ZCT98, BTKVG99, Bha99, CMA+99, FT96, FT97a, SC96b]. **Actually** [Sta98c]. **Acylation**

SAL^{+}94, vH96b, Sta95, Sta96a, SL97, SDG97, SPR94, SJ91, SJR91, Tal93, TJ95, Tos95, Tri97, VABM94, VV95, VIK98, VAVN91, WD95, WZW96]. **Calculations** [WB94, Wen96b, Wen96a, WP90, Wil96, YNY99, ZO94, ZO95, ZC95, dVJ93, AMC97, BK97, Bla99, BT96b, Boe97, BJA99, Bou96c, BB97a, DV96, Egu96c, ELMY96, FWS97, FFD96a, Gur99, HR99, HS99, Jac98, KLO^{+}98, KH96a, KKNY99, KF96c, LMC97b, LFD99, LBL98, LXWZ99, MKRW99, MVS97, MECE97, MSS99b, NV97a, Ort98a, Ort99, PWL98, PSBL98, RP98b, SGGC99, SEKEB98, Sta96b, Sta98d, Sta98e, SZ97b, Sut99b, ZDO99, ZWD98a, ZWD98b, Van96, vMVvLvD97, SJ97, WGP99]. **Calculus** [Kin96, Ney95b]. **Call** [Ano98b, Ano98c, Ano98d, Ano98e, Ano98f, Ano98g, Ano98h, Ano98i, Ano98j, Ano98k, Ano98l, Ano98m]. **Callaway** [Tri95]. **cam** [CL90]. **Camphor** [CL90]. **Can** [Bau98, GVK99]. **Cancer** [LFB96, Lad97a]. **Cannabinoid** [RFM90, Reg92]. **Cannabinoids** [PHBB95]. **Canonical** [FK94]. **capacities** [NOY98]. **Capacity** [Pal93a]. **Capping** [ZLWES99]. **Capture** [BMA93, BF96, KSW98, SK99a]. **Car** [Kry93]. **Carbanions** [OKI98]. **Carbene** [Cio93, Sak98]. **Carbenes** [SG97, SGB98]. **Carbides** [SGB97]. **Carbon** [AMRT94, AMKS93, BKS96, BF95, KL94, MR92, Suh93, TAY^{+}97, VMCK97, WTSN94, XR94]. **Carbon-** [Suh93]. **Carbon-Carbon** [BF95]. **Carbonic** [BAK97]. **Carbonyl** [ET97, VBUS99, GS97b]. **Carbonyls** [SZL95, SG96a, SG96b, SG97, SGB98, MSMR99, SG96c, Van96]. **Carborane** [RA91]. **Carborane-Hydrocarbon** [RA91]. **Carboranes** [PK77]. **Carboxyl** [KVS98]. **Carboxylic** [MBP97, MKBP97]. **carbyne** [DM98, DM99]. **Carcinogen** [WP90]. **Carcinogens** [LP97b]. **Cardiac** [MBV^{+}98]. **Career** [Kas99]. **Carlo** [ACB^{+}99, ACAT92, ACHT95, BBMM99, BBC^{+}94, BBC^{+}96b, BRA^{+}99, BRV99, Cor97, CDC98, KNN96b, KNN96c, KNN96d, KKNN97, KI94, Kid99, MB97b, Rey90, Rot96, Rot97, UBA92, VBD^{+}98]. **Carotenoids** [TCM98]. **Carriers** [LTSL96c, LTSL96a, LTSL96b]. **Cartesian** [Sch92, KA95b, Le 97, SF95b]. **CAS** [PPP97, YNY99]. **CAS-SCF** [YNY99]. **Case** [BA91, CT95, LB96b, LB96d, RRC94, BBMM99, LB96c, MVS97, PCD99, SC99, TMA97, Whi99]. **cases** [hJH97]. **Casimir** [Mon94]. **CASMP2** [YTYS97]. **CASPT2** [BBC^{+}96a]. **CASSCF** [BBOR96, BBC^{+}96a, GMMH97, LHNK99, MCOS94, Pra97, SG93, XLW^{+}99, YTYS97]. **CASVB** [CTG97, TC98b]. **Catacondensed** [Ran97]. **Catalysis** [FB96, MÅ96, SNMB97, SPG97, Tch96b, KÅ99]. **Catalysts** [EZ93, SDE94]. **Catalytic** [CJX^{+}92, EZ92, HBH98, NHN97, PB95b, Ryd94, DD99, FNSV99, GWB97, XYC98]. **Catalyzed** [BT96a, BT96c, PHBB94, SJ91, BT96b, KKS99, WJC^{+}98, WJC^{+}99]. **Catastrophe** [MS90]. **Cathodic** [HDY^{+}91]. **Cation** [AKD96, BLC95, GKKM96, GMS97, Jur99a, Yam97, Gal98, YNNR97]. **Cationic** [Bou94, FW92a, FW92b]. **Cations** [BSHP97, HDB^{+}95, LE92, MKM93b, Pro95]. **Cauchy** [BOX94]. **Caused** [TMDB98]. **causing** [Hag99b]. **Cavities** [PB95b, RPJZW96, ZWJP95]. **Cavity** [CDD^{+}99]. **CBC** [KJ95]. **cc** [GR95a]. **CCCH** [CMF^{+}98]. **CCD**

PMS94, RW92, Spr96, TFSZ95, TZCT97, XSG97, BL99, BGS99, BT96b, Dia99, FMD^{+}96, Fra99, GJDD97, KP96, Li97, MECE97, PS99a, SZCO99, TST^{+}99, WG99, BHGC99, KJ97]. Students [Ano99n]. Studied [FWT^{+}96, LSGS91, PIG94, RHC96, Ryd94, SAFK97, TNSE94, ZY94, GZSvD99, hJH97]. Studies [ART94a, dAdM95, AK97, BKWL97, BJMT94, BHH92, BZQ95, BCS96, BDH^{+}97, Cai93, CL97, CCC^{+}95a, CPBC95, CBSR^{+}98, CXL97, CDC98, EZ92, FF94a, FF94b, FT95, FB96, FLF96, GBVM93, GJLA99, GL96a, GL96b, HCR94, Har97a, HS92a, HHKM95, HBH98, JY94, Jur98b, KSR95, Kar90, KS94b, KN92, KL92, LKM99, LYSL95, LSS96a, LSS96b, Les92, LX95, LB94, LC93, Löw68b, LG71, LKU90, LCP^{+}91, MZ95, MR92, MZ93, MGK99, MC95, Mor98a, MFCA93, NNMH96, NONY97, Nak92, NHN97, Pau92, PVLG93, PBB94a, PS68, PCF94, PS94b, RKPE95, RKG96, Sak97, SA96, SP92, SCP93, SSM90, Spr93, Sta98a, SZ98, TZCT97, TCZ91, TSPK96, TB95, TD96b, WY95, WP92, YOTY93, YXX99, YTYS97, ZYY95, BH99, CP99b, DA97, DP96, FT96, FF96, FT97a, GFY^{+}99, GL96c, Hag99a, HWB97b, HWB97a]. studies [LSS96c, NMN^{+}99, NL96b, RC99, Tri98c, WJC^{+}99]. Study [AL95, ADB95, AKD96, AP93, ANB94, AMT^{+}99, AHI96, AR96, AMKS93, ABCM93, ADPS98, BLC95, BAR94, BA97b, BAN97, Bat92, BBOR96, BTTS97, BJ98, BILA95, BEG94, BCLS94, BLE96, BBC^{+}96a, BSP97, BSHP97, BHX96, Boč96, BP92, BHH92, BjH97, BAK96a, BAK96b, BAK97, BCRL94, BPL97b, BRA^{+}99, Bra97b, BHPB93, BHPB95, BVV91, BMVV93, BS95, BMG95, Bue96, BLG95, BDD93, BK94c, BvL96, CBAM97, CWX93, Cai94, CdBKZ99, CPN91, CRSP93, CCC^{+}95b, CCB^{+}97, Che96, Che97, CL92, CA97, CCZ97, DS96, DD97a, DN96, DDRB96, DAR^{+}96a, DB94a, DSS90, DD96a, DD96c, DZ96a, DV91, DZ97, DD93, DDC97, Dun99, ESP98, EMMK94, ET97, ET99, EDF^{+}98, FY95, FLRV97, FMDA94, FDF97, FGM90, FL95, FDD^{+}93, FWBT94, FKR92, Gal96, GG97a, GD96, GBL97, GL98, HK95a, HDY^{+}91, HP97]. Study [II94, JGCJ96a, JGCJ96c, JKK^{+}92, Jai70, JKRW98, JGR98, JMR98, JDJP99, JMS95, JSKC95, Jur96b, Jur97f, Jur99b, Jur99a, KW92, KSN93, KI94, KH96a, Kry98, KGVM97, KG99, KL97c, LV93, LJ95, LMV92, Les91, LHL91, LGT94, LH94, Lio92, LFD94, LSC98, Lu99, LBG95, MKK96a, MKK96b, MKK98, MRT97, MCOS94, MKDL93, MMRSN92, MLA93, MALT96, MTP^{+}98, MDD93, Mav98, MB98, MG93b, MRL99, MTD93, MDJ98, MY99, MK99, MC94, MKM96, Mor97a, MBML91, MCA95, MS90, MBP97, NSS^{+}95, NN94, NFVM94, NM95, OTS^{+}95, Oli99, Pal94, Pan93, PMM97, PP98a, PHH94, PFMC97, PLV92, PPP97, PM93, PBB92, PB95b, PZ95, PMJM^{+}91, PHBB92, PBBH93, PHBB95, RL95, RTKP96a, RTKP96b, RM96, Réc90, RGHH94, RK91,

References

Avery:1993:CRQ

[AAS93] J. Avery, F. Antonsen, and I. Shim. 4-Currents in relativistic quantum chemistry. *International Journal of Quantum Chemistry*, 45(6):573–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Adams:1996:AAS

[AB96] Barry G. Adams and E. J. Brandas. Algebraic approach to simple quantum systems. *International Journal of Quantum Chemistry*, 57(2):259–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anglada:1997:RSM

[AB97] Josep Maria Anglada and Josep Maria Bofill. On the restricted step method coupled with the augmented Hessian for the search of stationary points of any continuous function. *International Journal of Quantum Chemistry*, 62(2): 153–165, March 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42498;`

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42498&PLACEBO=IE.pdf.

Amos:1999:NCF

[AB99] A. T. Amos and B. L. Burrows. A note on current flow in donor-bridge-acceptor systems. *International Journal of Quantum Chemistry*, 74(5):585–594, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62503009; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62503009&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Adhikari:1993:DDM

[ABB93] S. Adhikari, S. P. Bhattacharyya, and D. M. Bhattacharyya. Decay dynamics of a metastable state in a time-varying electric field: A three-level prototypical system. *International Journal of Quantum Chemistry*, 47(3):213–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andres:1993:VDS

[ABCM93] J. Andres, A. Beltran, J. Carda, and G. Monros. V^{4+} doping into SiO_2, ZrO_2 and $ZrSiO_4$ structures. an ab initio perturbed ion study. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:175–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Andres:1994:VSE

[ABDM94] J. L. Andres, J. Bertran, M. Duran, and J. Marti. Vibrational Stark effect and vibrational static electric properties of N_2O. *International Journal of Quantum Chemistry*, 52(1):9–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Avery:1997:FTA

[ABLA97] John Avery, Wensheng Bian, John Loeser, and Frank Antonsen. Fourier transform approach to potential harmonics. *International Journal of Quantum Chemistry*, 63(1):5–14, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42574;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42574&PLACEBO=IE.pdf.

Alonso:1995:NFE

[ABR95] J. A. Alonso, L. C. Balbas, and A. Rubio. Nonlocal functionals for exchange and correlation in density functional theory: Application to atoms and to small atomic clusters. *International Journal of Quantum Chemistry*, 56(5):499–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Angyan:1994:CAM

[ÁC94] János G. Ángyán and Christophe Chipot. A comprehensive approach to molecular charge density models: From distributed multipoles to fitted atomic charges. *International Journal of Quantum Chemistry*, 52(1):17–37, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alonso:1995:ECD

[AC95] J. A. Alonso and N. A. Cordero. Exchange and correlation in density functional theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:49–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Alexander:1997:AWF

[AC97] S. A. Alexander and R. L. Coldwell. Atomic wave function forms. *International Journal of Quantum Chemistry*, 63(5):1001–1022, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42649; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42649&PLACEBO=IE.pdf.

Alexander:1992:CAM

[ACAT92] S. A. Alexander, R. L. Coldwell, G. Aissing, and A. J. Thakkar. Calculating atomic and molecular properties using variational Monte Carlo methods. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:213–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Akhmatskaya:1999:MCS

[ACB+99] Elena V. Akhmatskaya, Matthew D. Cooper, Neil A. Burton, Andrew J. Masters, and Ian H. Hillier. Monte Carlo simulations of water clusters on a parallel computer using an ab initio potential. *International Journal of Quantum Chemistry*, 74(6):709–719, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001787; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001787&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Alexander:1995:HEE

[ACHT95] S. A. Alexander, R. L. Coldwell, R. E. Hoffmeyer, and A. J. Thakkar. High-energy electron and X-ray scattering from H_2 using Monte Carlo techniques. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:627–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Anusooya:1998:RCC

[ACPR98] Y. Anusooya, Aparna Chakrabarti, Swapan K. Pati, and S. Ramasesha. Ring currents in condensed ring systems. *International Journal of Quantum Chemistry*, 70(3):503–513, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75017; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75017&PLACEBO=IE.pdf.

Avram:1997:FCF

[AD97] N. M. Avram and Gh. E. Drăgănescu. Franck–Condon factors for the Morse potential. *International Journal of Quantum Chemistry*, 64(6):655–660, September 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42726; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42726&PLACEBO=IE.pdf.

Adams:1990:PTI

[Ada90] W. H. Adams. Perturbation theory of intermolecular interactions: What is the problem, are there solutions? *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:531–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Adamowicz:1991:OSO

[Ada91a] Ludwik Adamowicz. Optimized second-order correlation orbital manifold for single excitations in the coupled-cluster method. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:71–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Adams:1991:PTI

[Ada91b] William H. Adams. Perturbation theory of intermolecular interactions: Are second-order Rayleigh–Schrödinger energies meaningful? *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:165–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Adams:1996:IPTa

[Ada96a] W. H. Adams. Intermolecular perturbation theory: Renormalized interaction energies. *International Journal of Quantum Chemistry*, 60(7):67–??, 1996. CODEN IJQCB2.

Adams:1996:IPTc

[Ada96b] W. H. Adams. Intermolecular perturbation theory: Renormalized interaction energies. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):67–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Adams:1996:IPTb

[Ada96c] William H. Adams. Intermolecular perturbation theory: Renormalized interaction energies. *International Journal of Quantum Chemistry*, 60(7):1279–1289, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60739`.

Adams:1996:LVS

[Ada96d] William H. Adams. On the limits of validity of the symmetrized Rayleigh–Schrödinger perturbation theory. *International Journal of Quantum Chemistry*, 60(1):273–285, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60590`.

Adams:1999:DES

[Ada99] William H. Adams. Definition of eigenproblems suited to intermolecular perturbation theory. *International Journal of Quantum Chemistry*, 72(4):393–404, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006317; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006317&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Adant:1995:ISN

[ADB95] C. Adant, M. Dupuis, and J. L. Brédas. Ab initio study of the nonlinear optical properties of urea: Electron correlation and dispersion effect. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:497–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Adhikari:1996:ALG

[ADB96] S. Adhikari, P. Dutta, and S. P. Bhattacharyya. Applications of a local grid method for modeling chemical dynamics at a mean-field level. *International Journal of Quantum Chemistry*, 59(2):109–117, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60531.

Ayers:1998:ADF

[ADM98] Paul W. Ayers, Orville W. Day Jr., and Robert C. Morrison. Analysis of density functionals and their density tails in H_2. *International Journal of Quantum Chemistry*, 69(4):541–550, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30008; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30008&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Andres:1998:CTS

[ADPS98] J. Andres, L. R. Domingo, M. T. Picher, and V. S. Safont. Comparative theoretical study of transition structures, barrier heights, and reaction energies for the intramolecular tautomerization in acetaldehyde/vinyl alcohol and acetaldimine/

vinylamine systems. *International Journal of Quantum Chemistry*, 66(1):9–24, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29835; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29835&PLACEBO=IE.pdf.

Abu-Eittah:1999:EAS

[AEAO99] Rafie H. Abu-Eittah and A. M. Al-Omar. Electronic absorption spectra of some highly perturbed N-sulfinylanilines: Molecular orbital treatment. *International Journal of Quantum Chemistry*, 72(1):1–13, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002298; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002298&PLACEBO=IE.pdf.

Amovilli:1999:TMS

[AFM99] Claudio Amovilli, Franca Maria Floris, and Benedetta Mennucci. Theoretical modeling of the symmetric (C_{2v}) electrophilic attachment of chlorine to ethylene in aqueous solution. *International Journal of Quantum Chemistry*, 74(1):59–67, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62000139; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62000139&PLACEBO=IE.pdf.

Arimoto:1997:SAC

[AFO+97] Shigeru Arimoto, Kenichi Fukui, Hiromu Ohno, Keith F. Taylor, and Paul G. Mezey. Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. III. *International Journal of Quantum Chemistry*, 63(1):149–163, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42561; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42561&PLACEBO=IE.pdf.

Arimoto:1995:SACa

[AFTM95a] S. Arimoto, K. Fukui, K. F. Taylor, and P. G. Mezey. Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. I. *International Journal of Quantum Chemistry*, 53(4):375–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arimoto:1995:SACb

[AFTM95b] S. Arimoto, K. Fukui, K. F. Taylor, and P. G. Mezey. Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. II. *International Journal of Quantum Chemistry*, 53(4):387–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arimoto:1998:SAC

[AFTM98] Shigeru Arimoto, Kenichi Fukui, Keith F. Taylor, and Paul G. Mezey. Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. IV. *International Journal of Quantum Chemistry*, 67(1):57–69, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29885`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29885&PLACEBO=IE.pdf`.

Arimoto:1999:SAC

[AFZ+99] Shigeru Arimoto, Kenichi Fukui, Peter Zizler, Keith F. Taylor, and Paul G. Mezey. Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. V. *International Journal of Quantum Chemistry*, 74 (6):633–644, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001780`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001780&PLACEBO=IE.pdf`. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Alagona:1998:IRS

[AGAP98] Giuliano Alagona, Caterina Ghio, Alessandro Agresti, and Riccardo Pratesi. Ab initio relative stability of a few conformers of bilirubin *in vacuo* and in aqueous solution

(PCM). *International Journal of Quantum Chemistry*, 70 (2):395–405, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75009; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75009&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Aagren:1997:BTV

[ÅGL97] Hans Ågren, Faris Gel'Mukhanov, and Christoph Liegener. Band theory vs. exciton theory interpretations of X-ray spectra of oligomers and polymers. *International Journal of Quantum Chemistry*, 63(2):313–332, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42604; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42604&PLACEBO=IE.pdf.

Alagona:1999:ISP

[AGM99] Giuliano Alagona, Caterina Ghio, and Susanna Monti. Ab initio study of preferential interactions between aromatic side chains. *International Journal of Quantum Chemistry*, 73 (2):175–186, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003515; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003515&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998*. Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Avery:1996:MSP

[AH96] John Avery and Tom Børsen Hansen. A momentum-space picture of the chemical bond. *International Journal of Quantum Chemistry*, 60(1):201–211, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60584.

Andrae:1997:NES

[AH97] Dirk Andrae and Juergen Hinze. Numerical electronic structure calculations for atoms. I generalized variable transformation and nonrelativistic calculations. *International Journal of Quantum Chemistry*, 63(1):65–91, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42554; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42554&PLACEBO=IE.pdf.

Altmann:1996:SPN

[AHI96] Julianna A. Altmann, Nicholas C. Handy, and Victoria E. Ingamells. A study of the performance of numerical basis sets in DFT calculations on sulfur-containing molecules. *International Journal of Quantum Chemistry*, 57(4):533–542, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60399.

AbuEittah:1997:EAS

[AHM97] R. H. Abu Eittah, M. M. Hamed, and A. A. Mohamed. Electronic absorption spectra of some nicotinamides and nicotinic acids. molecular orbital treatment. *International Journal of Quantum Chemistry*, 64(6):689–701, September 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42730; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42730&PLACEBO=IE.pdf.

Avery:1996:SBS

[AHWA96] John Avery, Tom Børsen Hansen, Minchang Wang, and Frank Antonsen. Sturmian basis sets in momentum space. *International Journal of Quantum Chemistry*, 57(3):401–411, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60377.

Aoki:1999:SRF

[AI99] Yuriko Aoki and Akira Imamura. A simple rule to find nondisjoint NBMO degenerate systems for designing high-spin organic molecules. *International Journal of Quantum Chemistry*, 74(5):491–502, ???? 1999. CODEN IJQCB2. ISSN

0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62503001; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62503001&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Arulmozhiraja:1997:SCH

[AK97] S. Arulmozhiraja and P. Kolandaivel. Studies of chemical hardness and chemical potential on isomers and hardness profiles of hydrogen-bonded systems. *International Journal of Quantum Chemistry*, 64(2):231–242, August 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42671; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42671&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Aida:1996:IMS

[AKD96] Misako Aida, Motohisa Kaneko, and Michel Dupuis. An ab initio MO study on the thymine dimer and its radical cation. *International Journal of Quantum Chemistry*, 57(5):949–957, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60433.

Akagi:1990:GES

[AKS+90] K. Akagi, T. Kadokura, H. Shirakawa, H. Teramae, and A. Imamura. Geometrical and electronic structures of polyacetylene chlorinated via prolonged chemical doping. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:41–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Adamo:1995:SPS

[AL95] C. Adamo and J. Lelj. Stationary point structure and energetics: Density functional study including solvent effects on the tautomerization of formamide and 2-pyridone. *International Journal of Quantum Chemistry*, 56(5):645–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alacid:1998:DCL

[AL98] Mercedes Alacid and Claude Leforestier. Direct calculation of long time correlation functions using an optical potential. *International Journal of Quantum Chemistry*, 68 (5):317–328, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29952; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29952&PLACEBO=IE.pdf.

Alexander:1995:SDF

[Ale95] S. A. Alexander. State decay in finite and infinite discrete systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:145–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Alikhani:1999:SVB

[Ali99] M. E. Alikhani. Structural, vibrational, and bonding analysis of $M_2 — SiO$ (M = Li or Ag) using density functional theory. *International Journal of Quantum Chemistry*, 71 (6):499–503, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=15000348; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=15000348&PLACEBO=IE.pdf.

Allen:1994:CE

[All94] L. C. Allen. Chemistry and electronegativity. *International Journal of Quantum Chemistry*, 49(3):253–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Azavant:1996:QMC

[ALRP96] Patrick Azavant, Albert Lichanot, Michel Rerat, and Cesare Pisani. A quantum-mechanical calculation of the dynamic structure factors of magnesium difluoride. *International Journal of Quantum Chemistry*, 58(4):419–429, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60488.

Altmann:1996:CAS

[Alt96] S. L. Altmann. Clifford algebra, symmetries, and vectors. *International Journal of Quantum Chemistry*, 60(1):359–372, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60598.

Arteca:1990:QAS

[AM90] G. A. Arteca and P. G. Mezey. A quantitative approach to structural similarity from molecular topology of reaction paths. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:1–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Aissing:1993:RES

[AM93] G. Aissing and H. J. Monkhorst. On the removal of the exchange singularity in extended systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27: 81–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Almeida:1997:ESG

[AM97] Rafael Almeida and Daniel A. Morales. Exact solution to a general quantum mechanical problem with time-dependent boundary conditions. *International Journal of Quantum Chemistry*, 63(4):827–833, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42633; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42633&PLACEBO=IE.pdf.

Amovilli:1998:KED

[AM98a] C. Amovilli and N. H. March. Kinetic energy density in terms of electron density for closed-shell atoms in a bare Coulomb field. *International Journal of Quantum Chemistry*, 66(4):281–283, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29863; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29863&PLACEBO=IE.pdf.

Arakane:1998:RFM

[AM98b] Fusanori Arakane and Osamu Matsuoka. Recurrence formulas for molecular integrals over Laguerre Gaussian-type functions. *International Journal of Quantum Chemistry*, 66 (4):273–279, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29862; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29862&PLACEBO=IE.pdf.

Actis:1997:ILN

[AMC97] M. Actis and F. Michel-Calendini. Impurity levels and nonlinear optical properties of doped $BaTiO_3$ from extended cluster LDA calculations. *International Journal of Quantum Chemistry*, 61(4):657–664, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42452; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42452&PLACEBO=IE.pdf.

Aguilar:1997:IVB

[AMD+97] J. G. Aguilar, A. Mananes, F. Duque, M. J. López, M. P. Iniguez, and J. A. Alonso. Ionic vibrational breathing mode of metallic clusters. *International Journal of Quantum Chemistry*, 61(4):613–626, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42447; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42447&PLACEBO=IE.pdf.

Aissing:1993:RIS

[AMH93] G. Aissing, H. J. Monkhorst, and C. Hu. Rules for intrinsically (super) conducting polymers. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:245–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Andres:1993:TSE

[AMKS93] J. Andrés, V. Moliner, J. Krechl, and E. Silla. A theoretical study of the effect of basis sets on stationary structures for the addition of carbon dioxide to methylamine: A relation among geometries, energy status, and electronic structures. *International Journal of Quantum Chemistry*, 45(5):433–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aguilar:1995:VFS

[AML+95] J. G. Aguilar, A. Mananes, M. J. Lopez, M. P. Iniguez, and J. A. Alonso. Vibrational frequencies of sodium clusters. *International Journal of Quantum Chemistry*, 56(5):589–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Amos:1996:BPU

[Amo96] A. T. Amos. Bond properties using a modern version of the Drude model. *International Journal of Quantum Chemistry*, 60(1):67–74, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60626`.

Abashkin:1994:DFT

[AMRT94] Y. Abashkin, F. Mele, N. Russo, and M. Toscano. Density functional treatment of water-carbon dioxide van der Waals complex. *International Journal of Quantum Chemistry*, 52(4):1011–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Almeida:1999:TSW

[AMT+99] A. L. Almeida, J. B. L. Martins, C. A. Taft, E. Longo, and W. A. Lester Jr. Theoretical study of water coverage on MgO surfaces. *International Journal of Quantum Chemistry*, 71(2):153–165, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000023; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000023&PLACEBO=IE.pdf`.

Alemany:1994:CSS

[ANB94] P. Alemany, J. J. Novoa, and L. Bengtsson. A comparative study on the structure of M_2Se and M_2I0^+ (M = Ag, Au) using pseudopotentials and full ab initio methods. *International Journal of Quantum Chemistry*, 52(1):1–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Adhikari:1996:GRO

[ANB96] S. Adhikari, D. N. Nath, and S. P. Bhattacharyya. Generalized Rabi oscillations in a three-level metastable system under periodic and quasiperiodic perturbations. *International Journal of Quantum Chemistry*, 58(1):3–10, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60457`.

Andre:1990:OSO

[And90] J.-M. André. Orbital symmetry and orbital interactions in polymeric band structures: Examples of polyethylene and polysilane. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:65–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Andersson:1993:MTP

[And93a] N. Andersson. A multiple-transient-point WKB investigation of complex energy resonances. *International Journal of Quantum Chemistry*, 46(3):375–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andre:1993:ECG

[And93b] J. André. Enrico clementi: Gradus ad parnassum. *International Journal of Quantum Chemistry*, 45(6):507–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anderson:1994:EDD

[And94] A. B. Anderson. Electron density distribution functions and the ASED-Mo theory. *International Journal of Quantum Chemistry*, 49(5):581–??, February 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Angyan:1993:RSP

[Áng93] János G. Ángyán. Rayleigh–Schrödinger perturbation theory for nonlinear Schrödinger equations with linear perturbation. *International Journal of Quantum Chemistry*, 47(6):469–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1992:DMJ

[Ano92a] Anonymous. Dewar, Michael J. S. *International Journal of Quantum Chemistry*, 44(4):419–??, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1992:LP

[Ano92b] Anonymous. List of participants. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:ix, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Anonymous:1993:GPEa

[Ano93a] Anonymous. Guidelines for preparing an electronic manuscript. *International Journal of Quantum Chemistry*, 45(3):329–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1993:GPEb

[Ano93b] Anonymous. Guidelines for preparing an electronic manuscript. *International Journal of Quantum Chemistry*, 45(4):405–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1993:LP

[Ano93c] Anonymous. List of participants. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:xi, 1993. CODEN IJQSDI. ISSN 0161-3642.

Anonymous:1994:BIR

[Ano94a] Anonymous. Biographical information for Robert G. Parr. *International Journal of Quantum Chemistry*, 49(3):133–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1994:RGP

[Ano94b] Anonymous. Robert G. parr. *International Journal of Quantum Chemistry*, 49(3):131–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1995:DSIa

[Ano95a] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 54(4):I, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1995:DSIb

[Ano95b] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 54(5):I, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1995:DSIc

[Ano95c] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 54(6):VII, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1995:DSId

[Ano95d] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 55(1):I, July 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1995:DSIe

[Ano95e] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 55(2):I, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1995:DSIf

[Ano95f] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 55(4):I, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1995:DSIg

[Ano95g] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 55(5):I, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1995:DSIh

[Ano95h] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 56(1):I, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1995:DSIi

[Ano95i] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 56(2):I, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1995:DSIj

[Ano95j] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 56(3):I, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1995:DSIk

[Ano95k] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 56(4):III, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1995:DSIl

[Ano95l] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 56(5):III, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1995:VTC

[Ano95m] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 54(6):I, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1995:VTP

[Ano95n] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 54(6):393–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIa

[Ano96a] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 57(1):I, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIb

[Ano96b] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 57(2):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIc

[Ano96c] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 57(5):I–??, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSId

[Ano96d] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 57(6):XIII–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIe

[Ano96e] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 58(1):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIf

[Ano96f] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 58(2):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIg

[Ano96g] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 58(3):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIh

[Ano96h] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 58(4):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIi

[Ano96i] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 58(5):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIj

[Ano96j] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 58(6):IX–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIk

[Ano96k] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 59(1):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIl

[Ano96l] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 59(2):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIm

[Ano96m] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 59(3):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIn

[Ano96n] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 59(4):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIo

[Ano96o] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 59(5):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIp

[Ano96p] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 59(6):VII–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIq

[Ano96q] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 60(1):I–??, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIr

[Ano96r] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 60(2):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIs

[Ano96s] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 60(3):I, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIt

[Ano96t] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 60(4):I, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIu

[Ano96u] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 60(6):XIII, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:DSIv

[Ano96v] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 23(??):vii–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

Anonymous:1996:PS

[Ano96w] Anonymous. Published symposia. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 23(??):i–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

Anonymous:1996:VTCa

[Ano96x] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 57(6):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:VTCb

[Ano96y] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 58(6):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:VTCc

[Ano96z] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 59(6):I–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:VTCd

[Ano96-27] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 60(6):I, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:VTPa

[Ano96-28] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 57(6):1135–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:VTPb

[Ano96-29] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 58(6):733–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:VTPc

[Ano96-30] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 59(6):507–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1996:VTPd

[Ano96-31] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 60(6):1201–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:DSIa

[Ano97a] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 61(1):I, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:DSIb

[Ano97b] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 61(2):I, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:DSIc

[Ano97c] Anonymous. Diskette submission instructions. *International Journal of Quantum Chemistry*, 61(3):I, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:GESa

[Ano97d] Anonymous. Guidelines for electronic submission. *International Journal of Quantum Chemistry*, 61(4):I, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:GESb

[Ano97e] Anonymous. Guidelines for electronic submission. *International Journal of Quantum Chemistry*, 61(5):I, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:GESc

[Ano97f] Anonymous. Guidelines for electronic submission. *International Journal of Quantum Chemistry*, 61(6):XIII, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:GESd

[Ano97g] Anonymous. Guidelines for electronic submission. *International Journal of Quantum Chemistry*, 62(1):I–??, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:GESe

[Ano97h] Anonymous. Guidelines for electronic submission. *International Journal of Quantum Chemistry*, 62(3):i–??, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:GESf

[Ano97i] Anonymous. Guidelines for electronic submission. *International Journal of Quantum Chemistry*, 62(4):i–??, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:GESg

[Ano97j] Anonymous. Guidelines for electronic submission. *International Journal of Quantum Chemistry*, 62(5):i–??, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:GESh

[Ano97k] Anonymous. Guidelines for electronic submission. *International Journal of Quantum Chemistry*, 63(1):I–??, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:GESi

[Ano97l] Anonymous. Guidelines for electronic submission. *International Journal of Quantum Chemistry*, 63(6):XI–??, July 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:I

[Ano97m] Anonymous. Introduction. *International Journal of Quantum Chemistry*, 64(1):1–5, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42657; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42657&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Anonymous:1997:LP

[Ano97n] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 64(5):497–499, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42714; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42714&PLACEBO=IE.pdf. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

Anonymous:1997:PS

[Ano97o] Anonymous. Published symposia. *International Journal of Quantum Chemistry*, 65(6):XIII–??, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:VTCa

[Ano97p] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 61(6):I, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:VTCb

[Ano97q] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 63(6):I–??, July 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:VTCd

[Ano97r] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 64(6):I–??, September 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:VTCe

[Ano97s] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 65(6):I–??, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:VTPa

[Ano97t] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 61(6):1003–??, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:VTPb

[Ano97u] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 63(6):1135–??, July 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:VTPc

[Ano97v] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 64(6):739–??, September 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1997:VTPd

[Ano97w] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 65(6):1179–??, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:BR

[Ano98a] Anonymous. Books received. *International Journal of Quantum Chemistry*, 70(3):527, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75019; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75019&PLACEBO=IE.pdf`.

Anonymous:1998:CCa

[Ano98b] Anonymous. Call for contributions. *International Journal of Quantum Chemistry*, 68(6):431–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:CCb

[Ano98c] Anonymous. Call for contributions. *International Journal of Quantum Chemistry*, 68(6):433–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:CCc

[Ano98d] Anonymous. Call for contributions. *International Journal of Quantum Chemistry*, 69(1):137–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:CCd

[Ano98e] Anonymous. Call for contributions. *International Journal of Quantum Chemistry*, 69(1):139–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:CCe

[Ano98f] Anonymous. Call for contributions. *International Journal of Quantum Chemistry*, 69(1):141–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:CCf

[Ano98g] Anonymous. Call for contributions. *International Journal of Quantum Chemistry*, 69(1):143–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:CCg

[Ano98h] Anonymous. Call for contributions. *International Journal of Quantum Chemistry*, 69(2):219–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:CCh

[Ano98i] Anonymous. Call for contributions. *International Journal of Quantum Chemistry*, 69(2):221–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:CCi

[Ano98j] Anonymous. Call for contributions. *International Journal of Quantum Chemistry*, 69(2):223–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:CCj

[Ano98k] Anonymous. Call for contributions. *International Journal of Quantum Chemistry*, 69(2):225–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:CCk

[Ano98l] Anonymous. Call for contributions. *International Journal of Quantum Chemistry*, 69(3):435–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:CCl

[Ano98m] Anonymous. Call for contributions. *International Journal of Quantum Chemistry*, 69(3):437–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:Ia

[Ano98n] Anonymous. Introduction. *International Journal of Quantum Chemistry*, 70(4-5):529, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75033; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75033&PLACEBO=IE.pdf`.

Anonymous:1998:Ib

[Ano98o] Anonymous. Introduction. *International Journal of Quantum Chemistry*, 70(6):1099, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75079; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75079&PLACEBO=IE.pdf`.

Anonymous:1998:PS

[Ano98p] Anonymous. Published symposia. *International Journal of Quantum Chemistry*, 70(6):XII–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:VTCa

[Ano98q] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 66(6):I–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:VTCb

[Ano98r] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 67(6):I–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:VTCc

[Ano98s] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 68(6):I–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:VTCd

[Ano98t] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 69(6):I–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:VTCe

[Ano98u] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 70(6):I–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:VTPa

[Ano98v] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 66(6):459–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:VTPb

[Ano98w] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 67(6):411–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:VTPc

[Ano98x] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 68(6):435–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:VTPd

[Ano98y] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 69(6):761–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1998:VTPe

[Ano98z] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 70(6):1217–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1999:BPA

[Ano99a] Anonymous. Bernard Pullman and Alberte Pullman. *International Journal of Quantum Chemistry*, 75(3):135, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000675/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000675&PLACEBO=IE.pdf.

Anonymous:1999:B

[Ano99b] Anonymous. Bibliography. *International Journal of Quantum Chemistry*, 75(3):139, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000655/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000655&PLACEBO=IE.pdf.

Anonymous:1999:BSL

[Ano99c] Anonymous. Biographical sketch — Lionel Goodman. *International Journal of Quantum Chemistry*, 72(4):239, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006324; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006324&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Anonymous:1999:GGH

[Ano99d] Anonymous. George G. Hall. *International Journal of Quantum Chemistry*, 74(5):437, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62503011; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62503011&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Anonymous:1999:IMB

[Ano99e] Anonymous. Introduction: In Memory of Bernard Pullman (1919–1996). *International Journal of Quantum Chemistry*, 75(3):137–138, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000654/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000654&PLACEBO=IE.pdf.

Anonymous:1999:JG

[Ano99f] Anonymous. J. Gerratt. *International Journal of Quantum Chemistry*, 74(2):69, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003371; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003371&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Anonymous:1999:LG

[Ano99g] Anonymous. Lionel Goodman. *International Journal of Quantum Chemistry*, 72(4):235–??, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1999:LGP

[Ano99h] Anonymous. Lionel Goodman — publications. *International Journal of Quantum Chemistry*, 72(4):241–244, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006325; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006325&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Anonymous:1999:LPa

[Ano99i] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 72(4):247, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006327; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006327&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Anonymous:1999:LPb

[Ano99j] Anonymous. List of Participants. *International Journal of Quantum Chemistry*, 73(2):255–263, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003523; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003523&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998*. Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Anonymous:1999:LPc

[Ano99k] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 75(3):327–330, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000673/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000673&PLACEBO=IE.pdf.

Anonymous:1999:LPd

[Ano99l] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 75(4–5):335–359, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004993/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004993&PLACEBO=IE.pdf.

Anonymous:1999:LPe

[Ano99m] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 75(6):969–993, December 20, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004793/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004793&PLACEBO=IE.pdf.

Anonymous:1999:PSP

[Ano99n] Anonymous. PhD students and post-doctoral fellows of Lionel Goodman. *International Journal of Quantum Chem-*

istry, 72(4):245, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006326; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006326&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Anonymous:1999:PLG

[Ano99o] Anonymous. Photo of Lionel Goodman. *International Journal of Quantum Chemistry*, 72(4):235, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006302; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006302&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Anonymous:1999:SPJ

[Ano99p] Anonymous. Scientific publications of J. Gerratt. *International Journal of Quantum Chemistry*, 74(2):77–81, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003352; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003352&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Anonymous:1999:VTCa

[Ano99q] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 71(6):i–??, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1999:VTCb

[Ano99r] Anonymous. Volume table of contents. *International Journal of Quantum Chemistry*, 72(6):I–??, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1999:VTPa

[Ano99s] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 71(6):515–??, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:1999:VTPb

[Ano99t] Anonymous. Volume title page. *International Journal of Quantum Chemistry*, 72(6):605–??, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aucar:1993:RTI

[AO93] G. A. Aucar and J. Oddershede. Relativistic theory for indirect nuclear spin-spin couplings within the polarization propagator approach. *International Journal of Quantum Chemistry*, 47(6): 425–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alfredsson:1996:CHF

[AOH96] Maria Alfredsson, Lars Ojamäe, and K. G. Hermansson. A comparison of Hartree–Fock, MP2, and DFT results for the HCN dimer and crystal. *International Journal of Quantum Chemistry*, 60(3):767–778, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60643`.

Aono:1998:RBB

[Aon98] Shigeyuki Aono. Relation between BCS Hamiltonian and Ginzburg–Landau equation. *International Journal of Quantum Chemistry*, 69(6):693–703, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74986; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74986&PLACEBO=IE.pdf`.

Aono:1999:TOR

[Aon99] Shigeyuki Aono. Theory of optical rotation, Faraday effect, and inverse Faraday effect. *International Journal of Quantum Chemistry*, 75(1):33–45, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63003147; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63003147&PLACEBO=IE.pdf`.

Aleman:1993:HRP

[AP93] C. Aleman and J. J. Perez. Helical region of the potential energy surface of alpha-aminoisobutyric acid: A theoretical study. *International Journal of Quantum Chemistry*, 47(3):231–??, 1993.

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

Alkorta:1996:MPP

[AP96] Ibon Alkorta and Juan J. Perez. Molecular polarization potential maps of the nucleic acid bases. *International Journal of Quantum Chemistry*, 57(1):123–135, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60351.

Aquino:1995:AEE

[Aqu95] N. A. Aquino. Accurate energy eigenvalues for enclosed hydrogen atom within spherical impenetrable boxes. *International Journal of Quantum Chemistry*, 54(2):107–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anderson:1993:MSO

[AR93] K. Anderson and B. O. Roos. Multiconfigurational second-order perturbation theory: A test of geometries and binding energies. *International Journal of Quantum Chemistry*, 45(6):591–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andreev:1996:QCS

[AR96] Ye. A. Andreev and I. V. Repyakh. Quantum chemical study of self-organized water fractals. *International Journal of Quantum Chemistry*, 57(4):767–773, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60415.

Angulo:1999:EIU

[AR99a] J. C. Angulo and E. Romera. Erratum: Improved upper bounds for the atomic ionization potential. *International Journal of Quantum Chemistry*, 73(6):519, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61007369; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61007369&PLACEBO=IE.pdf. See [AR99b].

Angulo:1999:IUB

[AR99b] J. C. Angulo and E. Romera. Improved upper bounds for the atomic ionization potential. *International Journal of Quantum

Chemistry, 71(2):185–189, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000026; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000026&PLACEBO=IE.pdf. See erratum [AR99a].

Arai:1994:ECT

[Ara94] Tadashi Arai. Electron correlations and transport effective mass in narrow-band systems and the Hubbard model. *International Journal of Quantum Chemistry*, 49(5):727–??, February 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Albuquerque:1995:DNP

[ARdAB95] M. G. Albuquerque, C. R. Rodrigues, R. B. de Alencastro, and E. J. Barreiro. Design of new potential 5-Lipoxygenase inhibitors, dual thromboxane synthase inhibitors, and thromboxane A2 receptor antagonists by AM1. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):181–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Ackermann:1992:EMP

[ARDP92] L. Ackermann, N. Rosch, B. I. Dunlap, and G. Pacchioni. Electronic and magnetic properties of organometallic clusters: From the molecular to the metallic state. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:605–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Arteca:1993:AMS

[Art93] G. A. Arteca. Assessment of molecular shape fluctuations along dynamic trajectories. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:547–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Abashkin:1994:TSE

[ART94a] Y. Abashkin, N. Russo, and M. Toscano. Transition states and energy barriers from density functional studies: Representative isomerization reactions. *International Journal of Quantum Chemistry*, 52(4):695–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arteca:1994:CED

[Art94b] G. A. Arteca. Complexity of entanglements and degree of folding in branched polymers with excluded-volume interaction. *International Journal of Quantum Chemistry. Symposium*, 28: 433–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Arteca:1996:MSTa

[Art96a] G. A. Arteca. Molecular shape transitions in grafted polymers under geometrical confinement. *International Journal of Quantum Chemistry*, 60(7):303–??, 1996. CODEN IJQCB2.

Arteca:1996:MSTc

[Art96b] G. A. Arteca. Molecular shape transitions in grafted polymers under geometrical confinement. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):303–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Arteca:1996:MSTb

[Art96c] Gustavo A. Arteca. Molecular shape transitions in grafted polymers under geometrical confinement. *International Journal of Quantum Chemistry*, 60(7):1515–1523, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60711`.

Arteca:1997:STP

[Art97] Gustavo A. Arteca. Shape transitions in polymer mushrooms compressed by a finite-size obstacle. *International Journal of Quantum Chemistry*, 65(5):519–530, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42781`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42781&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Arteca:1998:ATD

[Art98] Gustavo A. Arteca. Analysis of three-dimensional molecular shape using surface area and molecular volume scaling descriptors. *International Journal of Quantum Chemistry*, 70

(4-5):981–992, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75076; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75076&PLACEBO=IE.pdf.

Acrivos:1993:SWF

[AS93] J. V. Acrivos and O. Stradella. SCF wave functions for $(CuO_2)_n$ lamella in crystal field of TprimesbondNd$_2$CuO$_4$. *International Journal of Quantum Chemistry*, 46(1):55–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Animalu:1995:NIR

[AS95] A. O. E. Animalu and R. M. Santilli. Nonlocal isotopic representation of the Cooper pair in superconductivity. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:175–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Anderson:1996:NMH

[AS96] Norman Anderson and Brian T. Sutcliffe. The nuclear motion Hamiltonian for a tetratomic molecule considered as a combination of an atom and a triatom. *International Journal of Quantum Chemistry*, 60(1):37–46, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60603.

Aihara:1999:KSC

[AS99] Jun-Ichi Aihara and Atsushi Sakurai. Kinetic stability of C_{78} fullerene isomers as revealed by the bond resonance energy method. *International Journal of Quantum Chemistry*, 74(6):753–760, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001791; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001791&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Aiga:1994:FDH

[ASI94a] F. Aiga, K. Sasagane, and R. Itoh. Frequency-dependent hyperpolarizabilities in the Brueckner coupled-cluster theory. *In-*

ternational Journal of Quantum Chemistry, 51(2):87–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aoki:1994:DFE

[ASI94b] Y. Aoki, S. Suhai, and A. Imamura. A density functional elongation method for the theoretical synthesis of aperiodic polymers. *International Journal of Quantum Chemistry*, 52(2):267–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aray:1991:CDE

[ASM91] Yosslen Aray, Humberto Soscun, and Juan Murgich. The charge distribution and the electric field gradient at the nuclei of two-coordinated N atoms. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:587–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Aguado:1997:ASO

[ASP97] Alfredo Aguado, Virgilio Sanz, and Miguel Paniagua. Application of second-order density functional methods to the calculation of the BeFH potential energy surface. *International Journal of Quantum Chemistry*, 61(3):491–497, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42417; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42417&PLACEBO=IE.pdf.

Arnau:1993:IRC

[AST93] A. Arnau, E. Silla, and I. Tunon. Ab initio rotational constants of interstellar species: Cyanoacetylene hydrogenated derivatives. *International Journal of Quantum Chemistry*, 46(2):231–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Apell:1995:PCP

[AST95] S. P. Apell, J. R. Sabin, and S. B. Trickey. Prediction of crystalline properties from ultrathin layered systems: Energy deposition. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:153–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Antoniou:1993:GSD

[AT93] I. Antoniou and S. Tasaki. Generalized spectral decompositions of mixing dynamical systems. *International Journal of Quantum Chemistry*, 46(3):425–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aiga:1999:MCM

[AT99] Fumihiko Aiga and Tsukasa Tada. Multiple cluster model (MCM) for surface reaction systems. *International Journal of Quantum Chemistry*, 71(5):403–413, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10050250; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10050250&PLACEBO=IE.pdf.

Atabek:1994:IEL

[Ata94] O. Atabek. Isotope effects in laser-induced multiphoton molecular dynamics. *International Journal of Quantum Chemistry. Symposium*, 28:113–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Atabek:1997:LIA

[Ata97a] O. Atabek. Laser-induced alignment dynamics in multiphoton dissociation of H_2^+. *International Journal of Quantum Chemistry*, 65(5):617–624, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42792; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42792&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Atabek:1997:NEM

[Ata97b] O. Atabek. Nonadiabatic effects in multiphoton dissociation dynamics. *International Journal of Quantum Chemistry*, 64(1):53–61, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42665; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42665&PLACEBO=IE.pdf. Special Issue: *Second Triennial*

Congress of the International Society for Theoretical Chemical Physics. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Aoki:1997:MOA

[ATI97] Yuriko Aoki, Tomofumi Tada, and Akira Imamura. Molecular orbital approach to the Peierls instability in polyenes and its application to model crystals of charge-transfer complexes. *International Journal of Quantum Chemistry*, 64 (3):325–336, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42690; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42690&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Alpert:1996:DHB

[ATP+96] Bernard Alpert, Véronique Le Tilly, Serge Pin, Olivier Sire, and Christian Zentz. Do the hemeproteins behave as a dissipative structure? *International Journal of Quantum Chemistry*, 59(4):281–289, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60548.

Alkorta:1992:QMP

[AV92] I. Alkorta and H. O. Villar. Quantum mechanical parametrization of a conformationally dependent hydrophobic index. *International Journal of Quantum Chemistry*, 44(2):203–??, September 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Avery:1979:TIDb

[Ave79a] J. Avery. Transferable integrals in a deformation density approach to crystal orbital calculations. I. *International Journal of Quantum Chemistry*, 16(??):1265–1277, ?? 1979. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Avery:1979:TIDd

[Ave79b] J. Avery. Transferable integrals in a deformation density approach to crystal orbital calculations. II. *International Journal of Quantum Chemistry*, 16(??):1279–1299, ?? 1979. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Avery:1979:TIDa

[Ave79c] J. Avery. Transferable integrals in a deformation density approach to crystal orbital calculations. III. *International Journal of Quantum Chemistry*, S13(??):403–412, ?? 1979. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Avery:1980:TID

[Ave80] J. Avery. Transferable integrals in a deformation density approach to crystal orbital calculations. IV. *International Journal of Quantum Chemistry*, ??(??):??, ?? 1980. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Angulo:1996:MPA

[AYDR96] J. C. Angulo, R. J. Yañez, J. S. Dehesa, and E. Romera. Monotonicity properties of the atomic charge density function. *International Journal of Quantum Chemistry*, 58(1):11–21, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60459`.

Armour:1999:CBO

[AZ99] E. A. G. Armour and V. Zeman. Corrections to the Born–Oppenheimer approximation as applied to a system made up of hydrogen and antihydrogen. *International Journal of Quantum Chemistry*, 74(6):645–652, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001781; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001781&PLACEBO=IE.pdf`. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Antolin:1997:MEA

[AZAC97] J. Antolín, A. Zarzo, J. C. Angulo, and J. C. Cuchí. Maximum-entropy analysis of momentum densities in diatomic molecules. *International Journal of Quantum Chemistry*, 61(1):77–83, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42388; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42388&PLACEBO=IE.pdf`.

Bishop:1990:CES

[BA90] R. F. Bishop and J. S. Arponen. Correlations in extended systems: A microscopic multilocal method for describing both local and global properties. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:197–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Banerjee:1991:PIA

[BA91] Ajit Banerjee and Noah P. Adams. Path integral approach to chemical dynamics: A test case of H + O_2 darlr OH + O reaction. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:311–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Brandas:1993:PCN

[BA93] E. J. Brändas and I. E. Antoniou. On the positivity condition in the nonunitary transformation theory of irreversibility. *International Journal of Quantum Chemistry*, 46(3):419–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barone:1997:FRT

[BA97a] Vincenzo Barone and Carlo Adamo. First-row transition-metal hydrides: A challenging playground for new theoretical approaches. *International Journal of Quantum Chemistry*, 61(3):443–451, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42412; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42412&PLACEBO=IE.pdf.

Barone:1997:TGP

[BA97b] Vincenzo Barone and Carlo Adamo. Toward a general protocol for the study of static and dynamic properties of hydrogen-bonded systems. *International Journal of Quantum Chemistry*, 61(3):429–442, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42411; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42411&PLACEBO=IE.pdf.

Bader:1994:WDA

[Bad94] R. F. W. Bader. Why define atoms in real space? *International Journal of Quantum Chemistry*, 49(3):299–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bader:1995:CNS

[Bad95] R. F. W. Bader. Chemistry and the near-sighted nature of the one-electron density matrix. *International Journal of Quantum Chemistry*, 56(4):409–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burrows:1999:ATC

[BAD99] B. L. Burrows, A. T. Amos, and S. G. Davison. Approximations in the theory of charge transfer through bridged systems. *International Journal of Quantum Chemistry*, 72 (3):207–220, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40003033; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40003033&PLACEBO=IE.pdf`.

Barriuso:1997:MIO

[BADM97] M. T. Barriuso, J. A. Aramburu, C. Daul, and M. Moreno. A microscopic insight into oscillator strengths: The charge transfer bands for $CuCl_4^{2-}$. *International Journal of Quantum Chemistry*, 61(3):563–570, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42427; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42427&PLACEBO=IE.pdf`.

Bernholdt:1995:PCC

[BAF+95] D. E. Bernholdt, E. Apra, H. A. Fruchtl, M. F. Guest, R. J. Harrison, R. A. Kendall, R. A. Kutteh, X. Long, J. B. Nicholas, J. A. Nichols, H. L. Taylor, A. T. Wong, G. I. Fann, R. J. Littlefield, and J. Nieplocha. Parallel computational chemistry made easier: The development of NWChem. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29: 475–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Bohm:1996:MDM

[BAK96a] Stanislav Böhm, Diana Antipova, and Josef Kuthan. Methanediol decomposition mechanisms: A study considering various ab initio approaches. *International Journal of Quantum Chemistry*, 58(1):47–55, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60463.

Bohm:1996:SMD

[BAK96b] Stanislav Böhm, Diana Antipova, and Josef Kuthan. A study of methanetriol decomposition mechanisms. *International Journal of Quantum Chemistry*, 60(2):649–655, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60632.

Bohm:1997:SMD

[BAK97] Stanislav Böhm, Diana Antipova, and Josef Kuthan. A study of methanetetraol dehydration to carbonic acid. *International Journal of Quantum Chemistry*, 62(3):315–322, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42507; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42507&PLACEBO=IE.pdf.

Ballhausen:1996:O

[Bal96] C. J. Ballhausen. Overture. *International Journal of Quantum Chemistry*, 58(6):539–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barreiro:1997:SSL

[BAN97] Gabriela Barreiro, Ricardo Bicca De Alencastro, and Joaquim Delphino Da Motta Neto. A semiempirical study on leupeptin: An inhibitor of cysteine proteases. *International Journal of Quantum Chemistry*, 65(6):1125–1134, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42838; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42838&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on the Application* *of Fundamental Theory to Problems of Biology and Pharmocolgy*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Bardo:1990:CEL

[Bar90] R. D. Bardo. Coupling of electrons and lattice wave packets in superconducting metastable states formed at high pressure. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:717–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Barone:1994:DFT

[BAR94] V. Barone, C. Adamo, and N. Russo. Density functional theory: An effective theoretical tool for the study of radicals. *International Journal of Quantum Chemistry*, 52(4):963–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Batra:1992:ATF

[Bat92] I. P. Batra. Application of thin films method in the study of alkali-semiconductor interaction. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:643–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Bauschlicher:1997:EEF

[Bau97] Charles W. Bauschlicher Jr. The effect of an electric field on the vibrational frequency of CN. *International Journal of Quantum Chemistry*, 61(5):859–863, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42458; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42458&PLACEBO=IE.pdf`.

Bauschlicher:1998:QBC

[Bau98] Charles W. Bauschlicher Jr. QCISD(T) and B3LYP can correctly describe the EA of B, Al, and Ga. *International Journal of Quantum Chemistry*, 66(4):285–286, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29864; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29864&PLACEBO=IE.pdf`.

Bartlett:1971:GSR

[BB71] R. J. Bartlett and E. J. Brändas. Geometric sumrule and the reduced partitioning procedure. *International Journal of Quan-*

tum Chemistry, 5(??):151–??, ?? 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boehm:1993:IIV

[BB93] R. C. Boehm and A. Banerjee. Ab initio investigation of void stabilization: Oxygen in nickel. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:163–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Boudreaux:1994:SMM

[BB94] E. A. Boudreaux and E. Baxter. SC-MEH-MO calculations on lanthanide systems. I. Sm(Cp0*)$_2$, bis(Pentamethyl-Cyclopentaldienyl)Sm(II). *International Journal of Quantum Chemistry. Symposium*, 28:565–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Boudreaux:1995:SMM

[BB95] E. A. Boudreaux and E. Baxter. SC-MEH-MO calculations on lanthanide systems. II. (sm(cp*)$^+$), sm(cp*)$^{2+}$, and the [sm(cp*)]$_4^{8+}$ tetrameter. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:605–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Boudreaux:1997:QSM

[BB97a] E. A. Boudreaux and E. Baxter. QR-SCMEH-MO calculations on lanthanide systems. IV. The [SmCp*]$_4$ cluster. *International Journal of Quantum Chemistry*, 64(3): 297–300, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42688; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42688&PLACEBO=IE.pdf`. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Bracken:1997:CGI

[BB97b] Paul Bracken and Rodney J. Bartlett. Calculation of Gaussian integrals using symbolic manipulation. *International Journal of Quantum Chemistry*, 62(6):557–570, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42542; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42542&PLACEBO=IE.pdf`.

Boudreaux:1992:SMC

[BBC92] E. A. Boudreaux, E. Baxter, and K. Chin. SC-MEH-Cl calculations on the $(NH_4)_4CuCl_6$ (D_{2h}) cluster in (NH_{42} $CuCl_4$). *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:543–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Bianchi:1994:QMC

[BBC+94] R. Bianchi, D. Bressanini, P. Cremaschi, M. Mella, and G. Morosi. A quantum Monte Carlo simulation of the two-dimensional H_2 molecule. *International Journal of Quantum Chemistry*, 50 (6):401–??, June 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bernardi:1996:ISD

[BBC+96a] Fernando Bernardi, Andrea Bottoni, Rita Casadio, Piero Fariselli, and Adelio Rigo. An ab initio study of the dioxygen binding site of hemocyanin: A comparison between CASSCF, CASPT2, and DFT approaches. *International Journal of Quantum Chemistry*, 58(1):109–119, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60458`.

Bianchi:1996:WFO

[BBC+96b] R. Bianchi, D. Bressanini, P. Cremaschi, M. Mella, and G. Morosi. Wave-function optimization by least squares fitting of the exact wave function sampled by quantum Monte Carlo. *International Journal of Quantum Chemistry*, 57(3):321–325, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60393`.

Bruno-Blanch:1995:QCQ

[BBE95] L. Bruno-Blanch and G. L. Estiu. Quantum chemistry in QSAR: Anticonvulsivant activity of VPA derivatives. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):39–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Bonchev:1994:MCC

[BBLK94] D. Bonchev, A. T. Balaban, X. Liu, and D. J. Klein. Molecular cyclicity and centricity of polycyclic graphs. I cyclicity based on resistance distance or reciprocal distances. *International Journal of Quantum Chemistry*, 50(1):1–??, March 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bertini:1999:LEC

[BBMM99] Luca Bertini, Dario Bressanini, Massimo Mella, and Gabriele Morosi. Linear expansions of correlated functions: Variational Monte Carlo case study. *International Journal of Quantum Chemistry*, 74(1):23–33, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62000135; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62000135&PLACEBO=IE.pdf`.

Bearpark:1996:PES

[BBOR96] Michael J. Bearpark, Fernando Bernardi, Massimo Olivucci, and Michael A. Robb. Potential energy surfaces of pseudoaromatic molecules: An MMVB and CASSCF study of pentalene. *International Journal of Quantum Chemistry*, 60(1):505–512, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60613`.

Boettger:1994:QSE

[BBRT94] J. C. Boettger, U. Birkenheuer, N. Roesch, and S. B. Trickey. Quantum size effects in hexagonal aluminum films. *International Journal of Quantum Chemistry. Symposium*, 28:675–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Bernholc:1997:RSM

[BBS+97] J. Bernholc, E. L. Briggs, D. J. Sullivan, C. J. Brabec, M. Buongiorno Nardelli, K. Rapcewicz, C. Roland, and M. Wensell. Real-space multigrid methods for large-scale electronic structure problems. *International Journal of Quantum Chemistry*, 65(5):531–543, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42782; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42782&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the*

International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Bagdassarian:1996:QMMc

[BBSS96a] C. K. Bagdassarian, B. B. Braunheim, V. L. Schramm, and S. D. Schwartz. Quantitative measures of molecular similarity: Methods to analyze transition-state analogs for enzymatic reactions. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 23 (??):73–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

Bagdassarian:1996:QMMa

[BBSS96b] C. K. Bagdassarian, B. B. Braunhelm, V. L. Schramm, and S. D. Schwartz. Quantitative measures of molecular similarity: Methods to analyze transition-state analogs for enzymatic reactions. *International Journal of Quantum Chemistry*, 60(8): 73–??, 1996. CODEN IJQCB2.

Bagdassarian:1996:QMMb

[BBSS96c] Carey K. Bagdassarian, Benjamin B. Braunheim, Vern L. Schramm, and Steven D. Schwartz. Quantitative measures of molecular similarity: Methods to analyze transition-state analogs for enzymatic reactions. *International Journal of Quantum Chemistry*, 60(8):1797–1804, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60751`.

Barone:1997:CBP

[BBTU97] Vincenzo Barone, Alessandro Bencini, Federico Totti, and Myriam G. Uytterhoeven. Comparison between post-Hartree–Fock and DFT methods for the study of strength and mechanism of cleavage of Hg — C bond. *International Journal of Quantum Chemistry*, 61(3):361–367, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42410`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42410&PLACEBO=IE.pdf`.

Bendale:1991:CES

[BBZ91] Rajiv D. Bendale, John David Baker, and Michael C. Zerner. Calculations on the electronic structure and spectroscopy of C_{60} and C_{70} cage structures. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:557–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Brown:1993:SME

[BC93] R. G. Brown and M. Ciftan. Statistical microdynamics of extended systems in natural function spaces. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:363–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Bracken:1995:ISC

[BČ95] P. Bracken and J. Čížek. Investigation of the $^1E_{2g}^-$ states in cyclic polyenes. *International Journal of Quantum Chemistry*, 53(5):467–471, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baxter:1996:MFH

[BC96a] Carol A. Baxter and David B. Cook. Molecular fragments and the hybrid basis. *International Journal of Quantum Chemistry*, 60(1):173–183, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60580`.

Bracken:1996:IPT

[BČ96b] P. Bracken and J. Čížek. Interpolant polynomial technique applied to the PPP model. I. asymptotics for excited states of cyclic polyenes in the finite cyclic Hubbard model. *International Journal of Quantum Chemistry*, 57(6):1019–1031, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60446`.

Benson:1997:LTM

[BC97a] Michael T. Benson and Thomas R. Cundari. Late transition-metal multiple bonding: Platinum phosphinidenes and ruthenium alkylidenes. *International Journal of Quantum Chemistry*, 65(5):987–996, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42830; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42830&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Blaudeau:1997:OGB

[BC97b] J.-P. Blaudeau and L. A. Curtiss. Optimized Gaussian basis sets for use with relativistic effective (core) potentials: K, Ca, Ga–Kr. *International Journal of Quantum Chemistry*, 61(6):943–952, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42478; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42478&PLACEBO=IE.pdf.

Bandrauk:1999:MNW

[BCC99] A. D. Bandrauk, S. Chelkowski, and P. B. Corkum. Measuring nuclear wave functions by laser Coulomb explosion imaging. *International Journal of Quantum Chemistry*, 75(4–5):951–959, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004989/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004989&PLACEBO=IE.pdf.

Brandas:1995:FLS

[BCD95] E. J. Brändas and C. A. Chatzidimitriou-Dreismann. Fundamentals, logical structure, and unification of natural sciences. *International Journal of Quantum Chemistry*, 53(1):95–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burke:1998:UEC

[BCL98] Kieron Burke, Federico G. Cruz, and Kin-Chung Lam. Unambiguous exchange — correlation energy density for Hooke's atom. *International Journal of Quantum Chemistry*, 70(4-5):583–589, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75036;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75036&PLACEBO=IE.pdf.

Benson:1994:ECP

[BCLS94] M. T. Benson, T. R. Cundari, Y. Li, and L. A. Strohecker. Effective core potential study of multiply bonded transition metal complexes of the heavier main group elements. *International Journal of Quantum Chemistry. Symposium*, 28:181–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Bergson:1997:VMI

[BCMÖ97] Göran Bergson, Jean-Louis Calais, Jorge Morales, and Yngve Öhrn. Vibrational motion in isotopomers of the HeH^+ molecular ion: An application of the electron nuclear dynamics method. *International Journal of Quantum Chemistry*, 63 (2):415–424, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42585; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42585&PLACEBO=IE.pdf.

Bohr:1994:DFS

[BCRL94] F. Bohr, H. Chermette, and M. F. Ruiz-Lopez. A density functional study of pseudotetrahedral metal-nitrosyl complexes. *International Journal of Quantum Chemistry*, 52(4):1039–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bu:1996:ISH

[BCS96] Yuxiang Bu, Zhaohua Cao, and Xinyu Song. Ab initio studies on hydrogen-transfer tunneling for Cl + HCl abstraction hydrogen reaction. *International Journal of Quantum Chemistry*, 57(1):95–104, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60348.

Bu:1995:ISR

[BCY95] Y. Bu, Z. Cao, and Z. Yang. The inner-sphere reorganization energies for AH_2 + ${AH_2}^{+(-)}$ (A = Al, Si, P, S) electron self-exchange reactions in electron-transfer processes from ab initio calculations. *International Journal of Quantum Chemistry*, 55 (4):329–337, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bian:1994:DSMa

[BD94a] W. Bian and C. Deng. Direct solution of the many-body Schrödinger equation in the hyperspherical formalism: Application of the HH-GLF method to the positronium ion e + e — e+. *International Journal of Quantum Chemistry*, 50(6):395–??, June 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bian:1994:DSMb

[BD94b] W. Bian and C. Deng. Direct solution of the many-body Schrödinger equation in the hyperspherical formalism: Formulation of the CFHH-GLF method. *International Journal of Quantum Chemistry*, 51(4):285–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bian:1994:DSMc

[BD94c] W. Bian and C. Deng. Direct solution of the many-body Schrödinger equation in the hyperspherical formalism: Formulation of the CFHH-GLF method. *International Journal of Quantum Chemistry*, 51(5):285–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bian:1995:TCD

[BD95] W. Bian and C. Deng. Theoretical and computational developments. *International Journal of Quantum Chemistry*, 54(5): 273–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandt:1996:PBQ

[BDC96] Siegmund Brandt, Hans Dieter Dahmen, and H. Carlsen. The Picture Book of Quantum Mechanics, 2nd ed. *International Journal of Quantum Chemistry*, 58(5):533–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bureau:1993:CSC

[BDD93] C. Bureau, M. Defranceschi, and J. Delhalle. Cluster-size convergence of some physical parameters of bare (Ni_n) and CH_3-Chemisorbed (CH_3-Ni_n) nickel (111) clusters: An ab initio study. *International Journal of Quantum Chemistry*, 46(1):87–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baeten:1996:PAA

[BDG96] A. Baeten, F. De Proft, and P. Geerlings. Proton affinity of amino acids: Their interpretation with density functional theory-based descriptors. *International Journal of Quantum Chemistry*, 60(4):931–939, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60651.

Bu:1997:NIS

[BDH+97] Yuxiang Bu, Yangjun Ding, Faxin He, Lifu Jiang, and Xinyu Song. Nonempirical ab initio studies on inner-sphere reorganization energies of $M^{2+}(H_2O)_6/M^{3+}(H_2O)_6$ redox couples at valence basis level. *International Journal of Quantum Chemistry*, 61(1):117–126, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42377; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42377&PLACEBO=IE.pdf.

Berthier:1997:FFD

[BDNT97] G. Berthier, M. Defranceschi, J. Navaza, and G. Tsoucaris. Form factors directly determined from momentum space Hartree–Fock solutions: H_2 and Li_2. *International Journal of Quantum Chemistry*, 63(2):451–457, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42589; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42589&PLACEBO=IE.pdf.

Bray:1997:RPL

[BDPS97] Mark R. Bray, Robert J. Deeth, Veronica J. Paget, and Paul D. Sheen. The relative performance of the local density approximation and gradient-corrected density functional theory for computing metal-ligand distances in Werner-type and organometallic complexes. *International Journal of Quantum Chemistry*, 61(1):85–91, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42373; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42373&PLACEBO=IE.pdf.

Berthier:1996:NOS

[BDT96] G. Berthier, M. Defranceschi, and G. Tsoucaris. Note on origin-shift invariants and phase constraints for momentum space wave functions. *International Journal of Quantum Chemistry*, 60(1):195–199, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60583`.

Bendazzoli:1993:CAF

[BE93] G. L. Bendazzoli and S. Evangelisti. Computation and analysis of the full configuration interaction wave function of some simple systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:287–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Bendazzoli:1995:PMA

[BE95] G. L. Bendazzoli and S. Evangelisti. The PPP model of alternant cyclic polyenes with modified boundary conditions. *International Journal of Quantum Chemistry*, 55(4):347–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bendazzoli:1998:ABR

[BE98] G. L. Bendazzoli and S. Evangelisti. Asymptotic behavior of the RHF energy of the PPP model of alternant cyclic polyenes. *International Journal of Quantum Chemistry*, 66 (6):397–407, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29875; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29875&PLACEBO=IE.pdf`.

Becke:1994:TTK

[Bec94] A. D. Becke. Thermochemical tests of a kinetic-energy dependent exchange-correlation approximation. *International Journal of Quantum Chemistry. Symposium*, 28:625–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Beck:1997:HSC

[Bec97a] Donald R. Beck. Hyperfine structure constants of $(d + s)^3$ states in La I and the Zr II and Hf II isoelectronic sequences. *International Journal of Quantum Chemistry*, 65

(5):555–564, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42785; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42785&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Beck:1997:RSM

[Bec97b] Thomas L. Beck. Real-space multigrid solution of electrostatics problems and the Kohn–Sham equations. *International Journal of Quantum Chemistry*, 65(5):477–486, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42776; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42776&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Beebe:1972:NSS

[Bee72] Nelson H. F. Beebe. A note on space spanning. *International Journal of Quantum Chemistry*, 6S:439–441, 1972. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Beebe:1976:SFS

[Bee76] Nelson H. F. Beebe. On the symmetry of filled shells. *International Journal of Quantum Chemistry*, 10:1007–1010, 1976. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Beebe:1979:MVO

[Bee79] Nelson H. F. Beebe. Modification of virtual orbitals. *International Journal of Quantum Chemistry*, 15:589–600, 1979. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bendazzoli:1994:FCI

[BEG94] G. L. Bendazzoli, S. Evangelisti, and L. Gagliardi. Full configuration interaction study of the ground state of closed-shell cyclic PPP polyenes. *International Journal of Quantum Chemistry*, 51(1):13–??, June 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bouferguene:1998:CDM

[BEJ98] Ahmed Bouferguene, Babak Etemadi, and Herbert W. Jones. Calculations on diatomic molecules with Slater-type orbital basis sets. *International Journal of Quantum Chemistry*, 70(1):89–93, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74372; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74372&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Bergson:1996:CIR

[Ber96a] G. Bergson. The Chairman's introductory remark. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):3–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Bergstrom:1996:QME

[Ber96b] R. Bergström. *Quantum Mechanical Electronic Structure Calculations with Chemical Accuracy.* edited by S. R. Langhoff. *International Journal of Quantum Chemistry*, 60(3):791–??, 1996. CODEN IJQCB2.

Berry:1996:MDP

[Ber96c] R. Stephen Berry. Many-dimensional potential surfaces: What they imply and how to think about them. *International Journal of Quantum Chemistry*, 58(6):657–670, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60519.

Berces:1997:DFC

[Bér97] Attila Bérces. Density functional calculations of dioxygen binding in mono- and dinuclear copper complexes. *International Journal of Quantum Chemistry*, 65(6):1077–1086, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42844; http://www3.

interscience.wiley.com/cgi-bin/fulltext?ID=42844&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on the Application of Fundamental Theory to Problems of Biology and Pharmocolgy*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Bouferguene:1994:SCA

[BF94] A. Bouferguene and M. Fares. Some convergence aspects of the one-center expansion methods. *International Journal of Quantum Chemistry*, 51(6):345–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barone:1995:TER

[BF95] V. Barone and S. Fliszar. Theoretical energies of representative carbon-carbon bonds. *International Journal of Quantum Chemistry*, 55(6):469–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bacchus-Montabonel:1996:SSE

[BF96] M. C. Bacchus-Montabonel and F. Fraija. State-selective electron capture processes in collisions involving boron ions. *International Journal of Quantum Chemistry*, 57(4):611–623, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60425.

Bouferguene:1996:SST

[BFH96] A. Bouferguene, M. Fares, and P. E. Hoggan. STOP: A Slater-type orbital package for molecular electronic structure determination. *International Journal of Quantum Chemistry*, 57(4): 801–810, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60418.

Broeckhove:1991:STD

[BFL91] J. Broeckhove, B. Feyen, and L. Lathouwers. Sensitivity of time-dependent vibrational dynamics to curve-crossing topology. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:141–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Brajczewska:1993:ESC

[BFP93] M. Brajczewska, C. Fiolhais, and J. P. Perdew. Energetics of small clusters of stabilized jellium: Continuum and shell-structure effects. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:249–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Broeckhove:1992:MAA

[BFV92] J. Broeckhove, B. Feyen, and P. Van Leuven. Multiphoton absorption in anharmonic systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:435–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Broeckhove:1993:QWD

[BFV+93] J. Broeckhove, B. Feyen, P. Van Leuven, R. Cimiraglia, and M. Persico. Quantum wavepacket dynamics for the ${}^1\Sigma^+$ states of boron hydride. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:517–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Broeckhove:1994:IRM

[BFV94] J. Broeckhove, B. Feyen, and P. Van Leuven. Influence of rotation on multiphoton processes in HF. *International Journal of Quantum Chemistry. Symposium*, 28:173–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Brandas:1970:CPS

[BG70] E. Brändas and O. Goscinski. Critical point, singularities, and extrapolations in the helium isoelectronic sequence. *International Journal of Quantum Chemistry*, 4(??):571–??, ?? 1970. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bochicchio:1995:MES

[BG95] R. C. Bochicchio and H. Grinberg. On master equations, spectral resolutions, and self-energy fields in propagator theories for quantum open systems. *International Journal of Quantum Chemistry*, 54(1):27–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bokanowski:1998:UDM

[BG98a] Olivier Bokanowski and Benoît Grebert. Utilization of deformations in molecular quantum chemistry and application to density functional theory. *International Journal of Quantum Chemistry*, 68(4):221–231, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29943; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29943&PLACEBO=IE.pdf.

Burton:1998:MEGa

[BG98b] P. J. Burton and M. D. Gould. Matrix elements of $U(2n)$ generators in a multishell spin-orbit basis. I. The del-operator MEs in a two-shell composite Gelfand–Paldus basis. *International Journal of Quantum Chemistry*, 66 (5):323–343, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29869; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29869&PLACEBO=IE.pdf.

Burton:1998:MEGb

[BG98c] P. J. Burton and M. D. Gould. Matrix elements of $U(2n)$ generators in a multishell spin-orbit basis. II. The two-shell nonzero shift ACCs and $U(2n)$ generator MEs. *International Journal of Quantum Chemistry*, 66(5):345–363, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29870; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29870&PLACEBO=IE.pdf.

Burton:1998:MEGc

[BG98d] P. J. Burton and M. D. Gould. Matrix elements of $U(2n)$ generators in a multishell spin-orbit basis. III. General formulas. *International Journal of Quantum Chemistry*, 66 (5):365–375, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29871; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29871&PLACEBO=IE.pdf.

Buendia:1997:HFW

[BGS97] E. Buendía, F. J. Gálvez, and A. Sarsa. Hartree–Fock wave functions with a modified GTO basis for atoms. *International Journal of Quantum Chemistry*, 65(1):59–64, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42741; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42741&PLACEBO=IE.pdf.

Buendia:1998:FWF

[BGS98] E. Buendía, F. J. Gálvez, and A. Sarsa. Factored wave function for bound S-type states of two-electron atomic systems. *International Journal of Quantum Chemistry*, 68 (6):405–413, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29958; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29958&PLACEBO=IE.pdf.

Baccarelli:1999:SSE

[BGS99] I. Baccarelli, F. A. Gianturco, and F. Schneider. Spatial structures and electronic excited states of small protonated helium clusters. *International Journal of Quantum Chemistry*, 74(2):193–212, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003364; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003364&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Brailsford:1971:SPO

[BH71] D. F. Brailsford and G. G. Hall. Symmetry properties of one- and two-electron molecular integrals. *International Journal of Quantum Chemistry*, 5(??):657–668, ?? 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bianco:1999:TSH

[BH99] Roberto Bianco and James T. Hynes. Theoretical studies of heterogeneous reaction mechanisms relevant for stratospheric ozone depletion. *International Journal of Quantum Chemistry*, 75(4–5):683–692, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004965/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004965&PLACEBO=IE.pdf.

Bhattacharjee:1999:IQC

[Bha99] Apurba K. Bhattacharjee. Ab initio quantum chemical analysis of stereoelectronic properties may explain *in vitro* antileishmanial activity of some macrocyclic bisbenzylisoquinoline alkaloids. *International Journal of Quantum Chemistry*, 75(6):995–1002, December 20, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004795/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004795&PLACEBO=IE.pdf`.

Brewster:1995:RRD

[BHB+95] M. E. Brewster, M.-J. Huang, C. Browne, M. Bodor, E. Pop, and A. T. Balaban. Relative reactivity of 1,4- and 1,6-Dihydronicotinic acid derivatives to radically mediated oxidation — A theoretical and experimental evaluation. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):161–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Bohr:1999:TSP

[BHGC99] F. Bohr, E. Henon, I. García, and M. Castro. Theoretical study of the peroxy radicals RO_2 self-reaction: Structures and stabilization energies of the intermediate RO_4 R for various R. *International Journal of Quantum Chemistry*, 75(4–5):671–682, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004964/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004964&PLACEBO=IE.pdf`.

Bodor:1992:NNS

[BHH92] N. Bodor, M.-J. Huang, and A. Harget. Neural network studies. 4. an extended study of the aqueous solubility of organic compounds. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:853–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Burk:1993:CTP

[BHKK93] P. Burk, K. Herodes, I. Koppel, and I. Koppel. Critical test of PM3-Calculated proton affinities. *International Journal of*

Quantum Chemistry. Quantum Chemistry Symposium, 27:633–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Bakker:1999:IAI

[BHL+99] Albert Bakker, Kersti Hermansson, Jan Lindgren, Michael M. Probst, and Philippe A. Bopp. Interaction of Aluminum(III) with water. An ab initio study. *International Journal of Quantum Chemistry*, 75(4–5):659–669, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004963/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004963&PLACEBO=IE.pdf`.

Brandas:1975:DRS

[BHM75] E. Brändas, M. Hehenberger, and H. V. McIntosh. Dispersion relations and spectral densities. *International Journal of Quantum Chemistry*, 9(??):103–117, ?? 1975. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brewster:1993:HSS

[BHPB93] M. E. Brewster, M.-J. Huang, E. Pop, and N. Bodor. Hydroxyl stretching in substituted phenols: An AM1 study. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:7–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Brewster:1995:IIT

[BHPB95] M. E. Brewster, M.-J. Huang, E. Pop, and N. Bodor. Isomeric interconversions in tamoxifen and related compounds: An AM1 study. *International Journal of Quantum Chemistry*, 53(3):343–??, February 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Broch:1996:IMIa

[BHV96a] H. Broch, A. Hamza, and D. Vasilescu. Ab initio modeling of the interaction between guanine-cytosine base pair and mustard alkylating agents. *International Journal of Quantum Chemistry*, 60(8):21–??, 1996. CODEN IJQCB2.

Broch:1996:IMIb

[BHV96b] H. Broch, A. Hamza, and D. Vasilescu. Ab initio modeling of the interaction between guanine-cytosine base pair and mustard alkylating agents. *International Journal of Quantum Chemistry*, 60(8):1745–1764, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60747.

Broch:1996:IMIc

[BHV96c] H. Broch, A. Hamza, and D. Vasilescu. Ab initio modeling of the interaction between guanine-cytosine base pair and mustard alkylating agents. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 23(??):21–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

Bishop:1996:MSQ

[BHX96] R. F. Bishop, R. G. Hale, and Y. Xian. A microscopic study of the quantum critical behavior of the spin-1/2 anisotropic Heisenberg models. *International Journal of Quantum Chemistry*, 57(5):919–927, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60430.

Beltran:1995:MSC

[BILA95] A. Beltran, J. A. Igualada, R. Llusar, and J. Andres. $MgAl_2O_4$ spinel crystal structure an ab initio perturbed ion study. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:685–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Beck:1997:MMD

[BIM97] Thomas L. Beck, Karthik A. Iyer, and Michael P. Merrick. Multigrid methods in density functional theory. *International Journal of Quantum Chemistry*, 61(2):341–348, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42398; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42398&PLACEBO=IE.pdf.

Belmiloud:1998:DSA

[BJ98] D. Belmiloud and M. Jacon. DVR study of the $A_2B_2 \leftarrow X^2A_1$ absorption spectrum of NO_2. *International Journal of Quantum Chemistry*, 70(3):475–489, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75015; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75015&PLACEBO=IE.pdf.

Boettger:1999:SPC

[BJA99] J. C. Boettger, M. D. Jones, and R. C. Albers. Structural properties of crystalline uranium from linear combination of Gaussian-type orbitals calculations. *International Journal of Quantum Chemistry*, 75(4–5):911–915, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004978/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004978&PLACEBO=IE.pdf.

Bodor:1997:TSS

[BjH97] Nicholas S. Bodor and Ming ju Huang. Theoretical study of the stereoisomers of tetrahydrocannabinols. *International Journal of Quantum Chemistry*, 61(1):127–135, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42378; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42378&PLACEBO=IE.pdf.

Bunge:1998:ODP

[BJLK98] Carlos F. Bunge, Rocio Jáuregui, and Eugenio Ley-Koo. Optimal decoupling of positive- and negative-energy orbitals in relativistic electronic structure calculations beyond Hartree–Fock. *International Journal of Quantum Chemistry*, 70(4-5):805–812, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75059; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75059&PLACEBO=IE.pdf.

Bernardinelli:1994:CSS

[BJMT94] G. Bernardinelli, C. W. Jefford, D. Maric, and C. Thomson. Computational studies of the structures and properties of potential antimalarial compounds based on the 1,2,4-Trioxane ring structure. I. artemisinin-like molecules. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21:117–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Bernotas:1994:SQC

[BK94a] A. Bernotas and J. Kaniauskas. Second quantization and coefficients of fractional parentage. *International Journal of Quantum Chemistry*, 50(4):293–??, May 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Blanke:1994:NNE

[BK94b] G. Blanke and H. Kleindienst. Nonadiabatic NO expansions for the ground state wave function of H_2^+. *International Journal of Quantum Chemistry*, 51(1):3–??, June 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burk:1994:TSS

[BK94c] P. Burk and I. Koppel. Theoretical study of structure and basicity of some alkali metal oxides, hydroxides, and amides. *International Journal of Quantum Chemistry*, 51(4 (or 5??)): 313–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bleil:1995:CRL

[BK95] R. Bleil and S. Kais. Charge renormalization at the large-D limit for atoms and molecules. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:349–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Bader:1996:UEC

[BK96] R. F. W. Bader and T. A. Keith. Use of electron charge and current distributions in the determination of atomic contributions to magnetic properties. *International Journal of Quantum Chemistry*, 60(1):373–379, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60599.

Bellaiche:1997:AEC

[BK97] L. Bellaiche and K. Kunc. All-electron calculations with plane waves in solid lithium hydride. *International Journal of Quantum Chemistry*, 61(4):647–656, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42451; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42451&PLACEBO=IE.pdf.

Bytautas:1998:SAN

[BK98] L. Bytautas and D. J. Klein. Symmetry aspects of non-rigid molecules and transition structures in chemical reactions. *International Journal of Quantum Chemistry*, 70 (1):205–217, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74366; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74366&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Backer:1994:RST

[BKEMM94] T. Backer, M. Klessinger, M. Eckert-Makosic, and Z. B. Maksic. The relative stability of the tautomers of alpha-hydroxytetronic acid. *International Journal of Quantum Chemistry*, 50(6):385–??, June 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barrois:1997:ANEa

[BKL97] René Barrois, Heinz Kleindienst, and Arne Lüchow. Accurate nonrelativistic energies for $^2\mathrm{P}^o$ states of the Li isoelectronic series. *International Journal of Quantum Chemistry*, 61(1):107–116, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42376; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42376&PLACEBO=IE.pdf.

Busse:1998:NEA

[BKL98] Georg Büsse, Heinz Kleindienst, and Arne Lüchow. Nonrelativistic energies for the Be atom: Double-linked Hylleraas-CI calculation. *International Journal of Quantum Chemistry*, 66 (3):241–247, January 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29857; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29857&PLACEBO=IE.pdf.

Broeckhove:1994:AGS

[BKLV94] J. Broeckhove, W. Keutgens, L. Lathouwers, and P. Van Leuven. Application of the GCA to a series of curve crossing topologies. *International Journal of Quantum Chemistry*, 52(1):49–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Broeckhove:1995:DNE

[BKLv95] J. Broeckhove, W. Keutgens, L. Lathouwers, and P. van Leuven. On the definition of nonadiabatic effects in curve-crossing problems. *International Journal of Quantum Chemistry*, 55(1): 3–??, July 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bonchev:1993:SRW

[BKM93] D. Bonchev, L. B. Kier, and O. Mekenyan. Self-returning walks and fractional electronic charges of atoms in molecules. *International Journal of Quantum Chemistry*, 46(5):635–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balawender:1997:ABM

[BKR97] Robert Balawender, Ludwik Komorowski, and Szczepan Roszak. Acidic and basic molecular hardness in LCAO approximation. *International Journal of Quantum Chemistry*, 61(3):499–505, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42418; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42418&PLACEBO=IE.pdf.

Balaban:1996:HDC

[BKS96] Alexandru T. Balaban, Douglas J. Klein, and William A. Seitz. Holes in diamond or carbon nitride lattices. *International Journal of Quantum Chemistry*, 60(5):1065–1068, December 5, 1996.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60665.

Bajdor:1997:ETS

[BKWL97] Krzysztof Bajdor, Piotr Koczoń, Ewa Wieckowska, and Włodzimierz Lewandowski. Experimental and theoretical studies on vibrational structure of metal complexes with m-halogenobenzoic acids. *International Journal of Quantum Chemistry*, 62(4):385–392, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42525; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42525&PLACEBO=IE.pdf.

Belousov:1999:IPM

[BKY99] A. V. Belousov, V. A. Kovarsky, and B. S. Yastrebov. Influence of the polar medium fluctuation on the nonradiative electron transfer in molecules. *International Journal of Quantum Chemistry*, 74(4):381–386, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62502088; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62502088&PLACEBO=IE.pdf.

Beebe:1972:POT

[BL72] Nelson H. F. Beebe and Sten Lunell. A projection operator technique for orbital basis variation. *International Journal of Quantum Chemistry*, 6:1149–1155, 1972. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Beebe:1977:STE

[BL77] Nelson H. F. Beebe and Jan Linderberg. Simplifications in the two-electron integral array in molecular calculations. *International Journal of Quantum Chemistry*, 12(4):683–705, October 1977. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Braga:1992:CLR

[BL92] M. Braga and S. Larsson. Calculation of the long-range coupling between electrons in lone pairs and double bonds using semiempirical and ab initio methods. *International Journal of*

Quantum Chemistry, 44(5):839–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bustad:1998:SCI

[BL98] J. Bustad and S. Lunell. Semiempirical configuration interaction calculations of XPS shake-up satellites in $Ni(CO)_4$. *International Journal of Quantum Chemistry*, 69(5):649–657, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30029; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30029&PLACEBO=IE.pdf`.

Babinec:1999:ISS

[BL99] Peter Babinec and Jerzy Leszczynski. An ab initio study of the structures and properties of the ${XH_4}^{2+}$ and ${XH_6}^{2+}$ (X = C, Si, Ge) dications. *International Journal of Quantum Chemistry*, 72(4):319–324, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006307; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006307&PLACEBO=IE.pdf`. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Blado:1996:STP

[Bla96] Gardo Garnet Blado. Supersymmetric treatment of a particle subjected to a ring-shaped potential. *International Journal of Quantum Chemistry*, 58(5):431–439, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60498`.

Blaney:1999:HMI

[Bla99] Frank E. Blaney. Homology modeling and ab initio calculations identify a basis for ligand selectivity for the PPARγ nuclear hormone receptor. *International Journal of Quantum Chemistry*, 73(2):97–111, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003509; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003509&PLACEBO=IE.pdf`. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba*

(Italy), September 8-11, 1998. Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Bittererova:1995:ICS

[BLB95] M. Bittererova, H. Lischka, and S. Biskupic. Ab initio calculation of stationary points for the ground and the first excited state of HCO. *International Journal of Quantum Chemistry*, 55(3):261–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bersuker:1997:MCQ

[BLBP97] I. B. Bersuker, M. K. Leong, J. E. Boggs, and R. S. Pearlman. A method of combined quantum mechanical (QM)/molecular mechanics [MM] treatment of large polyatomic systems with charge transfer between the QM and MM fragments. *International Journal of Quantum Chemistry*, 63(6):1051–??, July 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bahn:1995:TSL

[BLC95] C. S. Bahn, C. J. Lauderdale, and R. T. Carlin. A theoretical study of lithium ion and aromatic organic cation graphite intercalates. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:533–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Bergstrom:1996:CSD

[BLE96] Robert Bergström, Sten Lunell, and Leif A. Eriksson. Comparative study of DFT methods applied to small titanium/oxygen compounds. *International Journal of Quantum Chemistry*, 59(6):427–443, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60562`.

Bundgen:1995:CIS

[BLG95] P. Bundgen, G. H. Lushington, and F. Grein. Configuration interaction study of relativistic corrections to the Zeeman effect in diatomic molecules. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:283–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Barrois:1997:ANEb

[BLK97] René Barrois, Arne Lüchow, and Heinz Kleindienst. Accurate nonrelativistic energies for ^{2}p^e states of the Li isoelectronic series. *International Journal of Quantum Chemistry*, 62(1):77–88, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42491; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42491&PLACEBO=IE.pdf.

Bockisch:1992:SAL

[BLRD92] F. Bockisch, D. Liotard, J.-C. Rayez, and B. Duguay. Simulated annealing to locate various stationary points in semiempirical methods. *International Journal of Quantum Chemistry*, 44(4):619–??, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Berendsen:1996:ANT

[BM96] Herman J. C. Berendsen and Janez Mavri. Approach to nonadiabatic transitions by density matrix evolution and molecular dynamics simulations. *International Journal of Quantum Chemistry*, 57(5):975–983, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60436.

Bacchus-Montabonel:1993:TTE

[BMA93] M. C. Bacchus-Montabonel and K. Amezian. Theoretical treatment of electron capture processes for closed- and open-shell systems. *International Journal of Quantum Chemistry*, 45(6):709–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burrows:1999:AAS

[BMA99] B. L. Burrows, F. M. Moideen, and A. T. Amos. Approximate analytical solutions for two-state time-dependent problems. *International Journal of Quantum Chemistry*, 74(5):559–571, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62503007; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62503007&PLACEBO=IE.pdf. Special Issue: *The Role of*

Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II). Issue Edited by Don Rees, Hiroshi Fujimotoi.

Bruna:1995:SBI

[BMG95] P. J. Bruna, R. C. Mawhinney, and F. Grein. Stability of BN and its ions, from BN_3^+ to BN_2^-. an ab initio MRD-CI study. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:455–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Butler:1998:SAD

[BMG+98] Leslie G. Butler, Andrew W. Maverick, Cenobio H. Gallegos, Jeffrey D. Goettee, Bruce R. Marshall, C. Maxwell Fowler, Dwight G. Rickel, Joseph M. Gonzales, and Leonard J. Tabaka. Some aspects of data processing for an optical absorption experiment in a pulsed 1000-Tesla magnet. *International Journal of Quantum Chemistry*, 70(4-5):797–804, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75058; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75058&PLACEBO=IE.pdf.

Blumhagen:1996:DTD

[BMK96] K. Blumhagen, I. Muegge, and E. W. Knapp. Diffusion of two different water models and thermal conductivity in a protein-water system. *International Journal of Quantum Chemistry*, 59(4):271–279, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60547.

Boone:1998:SPE

[BML98] Amy J. Boone, David H. Magers, and Jerzy Leszczyński. Searches on the potential energy hypersurfaces of $GeCH_2$, $GeSiH_2$, and Ge_2 H_2. *International Journal of Quantum Chemistry*, 70(4-5):925–932, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75070; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75070&PLACEBO=IE.pdf.

Brinck:1992:SEP

[BMP92] T. Brinck, J. S. Murray, and P. Politzer. Surface electrostatic potentials of halogenated methanes as indicators of directional intermolecular interactions. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:57–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Brinck:1993:MSE

[BMP93] R. Brinck, J. S. Murray, and P. Politzer. Molecular surface electrostatic potentials and local ionization energies of group V-VII hydrides and their anions: Relationships for aqueous and gas-phase acidities. *International Journal of Quantum Chemistry*, 48(2):73–??, October 15, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Broch:1993:EPG

[BMVV93] H. Broch, M. Msellem, R. Viani, and D. Vasilescu. Electrostatic properties of glutathione: A quantum molecular study. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:49–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Beck:1974:EEC

[BN74] D. R. Beck and C. A. Nicolaides. The effect of electron correlation on atomic properties. *International Journal of Quantum Chemistry*, S8(??):17–28, ?? 1974. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bettega:1996:NGG

[BNLF96] Márcio H. F. Bettega, Alexandra P. P. Natalense, Marco A. P. Lima, and Luiz G. Ferreira. Note on the generation of Gaussian bases for pseudopotential calculations. *International Journal of Quantum Chemistry*, 60(4):821–824, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60654`.

BiccadeAlencastro:1994:SEE

[BNZ94] R. Bicca de Alencastro, J. D. Da Motta Neto, and M. C. Zerner. Solvent effects on the electronic spectrum of Reichardt's dye. *International Journal of Quantum Chemistry. Symposium*, 28: 361–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Brzeska:1993:CPF

[BO93] D. Brzeska and S. Olszewski. Closure property for free electrons. *International Journal of Quantum Chemistry*, 45(1):105–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boca:1996:PCO

[Boč96] Roman Boča. Platinum-centered octakis (triphenylphosphino gold) clusters: A relativistic MO study. *International Journal of Quantum Chemistry*, 57(4):735–740, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60412`.

Boettger:1991:TPL

[Boe91] J. C. Boettger. Theoretical properties of a 3-layer film of $LiBeH_3$. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:629–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Boettger:1992:CTD

[Boe92] J. C. Boettger. Calculations of thickness dependencies in the properties of ultra-thin films. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:633–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Boettger:1993:SPL

[Boe93] J. C. Boettger. Spin-polarized LCGTO-FF band structure technique: Application to 3d transition metal monolayers. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:147–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Boettger:1995:ESC

[Boe95] J. C. Boettger. Equation of state calculations using the LCGTO-FF method: Equilibrium properties of hcp beryllium. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:197–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Boettger:1996:GFFa

[Boe96a] J. C. Boettger. Gaussian fitting function basis sets for crystalline silicon: Bond-centered s-type vs. site-centered f-type.

International Journal of Quantum Chemistry, 60(7):133–??, 1996. CODEN IJQCB2.

Boettger:1996:GFFc

[Boe96b] J. C. Boettger. Gaussian fitting function basis sets for crystalline silicon: Bond-centered *s*-type vs. site-centered *f*-type. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):133–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Boettger:1996:GFFb

[Boe96c] Jonathan C. Boettger. Gaussian fitting function basis sets for crystalline silicon: Bond-centered *s*-type vs. site-centered *f*-type. *International Journal of Quantum Chemistry*, 60 (7):1345–1349, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60692`.

Boettger:1997:SRL

[Boe97] Jonathan C. Boettger. Scalar-relativistic LCGTO DFT calculations for atoms using the Douglas–Kroll transformation. *International Journal of Quantum Chemistry*, 65(5): 565–574, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42786; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42786&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Boettger:1998:RES

[Boe98] J. C. Boettger. Relativistic effects on the structural phase stability of molybdenum. *International Journal of Quantum Chemistry*, 70(4-5):825–830, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75061; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75061&PLACEBO=IE.pdf`.

Borstnik:1994:CCD

[Bor94] B. Borstnik. The character of the correlations in DNA sequences. *International Journal of Quantum Chemistry*, 52(2):

457–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boustani:1994:SLI

[Bou94] I. Boustani. Systematic LSD investigations on cationic boron clusters: B0+n ($n = 2 - 14$). *International Journal of Quantum Chemistry*, 52(4):1081–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boudreaux:1996:SMCa

[Bou96a] E. A. Boudreaux. SCMEH-MO calculations on lanthanide systems. III. $Ln(CO)_6$, $Ln(OC)_6$ (Ln = Nd, Sm). *International Journal of Quantum Chemistry*, 60(7):461–??, 1996. CODEN IJQCB2.

Boudreaux:1996:SMCc

[Bou96b] E. A. Boudreaux. SCMEH-MO calculations on lanthanide systems. III. $Ln(CO)_6$, $Ln(OC)_6$ (Ln = Nd, Sm). *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):461–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Boudreaux:1996:SMCb

[Bou96c] Edward A. Boudreaux. SCMEH-MO calculations on lanthanide systems. III. $Ln(CO)_6$, $Ln(OC)_6$ (Ln = Nd, Sm). *International Journal of Quantum Chemistry*, 60(7):1673–1677, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60728`.

Bartolotti:1994:QOC

[BOX94] L. J. Bartolotti, L. Ortiz, and Q. Xie. Quadrupole and octupole Cauchy moments of the atoms through argon. *International Journal of Quantum Chemistry*, 49(4):449–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bodor:1992:IBR

[BP92] N. Bodor and L. Prokai. Intermediates of the borane reduction of some imidazolidines: An am1 study. *International Journal of Quantum Chemistry*, 44(5):795–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bishop:1993:DQOb

[BP93a] D. M. Bishop and J. Pipin. Dipole, quadrupole, octupole, and dipole-dipole-quadrupole polarizabilities and second hyperpolarizabilities at real and imaginary frequencies for helium in the 2^3 state. dispersion-energy coefficients for interactions between He(2^3S) and H(1^2S), He(1^1S), He(2^3S), or $H_2(X^1\Sigma_g^+)$. *International Journal of Quantum Chemistry*, 47(2):129–??, July 15, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bishop:1993:DQOa

[BP93b] D. M. Bishop and J. Pipin. Dipole, quadrupole, octupole, and dipole-octupole polarizabilities at real and imaginary frequencies for H, he, and H_2 and the dispersion-energy coefficients for interactions between them. *International Journal of Quantum Chemistry*, 45(4):349–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boughton:1993:TUL

[BP93c] J. W. Boughton and P. Pulay. The tautomers of uracil: A local correlation treatment. *International Journal of Quantum Chemistry*, 47(1):49–??, July 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burke:1995:RSA

[BP95] K. Burke and J. P. Perdew. Real-space analysis of the exchange-correlation energy. *International Journal of Quantum Chemistry*, 56(4):199–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhattacharyya:1996:DOD

[BP96a] K. Bhattacharyya and R. K. Pathak. Degeneracy in one dimension: Role of singular potentials. *International Journal of Quantum Chemistry*, 59(3):219–226, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60541`.

Bishop:1996:HOM

[BP96b] David M. Bishop and Janusz Pipin. High-order multipolar hyperpolarizabilities with imaginary frequency for H and He. *International Journal of Quantum Chemistry*, 59(2):103–108,

???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60530.

Bonapasta:1996:HIS

[BP96c] Aldo Amore Bonapasta and Lorenzo Pavesi. Hydrogen interaction with shallow and deep centers in GaAs. *International Journal of Quantum Chemistry*, 57(5):823–841, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60437.

Burke:1997:WGG

[BPE97] Kieron Burke, John P. Perdew, and Matthias Ernzerhof. Why the generalized gradient approximation works and how to go beyond it. *International Journal of Quantum Chemistry*, 61 (2):287–293, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42392; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42392&PLACEBO=IE.pdf.

Brewster:1996:ABMc

[BPHB96a] M. E. Brewster, E. Pop, M.-J. Huang, and M. Bodor. AM1-based model system for estimation of brain/blood concentration ratios. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 23 (??):51–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

Brewster:1996:ABMa

[BPHB96b] M. E. Brewster, E. Pop, M.-J. Huang, and N. Bodor. AM1-based model system for estimation of brain/blood concentration ratios. *International Journal of Quantum Chemistry*, 60(8):51–??, 1996. CODEN IJQCB2.

Brewster:1996:ABMb

[BPHB96c] Marcus E. Brewster, Emil Pop, Ming-Ju Huang, and Nicholas Bodor. AM1-based model system for estimation of brain / blood concentration ratios. *International Journal of Quantum Chemistry*, 60(8):1775–1787, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60749.

Bouyer:1994:GSC

[BPL94] F. Bouyer, G. Picard, and J.-J. Legendre. Geometrical and spectroscopical characterizations of some complex entities of aluminum(III) with fluoride ions by LDF-based calculations. *International Journal of Quantum Chemistry*, 52(4):927–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borstnik:1997:CSD

[BPL97a] B. Borštnik, D. Pumpernik, and D. Lukman. Computer simulation of DNA sequential correlations. *International Journal of Quantum Chemistry*, 64(3):387–392, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42694; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42694&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Bouyer:1997:CAC

[BPL97b] Frédéric Bouyer, Gérard Picard, and Jean-Jacques Legendre. Computational and analytical chemistry: Methodology to study chemical reactions between sodium, calcium, and aluminum fluorides in molten cryolite. *International Journal of Quantum Chemistry*, 61(3):507–514, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42419; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42419&PLACEBO=IE.pdf.

Bouferguene:1994:NSC

[BR94] A. Bouferguene and D. Rinaldi. A new single-center method to compute molecular integrals of quantum chemistry in Slater-type orbital basis of functions. *International Journal of Quantum Chemistry*, 50(1):21–??, March 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Berrondo:1997:RAS

[BR97] M. Berrondo and J. Récamier. Resonances and antibound states in a Morse potential. *International Journal of Quantum Chemistry*, 62(3):239–244, ???? 1997. CODEN IJQCB2. ISSN

0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42506; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42506&PLACEBO=IE.pdf.

Brandas:1968:SAC

[Brä68] 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(??):37–??, ?? 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandow:1975:FTE

[Bra75] B. H. Brandow. Formal theory of effective π-electron Hamiltonians. *International Journal of Quantum Chemistry*, ??(??):??, ?? 1975. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:1993:RMI

[Brä93a] E. J. Brändas. Resonances and microscopic irreversibility: An introduction. *International Journal of Quantum Chemistry*, 46 (3):339–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:1993:SCH

[Brä93b] E. J. Brändas. Some comments on H-Bond dynamics in DNA base pairs. *International Journal of Quantum Chemistry*, 46 (3):499–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bracken:1996:ISS

[Bra96] P. Bracken. Investigation of some soluble lattice spin models. *International Journal of Quantum Chemistry*, 57(2):235–243, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60362.

Bracken:1997:NSG

[Bra97a] P. Bracken. Numerical solution for the ground-state energy of the anisotropic Heisenberg model. *International Journal of Quantum Chemistry*, 62(1):13–21, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL

http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42485; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42485&PLACEBO=IE.pdf.

Branchadell:1997:DFS

[Bra97b] Vicenç Branchadell. Density functional study of Diels–Alder reactions between cyclopentadiene and substituted derivatives of ethylene. *International Journal of Quantum Chemistry*, 61(3):381–388, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42431; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42431&PLACEBO=IE.pdf.

Brandas:1998:BRA

[Brä98a] Erkki J. Brändas. Book review: *Atoms and their spectroscopic properties*, by V. P. Shevelko. *International Journal of Quantum Chemistry*, 68(1):73, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29924; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29924&PLACEBO=IE.pdf.

Brandas:1998:BRP

[Brä98b] Erkki J. Brändas. Book review: *The physics of atoms and quanta: Introduction to experiments and theory; Molecular physics and elements of quantum chemistry: Introduction to experiments and theory*, by H. Haken and H. C. Wolf. *International Journal of Quantum Chemistry*, 66(1):109, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29833; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29833&PLACEBO=IE.pdf.

Brandas:1998:BRX

[Brä98c] Erkki J. Brändas. Book review: *X-Ray Radiation of Highly Charged Ions*, by H. F. Beyer, H-J Kluge, and V. P. Shevelko. *International Journal of Quantum Chemistry*, 68(1):73–??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bouzida:1999:CSL

[BRA+99] Djamal Bouzida, Paul A. Rejto, Sandra Arthurs, Anthony B. Colson, Stephan T. Freer, Daniel K. Gehlhaar, Veda Larson, Brock A. Luty, Peter W. Rose, and Gennady M. Verkhivker. Computer simulations of ligand-protein binding with ensembles of protein conformations: A Monte Carlo study of HIV-1 protease binding energy landscapes. *International Journal of Quantum Chemistry*, 72 (1):73–84, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002304; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002304&PLACEBO=IE.pdf`.

Bredow:1999:EEC

[Bre99] Thomas Bredow. Effect of embedding and cluster size on the ab initio study of potassium adsorption at rutile(110). *International Journal of Quantum Chemistry*, 75(2):127–132, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=64000657; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=64000657&PLACEBO=IE.pdf`.

Broer:1993:UCO

[Bro93] R. Broer. On the use of corresponding orbitals for the construction of mutually orthogonal orbital sets. *International Journal of Quantum Chemistry*, 45(6):587–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Broyles:1995:DRH

[Bro95] A. A. Broyles. The derivation of the relativistic Hamiltonian for molecules. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:257–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Broo:1996:BSCa

[Bro96a] A. Broo. Basis set and correlation effects on geometry of octahedral second-row transition-metal complexes. *International Journal of Quantum Chemistry*, 60(7):119–??, 1996. CODEN IJQCB2.

Broo:1996:BSCc

[Bro96b] A. Broo. Basis set and correlation effects on geometry of octahedral second-row transition-metal complexes. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):119–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Broo:1996:BSCb

[Bro96c] Anders Broo. Basis set and correlation effects on geometry of octahedral second-row transition-metal complexes. *International Journal of Quantum Chemistry*, 60(7):1331–1343, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60691`.

Berrondo:1995:SST

[BRS95] M. Berrondo and J. F. Rivas-Silva. Stokes shifts in Tl-doped alkali halides. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:253–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Berrondo:1996:CMI

[BRS96] M. Berrondo and J. F. Rivas-Silva. Cluster models of ionic crystals: Band gaps. *International Journal of Quantum Chemistry*, 57(6):1115–1119, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60455`.

Bouzida:1999:MCS

[BRV99] Djamal Bouzida, Paul A. Rejto, and Gennady M. Verkhivker. Monte Carlo study of ligand-protein binding energy landscapes with the weighted histogram analysis method. *International Journal of Quantum Chemistry*, 73(2):113–121, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003510`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003510&PLACEBO=IE.pdf`. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998.* Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Bandrauk:1997:CEI

[BRZY97] André D. Bandrauk, J. Ruel, Tao Zuo, and Hengtai Yu. Controlling electrons with intense laser and magnetic fields. *International Journal of Quantum Chemistry*, 64(5):613–617, September 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42710; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42710&PLACEBO=IE.pdf`. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

Bartlett:1975:SAD

[BS75] R. J. Bartlett and D. M. Silver. Some aspects of diagrammatic perturbation theory. *International Journal of Quantum Chemistry*, S9(??):183–198, ?? 1975. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balendiran:1991:SBD

[BS91] K. Balendiran and M. Sundaralingam. Structure of the B-DNA dodecamer with the reversed central sequence d(CGCGTTAACGCG) and its netropsin complex. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:199–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Broclawik:1992:QES

[BS92] E. Broclawik and D. R. Salahub. Quintet electronic states of MoO: Gaussian density functional calculations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:393–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Banacky:1993:DCD

[BS93] P. Banacky and M. Svrcek. Dissipative and coherent dynamics induced by a nonadiabatic electron-phonon coupling: Aspects of superconductivity. *International Journal of Quantum Chemistry*, 46(3):475–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Broclawik:1994:ESM

[BS94] E. Broclawik and D. R. Salahub. On the electronic structure of MoO: Spin-polarized density functional calculations of spectroscopic properties of low-lying quintet, triplet, and septet states.

International Journal of Quantum Chemistry, 52(4):1017–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brummel:1995:SSB

[BS95] H. A. Brummel and G. C. Shields. Semiempirical study of the Bergman reaction: Towards a computationally efficient and accurate method for modeling the enediyne anticancer antibiotics. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):51–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Beljonne:1994:TET

[BSB94] D. Beljonne, Z. Shuai, and J. L. Brédas. Theoretical evolution of the third-order molecular polarizabilities as a function of chain length in thiophene and pyrrole oligomers. *International Journal of Quantum Chemistry*, 52(1):39–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bischof:1997:QCS

[BSHP97] Gerhard Bischof, Alexander Silbernagl, Kersti Hermansson, and Michael Probst. Quantum chemical study of the molecular dynamics of hydrated li+ and Be_2^+ cations. *International Journal of Quantum Chemistry*, 65(5):803–816, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42812; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42812&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Berthier:1997:TSB

[BSP97] G. Berthier, R. Savinelli, and A. Pullman. Theoretical study of the binding of the chloride anion to water and alcohols. *International Journal of Quantum Chemistry*, 63(2):567–574, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42600;`

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42600&PLACEBO=IE.pdf.

Bohm:1998:NAT

[BSP98] Michael C. Böhm, Johannes Schütt, and Sabine Philipp. New aspects in the theory of π electron systems on the basis of quantum statistical considerations. *International Journal of Quantum Chemistry*, 69(6):727–752, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74990; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74990&PLACEBO=IE.pdf.

Banacky:1996:ENF

[BSS96] Pavol Baňacký, Michal Svrček, and Vojtech Szöcs. Effect of nonadiabaticity on the Fermi-edge photoemission and tunneling spectra of superconductors. *International Journal of Quantum Chemistry*, 58(5):487–496, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60503.

Barysz:1997:NTO

[BSS97a] Maria Barysz, Andrzej J. Sadlej, and Jaap G. Snijders. Nonsingular two/one-component relativistic Hamiltonians accurate through arbitrary high order in α^2. *International Journal of Quantum Chemistry*, 65(3):225–239, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42760; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42760&PLACEBO=IE.pdf.

Bohm:1997:BFE

[BSS+97b] Michael C. Böhm, Joachim Schulte, Johannes Schütt, Thomas Schedel-Niedrig, Harald Werner, and Robert Schlögl. Ba_xC_{60} fullerides: π Electronic peculiarities of the C_{60} molecule and their consequences for the solid state. *International Journal of Quantum Chemistry*, 65(4):333–373, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42770; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42770&PLACEBO=IE.pdf.

Babic:1995:REF

[BT95] D. Babić and N. Trinajstić. Resonance energies of fullerenes with 4-membered rings. *International Journal of Quantum Chemistry*, 55(4):309–314, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boegel:1996:DCAa

[BT96a] H. Boegel and S. Tobisch. DFT calculations of alternative structures in the allyl-nickel catalyzed polymerization of butadiene. *International Journal of Quantum Chemistry*, 60(7): 197–??, 1996. CODEN IJQCB2.

Boegel:1996:DCAb

[BT96b] H. Boegel and S. Tobisch. DFT calculations of alternative structures in the allyl-nickel catalyzed polymerization of butadiene. *International Journal of Quantum Chemistry*, 60(7):1409–1417, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60700`.

Boegel:1996:DCAc

[BT96c] H. Boegel and S. Tobisch. DFT calculations of alternative structures in the allyl-nickel catalyzed polymerization of butadiene. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):197–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Baeten:1999:UHP

[BTKVG99] A. Baeten, M. Tafazoli, M. Kirsch-Volders, and P. Geerlings. Use of the HSAB principle in quantitative structure-activity relationships in toxicological research: Application to the genotoxicity of chlorinated hydrocarbons. *International Journal of Quantum Chemistry*, 74(3):351–355, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62004765; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62004765&PLACEBO=IE.pdf`. Special Issue: *Biophysics Quarterly*.

Bogel:1998:DIS

[BTN98] Horst Bögel, Sven Tobisch, and Thomas Nowak. DFT investigations of the structure and bonding between transition metals and olefins. *International Journal of Quantum Chemistry*, 69(3):387–396, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29993; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29993&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Bell:1997:DID

[BTTS97] Robert L. Bell, Deni L. Taveras, Thanh N. Truong, and Jack Simons. A direct ab initio dynamics study of the water-assisted tautomerization of formamide. *International Journal of Quantum Chemistry*, 63(4):861–874, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42637; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42637&PLACEBO=IE.pdf.

Buemi:1996:CAR

[Bue96] Giuseppe Buemi. Conformational analysis and rotation barriers of 2-aminoethanethiol and 2-aminoethanol: An ab initio study. *International Journal of Quantum Chemistry*, 59(3):227–237, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60542.

Bencini:1994:ESP

[BUZ94] A. Bencini, M. G. Uytterhoeven, and C. Zanchini. Electronic structure of paramagnetic clusters of transition metal ions. 3. magnetic properties and scattered wave description of the electronic structure of the hexanuclear octahedral cluster $[Fe_6(3S)_8(PEt_3)_6](BPh_4)_2$. *International Journal of Quantum Chemistry*, 52(4):903–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brown:1993:QMI

[BV93] F. K. Brown and J. M. Veal. A quantum mechanical investigation of the annealing energy for phosphodiester, formacetal, and thioformacetal backbones. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quan-*

tum Pharmacology., 20:37–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Byrman:1996:VBS

[BvL96] Carsten P. Byrman and Joop H. van Lenthe. A valence bond study of the oxygen molecule. *International Journal of Quantum Chemistry*, 58(4):351–360, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60491.

Broch:1991:QMS

[BVV91] H. Broch, R. Viani, and D. Vasilescu. Quantum molecular study of the alkylating agent mechlorethamine. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:119–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Brink:1990:SRC

[BW90] H. Brink and P. Winkler. Siegert resonance calculations — real and divergence-free. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:321–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Berggren:1997:DOD

[BW97] Karl-Fredrik Berggren and Chuan-Kui Wang. Different orbitals for different electrons in a system of intersecting quantum wires. *International Journal of Quantum Chemistry*, 63(3):667–673, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42628; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42628&PLACEBO=IE.pdf.

Badenhoop:1999:NSA

[BW99] J. K. Badenhoop and F. Weinhold. Natural steric analysis of internal rotation barriers. *International Journal of Quantum Chemistry*, 72(4):269–280, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006330; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006330&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Bishop:1994:CCT

[BX94] R. F. Bishop and Y. Xian. The coupled cluster theory of quantum lattice systems. *International Journal of Quantum Chemistry. Symposium*, 28:155–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Bishop:1995:MCC

[BXZ95] R. F. Bishop, Y. Xian, and C. Zeng. A microscopic coupled-cluster treatment of electronic correlations in Hubbard models. *International Journal of Quantum Chemistry*, 55(2):181–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Broclawik:1997:DFS

[BYE+97] Ewa Broclawik, Ryo Yamauchi, Akira Endou, Momoji Kubo, and Akira Miyamoto. Density functional study on the activation of methane over Pd_2, PdO, and Pd_2 O clusters. *International Journal of Quantum Chemistry*, 61(4): 673–682, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42454; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42454&PLACEBO=IE.pdf.

Bulut:1999:QWP

[BYGA99] Niyazi Bulut, Abdulkadir Yildiz, Fahrettin Gögtaş, and Sinan Akpinar. Quantum wave packet study of O(^{1}D) + HCl(v) $\to$ ClO($v\prime$) + H reaction. *International Journal of Quantum Chemistry*, 73(5):425–432, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61004333; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61004333&PLACEBO=IE.pdf.

Bu:1995:TSI

[BZQ95] Y. Bu, Y. Zhang, and L. Qiu. Theoretical studies on the inner-sphere reorganization energies for the self-exchange reactions of gas-phase diatomic molecules HA (A = Mg, Al, Si, P, S, Cl). *International Journal of Quantum Chemistry*, 54(4):249–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Champagne:1990:MCP

[CA90a] B. Champagne and J.-M. André. Model calculations of polarizabilities of polyene chains: Oligomers and infinite polymers. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:859–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Contreras:1990:TMO

[CA90b] R. R. Contreras and A. J. Aizman. Theory of molecular orbital energy shifting induced by electrostatic external effects. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:89–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Contreras:1991:ISE

[CA91] Renato R. Contreras and Arie J. Aizman. Ion solvation energies from density functional theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:281–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Cordero:1997:DFS

[CA97] N. A. Cordero and J. A. Alonso. Density functional study of atomic electron affinities using a nonlocal exchange and a local correlation functional. *International Journal of Quantum Chemistry*, 61(2):253–261, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42406; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42406&PLACEBO=IE.pdf`.

Cabral:1996:CPE

[Cab96] B. J. Costa Cabral. Condensed-phase effects on the conformational equilibrium of ethylene glycol. *International Journal of Quantum Chemistry*, 60(7):1651–1660, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60726`.

Cai:1993:MSF

[Cai93] Z.-L. Cai. The MRSDCI studies of four low-lying electronic states of the BF_2 radical. *International Journal of Quantum Chemistry*, 45(3):295–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cai:1994:ISL

[Cai94] Z.-L. Cai. Ab initio study of the low-lying electronic states of the CH_2NO_2 radical. *International Journal of Quantum Chemistry*, 49(6):781–??, March 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chrysos:1995:SAG

[CAJ95] M. Chrysos, M. E. Alikhani, and M. Jacon. On the stability of the autodissociative ground electronic state of BeH^{2+}. *International Journal of Quantum Chemistry*, 53(1):57–65, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cardenas:1996:PIT

[CAK+96] R. Cardenas, J. Andres, J. Krechl, M. Campillo, and O. Tapia. On a possible invariance of a transition structure to the effects produced by ancillary H-bonding molecules: Modeling the effects of Ser-48 in the hydride-transfer step of liver alcohol dehydrogenase. *International Journal of Quantum Chemistry*, 57(2):245–257, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60363`.

Calais:1993:DFT

[Cal93] J.-L. Calais. *Density-Functional Theory of Atoms and Molecules*, by R. G. Parr and W. Yang. *International Journal of Quantum Chemistry*, 47(1):101–??, July 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Calais:1996:FES

[Cal96a] Jean-Louis Calais. Finite and extended systems. *International Journal of Quantum Chemistry*, 58(3):307–313, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60484`.

Calais:1996:WSQ

[Cal96b] Jean-Louis Calais. Wavelets — something for quantum chemistry? *International Journal of Quantum Chemistry*, 58(6):541–548, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60507`.

Castillo:1997:SSR

[CAM+97] R. Castillo, J. Andrés, V. Moliner, V. S. Safont, and M. Oliva. A semiempirical study on the ring-opening process for the cyclopropanone, 2,2-dimethylcyclopropanone, *trans*-2,3-di-*tert*-butylcyclopropanone, and spiro(bicyclo[2.2.1]heptane-2.1′-cyclopropan)-2′-one systems in solution. *International Journal of Quantum Chemistry*, 65(5):729–738, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42805; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42805&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Canuto:1994:EEC

[Can94] S. Canuto. Extreme electron correlation effects on the electric properties of atomic anions. *International Journal of Quantum Chemistry. Symposium*, 28:265–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Canuto:1997:ECE

[Can97] Sylvio Canuto. Electron correlation effects on the angular momentum anisotropies of the dipole polarizabilities of the first-row stable atomic anions. *International Journal of Quantum Chemistry*, 63(2):459–463, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42590; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42590&PLACEBO=IE.pdf.

Champagne:1996:IDP

[CAÖ96] Benoît Champagne, Jean-Marie André, and Yngve Öhrn. Ab initio dynamic polarizabilities of polymers. I. hydrogen chain models. *International Journal of Quantum Chemistry*, 57(5): 811–821, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60427.

Castleman:1991:SES

[Cas91] A. W. Castleman. Solvation effects on the structure and reactivity of clusters. *International Journal of Quantum Chem-*

istry. Quantum Chemistry Symposium, 25:527–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Castro:1997:RJT

[Cas97] Miguel Castro. The role of the Jahn–Teller distortions on the structural, binding, and magnetic properties of small Fe_n clusters, $n \leq 7$. *International Journal of Quantum Chemistry*, 64(2):223–230, August 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42684; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42684&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Chandra:1993:PES

[CB93a] A. K. Chandra and K. Bhattacharyya. Perturbation expansions, Symanzik scaling, and Padé-Type approximants: The anharmonic oscillator problem. *International Journal of Quantum Chemistry*, 45(3):251–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chang:1993:QFS

[CB93b] J. Chang and N. J. Brown. Quantum functional sensitivity analysis for the 3-D (J = O) H + H_2 reaction. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:567–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Chang:1994:EQF

[CB94a] J. Chang and N. J. Brown. Erratum: Quantumn functional sensitivity analysis for the 3-D (J = O) H + H_2. *International Journal of Quantum Chemistry*, 51(1):53–??, June 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cybulski:1994:TRD

[CB94b] S. M. Cybulski and D. M. Bishop. Theory of relaxed density matrices: Application to second-order response properties. *International Journal of Quantum Chemistry*, 49(4):371–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chelkowski:1996:WFSa

[CB96a] S. Chelkowski and A. D. Bandrauk. Wave-function splitting technique for calculating above-threshold ionization electron spectra. *International Journal of Quantum Chemistry*, 60(7): 473–??, 1996. CODEN IJQCB2.

Chelkowski:1996:WFSb

[CB96b] S. Chelkowski and A. D. Bandrauk. Wave-function splitting technique for calculating above-threshold ionization electron spectra. *International Journal of Quantum Chemistry*, 60 (7):1685–1689, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60731`.

Chelkowski:1996:WFSc

[CB96c] S. Chelkowski and A. D. Bandrauk. Wave-function splitting technique for calculating above-threshold ionization electron spectra. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):473–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Cizek:1996:IPT

[ČB96d] J. Čížek and P. Bracken. Interpolant polynomial technique applied to the PPP model. II. testing the interpolant technique on the Hubbard model. *International Journal of Quantum Chemistry*, 57(6):1033–1048, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60448`.

Chaudhury:1999:BSS

[CB99] Pinaki Chaudhury and S. P. Bhattacharyya. Bound states in screened and bare Coulomb potentials: A nonorthogonal CI-based route to effective Hamiltonians for two-electron systems. *International Journal of Quantum Chemistry*, 74 (2):153–161, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003361; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003361&PLACEBO=IE.pdf`. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Cabria:1997:NAI

[CBAM97] I. Cabria, M. T. Barriuso, J. A. Aramburu, and M. Moreno. Neutral atoms in ionic lattices: Study of KCl:Ag^0. *International Journal of Quantum Chemistry*, 61(4):627–634, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42448; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42448&PLACEBO=IE.pdf.

Calamante:1994:FPI

[CBG94] F. Calamante, R. C. Bochicchio, and H. Grinberg. Feynman path integral representation for many-Fermion interacting systems. *International Journal of Quantum Chemistry*, 49(6):789–??, March 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cheng:1995:QMS

[CBL95] H.-P. Cheng, R. N. Barnett, and U. Landman. Quantum mechanical simulations of water and ammonia molecules and their clusters. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:615–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Castillo:1998:TSH

[CBSR+98] S. Castillo, V. Bertin, E. Solano-Reyes, H. Luna-Garcia, A. Cruz, and E. Poulain. Theoretical studies on hydrogen activation by iridium dimers. *International Journal of Quantum Chemistry*, 70(4-5):1029–1035, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75025; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75025&PLACEBO=IE.pdf.

Cann:1993:ECE

[CBT93a] N. M. Cann, R. J. Boyd, and A. J. Thakkar. Electron correlation effects in the Rydberg-like 3^3D and 3^1D states of helium-like ions. *International Journal of Quantum Chemistry*, 48(1):1–??, October 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cann:1993:SEC

[CBT93b] N. M. Cann, R. J. Boyd, and A. J. Thakkar. Statistical electron correlation coefficients for 29 states of the heliumlike ions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:33–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Cioslowski:1991:MSO

[CC91] Jerzy Cioslowski and Matt Challacombe. Maximum similarity orbitals for analysis of the electronic excited states. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:81–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Cassam-Chenai:1995:ERD

[CC95] P. Cassam-Chenai. Ensemble representable densities for atoms and molecules. I. general theory. *International Journal of Quantum Chemistry*, 54(4):201–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cundari:1996:SEM

[CC96] Thomas R. Cundari and Scot Curtiss. Substituent effects on methane activation and elimination by high-valent Zr complexes. *International Journal of Quantum Chemistry*, 60(3): 779–788, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60644.

Chibotaru:1997:VIM

[CC97a] L. F. Chibotaru and F. Cimpoesu. Vibronic instability of molecular configurations in, the Hartree–Fock–Roothaan approximation. *International Journal of Quantum Chemistry*, 65(1):37–48, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42739; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42739&PLACEBO=IE.pdf.

Clementi:1997:NAC

[CC97b] Enrico Clementi and Giorgina Corongiu. Note on the atomic correlation energy. *International Journal of Quantum Chemistry*, 62(6):571–591, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42543;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42543&PLACEBO=IE.pdf.

Cassam-Chenai:1998:SBS

[CC98] P. Cassam-Chenaï. Symmetrizing broken symmetry wave functions in quantum chemistry. *International Journal of Quantum Chemistry*, 68(2):91–101, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29929; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29929&PLACEBO=IE.pdf.

Castillo:1997:TSP

[CCB+97] S. Castillo, A. Cruz, V. Bertin, E. Poulain, J. S. Arellano, and G. Del Angel. Theoretical study on Pd dimer and trimer interaction with the hydrogen molecule. *International Journal of Quantum Chemistry*, 62(1):29–45, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42487; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42487&PLACEBO=IE.pdf.

Cassam-Chenai:1993:SUC

[CCC93] P. Cassam-Chenai and G. S. Chandler. Spin-unrestricted calculations in quantum chemistry. *International Journal of Quantum Chemistry*, 46(5):593–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:1995:BSS

[CCC+95a] Y. Cao, L. Chen, B. Chen, J. Fen, W. Chen, and Y-K Pan. Band structure studies on crystalline C_{60}, Ca_3C_{60}, and Ca_5C_{60}. *International Journal of Quantum Chemistry*, 54(4):265–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Castillo:1995:TSR

[CCC+95b] S. Castillo, A. Cruz, A. Cuan, A. Ramirez-Solis, E. Poulain, and G. Del Angel. Theoretical study of the rhodium dimer interaction with the hydrogen molecule. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29: 549–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Clementi:1993:TSO

[CCE+93] E. Clementi, G. Corongiu, D. Estrin, E. Hollauer, and O. G. Stradella. Time scales and other problems in linking simulations of simple chemical systems to more complex ones. *International Journal of Quantum Chemistry*, 45(6):511–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cunningham:1996:CBO

[CCG+96] Terence P. Cunningham, David L. Cooper, Joseph Gerratt, Peter B. Karadakov, and Mario Raimondi. Chemical bonding in oxohalides of hypercoordinate nitrogen and phosphorus. *International Journal of Quantum Chemistry*, 60(1):393–400, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60601`.

Cammi:1996:EED

[CCM+96] Roberto Cammi, Maurizio Cossi, Benedetta Mennucci, Christian Silvio Pomelli, and Jacopo Tomasi. Energy and energy derivatives for molecular solutes: Perspectives of application to hybrid quantum and molecular methods. *International Journal of Quantum Chemistry*, 60(6):1165–1178, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60681`.

Casida:1998:ESP

[CCS98] Mark E. Casida, Kim C. Casida, and Dennis R. Salahub. Excited-state potential energy curves from time-dependent density-functional theory: A cross section of formaldehyde's $^1A_1$ manifold. *International Journal of Quantum Chemistry*, 70(4-5):933–941, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75071; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75071&PLACEBO=IE.pdf`.

Cisneros:1999:DSS

[CCS99] G. Andrés Cisneros, Miguel Castro, and Dennis R. Salahub. DFT study of the structural and electronic properties of small Ni_n (n = 2–4) clusters. *International Journal of Quantum Chemistry*, 75(4–5):847–861, November 15,

1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004981/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004981&PLACEBO=IE.pdf`.

Chuang:1998:IES

[CCT98] Yao-Yuan Chuang, Christopher J. Cramer, and Donald G. Truhlar. The interface of electronic structure and dynamics for reactions in solution. *International Journal of Quantum Chemistry*, 70(4-5):887–896, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75066`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75066&PLACEBO=IE.pdf`.

Cassam-Chenai:1996:ERD

[CCWCF96] P. Cassam-Chenaï, S. K. Wolff, G. S. Chandler, and B. N. Figgis. Ensemble-representable densities for atoms and molecules. II. Application to $CoCl_4^{2-}$. *International Journal of Quantum Chemistry*, 60(2):667–680, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60634`.

Coutinho:1997:CAS

[CCZ97] Kaline Coutinho, Sylvio Canuto, and M. C. Zerner. Calculation of the absorption spectrum of benzene in condensed phase. A study of the solvent effects. *International Journal of Quantum Chemistry*, 65(5):885–891, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42820`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42820&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Cundari:1990:AH

[CD90] T. R. Cundari and R. S. Drago. Alkane hydroxylations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:665–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Chatzidimitriou-Dreismann:1993:PDQ

[CD93] C. Chatzidimitriou-Dreismann. Protonic delocalization and quantum correlations in the H-bond dynamics of G–C and $\kappa-\pi$ DNA base pairs. *International Journal of Quantum Chemistry*, 46(3):483–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cances:1999:SRM

[CDB99] Eric Cances, Mireille Defranceschi, and Claude Le Bris. Some recent mathematical contributions to quantum chemistry. *International Journal of Quantum Chemistry*, 74 (5):553–557, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62503006; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62503006&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II).* Issue Edited by Don Rees, Hiroshi Fujimotoi.

Caneschi:1999:MRP

[CdBKZ99] Andrea Caneschi, Fabrizia Fabrizi de Biani, Lars Kloo, and Piero Zanello. Magnetic and redox properties in hydroxo- and alkoxo-bridged Fe(III) binuclear complexes: A density functional study. *International Journal of Quantum Chemistry*, 72(1):61–71, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002303; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002303&PLACEBO=IE.pdf.

Coutinho:1998:SCM

[CDC98] Kaline Coutinho, M. J. De Oliveira, and Sylvio Canuto. Sampling configurations in Monte Carlo simulations for quantum mechanical studies of solvent effects. *International Journal of Quantum Chemistry*, 66(3):249–253, January 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29858; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29858&PLACEBO=IE.pdf.

Catalan:1999:SFI

[CDD+99] Javier Catalán, Juan Carlos Del Valle, Cristina Díaz, Jose Palomar, Jose L. G. De Paz, and Michael Kasha. Solvatochromism of fluorophores with an intramolecular hydrogen bond and their use as probes in biomolecular cavity sites. *International Journal of Quantum Chemistry*, 72 (4):421–438, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006320; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006320&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Chaudhuri:1996:SAC

[CDDM96] R. Chaudhuri, B. Datta, K. Das, and D. Mukherjee. A spin-adapted coupled-cluster based linear response theory for double ionization potentials. *International Journal of Quantum Chemistry*, 60(1):347–358, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60597.

Culot:1993:TEA

[CDDV93] C. Culot, M. Dory, F. Durant, and D. P. Vercauteren. Theoretical evaluation of atomic charges to be integrated into conformational analyses of neutral lipids. *International Journal of Quantum Chemistry*, 46(1):211–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Culot:1994:CAP

[CDMA94] C. Culot, F. Durant, D. H. Mosley, and J.-M. André. Conformational analyses of the polymorphism of triglycerides. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21:57–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Cruz:1999:TSP

[CDP+99] A. Cruz, G. Del Angel, E. Poulain, J. M. Martínez-Magadán, and M. Castro. Theoretical study for the Pt_2 Au- and $PtAu_2$-ethylene interaction. *International Journal of Quantum Chemistry*, 75(4–5):699–707, November 15,

1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004967/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004967&PLACEBO=IE.pdf.

Czerminski:1990:SAW

[CE90] R. Czerminski and R. Elber. Self-avoiding walk between two fixed points as a tool to calculate reaction paths in large molecular systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:167–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Cederbaum:1990:GFT

[Ced90] L. S. Cederbaum. On Green's functions and their applications. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:393–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Cedillo:1994:NRG

[Ced94] A. Cedillo. A new representation for ground states and its Legendre transforms. *International Journal of Quantum Chemistry. Symposium*, 28:231–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Corongiu:1996:RPE

[CEM+96] G. Corongiu, D. Estrin, G. Murgia, L. Paglieri, L. Pisani, G. Suzzi Valli, J. D. Watts, and E. Clementi. Revisiting the potential energy surface for [$H_3N \cdots HCl$]: An ab initio and density functional theory investigation. *International Journal of Quantum Chemistry*, 59(2):119–134, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60532.

Cheranovskii:1999:EDG

[CEZ+99] V. O. Cheranovskii, E. V. Ezerskaya, O. A. Zhikol, A. Kinal, and H. O. Pamuk. Effect of doping on the ground-state spin of stacked organometallic ferromagnets. *International Journal of Quantum Chemistry*, 73(6):511–517, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61007368; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61007368&PLACEBO=IE.pdf.

Cohen:1993:IET

[CF93] J. M. Cohen and G. R. Famini. An improved eikonal treatment of rotationally inelastic He–H_2 scattering. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27: 527–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Cotton:1996:ESM

[CF96] F. Albert Cotton and Xuejun Feng. Electronic structure and metal-metal interaction in edge- and face-sharing bioctahedral compounds of molybdenum. *International Journal of Quantum Chemistry*, 58(6):671–680, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60520.

Cundari:1999:RPM

[CF99] Thomas R. Cundari and Wentao Fu. Reaction pathways for model II-VI precursors: A computational study. *International Journal of Quantum Chemistry*, 71(1):47–56, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000012; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000012&PLACEBO=IE.pdf.

Chelkowski:1997:ENC

[CFB97] S. Chelkowski, C. Foisy, and A. D. Bandrauk. Exact numerical calculations of dissociative-ionization of molecular ions in intense laser fields: Non-Born–Oppenheimer dynamics. *International Journal of Quantum Chemistry*, 65(5): 503–512, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42779; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42779&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Caldas:1990:AAD

[CFDS90] M. J. Caldas, A. Fazzio, J. Dabrowski, and M. Scheffler. Anion-antisite defects in GaAs: As and Sb. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:563–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Champagne:1995:CEL

[CFMA95] B. Champagne, J. G. Fripiat, D. H. Mosley, and J.-M. André. On the convergence of the exchange-like sums in the random phase approximation applied to stereoregular polymers. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:429–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Cheng:1996:ISS

[CFR96] Vincent K. W. Cheng, Michaela Flock, and Michael Ramek. Ab initio SCF structure investigation of β-hydroxypropionic acid and 3-Aminopropionamide. *International Journal of Quantum Chemistry*, 57(5):929–941, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60431`.

Calamante:1995:PAE

[CG95] F. Calamante and H. Grinberg. Padé approximants to the evolution operator through the Lippmann Schwinger variational principle. *International Journal of Quantum Chemistry*, 54(3):137–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cohen:1996:UAM

[CG96] Joel M. Cohen and David Z. Goodson. Unified approach to molecular structure and molecular vibrations. *International Journal of Quantum Chemistry*, 59(6):445–456, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60563`.

Capelle:1997:DFT

[CG97a] K. Capelle and E. K. U. Gross. Density functional theory for triplet superconductors. *International Journal of Quantum Chemistry*, 61(2):325–332, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42396; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42396&PLACEBO=IE.pdf`.

Cioslowski:1997:TIS

[CG97b] Jerzy Cioslowski and Xiang Gao. Transannular interactions in ${S_8}^{2+}$ and ${Se_8}^{2+}$: Reality or artifact? *International Journal of Quantum Chemistry*, 65(5):609–616, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42791; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42791&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Chandrasekher:1996:SBE

[CGG96] Charu A. Chandrasekher, K. S. Griffith, and Gregory I. Gellene. Symmetry breaking and electron correlation in O_2^-, O_2, and O_2^+: A comparison of coupled cluster and quadratic configuration interaction approaches. *International Journal of Quantum Chemistry*, 58(1):29–39, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60461`.

Chattaraj:1996:ECP

[CGLP96] Pratim K. Chattaraj, Swapan K. Ghosh, Shubin Liu, and Robert G. Parr. Exchange-correlation potential and excited-state density functional theory. *International Journal of Quantum Chemistry*, 60(1):535–543, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60617`.

Caballol:1974:GOS

[CGR74] R. Caballol, R. Gallifa, J. M. Carbo Riera, and R. ??? Generalized open shell SCF theory. *International Journal of Quantum Chemistry*, 8(??):373–394, ?? 1974. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cordero:1994:IPA

[CGRB94] N. A. Cordero, O. V. Gritsenko, A. Rubio, and L. C. Balbas. Ionization potentials of atoms calculated with a nonlocal exchange and a local correlation functional. *International Journal of Quantum Chemistry*, 52(4):993–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cecilia:1994:NPE

[CGSP94] J. Cecilia, J. Galceran, J. Salvador, and J. Puy. Numerical procedures in electrochemical simulation. *International Journal of Quantum Chemistry*, 51(6):357–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Clementi:1994:CHH

[CH94] E. Clementi and D. W. M. Hofman. Coulomb-Hole-Hartree–Fock functional. *International Journal of Quantum Chemistry*, 52(4):849–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaka:1995:SIM

[Cha95] A. M. Chaka. A semiempirical investigation of the mechanisms for the alkylation of arylamines. *International Journal of Quantum Chemistry*, 53(6):617–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Champagne:1997:VVE

[Cha97] Benoît Champagne. Vibrational versus electronic first hyperpolarizabilities of mono- and disubstituted benzenes: An ab initio coupled Hartree–Fock investigation. *International Journal of Quantum Chemistry*, 65(5):689–696, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42801; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42801&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Chan:1998:GHD

[Cha98] Garnet Kin-Lic Chan. General hybrid density functional theory. *International Journal of Quantum Chemistry*, 69(4):497–502, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30022; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30022&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Cheranovskii:1993:ESH

[Che93] V. O. Cheranovskii. Electron structure of a high-spin hydrocarbon polyallyl: Hubbard approximation with a strong electron repulsion. *International Journal of Quantum Chemistry*, 46(4): 577–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:1996:AMS

[Che96] P. C. Chen. Absorption maxima study of chromophores of indigoid dyes. *International Journal of Quantum Chemistry*, 60(2):681–687, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60635`.

Chen:1997:IRS

[Che97] P. C. Chen. Internal rotation study of some sixfold barrier molecules. *International Journal of Quantum Chemistry*, 62 (2):213–221, March 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42504`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42504&PLACEBO=IE.pdf`.

Carsky:1995:CGGa

[CHM95a] P. Carsky, V. Hrouda, and J. Michl. Cubic-grid Gaussian basis sets for electron scattering calculations. I. definition and construction. *International Journal of Quantum Chemistry*, 53(4): 419–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carsky:1995:CGGb

[CHM95b] P. Carsky, V. Hrouda, and J. Michl. Cubic-grid Gaussian basis sets for electron scattering calculations. II. matrix elements. *International Journal of Quantum Chemistry*, 53(4):431–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carsky:1995:CGGc

[CHMA95] P. Carsky, V. Hrouda, J. Michl, and D. Antic. Cubic-grid Gaussian basis sets for electron scattering calculations. III. effect of basis-set translation and size on the calculated cross section. *International Journal of Quantum Chemistry*, 53(4):437–??, 1995.

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

Christov:1994:TTK

[Chr94] S. G. Christov. Two types of Kramers rate equations for reactions in condensed media. *International Journal of Quantum Chemistry*, 52(5):1219–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Christov:1997:TAS

[Chr97] S. G. Christov. Two approaches to stochastic rate theory. *International Journal of Quantum Chemistry*, 64(4): 393–401, September 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42696; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42696&PLACEBO=IE.pdf.

Chun:1999:UIT

[Chu99] Paul W. Chun. Uncovering the innate thermodynamic quantities in protein unfolding. *International Journal of Quantum Chemistry*, 75(6):1027–1042, December 20, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004790/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004790&PLACEBO=IE.pdf.

Cimiraglia:1996:MBM

[Cim96] Renzo Cimiraglia. Many-body multireference Møller–Plesset and Epstein–Nesbet perturbation theory: Fast evaluation of second-order energy contributions. *International Journal of Quantum Chemistry*, 60(1):167–171, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60579.

Cioslowski:1990:IOT

[Cio90] J. Cioslowski. Isopycnic orbital transformations and localization of natural orbitals. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:15–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Cioslowski:1993:RIE

[Cio93] J. Cioslowski. Rigorous interpretation of electronic wavefunctions. IV origins of the unusual stability of the 1,3-dimethylimidazol-2-ylidene carbene. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:309–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Cioslowski:1994:ESB

[Cio94] J. Cioslowski. Electronic structure of the Benzene-Tetracyanoethylene complex: A synthesis of molecular orbital and density functional descriptions. *International Journal of Quantum Chemistry*, 49(4):463–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cave:1994:CED

[CJA94] R. J. Cave, J. L. Johnson, and M. A. Anderson. Calculation of electric dipole transition moments using quasi-degenerate variational perturbation theory and averaged coupled-pair functional theory. *International Journal of Quantum Chemistry*, 50(2):135–??, April 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Christiansen:1998:RFF

[CJH98] Ove Christiansen, Poul Jørgensen, and Christof Hättig. Response functions from Fourier component variational perturbation theory applied to a time-averaged quasienergy. *International Journal of Quantum Chemistry*, 68(1):1–52, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29921; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29921&PLACEBO=IE.pdf`.

Chen:1992:ESK

[CJX+92] T. L. Chen, J. Ji, S. X. Xiao, T. X. Cai, and G. S. Yan. The electronic structure of Keggin anion $(PW_{12}O_{40})^{3-}$ and catalytic properties. *International Journal of Quantum Chemistry*, 44(6):1015–??, December 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Collins:1990:EFC

[CL90] J. R. Collins and G. H. Loew. Effect of fluorination of camphor on its binding orientation in P450sub cam. *International*

Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology., 17:161–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Collins:1992:CCM

[CL92] J. R. Collins and G. H. Loew. Comparison of computational models for simulating heme proteins: A study of cytochrome C peroxidase. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:87–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Couty:1994:DEO

[CL94] M. Couty and B. Levy. On the determination of effective one-electron Hamiltonians to be used for studying large molecules. *International Journal of Quantum Chemistry*, 52(1): 59–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cundari:1995:ECP

[CL95] T. R. Cundari and Y. Li. Effective core potential modeling of group IVA-group IVB chemical vapor deposition. *International Journal of Quantum Chemistry*, 55(4):315–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cai:1997:SBS

[CL97] Shu-Hui Cai and Chun-Wan Liu. Studies on the band structures of some low-temperature superconductors. *International Journal of Quantum Chemistry*, 64(4):459–472, September 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42704; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42704&PLACEBO=IE.pdf`.

Camper:1990:SEC

[CLC90] D. L. Camper, G. H. Loew, and J. R. Collins. Steric and electronic criteria for teratogenicity of short chain aliphatic acids. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17:173–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Cruz:1995:VCH

[CLKMTA95] S. A. Cruz, E. Ley-Koo, J. L. Marin, and A. Taylor-Armitage. Variational calculations for the hydrogen atom confined in spaces with paraboloidal and spheroidal boundaries. *International Journal of Quantum Chemistry*, 54(1):3–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cardenas:1998:ISR

[CLOFR98] R. Cárdenas, J. Lagúnez-Otero, and A. Flores-Rivero. Ab initio study of the reaction mechanism of water dissociation into the ionic species OH^- and H_3 O^+. *International Journal of Quantum Chemistry*, 68(4):253–259, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29945`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29945&PLACEBO=IE.pdf`.

Chang:1993:BFL

[CLR+93] Y.-T. Chang, G. H. Loew, A. E. Rettie, T. A. Baillie, and P. R. Sheffels. Binding of flexible ligands to proteins: Valproic acid and its interaction with cytochrome P450cam. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:161–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Casanovas:1994:CEG

[CLSI94] J. Casanovas, A. Lorda, C. Sousa, and F. Illas. Character of the electronic ground state and of charge-transfer excited states in ionic solids: An ab initio cluster model approach. *International Journal of Quantum Chemistry*, 52(2):281–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cardenas-Lailhacar:1995:STS

[CLZ95] C. Cardenas-Lailhacar and M. C. Zerner. Searching for transition states: The Line-Then-Plane (LTP) approach. *International Journal of Quantum Chemistry*, 55(6):429–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cardenas-Lailhacar:1999:GSA

[CLZ99] Cristian Cardenas-Lailhacar and Michael C. Zerner. Generalized symmetry-adapted interpolation procedure for finding transition states in internal rotations. *International Journal of Quantum Chemistry*, 75(4–5):563–576, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004951/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004951&PLACEBO=IE.pdf.

Cortona:1994:SCC

[CM94a] P. Cortona and A. V. Monteleone. Self-consistent calculations of total energies and charge densities of solids without solving the band-structure problem. *International Journal of Quantum Chemistry*, 52(4):987–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Costa:1994:SCC

[CM94b] H. F. M. Da Costa and D. A. Micha. Self-consistent coupling of atomic orbitals to a moving charge. *International Journal of Quantum Chemistry. Symposium*, 28:49–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Cacelli:1996:DPC

[CM96a] I. Cacelli and R. Moccia. Differential photoionization cross section calculations for HI using the random-phase approximation with L^2 basis functions. *International Journal of Quantum Chemistry*, 60(1):409–419, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60604.

Campbell:1996:IFE

[CM96b] Loudon Campbell and F. A. Matsen. The Ising free-energy functional. *International Journal of Quantum Chemistry*, 59(5):391–400, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60557.

Chiu:1999:FTS

[CM99] Lue-Yung Chow Chiu and Mohammad Moharerrzadeh. Fourier transform of spherical Laguerre Gaussian functions and its application in molecular integrals. *International Journal of Quantum Chemistry*, 73(3):265–273, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL

http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003694; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003694&PLACEBO=IE.pdf.

Champagne:1993:ICU

[CMA93] B. Champagne, D. H. Mosley, and J.-M. André. Ab initio coupled and uncoupled Hartree–Fock calculations of the polarizabilities of finite and infinite polyacetylene chains. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:667–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Cogordan:1999:NAT

[CMA+99] J. A. Cogordan, M. Mayoral, E. Angeles, R. A. Toscano, and R. Martínez. Neuroleptic and antidepressant tricyclic compounds: Theoretical study for predicting their biological activity by semiempirical, density functional, and Hartree–Fock methods. *International Journal of Quantum Chemistry*, 71 (5):415–432, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10050251; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10050251&PLACEBO=IE.pdf.

Cartier:1996:CEM

[CMCR96] Alain Cartier, Marilia T. C. Martins-Costa, and Daniel Rinaldi. Computation of electronic molecular polarizabilities by a variational method at the CISD level. *International Journal of Quantum Chemistry*, 60(4):883–895, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60648.

Cardelino:1998:ICD

[CMF+98] B. H. Cardelino, C. E. Moore, D. O. Frazier, D. G. Musaev, and K. Morokuma. Ab initio calculations on the diacetylene dimer: HCCCC(H)C(H)CCCH. *International Journal of Quantum Chemistry*, 66(3):189–202, January 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29853; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29853&PLACEBO=IE.pdf.

Champagne:1993:IDP

[CMFA93] B. Champagne, D. H. Mosley, J. G. Fripiat, and J. M. André. Ab initio determination of polarizabilities per subunit in polymeric systems using the polarization propagator: Application to model hydrogen chains. *International Journal of Quantum Chemistry*, 46(1):1–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cometta-Morini:1992:SER

[CML92] C. Cometta-Morini and G. H. Loew. Structural and electronic requirements for binding at the mu-opioid receptor. *International Journal of Quantum Chemistry*, 44(2):235–??, September 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cometta-Morini:1993:PTU

[CMSF93] C. Cometta-Morini, C. Scharnagl, and S. F. Fischer. Proton transfer to ubiquinone Q_B in the photosynthetic reaction center of rps. viridis: The role of electrostatic interactions. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:89–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Chattaraj:1994:EDC

[CN94] P. K. Chattaraj and S. Nath. Electronegativity dynamics in a chemical reaction. *International Journal of Quantum Chemistry*, 49(5):705–??, February 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cadilhe:1999:CFB

[CN99] M. W. Cadilhe and J. J. Soares Neto. Classical four-body problem in hyperspherical coordinates. *International Journal of Quantum Chemistry*, 71(1):15–24, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000009`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000009&PLACEBO=IE.pdf`.

Cohen:1997:DFT

[Coh97] Marvin L. Cohen. Density functional theory and pseudopotentials: A panacea for calculating properties of materials. *International Journal of Quantum Chemistry*, 61

(4):603–611, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42439; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42439&PLACEBO=IE.pdf.

Coleman:1971:RRF

[Col71] A. J. Coleman. Recent results on Fermion N-representability. *International Journal of Quantum Chemistry*, 4(??):355–??, ?? 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Coleman:1997:AMF

[Col97] A. John Coleman. The AGP model for Fermion systems. *International Journal of Quantum Chemistry*, 63 (1):23–30, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42576; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42576&PLACEBO=IE.pdf.

Conrad:1992:QMC

[Con92] M. Conrad. Quantum molecular computing: The self-assembly model. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19: 125–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Cooper:1994:RBK

[Coo94] I. L. Cooper. On the relation between the Kratzer molecular potential and a set of displaced Morse oscillator potentials. *International Journal of Quantum Chemistry*, 49(1):25–??, January 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cook:1995:ECP

[Coo95] D. B. Cook. Effective core potentials and the structures of metallocenes. *International Journal of Quantum Chemistry*, 53 (3):309–??, February 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cook:1996:VO

[Coo96] David B. Cook. Virtual orbitals. *International Journal of Quantum Chemistry*, 60(4):793–801, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60646`.

Cordeiro:1997:CNH

[Cor97] João M. Marques Cordeiro. C — H···O and N — H···O hydrogen bonds in liquid amides investigated by Monte Carlo simulation. *International Journal of Quantum Chemistry*, 65 (5):709–717, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42803; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42803&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

CostaCabral:1996:CPEa

[Cos96a] B. J. Costa Cabral. Condensed-phase effects on the conformational equilibrium of ethylene glycol. *International Journal of Quantum Chemistry*, 60(7):439–??, 1996. CODEN IJQCB2.

CostaCabral:1996:CPEb

[Cos96b] B. J. Costa Cabral. Condensed-phase effects on the conformational equilibrium of ethylene glycol. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??): 439–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Clarkson:1992:LTS

[CP92] M. E. Clarkson and H. O. Pritchard. A Laplace transform solution of Schrödinger's equation using symbolic algebra. *International Journal of Quantum Chemistry*, 41(6):829–844, March 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Champagne:1999:BLA

[CP99a] Benoît Champagne and Eric A. Perpète. Bond length alternation effects on the static electronic polarizability and second hyperpolarizability of polyacetylene chains. *International*

Journal of Quantum Chemistry, 75(4–5):441–447, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004995/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004995&PLACEBO=IE.pdf.

Cho:1999:IDF

[CP99b] Soo Gyeong Cho and Bang Sam Park. Ab initio and density functional studies on bonding nature of the N — N bonds in 1,2,5-trinitroimidazole and 1,2,4,5-tetranitroimidazole. *International Journal of Quantum Chemistry*, 72(2):145–154, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002781; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002781&PLACEBO=IE.pdf.

Contreras:1995:DFT

[CPA95] R. Contreras, P. Perez, and A. Aizman. A density functional theory formulation of the reaction field model of solvent effects. *International Journal of Quantum Chemistry*, 56(5):433–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Champagne:1998:NFD

[CPA98] Benoît Champagne, Éric A. Perpète, and Jean-Marie André. Nonresonant frequency dispersion of the electronic second hyperpolarizability of *all-trans* polysilane chains: An ab initio TDHF oligomeric approach. *International Journal of Quantum Chemistry*, 70(4-5):751–761, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75053; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75053&PLACEBO=IE.pdf.

Castillo:1995:TSI

[CPBC95] S. Castillo, E. Poulain, V. Bertin, and A. Cruz. Theoretical studies of the interaction of PtSn systems with H_2. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:207–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Cruz:1998:TCH

[CPD+98] A. Cruz, E. Poulain, G. Del Angel, S. Castillo, and V. Bertin. Theoretical characterization of H_2 adsorption on AuPt clusters. *International Journal of Quantum Chemistry*, 67(6): 399–409, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29919; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29919&PLACEBO=IE.pdf.

Czaplewski:1999:GPC

[CPGC99] Cezary Czaplewski, Marta Pasenkiewicz-Gierula, and Jerzy Ciarkowski. G Protein-coupled receptor-bioligand interactions modeled in a phospholipid bilayer. *International Journal of Quantum Chemistry*, 73(2):61–70, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003506; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003506&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998*. Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Castillo:1991:TSP

[CPN91] S. Castillo, E. Poulain, and O. Novaro. A theoretical study of the photochemistry of methylcopper hydride: II. formation and stability of the HCuCHsub 3 intermediate complex. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:577–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Cooper:1996:PPE

[CPTR96] David L. Cooper, Robert Ponec, Thorstein Thorsteinsson, and Guido Raos. Pair populations and effective valencies from ab initio SCF and spin-coupled wave functions. *International Journal of Quantum Chemistry*, 57(3):501–518, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60389.

Chandra:1993:TDH

[CR93] A. K. Chandra and V. S. Rao. Temperature dependence of hydrogen transfer reactions via tunneling at low temperatures. *International Journal of Quantum Chemistry*, 47(6):437–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chakrabarti:1996:PLL

[CR96a] Aparna Chakrabarti and S. Ramasesha. Properties of the low-lying electronic states of phenanthrene: Exact PPP results. *International Journal of Quantum Chemistry*, 60(1):381–391, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60600`.

Chandra:1996:NSB

[CR96b] A. K. Chandra and V. Sreedhara Rao. Nonperfect synchronization of bond-forming and bond-rupturing processes in the reaction $H + H_2 \rightarrow H_2 + H$. *International Journal of Quantum Chemistry*, 58(1):57–65, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60464`.

Castillo:1993:TSR

[CRSP93] S. Castillo, A. Ramirez-Solis, and E. Poulain. Theoretical study of the reaction of Cd (^{1}S, ^{3}P, ^{1}P) with the methane molecule. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:587–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Chen:1996:CTCa

[CS96a] C. Chen and K.-C. Sun. Comparisons of the theoretical calculation of nitrogen clusters by semiempirical MO method. *International Journal of Quantum Chemistry*, 60(7):497–??, 1996. CODEN IJQCB2.

Chen:1996:CTCc

[CS96b] C. Chen and K.-C. Sun. Comparisons of the theoretical calculation of nitrogen clusters by semiempirical MO method. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):497–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Chen:1996:CTCb

[CS96c] Cheng Chen and Kuang-Chung Sun. Comparisons of the theoretical calculation of nitrogen clusters by semiempirical MO method. *International Journal of Quantum Chemistry*, 60 (7):1709–1718, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60734`.

Cook:1996:RM

[CS96d] D. Cook and B. T. Sutcliffe. Roy McWeeny. *International Journal of Quantum Chemistry*, 60(1):1–??, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Crawford:1998:IAT

[CS98] T. Daniel Crawford and John F. Stanton. Investigation of an asymmetric triple-excitation correction for coupled-cluster energies. *International Journal of Quantum Chemistry*, 70 (4-5):601–611, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75038; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75038&PLACEBO=IE.pdf`.

Chen:1999:TSSa

[CS99] Cheng Chen and Shuang-Fuh Shyu. Theoretical study of single-bonded nitrogen cluster-type molecules. *International Journal of Quantum Chemistry*, 73(4):349–356, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61000531; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61000531&PLACEBO=IE.pdf`.

Csavinszky:1990:AVD

[Csa90a] P. Csavinszky. Addendum to: "A variational density-functional calculation of the total atomic binding energy with recently proposed kinetic-energy and exchange-energy functionals". *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:83–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Csavinszky:1990:ISG

[Csa90b] P. Csavinszky. Investigation of the spatial generalization of Kato's theorem by a variational density-functional approach.

International Journal of Quantum Chemistry. Quantum Chemistry Symposium, 24:557–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Csavinszky:1991:CTA

[Csa91] P. Csavinszky. Calculation of the total atomic binding energy with recently proposed kinetic-, exchange-, and correlation-energy functionals. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:261–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Csavinszky:1992:PNI

[Csa92] P. Csavinszky. Precision in the numerical integration of the Thomas–Fermi–Dirac kinetic-energy and exchange-energy functionals using a modeled electron density. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26: 371–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Csavinszky:1993:DIA

[Csa93] P. Csavinszky. Determinantal inequalities among $< r^n >$. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:377–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Csavinszky:1994:CSL

[Csa94] P. Csavinszky. Convergence of a sequence of lower bounds for $< 1/r >$ for the noble gas, alkali, and alkaline earth atoms. *International Journal of Quantum Chemistry. Symposium*, 28: 227–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Csavinszky:1996:NIL

[Csa96] P. Csavinszky. Numerical investigation of a lower bound to the Thomas–Fermi kinetic energy and the validity of the Lieb conjecture for H^-, He, Li^+, $B3^+$, $O_6{}^+$, $Ne_8{}^+$, and $Mg_{12}{}^+$. *International Journal of Quantum Chemistry*, 57(3):449–452, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60382.

Carlsen:1999:QTA

[CSG99] Henrik Carlsen, Erik Sjöqvist, and Osvaldo Goscinski. Quantal trajectories for adiabatic and nonadiabatic regimes of vibronic systems. *International Journal of Quantum Chemistry*, 75(4–5):409–416, November 15, 1999. CODEN IJQCB2.

ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004939/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004939&PLACEBO=IE.pdf.

Chen:1999:TSSb

[CSH99] Cheng Chen, Shuang-Fuh Shyu, and Fu-Sheng Hsu. Theoretical study of salicylaldehyde conformal isomers and their intramolecular oxygen and hydrogen relations. *International Journal of Quantum Chemistry*, 74(4):395–404, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62502083; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62502083&PLACEBO=IE.pdf.

Chattaraj:1998:QFD

[CSP98] P. K. Chattaraj, S. Sengupta, and A. Poddar. Quantum fluid density functional theory of time-dependent processes. *International Journal of Quantum Chemistry*, 69 (3):279–291, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Cook:1993:SCC

[CSS93] D. B. Cook, J. A. Sordo, and T. L. Sordo. Some comments on the counterpoise correction for the basis set superposition error at the correlated level. *International Journal of Quantum Chemistry*, 48(6):375–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cory:1997:EES

[CSZ97] Marshall G. Cory, Krassimir K. Stavrev, and Michael C. Zerner. An examination of the electronic structure and spectroscopy of high- and low-spin model ferredoxin via several SCF and CI techniques. *International Journal of Quantum Chemistry*, 63(3):781–795, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42620;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42620&PLACEBO=IE.pdf.

Cammi:1995:NST

[CT95] R. Cammi and J. Tomasi. Nonequilibrium solvation theory for the polarizable continuum model: A new formulation at the SCF level with application to the case of the frequency-dependent linear electric response function. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:465–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Cammi:1996:TDV

[CT96] R. Cammi and J. Tomasi. Time-dependent variational principle for nonlinear Hamiltonians and its application to molecules in the liquid phase. *International Journal of Quantum Chemistry*, 60(1):297–306, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60593.

Cossi:1995:AEF

[CTC95] M. Cossi, J. Tomasi, and R. Cammi. Analytical expressions of the free energy derivatives for molecules in solution. application to the geometry optimization. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:695–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Cooper:1997:FVO

[CTG97] David L. Cooper, Thorstein Thorsteinsson, and Joseph Gerratt. Fully variational optimization of modern VB wave functions using the CASVB strategy. *International Journal of Quantum Chemistry*, 65(5):439–451, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42833; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42833&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Cullen:1991:EEB

[Cul91] John M. Cullen. An examination of the effects of basis set and charge transfer in hydrogen-bonded dimers with a constrained Hartree–Fock method. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:193–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Cullen:1995:RGV

[Cul95] J. M. Cullen. A rapid generalized valence-bond algorithm for semiempirical NDDO calculations. *International Journal of Quantum Chemistry*, 56(2):97–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cundari:1992:AEZ

[Cun92] T. R. Cundari. The activation and elimination of H_2 by Zr complexes. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:793–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Colmenero:1994:SCA

[CV94] F. Colmenero and C. Valdemoro. Self-consistent approximate solution of the second-order contracted Schrödinger equation. *International Journal of Quantum Chemistry*, 51(6):369–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Calderone:1998:CEH

[CV98] Anna Calderone and Jean-Pol Vigneron. Computation of the electromagnetic harmonics generation by stratified systems containing nonlinear layers. *International Journal of Quantum Chemistry*, 70(4-5):763–770, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75054`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75054&PLACEBO=IE.pdf`.

Cioslowski:1999:SAS

[CV99] Jerzy Cioslowski and Tereza Varnali. Systematic analysis of substituent effects. II. charges and energies of atoms in fluorochloroethanes. *International Journal of Quantum Chemistry*, 72(4):331–339, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006309`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006309&PLACEBO=IE.pdf`. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Cizek:1990:EAF

[CVP90] J. Cizek, F. Vinette, and J. Paldus. Explicit algebraic form of coupled cluster equations for the PPP model of benzene with an approximate inclusion of triexcited clusters. *International Journal of Quantum Chemistry*, 38(6):831–851, December 1990. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cizek:1991:SCP

[CVW91] J. Cizek, F. Vinette, and E. J. Weniger. Symbolic computation in physics and chemistry: Applications of the inner projection technique and of a new summation method for divergent series. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:209–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Calais:1997:FIB

[CW97] Jean-Louis Calais and Wolf Weyrich. Finite and infinite Born-von Kármán regions. *International Journal of Quantum Chemistry*, 63(1):223–227, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42567; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42567&PLACEBO=IE.pdf`.

Chen:1999:TSR

[CWJ+99] Xian-Yang Chen, Tao Wu, Quan Ju, Jie Ma, and Guan-Zhi Ju. Theoretical study of reactions between $AlH(^1\Sigma)$ and HF molecule. *International Journal of Quantum Chemistry*, 73 (5):417–424, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61004332; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61004332&PLACEBO=IE.pdf`.

Cai:1993:ISL

[CWX93] Z.-L. Cai, Y.-F. Wang, and H.-M. Xiao. An initio study of low-lying electronic states of the FNO_2 molecule. *International Journal of Quantum Chemistry*, 45(1):51–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:1998:CAS

[CWZ98a] Zexing Cao, Wei Wu, and Qianer Zhang. Construction and applications of symmetrized valence bond wave functions. *International Journal of Quantum Chemistry*, 66 (1):1–7, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29832; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29832&PLACEBO=IE.pdf.

Cao:1998:SCB

[CWZ98b] Zexing Cao, Wei Wu, and Qianer Zhang. Spectroscopic constants and bonding features of the low-lying states of LiB and LiB^+: Comparative study of VBSCF and MO theory. *International Journal of Quantum Chemistry*, 70 (2):283–290, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74996; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74996&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Chen:1999:AEI

[CXFP99] Jin-Quan Chen, Xiang-Jun Xin, Peng-Dong Fan, and Jia-Lun Ping. Algebraic expressions of irreducible bases for molecules C_{20} H_{20}, C_{80}, and C_{240}. *International Journal of Quantum Chemistry*, 73(3):283–297, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003696; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003696&PLACEBO=IE.pdf.

Chen:1997:SES

[CXL97] Tian-Lang Chen, Shen-Xiu Xiao, and Ping Li. Studies on the electronic structure and chemical bond of urea-nitrate. *International Journal of Quantum Chemistry*, 64(2): 247–248, August 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42673; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42673&PLACEBO=IE.pdf. Special Issue: *Second Triennial*

Congress of the International Society for Theoretical Chemical Physics. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Coleman:1995:PDS

[CYY95] A. J. Coleman, E. P. Yukalova, and V. I. Yukalov. Pairon distributions and the spectra of reduced Hamiltonians. *International Journal of Quantum Chemistry*, 54(4):211–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chacon:1993:PVM

[CZ93] M. R. Chacon and M. C. Zerner. Perturbation-variational methods revisited. *International Journal of Quantum Chemistry*, 47 (2):103–??, July 15, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Causa:1994:DFL

[CZ94a] M. Causa and A. Zupan. Density-functional LCAO calculations for solids: Comparison between Hartree–Fock and Kohn–Sham structural properties. *International Journal of Quantum Chemistry. Symposium*, 28:633–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Chacon:1994:EMC

[CZ94b] M. R. Chacon and M. C. Zerner. An efficient method for calculating static polarizabilities from a correlated wave function. *International Journal of Quantum Chemistry*, 49(5):601–??, February 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Czavinszky:1995:CDI

[Cza95] P. Czavinszky. Comparison of determinantal inequalities for lower bounds to $\langle 1/r \rangle$. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:303–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Czerwinski:1999:LDF

[Cze99] Marian Czerwiński. Local density functional theory applied to spin coupling in $Fe_6S_6{}^{5+}$ supercluster. *International Journal of Quantum Chemistry*, 72(1):39–51, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002301`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002301&PLACEBO=IE.pdf`.

Dixon:1991:ALD

[DA91] David A. Dixon and Anthony J. Arduengo. Application of local density functional theory to molecules containing a hypervalent bond. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:269–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

DaMottaNeto:1997:TSL

[DA97] Joaquim Delphino Da Motta Neto and Ricardo Bicca De Alencastro. Theoretical studies on local anesthetics: Procaine, lidocaine, tetracaine, bupivacaine, and dibucaine — neutral and monoprotonated. *International Journal of Quantum Chemistry*, 61(6):959–980, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42480; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42480&PLACEBO=IE.pdf.

Alencastro:1995:TSN

[dAdM95] R. B. de Alencastro and J. D. da Motta Neto. Theoretical studies on nonsteroidal antiinflammatory drugs benoxaprofen, chlorpromazine, and piroxicam. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):123–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

DeSantanna:1996:MMP

[DAF+96] Carlos M. R. De Sant'anna, Ricardo Bicca De Alencastro, Carlos A. M. Fraga, Eliezer J. Barreiro, and Joaquim Delphino Da Motta Neto. Molecular modeling on platelet-activating factor (PAF) and new proposed PAF antagonists. *International Journal of Quantum Chemistry*, 60(5):1069–1080, December 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60666.

DeSantAnna:1996:SSPb

[DAR+96a] C. M. R. De Sant'Anna, R. Bicca De Alencastro, C. R. Rodrigues, G. Barreiro, E. J. Barreiro, J. D. Da Motta Neto, and A. C. C. Freitas. A semiempirical study of pyrazole acylhydrazones as potential antimalarial agents. *International Journal of*

Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology., 23(??):111–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

DeSantanna:1996:SSP

[DAR+96b] Carlos M. R. De Sant'anna, Ricardo Bicca De Alencastro, Carlos R. Rodrigues, Gabriela Barreiro, Eliezer J. Barreiro, Joaquim Delphino Da Motta Neto, and Antônio Carlos C. Freitas. A semiempirical study of pyrazole acylhydrazones as potential antimalarial agents. *International Journal of Quantum Chemistry*, 60(8):1835–1843, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60743`.

Datta:1995:NDH

[Dat95] S. N. Datta. Near Dirac–Hartree–Fock results for first-row atoms calculated with GTO basis sets. *International Journal of Quantum Chemistry*, 56(2):91–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Daul:1994:DFT

[Dau94] C. Daul. Density functional theory applied to the excited states of coordination compounds. *International Journal of Quantum Chemistry*, 52(4):867–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Davidson:1998:HRP

[Dav98] Ernest R. Davidson. How robust is present-day DFT? *International Journal of Quantum Chemistry*, 69(3):241–245, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29998`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29998&PLACEBO=IE.pdf`. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Day:1995:LOE

[Day95] O. W. Day, Jr. A local one-electron operator for the generalized-overlap amplitudes. *International Journal of Quantum Chem-*

istry, 56(5):547–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Day:1996:EKT

[Day96] Orville W. Day Jr. The extended Koopmans' theorem Fock operator and the generalized overlap amplitude one-electron operator. *International Journal of Quantum Chemistry*, 57(3):391–399, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60376`.

Dehu:1994:TSC

[DB94a] C. Dehu and J. L. Brédas. Theoretical study of the conjugation length effect on the electronic and second-order nonlinear optical properties of amino-nitro diphenylacetylenes. *International Journal of Quantum Chemistry*, 52(1):89–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dutta:1994:ECR

[DB94b] P. Dutta and S. P. Bhattacharyya. On exact calculation of response properties of oscillators in static electric field: A Fourier grid Hamiltonian approach. I. one-dimensional systems. *International Journal of Quantum Chemistry*, 51(4 (or 5??)):293–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Defranceschi:1999:CME

[DB99] Mireille Defranceschi and Claude Le Bris. Computing a molecule in its environment: A mathematical viewpoint. *International Journal of Quantum Chemistry*, 71 (3):227–250, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10016709; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10016709&PLACEBO=IE.pdf`.

Davis:1992:NPB

[DBG92] L. P. Davis, L. W. Burggraf, and M. S. Gordon. Novel pentacoordinated bridged silicon anions. *International Journal of Quantum Chemistry*, 44(5):691–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Decleva:1994:CWL

[DBLV94] P. Decleva, M. Brosolo, A. Lisini, and M. Venuti. Continuum wavefunctions by least-squares scheme in a B-spline basis: Multicenter and multielectron formulations. *International Journal of Quantum Chemistry*, 52(2):507–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dunne:1999:WCE

[DBM99] Lawrence J. Dunne, Erkki J. Brändas, and John N. Murrell. D-wave condensate and essential phenomenological description of some properties of high T_c cuprate superconductors. *International Journal of Quantum Chemistry*, 74 (6):617–626, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001778; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001778&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Delhalle:1995:NVS

[DC95] J. Delhalle and J. Cizek. Note on the variation step in the iteration-variation approach: Illustration on the hydrogen atom. *International Journal of Quantum Chemistry*, 56(1):9–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deleuze:1997:CEV

[DC97] Michael S. Deleuze and Lorenz S. Cederbaum. Correlation effects in the valence X-ray photoionization spectra of ethylene, butadiene, and hexatriene. *International Journal of Quantum Chemistry*, 63(2):465–481, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42591; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42591&PLACEBO=IE.pdf.

Dive:1993:PCE

[DD93] G. Dive and D. Dehareng. Polarization correction of the electrostatic potential for aromatic compounds: Study of the nucleophilic attack. *International Journal of Quantum Chemistry*,

46(1):127–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deleuze:1996:TSXa

[DD96a] M. Deleuze and J. Delhalle. Theoretical study of the X-ray photoionization spectra of polycycloalkanes. *International Journal of Quantum Chemistry*, 60(7):293–??, 1996. CODEN IJQCB2.

Deleuze:1996:TSXb

[DD96b] M. Deleuze and J. Delhalle. Theoretical study of the X-ray photoionization spectra of polycycloalkanes. *International Journal of Quantum Chemistry*, 60(7):1505–1514, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60710.

Deleuze:1996:TSXc

[DD96c] M. Deleuze and J. Delhalle. Theoretical study of the X-ray photoionization spectra of polycycloalkanes. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30 (??):293–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Das:1997:SGE

[DD97a] G. P. Das and D. S. Dudis. Study of ground and excited states of doped polyacetylene. *International Journal of Quantum Chemistry*, 65(5):651–654, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42797; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42797&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Daul:1997:SNQ

[DD97b] Claude Daul and Stéphane Daul. Symmetrical "nonproduct" quadrature rules for a *fast* calculation of multicenter integrals. *International Journal of Quantum Chemistry*, 61 (2):219–230, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42403;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42403&PLACEBO=IE.pdf.

Dey:1998:FQF

[DD98a] Bijoy Kr. Dey and B. M. Deb. Femtosecond quantum fluid dynamics of helium atom under an intense laser field. *International Journal of Quantum Chemistry*, 70(3): 441–474, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75014; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75014&PLACEBO=IE.pdf.

Dey:1998:SIH

[DD98b] Bijoy Kr. Dey and B. M. Deb. Stripped ion-helium atom collision dynamics within a time-dependent quantum fluid density functional theory. *International Journal of Quantum Chemistry*, 67(4):251–271, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29904; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29904&PLACEBO=IE.pdf.

Dive:1999:SPC

[DD99] G. Dive and D. Dehareng. Serine peptidase catalytic machinery: Cooperative one-step mechanism. *International Journal of Quantum Chemistry*, 73(2):161–174, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003514; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003514&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998*. Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Doclo:1997:DFS

[DDC97] Karen G. Doclo, Claude A. Daul, and Steven Creve. A density functional study of ground-state and excited-state properties of $CoAl_2Cl_8(g)$. *International Journal of Quantum Chemistry*, 61(3):475–481, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42415;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42415&PLACEBO=IE.pdf.

Dehareng:1993:ACE

[DDG93] D. Dehareng, G. Dive, and J. M. Ghuysen. Analytical calculation of the electrostatic interaction energy within the CNDO framework. *International Journal of Quantum Chemistry*, 46 (6):711–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Daniel:1996:LCV

[DDH+96] C. Daniel, R. De Vivie-Riedle, M.-C. Heitz, J. Manz, and P. Saalfrank. From laser control of vibrationally mediated photodissociation to photodesorption: Model simulations of breaking metal-ligand bonds in organometallic molecules, clusters, and adsorbates at surfaces. *International Journal of Quantum Chemistry*, 57(4):595–609, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60424.

Dijkstra:1995:ECE

[DdJN95] F. Dijkstra, W. A. de Jong, and W. C. Nieuwpoort. Electron correlation effects on the f6-manifold of the (eu^{3+}) impurity in Ba_2GdNbO_6. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:609–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Dive:1996:PAM

[DDP96] G. Dive, D. Dehareng, and D. Peeters. Proposition for the acylation mechanism of serine proteases: A one-step process? *International Journal of Quantum Chemistry*, 58(1):85–107, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60466.

DeSantAnna:1996:SSPa

[DDRB96] C. M. R. De Sant'Anna, R. B. De Alencastro, C. R. Rodrigues, and G. Barreito. A semiempirical study of pyrazole acylhydrazones as potential antimalarial agents. *International Journal of Quantum Chemistry*, 60(8):111–??, 1996. CODEN IJQCB2.

DePrunele:1997:PSR

[De 97] E. De Prunelé. Power series with rational coefficients for two-electron atom energies. *International Journal of Quantum Chemistry*, 63(6):1079–1089, July 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42652; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42652&PLACEBO=IE.pdf`.

Dannenberg:1992:CEH

[DE92] J. J. Dannenberg and E. M. Evleth. A critical examination of H-bonding interactions calculated using the am1 molecular orbital method. *International Journal of Quantum Chemistry*, 44(5): 869–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DelBene:1992:HBM

[Del92] J. E. Del Bene. Hydrogen bonding: Methodology and applications to complexes of HF and HCl with HCN and CHsub 3 CN. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:527–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

DelRe:1996:CTB

[Del96] Giuseppe Del Re. Charge transfer between a molecule and an infinite electron reservoir in the MO scheme. *International Journal of Quantum Chemistry*, 60(1):141–146, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60576`.

Delley:1998:STA

[Del98] B. Delley. A scattering theoretic approach to scalar relativistic corrections on bonding. *International Journal of Quantum Chemistry*, 69(3):423–433, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29996; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29996&PLACEBO=IE.pdf`. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Deumens:1996:QQM

[Deu96] E. Deumens. Quaternionic quantum mechanics and quantum fields. by Stephen L. Adler. *International Journal of Quantum Chemistry*, 60(4):941–??, 1996. CODEN IJQCB2.

Deumens:1998:BRD

[Deu98a] Erik Deumens. Book review: *Dynamics of molecules and chemical reactions*, by Robert E. Wyatt and John Z. Zhang. *International Journal of Quantum Chemistry*, 67 (5):339, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29912; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29912&PLACEBO=IE.pdf.

Deumens:1998:BRQ

[Deu98b] Erik Deumens. Book review: *The Quantum Challenge*, by George Greenstein and Arthur G. Zajonc. *International Journal of Quantum Chemistry*, 69(5):689, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30033; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30033&PLACEBO=IE.pdf.

Deumens:1999:BR

[Deu99] Erik Deumens. Book Review. *International Journal of Quantum Chemistry*, 71(6):513–514, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=15000350; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=15000350&PLACEBO=IE.pdf.

Dewar:1992:SAC

[Dew92] M. J. S. Dewar. The semiempirical approach to chemistry. *International Journal of Quantum Chemistry*, 44(4):427–??, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Davidov:1999:VDP

[DFDK99] Genady Davidov, David Fuks, Simon Dorfman, and Genrich L. Krasko. Volume-dependent potential approach for tungsten. *International Journal of Quantum Chemistry*, 71

(4):343–348, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10049349; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10049349&PLACEBO=IE.pdf.

Dorfman:1998:SIP

[DFL98] Simon Dorfman, David Fuks, and Vlad Liubich. Sign of the interaction parameter in disordered Fe-Al alloys. *International Journal of Quantum Chemistry*, 70(4-5):1067–1073, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75029; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75029&PLACEBO=IE.pdf.

Deleuze:1992:SOG

[DHDP92] M. Deleuze, P. Horeczky, J. Delhalle, and B. T. Pickup. Second-order Green's function simulations of the valence XPS spectra of unsaturated hydrocarbons. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:31–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Daniel:1994:DPR

[DHLS94] C. Daniel, M. C. Heitz, L. Lehr, and T. Schroeder. Dynamics of photochemical reactions: Simulation by quantum calculations for transition metal hydrides. *International Journal of Quantum Chemistry*, 52(1):71–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dias:1999:AES

[Dia99] Jerry Ray Dias. Analysis of π-electronic structures of small alternant hydrocarbons to infinitely large polymeric strips: The aufbau principle and end-group effects. *International Journal of Quantum Chemistry*, 74(6):721–733, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001788; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001788&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Dahl:1995:DKP

[DJ95] J. P. Dahl and T. Jørgensen. On the Dirac–Kepler problem: The Johnson–Lippmann operator, supersymmetry, and normal-mode representations. *International Journal of Quantum Chemistry*, 53(2):161–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeBritoMota:1998:SEP

[DJF98] F. De Brito Mota, J. F. Justo, and A. Fazzio. Structural and electronic properties of silicon nitride materials. *International Journal of Quantum Chemistry*, 70(4-5):973–980, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75075; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75075&PLACEBO=IE.pdf`.

Dufty:1997:DMM

[DKBB97] James W. Dufty, Chang Sub Kim, Michael Bonitz, and Rolf Binder. Density matrix methods for semiconductor Coulomb dynamics. *International Journal of Quantum Chemistry*, 65 (5):929–940, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42824; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42824&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Derecskei-Kovacs:1996:NWF

[DKM96] Agnes Derecskei-Kovacs and Dennis S. Marynick. Nonempirical wave functions for very large molecules. I. The PRDDO/M method. *International Journal of Quantum Chemistry*, 58(2): 193–202, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60475`.

Derecskei-Kovacs:1997:NWFb

[DKM97] A. Derecskei-Kovacs and D. S. Marynick. Nonempirical wave functions for very large molecules. III. extension of the

PRDDO/M and PRDDO/M/FCP method to main-row elements Ga–Br. *International Journal of Quantum Chemistry*, 63(6):1091–??, July 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Diercksen:1994:MSC

[DKTZ94] G. H. F. Diercksen, M. Karelson, T. Tamm, and M. C. Zerner. Multicavity SCRF calculation of ion hydration energies. *International Journal of Quantum Chemistry. Symposium*, 28:339–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Derecskei-Kovacs:1997:NWFa

[DKWM97] Agnes Derecskei-Kovacs, David E. Woon, and Dennis S. Marynick. Nonempirical wave functions for very large molecules. II. the PRDDO/M/FCP method. *International Journal of Quantum Chemistry*, 61(1):67–76, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42387; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42387&PLACEBO=IE.pdf.

Du:1992:RAL

[DL92] P. Du and G. H. Loew. Role of axial ligand in the electronic structure of model compound I complexes. *International Journal of Quantum Chemistry*, 44(2):251–??, September 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dai:1999:LAA

[DlD99] Ying Dai and Shi liang Ding. Lie algebraic approach to multiphoton excitation of diatomic molecules in intense laser fields. *International Journal of Quantum Chemistry*, 71 (2):201–207, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000028; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000028&PLACEBO=IE.pdf.

Dorfman:1999:ISE

[DLF99] Simon Dorfman, Vlad Liubich, and David Fuks. Ab initio study of energy parameters in DO_3 phase of Fe-Al alloy. *International Journal of Quantum Chemistry*, 75(4–5):927–941, November

15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004987/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004987&PLACEBO=IE.pdf.

Decleva:1995:ACE

[DLV95] P. Decleva, A. Lisini, and M. Venuti. Accurate CI expansion in a spline basis of the helium ground-state wave function. *International Journal of Quantum Chemistry*, 56(1):27–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeLaVega:1993:GES

[DM93] J. M. Garcia De La Vega and B. Miguel. Gaussian expansions from STOs by the distance between subspaces. *International Journal of Quantum Chemistry*, 47(1):85–??, July 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Duch:1994:MSC

[DM94] W. Duch and J. Meller. On multireference superdirect configuration interaction in third order. *International Journal of Quantum Chemistry*, 50(4):243–??, May 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Datta:1995:DAD

[DM95] S. N. Datta and B. Mallik. Determination of the acid dissociation constants of p-benzohydroquinone by the INDO method. *International Journal of Quantum Chemistry*, 53(1):37–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Datta:1996:TEEa

[DM96] Sambhu N. Datta and Buddhadeb Mallik. Transport of excitation energy in a three-dimensional doped molecular crystal. IV. fourth-order propagation, exciton clothing, and exciton diffusion. *International Journal of Quantum Chemistry*, 59(2):147–165, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60534.

Datta:1997:MCC

[DM97a] Kakali Datta and Asok K. Mukherjee. Method for construction of characteristic polynomials via graph linearization. *International Journal of Quantum Chemistry*, 65(3): 199–204, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42757; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42757&PLACEBO=IE.pdf.

Datta:1997:TIR

[DM97b] Sambhu N. Datta and Buddhadeb Mallik. Theoretical investigation of the rates of electron transfer processes $Q_I^- + Q_{II} \rightarrow Q_I + Q_{II}^-$ and $Q_I^- + Q_{II}^- \rightarrow Q_I + Q_{II}^{2-}$ in photosynthesis. *International Journal of Quantum Chemistry*, 61 (5):865–879, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42459; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42459&PLACEBO=IE.pdf.

Dobrowolski:1998:CCK

[DM98] Jan Cz. Dobrowolski and Aleksander P. Mazurek. C_{60} carbyne knots (from 0_1 to 6_3): Theoretical NMR spectra. *International Journal of Quantum Chemistry*, 70(4-5): 1009–1015, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75022; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75022&PLACEBO=IE.pdf.

Dobrowolski:1999:CCL

[DM99] Jan Cz. Dobrowolski and Aleksander P. Mazurek. On the C_{60} carbyne links (from 2_1^2 to 6_3^2). *International Journal of Quantum Chemistry*, 75(4–5):839–846, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004980/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004980&PLACEBO=IE.pdf.

Dunne:1997:DLR

[DMB97] Lawrence J. Dunne, John N. Murrell, and Erkki J. Brändas. Off-diagonal long-range order, η-pairing, and Friedel oscillations in high T_c cuprate superconductors and the ground state of the extended Hubbard model. *International Journal of Quantum Chemistry*, 63(3):675–684, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42629; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42629&PLACEBO=IE.pdf`.

Dmitriev:1993:MCP

[DMFR93] Y. Yu. Dmitriev, A. O. Mitrushenkov, M. P. Fulscher, and B. O. Roos. A mutually consistent procedure for excitation energies and transition densities based on the Extended Brillouin's Theorem. *International Journal of Quantum Chemistry*, 47(2):155–??, July 15, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Neto:1992:PMM

[dMNZdA92] J. Delphino da Motta Neto, M. C. Zerner, and R. Bicca de Alencastro. A possible mechanism of molecular recognition for the reverse transcriptase of HIV-1. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:225–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

DaCosta:1996:IPLa

[DMR96a] H. F. M. DaCosta, D. A. Micha, and K. Runge. Intensity and polarization of light emitted in slow ion-atom collisions. *International Journal of Quantum Chemistry*, 60(7):257–??, 1996. CODEN IJQCB2.

DaCosta:1996:IPLc

[DMR96b] H. F. M. DaCosta, D. A. Micha, and K. Runge. Intensity and polarization of light emitted in slow ion-atom collisions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):257–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

DaCosta:1996:IPLb

[DMR96c] Herbert F. M. DaCosta, David A. Micha, and Keith Runge. Intensity and polarization of light emitted in slow ion-atom collisions. *International Journal of Quantum Chemistry*, 60 (7):1469–1477, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60705.

DeJong:1996:RCU

[DN96] W. A. De Jong and W. C. Nieuwpoort. Relativity and the chemistry of UF_6: A molecular Dirac–Hartree–Fock-CI study. *International Journal of Quantum Chemistry*, 58(2):203–216, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60476.

Duke:1990:FUI

[DO90] B. J. Duke and B. O'Leary. On the feasibility of using ab initio calculations, both crystal orbital and molecular orbital, to predict XPS chemical shifts in fluorinated polyethylenes. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:107–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Diz:1994:END

[DÖ94] A. Diz and Y. Öhrn. Electron-nuclear dynamics of molecular systems. *International Journal of Quantum Chemistry. Symposium*, 28:11–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Dobson:1998:PVW

[Dob98] John F. Dobson. Prospects for a van der Waals density functional. *International Journal of Quantum Chemistry*, 69 (4):615–618, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30016; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30016&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Datta:1993:TEE

[DP93] S. N. Datta and N. V. Prabhu. Transport of excitation energy in a doped molecular aggregate III. numerical investigation of exciton hopping with various exciton-depleting processes. *International Journal of Quantum Chemistry*, 46(2):295–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DelRe:1994:CES

[DP94] G. Del Re and A. Peluso. Chemical effects and surface properties: The nature of an absorbed complex. *International Journal of Quantum Chemistry*, 49(4):429–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Durand:1996:CST

[DP96] Philippe Durand and Ivana Paidarová. Convergence studies in the theory of effective Hamiltonians. *International Journal of Quantum Chemistry*, 58(4):341–350, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60490.

Deleuze:1997:CPE

[DP97] Michael S. Deleuze and Barry T. Pickup. The coupled perturbed electron propagator in the two-particle-hole and extended two-particle-hole Tamm–Dancoff approximations. *International Journal of Quantum Chemistry*, 63(2): 483–509, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42592; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42592&PLACEBO=IE.pdf.

Delchev:1994:SDF

[DPPM94] Y. I. Delchev, R. L. Pavlov, K. A. Pavlova, and L. P. Marinova. A semiclassical density functional evaluation of the smoothly varying part of the Hartree–Fock binding energy in atoms. *International Journal of Quantum Chemistry*, 52(6):1349–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dzegilenko:1997:TNA

[DQB97] Fedor N. Dzegilenko, Jianxin Qi, and Joel M. Bowman. Two novel applications of shepard-type interpolation for polyatomic systems: Reduced dimensionality HOCO and full dimensionality Ar-HCO. *International Journal of Quantum Chemistry*, 65(5):965–973, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42827; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42827&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Devemy:1996:SDM

[DRBE96] Jerome Devemy, Marie-Madeleine Rohmer, Marc Benard, and Rene Ernenwein. Standard and direct methods in ab initio Hartree–Fock calculations: Application to polyoxometallates, organometallic clusters, and polypeptides. *International Journal of Quantum Chemistry*, 58(3):267–281, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60481.

Delin:1998:FPO

[DREW98] Anna Delin, P. Ravindran, Olle Eriksson, and J. M. Wills. Full-potential optical calculations of lead chalcogenides. *International Journal of Quantum Chemistry*, 69 (3):349–358, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29990; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29990&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

DelBene:1990:CTM

[DS90] J. E. Del Bene and I. Shavitt. Comparison of theoretical methods for the determination of the lisup + affinities of neutral and anionic first- and second-row bases. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24: 365–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Duan:1992:MCP

[DS92] X. Duan and S. Scheiner. Modeling of coupled proton transfers by analytic functions. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the*

International Symposium on Quantum Biology and Quantum Pharmacology., 19:109–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Duan:1993:BIE

[DS93] X. Duan and S. Scheiner. Behavior of interaction energy and intramolecular bond stretch in linear and bifuricated hydrogen bonds. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:181–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Dahl:1996:SAP

[DS96] Tor Dahl and Per N. Skancke. Structural aspects of a possible transannular interaction in silatranes and azasilatranes: An ab initio study. *International Journal of Quantum Chemistry*, 60(1):567–578, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60620`.

Datta:1999:TEE

[DS99] S. N. Datta and Deepak Shah. Transport of excitation energy in a three-dimensional doped molecular aggregate. VII. Physical chemistry of exciton processes in thylakoid membrane. *International Journal of Quantum Chemistry*, 74(3):357–370, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62004766; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62004766&PLACEBO=IE.pdf`. Special Issue: *Biophysics Quarterly*.

Silva:1995:TDL

[dSdSN95] C. O. da Silva, E. C. da Silva, and M. A. C. Nascimento. Theoretical description of the low-lying valance states of the MgC molecule. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:639–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

DelBene:1990:TSC

[DSS90] J. E. Del Bene, E. A. Stahlberg, and I. Shavitt. A theoretical study of the complexes of N_2 O with hsup +, lisup +, and HF using various correlation methods. *International Journal* *of Quantum Chemistry. Quantum Chemistry Symposium*, 24: 455–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Duan:1993:MPT

[DSW93] X. Duan, S. Scheiner, and R. Wang. Modeling proton transfer potentials in angularly deformed hydrogen bonds. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:77–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Doerksen:1996:PHMa

[DT96a] R. J. Doerksen and A. J. Thakkar. Polarizabilities of heteroaromatic molecules: Azines revisited. *International Journal of Quantum Chemistry*, 60(7):421–??, 1996. CODEN IJQCB2.

Doerksen:1996:PHMc

[DT96b] R. J. Doerksen and A. J. Thakkar. Polarizabilities of heteroaromatic molecules: Azines revisited. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??): 421–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Doerksen:1996:PHMb

[DT96c] Robert J. Doerksen and Ajit J. Thakkar. Polarizabilities of heteroaromatic molecules: Azines revisited. *International Journal of Quantum Chemistry*, 60(7):1633–1642, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60724`.

DaSilva:1996:TCG

[DTA+96] Clarissa O. Da Silva, Fábio Eduardo C. Teixeira, José André T. Azevedo, Edilson C. Da Silva, and Marco Antonio Chaer Nascimento. Theoretical characterization of the ground state of the alkaline-earth monocarbides: Ordering of the two lower-lying states of the BeC, MgC, and CaC molecules. *International Journal of Quantum Chemistry*, 60(1):433–438, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60606`.

Datta:1996:TEEb

[DTM96] S. N. Datta, D. Tandon, and B. Mallik. Transfer of excitation energy in a three-dimensional-doped molecular crystal. V. self-consistency of the temporal processes involved in energy transfer in photosynthetic units. *International Journal of Quantum Chemistry*, 60(5):1045–1055, December 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60663.

Dacosta:1997:HTO

[DTS97] Herbert F. M. Dacosta, Milan Trsic, and Alfredo M. Simas. Hydrogen-type orbitals in terms of Gaussian functions. *International Journal of Quantum Chemistry*, 65 (2):143–150, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42751; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42751&PLACEBO=IE.pdf.

Duch:1990:TCI

[Duc90] W. Duch. Towards a configuration interaction method with flexible spaces. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:683–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Dunlap:1996:ADF

[Dun96] Brett I. Dunlap. Accurate density functional calculations on large systems. *International Journal of Quantum Chemistry*, 58(2):123–132, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60468.

Dunlap:1997:ADF

[Dun97] Brett I. Dunlap. Accurate density-functional calculations on large systems. *International Journal of Quantum Chemistry*, 64(2):193–203, August 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42681; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42681&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical*

Physics. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Dunlap:1998:QCM

[Dun98] Brett I. Dunlap. Quantum chemical molecular dynamics. *International Journal of Quantum Chemistry*, 69(3): 317–325, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29987; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29987&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Dunne:1999:AFT

[Dun99] Lawrence J. Dunne. Application of the field-theoretic method of Bohm and Pines to a study of the metal-insulator transition in doped dielectric media. *International Journal of Quantum Chemistry*, 71(1):111–120, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000008; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000008&PLACEBO=IE.pdf.

Dijkman:1991:PAS

[DV91] J. P. Dijkman and P. Th. Van Duijnen. Papain in aqueous solution and the role of Asp-158 in the mechanism: An ab initio SCF + DRF + BEM study. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:49–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

DeVries:1996:STA

[DV96] Alex H. De Vries and Piet Th. Van Duijnen. Solvatochromism of the $\pi* \leftarrow n$ transition of acetone by combined quantum mechanical–classical mechanical calculations. *International Journal of Quantum Chemistry*, 57(6):1067–1076, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60451.

Dijkstra:1998:REC

[DV98] Fokke Dijkstra and Joop H. Van Lenthe. On the rapid evaluation of cofactors in the calculation of nonorthogonal matrix elements. *International Journal of Quantum Chemistry*, 67(2):77–83, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29888; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29888&PLACEBO=IE.pdf.

Dijkstra:1999:ABB

[DV99] Fokke Dijkstra and Joop H. Van Lenthe. Aromaticity of bent benzene rings: A VBSCF study. *International Journal of Quantum Chemistry*, 74(2):213–221, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003365; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003365&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

deVries:1993:SPD

[dVJ93] A. H. de Vries, P. Th. Van Duijnen, and A. H. Juffer. Success and pitfalls of the dielectric continuum model in quantum chemical calculations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:451–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Derycke:1991:CST

[DVL+91] I. Derycke, J. P. Vigneron, Ph. Lambin, Th. Laloyaux, and A. A. Lucas. Computation of scanning tunneling microscope images. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:687–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Dai:1997:QFC

[DW97] Song-Tao Dai and Peter Winkler. A quadrature formula for correlation integrals. *International Journal of Quantum Chemistry*, 65(5):513–518, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?

ID=42780; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42780&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

DelBene:1998:SPN

[DWB98] Janet E. Del Bene, John D. Watts, and Rodney J. Bartlett. Structure and properties of ${NH_5}^{2+}$: A dication with two 2-electron 3-center bonds. *International Journal of Quantum Chemistry*, 70(4-5):1003–1007, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75021; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75021&PLACEBO=IE.pdf.

Davis:1999:ISC

[DWR99] William B. Davis, Michael R. Wasielewski, and Mark A. Ratner. Influence of substituents and chain length on the optical properties of poly(p-phenylenevinylene) oligomers. *International Journal of Quantum Chemistry*, 72(4):463–471, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006323; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006323&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Das:1996:TST

[DY96] G. P. Das and A. T. Yeates. Transport of solitons in *trans*-polyacetylene. *International Journal of Quantum Chemistry*, 59(3):251–257, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60544.

Das:1996:IDTa

[DYD96a] G. P. Das, A. T. Yeates, and D. S. Dudis. Iodine-doped trans-polyacetylene. *International Journal of Quantum Chemistry*, 60(7):287–??, 1996. CODEN IJQCB2.

Das:1996:IDTb

[DYD96b] G. P. Das, A. T. Yeates, and D. S. Dudis. Iodine-doped transpolyacetylene. *International Journal of Quantum Chem-*

istry, 60(7):1499–1504, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60709.

Das:1996:IDTc

[DYD96c] G. P. Das, A. T. Yeates, and D. S. Dudis. Iodine-doped trans-polyacetylene. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):287–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Deng:1994:DIR

[DZ94] L. Deng and T. Ziegler. The determination of intrinsic reaction coordinates by density functional theory. *International Journal of Quantum Chemistry*, 52(4):731–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dickson:1996:DFS

[DZ96a] Ross M. Dickson and Tom Ziegler. A density functional study of the electronic spectrum of permanganate. *International Journal of Quantum Chemistry*, 58(6):681–687, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60508.

Ding:1996:GEP

[DZ96b] Fu-Jiang Ding and Liang-Fu Zhang. Gauche effect and PM3 calculation of open-chain polyphosphorus hydrides. *International Journal of Quantum Chemistry*, 60(5):1037–1044, December 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60662.

Ding:1997:HNP

[DZ97] Fujiang Ding and Liangfu Zhang. $HNNH_3$, A new possible isomer of N_2H_4: An ab initio study. *International Journal of Quantum Chemistry*, 64(4):447–452, September 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42702; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42702&PLACEBO=IE.pdf.

Deng:1993:SAM

[DZF93] C. Deng, R. Zhang, and D. Feng. Solution of atomic and molecular Schrödinger equation described by hyperspherical coordinates. *International Journal of Quantum Chemistry*, 45(4):385–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolgounitcheva:1997:CEP

[DZO97] O. Dolgounitcheva, V. G. Zakrzewski, and J. V. Ortiz. Comparison of electron propagator methods for calculating electron detachment energies of anions. *International Journal of Quantum Chemistry*, 65(5):463–469, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42774; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42774&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Dolgounitcheva:1998:EPT

[DZOR98] O. Dolgounitcheva, V. G. Zakrzewski, J. V. Ortiz, and G. V. Ratovski. Electron propagator theory of conformational effects on anisole and thioanisole photoelectron spectra. *International Journal of Quantum Chemistry*, 70(4-5): 1037–1043, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75026; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75026&PLACEBO=IE.pdf`.

Evans:1997:BNS

[EB97] Jeremy N. S. Evans and C. R. Bowers. Biomolecular NMR spectroscopy. *International Journal of Quantum Chemistry*, 63 (5):1023–??, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Evangelisti:1995:CAS

[EBG95] S. Evangelisti, G. L. Bendazzoli, and L. Gagliardi. Complete active-space configuration interaction with optimized orbitals:

Application to Li_2. *International Journal of Quantum Chemistry*, 55(3):277–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esquivel:1992:SET

[EBMS92] J. L. Esquivel, D. Balmaceda, and J. F. Mata-Segreda. Solvation effect on the tunneling rates of proton transfer. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:807–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Elabsy:1996:CESc

[EC96a] A. M. Elabsy and P. Csavinszky. Combined effect of the screening of a donor ion and the conduction band non (??)arabolicity on the binding energy of a donor at the center of a spherical. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):507–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Elabsy:1996:CESa

[EC96b] A. M. Elabsy and P. Csavinszky. Combined effect of the screening of a donor ion and the conduction band nonparabolicity on the binding energy of a donor at the center of a spherical quantum dot. *International Journal of Quantum Chemistry*, 60(7): 507–??, 1996. CODEN IJQCB2.

Elabsy:1996:CESb

[EC96c] A. M. Elabsy and P. Csavinszky. Combined effect of the screening of a donor ion and the conduction band nonparabolicity on the binding energy of a donor at the center of a spherical quantum dot. *International Journal of Quantum Chemistry*, 60(7):1719–1722, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60735`.

Eurenius:1996:EMH

[ECBH96] Kirsten P. Eurenius, David C. Chatfield, Bernard R. Brooks, and Milan Hodoscek. Enzyme mechanisms with hybrid quantum and molecular mechanical potentials. I. theoretical considerations. *International Journal of Quantum Chemistry*, 60 (6):1189–1200, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60683`.

Ellis:1998:ECS

[EDF+98] Donald E. Ellis, Simon Dorfman, David Fuks, Ronit Evenhaim, and Kleber C. Mundim. Embedded cluster and supercell study of the structure of the interstitial Cu-C solid solutions. *International Journal of Quantum Chemistry*, 70 (4-5):1085–1092, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75031; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75031&PLACEBO=IE.pdf.

Eguiluz:1992:TFP

[EDH+92] A. G. Eguiluz, J. J. Deisz, M. Heinrichsmeier, A. Fleszar, and W. Hanke. Towards a first-principles implementation of density-functional theory at a metal surface. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:837–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Emery:1991:IDW

[EE91] Luke C. Emery and W. Daniel Edwards. Intermolecular dynamics for weakly bound donor-acceptor complexes. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:347–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Enkvist:1997:SCS

[EEL97] Christer Enkvist, David Edvardsson, and Sten Lunell. Spin coupling in shake-up processes. *International Journal of Quantum Chemistry*, 63(1):189–196, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42564; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42564&PLACEBO=IE.pdf.

Eguiluz:1996:LRQa

[Egu96a] A. G. Eguiluz. Linear response and quasiparticle calculations as probes of the Kohn–Sham eigenvalues in metals. *International Journal of Quantum Chemistry*, 60(7):245–??, 1996. CODEN IJQCB2.

Eguiluz:1996:LRQc

[Egu96b] A. G. Eguiluz. Linear response and quasiparticle calculations as probes of the Kohn–Sham eigenvalues in metals. *International*

Journal of Quantum Chemistry. Quantum Chemistry Symposium, 30(??):245–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Eguiluz:1996:LRQb

[Egu96c] Adolfo G. Eguiluz. Linear response and quasiparticle calculations as probes of the Kohn–Sham eigenvalues in metals. *International Journal of Quantum Chemistry*, 60(7):1457–1468, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60704.

Eid:1999:HOF

[Eid99] R. Eid. Higher order finite element solution of the one-dimensional Schrödinger equation. *International Journal of Quantum Chemistry*, 71(2):147–152, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000022; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000022&PLACEBO=IE.pdf.

Etemadi:1993:ALG

[EJ93] B. Etemadi and H. W. Jones. Accurate LCAO ground state calculations of HeH^{2+} using Slater-type orbitals. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:755–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Ekholm:1994:TIS

[EK94] M. Ekholm and Konschin. A theoretical investigation of some novel pilocarpine prodrugs. *International Journal of Quantum Chemistry*, 51(1):35–??, June 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Eliav:1994:RCC

[EKI94] E. Eliav, U. Kaldor, and Y. Ishikawa. Relativistic coupled cluster theory based on the No-Pair Dirac–Coulomb–Breit Hamiltonian: Relativistic pair correlation energies of the Xe atom. *International Journal of Quantum Chemistry. Symposium*, 28:205–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Elder:1973:UMS

[Eld73] M. Elder. Use of molecular symmetry in SCF calculations. *International Journal of Quantum Chemistry*, 7(??):75–85, ??

1973. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esseffar:1996:HLI

[ELMY96] M. Esseffar, A. Luna, O. Mó, and M. Yáñez. High-level ab initio calculations on CH_2^+ (^{2} A_1) + PO(^{2} II) reactions. *International Journal of Quantum Chemistry*, 57(4):559–566, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60420.

Emch:1997:FQM

[Emc97] Gérard G. Emch. Foundations of quantum mechanics: Building on von Neumann's heritage. *International Journal of Quantum Chemistry*, 65(5):379–387, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42784; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42784&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Eckert-Maksic:1994:PFA

[EMMK94] M. Eckert-Maksic, Z. B. Maksic, and M. Klessinger. Protonation of fused aromatic systems: Ab initio study of some model Wheland intermediates. *International Journal of Quantum Chemistry*, 49(4):383–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Eriksson:1994:ENG

[EMMS94] L. A. Eriksson, V. G. Malkin, O. L. Malkina, and D. R. Salahub. The effects of nonlocal gradient corrections in density functional calculations of hydrocarbon radical hyperfine structures. *International Journal of Quantum Chemistry*, 52(4):879–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Eriksson:1997:IMP

[EMMS97] Leif A. Eriksson, Olga L. Malkina, Vladimir G. Malkin, and Dennis R. Salahub. Investigation of Mössbauer parameters for a set of iodine compounds using gradient-corrected density functional theory. *International Journal of Quantum Chemistry*, 63(2):575–583, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42601; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42601&PLACEBO=IE.pdf.

Enchev:1996:TBD

[Enc96] Venelin Enchev. Tautomerism in 2,2′-bipyridyl-3,3′-diol. *International Journal of Quantum Chemistry*, 57(4):721–728, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60409.

Engdahl:1992:ESC

[Eng92] E. Engdahl. Extreme sensitivity of corrugation strength on diffraction resonance line-shapes for the gas-surface system He(21 meV)/Cu(115). *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:657–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Engel:1995:DFT

[Eng95] E. Engel. Density functional theory of field theoretical systems. *International Journal of Quantum Chemistry*, 56(4):217–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Enkvist:1997:SAQ

[Enk97] C. Enkvist. Strategies and applications in quantum chemistry: From molecular astrophysics to molecular engineering. edited by Y. Ellinger and M. Defranceschi. *International Journal of Quantum Chemistry*, 63(6):1133–??, July 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Edlund:1998:PGO

[EP98] Åke Edlund and Uri Peskin. A parallel Green's operator for multidimensional quantum scattering calculations. *International Journal of Quantum Chemistry*, 69(2):167–173, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29979; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29979&PLACEBO=IE.pdf.

Ernzerhof:1997:CCD

[EPB97] Matthias Ernzerhof, John P. Perdew, and Kieron Burke. Coupling-constant dependence of atomization energies. *International Journal of Quantum Chemistry*, 64(3):285–295, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42687; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42687&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Eriksson:1993:TCM

[Eri93] L. Eriksson. Theoretical and computational models for organic chemistry edited by S. J. Formosinho, I. G. Csizmadia, and L. G. Arnaut. *International Journal of Quantum Chemistry*, 45 (4):403–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ebner:1999:MDS

[ESHP99] Christoph Ebner, Roland Sansone, Sunantha Hengrasmee, and Michael Probst. Molecular dynamics study of an aqueous potassium nitrate solution. *International Journal of Quantum Chemistry*, 75(4–5):805–814, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004975/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004975&PLACEBO=IE.pdf.

Ebner:1998:QCS

[ESP98] Christoph Ebner, Roland Sansone, and Michael Probst. Quantum chemical study of the interaction of nitrate anion with water. *International Journal of Quantum Chemistry*, 70(4-5):877–886, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75065; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75065&PLACEBO=IE.pdf.

El-Sayed:1996:UPC

[ESTMK96] M. A. El-Sayed, I. Tanaka, Y. Molin, and J. L. Krause. Ultrafast processes in chemistry and photobiology. *International*

Journal of Quantum Chemistry, 60(2):713–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

El-Taher:1997:TSM

[ET97] S. El-Taher. A theoretical study of malononitrile addition to carbonyl compounds. *International Journal of Quantum Chemistry*, 62(4):419–426, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42528; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42528&PLACEBO=IE.pdf.

El-Taher:1999:TSG

[ET99] S. El-Taher. Theoretical study on the gas-phase reactivity of halogenated alkylperoxyl radicals toward alkenes. *International Journal of Quantum Chemistry*, 71(3):273–283, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10016711; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10016711&PLACEBO=IE.pdf.

Evarestov:1994:QCC

[ETV94] R. A. Evarestov, I. I. Tupitsin, and V. A. Veryazov. Quantum chemical calculation of nickel and copper atomic valencies in crystalline oxides. *International Journal of Quantum Chemistry*, 52(2):295–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Evangelisti:1997:ISC

[Eva97] Stefano Evangelisti. An ab initio study of the N_8 C_{12} heterofullerene. *International Journal of Quantum Chemistry*, 65(1):83–88, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42744; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42744&PLACEBO=IE.pdf.

Estiu:1992:SCB

[EZ92] G. L. Estiu and M. C. Zerner. Studies on CO bonding to Rh clusters using an intermediate neglect of differential overlap theory to model heterogeneous catalytic reactions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:587–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Estiu:1993:EGC

[EZ93] G. L. Estiu and M. C. Zerner. Electronic and geometric characteristics of precrystalline structures in highly dispersed Rh catalysts. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:195–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Fripiat:1991:ICS

[FADC91] J. G. Fripiat, J.-M. André, J. Delhalle, and J. L. Calais. An ab initio computational scheme for polymeric chains with fully converged Coulomb and exchange lattice sums. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:603–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Fano:1997:EAM

[Fan97] U. Fano. Evolution of atomic-molecular eigenchannels. *International Journal of Quantum Chemistry*, 64(1):31–33, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42662; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42662&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Faris:1997:DQP

[Far97] William G. Faris. Does quantum probability predict frequency? *International Journal of Quantum Chemistry*, 65 (5):389–398, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42795; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42795&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Friedemann:1996:TSD

[FB96] R. Friedemann and C. Breitkopf. Theoretical studies on the decarboxylation reaction in thiamin catalysis. *International Journal of Quantum Chemistry*, 57(5):943–948, March 5, 1996.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60432.

Flocke:1997:SGAa

[FBKD97a] N. Flocke, M. Barysz, J. Karwowski, and G. H. F. Diercksen. Symmetric group approach to relativistic CI. I. general formalism. *International Journal of Quantum Chemistry*, 61 (1):1–10, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42372; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42372&PLACEBO=IE.pdf.

Flocke:1997:SGAb

[FBKD97b] N. Flocke, M. Barysz, J. Karwowski, and G. H. F. Diercksen. Symmetric group approach to relativistic CI. II. reduction of matrices in the spin space. *International Journal of Quantum Chemistry*, 61(1):11–20, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42381; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42381&PLACEBO=IE.pdf.

Flocke:1997:SGAc

[FBKD97c] N. Flocke, M. Barysz, J. Karwowski, and G. H. F. Diercksen. Symmetric group approach to relativistic CI. III. matrix elements for spin-dependent operators. *International Journal of Quantum Chemistry*, 61(1):21–34, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42382; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42382&PLACEBO=IE.pdf.

Fan:1999:ASO

[FC99] Peng-Dong Fan and Jin-Quan Chen. Algebraic solutions for the octahedral group: Group chain $O \supset C_4$. *International Journal of Quantum Chemistry*, 74(1):7–22, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62000134; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62000134&PLACEBO=IE.pdf.

Fan:1999:UEA

[FCMB99] Peng-Dong Fan, Jin-Quan Chen, Luke Mcaven, and Philip Butler. Unique Euler angles and self-consistent multiplication tables for double point groups. *International Journal of Quantum Chemistry*, 75(1):1–9, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63003144; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63003144&PLACEBO=IE.pdf`.

Ferraro:1998:CMP

[FCVL98] M. B. Ferraro, M. C. Caputo, M. P. Béccar Varela, and P. Lazzeretti. Calculation of magnetic properties of HF, H_2O, NH_3, and CH_4 molecules using a longitudinal gauge for the vector potential. *International Journal of Quantum Chemistry*, 66(1):31–45, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29837; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29837&PLACEBO=IE.pdf`.

Fischer:1993:LAO

[FD93] P. Fischer and M. Defranceschi. Looking at atomic orbitals through Fourier and wavelet transforms. *International Journal of Quantum Chemistry*, 45(6):619–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuks:1996:EMP

[FD96a] David Fuks and Simon Dorfman. Effective mixing potentials and ordering thermodynamics of alloys. *International Journal of Quantum Chemistry*, 57(5):897–901, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60444`.

Fuks:1996:PDA

[FD96b] David Fuks and Simon Dorfman. Phase diagram of atom-vacancy solid solution. *International Journal of Quantum Chemistry*, 57(5):881–886, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60442`.

Fripiat:1990:DRP

[FDAC90] J. G. Fripiat, J. Dellhalle, J.-M. André, and J. L. Calais. Dependence of RHF properties of hydrogen and helium chains on the exchange lattice summations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:593–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Fazzio:1992:ESP

[FdCC92] A. Fazzio, C. R. Martins da Cunha, and S. Canuto. Electronic and structural properties of N and N_2 in type-IV semiconductors. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:667–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Fontaine:1993:PTS

[FDD+93] M. Fontaine, J. Delhalle, M. Defranceschi, G. Lecayon, and J. Boissel. Preliminary theoretical study of perfluorodimethyl ether and its protonated form. *International Journal of Quantum Chemistry*, 46(1):171–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuks:1995:NEP

[FDD95] D. Fuks, S. Dorfman, and G. Davidov. Nonempirical effective potential approach in consistent thermodynamics of solid and liquid tungsten. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:675–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Flamant:1997:NSE

[FDF97] I. Flamant, J. Delhalle, and J. G. Fripiat. Numerical study of the exchange effects in the valence and core energy bands of the metallic lithium chain. *International Journal of Quantum Chemistry*, 63(3):709–718, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42614`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42614&PLACEBO=IE.pdf`.

Fangstrom:1998:DFS

[FEE+98] Torbjörn Fangström, David Edvardsson, Marie Ericsson, Sten Lunell, and Christer Enkvist. Density functional study of chlorine-oxygen compounds related to the ClO self-reaction. *International Journal of Quantum Chemistry*, 66

(3):203–217, January 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29854; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29854&PLACEBO=IE.pdf.

Fernandez:1991:BEQ

[Fer91] Francisco M. Fernandez. Bounds to the energy of quantum-mechanical models from variational functionals. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:95–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Fernandez:1992:MMP

[Fer92] F. M. Fernandez. Moment-method perturbation theory for the hydrogen atom in parallel electric and magnetic fields and in inhomogeneous electric fields. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:117–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Ferenczy:1995:AEE

[Fer95] G. G. Ferenczy. Approximate energy-evaluating schemes for a system of weakly overlapping group functions. *International Journal of Quantum Chemistry*, 53(5):485–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ferenczy:1996:SCN

[Fer96] György G. Ferenczy. The self-consistent nonorthogonal group function approach in reduced basis frozen-core calculations. *International Journal of Quantum Chemistry*, 57(3):361–367, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60397.

Friedman:1990:TDE

[FF90] P. Friedman and K. F. Ferris. Theoretically-derived, energy-based criteria for aromaticity. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:843–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Fang:1994:ISI

[FF94a] D. C. Fang and X.-Y. Fu. Ab initio studies on the IRC and rate constant of the reaction between acetylene and the hydrogen atom. *International Journal of Quantum Chemistry*, 49(1):3–??, January 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fang:1994:ISM

[FF94b] D.-C. Fang and X.-Y. Fu. Ab initio studies on the mechanism of the cycloaddition reaction between ketene and allene. *International Journal of Quantum Chemistry*, 50(2):93–??, April 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fang:1996:ISM

[FF96] De-Cai Fang and Xiao-Yuan Fu. Ab initio studies on the mechanism of the fluoroketene-imine cycloaddition reaction: Via a *gauche* or *trans* intermediate. *International Journal of Quantum Chemistry*, 57(6):1107–1114, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60454.

Flamant:1996:FSAb

[FFD96a] I. Flamant, J. G. Fripiat, and J. Delhalle. Fourier space for accurate ab initio RHF band structure calculations on chainlike systems. *International Journal of Quantum Chemistry*, 60(7):1487–1497, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60708.

Flamant:1996:FSAc

[FFD96b] I. Flamant, J. G. Fripiat, and J. Delhalle. Fourier space for accurate ab initio RHF band structure calculations on chainlike systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):275–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Flamant:1996:FSAa

[FFD96c] L. Flamant, J. G. Fripiat, and J. Delhalle. Fourier space for accurate ab initio RHF band structure calculations on chainlike systems. *International Journal of Quantum Chemistry*, 60(7):275–??, 1996. CODEN IJQCB2.

Flamant:1998:AFS

[FFD98] I. Flamant, J. G. Fripiat, and J. Delhalle. Advantages of the Fourier space RHF band structure approach: Application to polyoxymethylene using a distributed basis set of s-type Gaussian functions. *International Journal of Quantum Chemistry*, 70(4-5):1045–1054, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75027; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75027&PLACEBO=IE.pdf.

Friedemann:1998:GMS

[FFN98] Rudolf Friedemann, Anne Von Fircks, and Stefan Naumann. GROMOS-MD simulations on the coenzyme thiamin diphosphate in apoenzyme environment. *International Journal of Quantum Chemistry*, 70(2):407–413, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75010; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75010&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Field:1996:RJC

[FG96] M. Field and J. Gao. Report for the Joint CECAM-NSF Planning Meeting. *International Journal of Quantum Chemistry*, 60(6):1093–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Faglioni:1999:GRR

[FG99] Francesco Faglioni and William A. Goddard III. GVB-RP: A reliable MCSCF wave function for large systems. *International Journal of Quantum Chemistry*, 73(1):1–22, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55001581; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55001581&PLACEBO=IE.pdf.

Flocco:1990:SCS

[FGM90] M. Flocco, X. Q. Gao, and L. Massa. A study of the Colle–Salvetti formula for the calculation of the correlation energy.

International Journal of Quantum Chemistry. Quantum Chemistry Symposium, 24:213–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Famulari:1998:IGO

[FGRS98] A. Famulari, E. Gianinetti, M. Raimondi, and M. Sironi. Implementation of gradient-optimization algorithms and force constant computations in BSSE-Free direct and conventional SCF approaches. *International Journal of Quantum Chemistry*, 69(2):151–158, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29977; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29977&PLACEBO=IE.pdf`.

Firestone:1994:LMS

[Fir94] R. A. Firestone. Least-motion stepwise $[2+2]$ ketene cycloaddition pathways predict the more hindered cis-Cycloadducts. *International Journal of Quantum Chemistry*, 49(1):21–??, January 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Friis-Jensen:1996:SFA

[FJR96] Britt Friis-Jensen and Sten Rettrup. Spin-free approach for evaluation of electronic matrix elements using character operators of $\updownarrow_\backslash$. *International Journal of Quantum Chemistry*, 60(5):983–991, December 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60670`.

Friis-Jensen:1997:ISC

[FJRS97] Britt Friis-Jensen, Sten Rettrup, and C. R. Sarma. Indexing scheme for classes of $\mathcal{S}_N$; partitions of N. *International Journal of Quantum Chemistry*, 64(4):421–426, September 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42700; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42700&PLACEBO=IE.pdf`.

Fakhreddine:1994:CFA

[FK94] K. Fakhreddine and H. Kobeissi. A “canonical functions” approach to the eigenvalues of a system of two coupled Schrödinger equations. *International Journal of Quantum Chemistry*, 49 (6):773–??, March 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Freund:1998:PRP

[FK98] Lars Freund and Martin Klessinger. Photochemical reaction pathways of ethylene. *International Journal of Quantum Chemistry*, 70(4-5):1023–1028, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75024; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75024&PLACEBO=IE.pdf`.

Fruchtl:1997:IRS

[FKHD97] Herbert A. Früchtl, Rick A. Kendall, Robert J. Harrison, and Kenneth G. Dyall. An implementation of RI-SCF on parallel computers. *International Journal of Quantum Chemistry*, 64(1):63–69, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42666; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42666&PLACEBO=IE.pdf`. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Fakhreddine:1999:BSC

[FKK99] Khaled Fakhreddine, Hafez Kobeissi, and Mahmoud Korek. Bound states of the coupled-channel Schrödinger equation: General eigenvalue function. *International Journal of Quantum Chemistry*, 73(4):325–332, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61000536; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61000536&PLACEBO=IE.pdf`.

Fox:1992:ESB

[FKR92] T. Fox, M. Kotzian, and N. Rosch. On the electronic structure of barrelene-based rigid organic donor-acceptor systems. an INDO model study including solvent effects. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:551–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Florian:1995:WCO

[FL95] J. Florian and J. Leszcynski. What changes occur in vibrational spectra of guanine and cytosine when they form the Watson–Crick base pair? A quantum chemical SCRF HF/6-31 G* study. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):207–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Fu:1996:TSE

[FLF96] Xiao-Yuan Fu, Qing-Ming Li, and De-Cai Fang. Theoretical studies on the elimination of hydrogen fluoride from alkyl fluoride and its substituent effect. *International Journal of Quantum Chemistry*, 57(4):715–719, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60408.

Farantos:1990:CDA

[FLHT90] S. C. Farantos, J. M. Gomez Llorente, O. Hahn, and H. S. Taylor. Classical dynamical analysis of the vibrational spectra for small polyatomic molecules. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:429–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Flock:1995:IHB

[Flo95] M. Flock. Intramolecular hydrogen bonding of d-hydroxypentanoic acid. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:585–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Flocke:1997:SGAd

[Flo97a] N. Flocke. Symmetric group approach to relativistic CI. IV. representations of one-electron spin operators and their products in a symmetric group-adapted basis of N-electron spin functions. *International Journal of Quantum Chemistry*, 61 (5):747–757, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42460; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42460&PLACEBO=IE.pdf.

Flocke:1997:SGAe

[Flo97b] N. Flocke. Symmetric group approach to relativistic CI. IV. Representations of one-electron spin operators and their products in a symmetric group-adapted basis of N-electron spin functions. *International Journal of Quantum Chemistry*, 64 (6):737, September 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42725; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42725&PLACEBO=IE.pdf.

Fetzer:1997:VIP

[FLRV97] Sharon M. Fetzer, Pierre R. Lebreton, Marie-Madelaine Rohmer, and Alain Veillard. Valence ionization potentials of anionic phosphate esters: An ab initio quantum mechanical study. *International Journal of Quantum Chemistry*, 65 (6):1095–1106, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42846; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42846&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on the Application of Fundamental Theory to Problems of Biology and Pharmocolgy*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Flamant:1996:RIE

[FMD+96] I. Flamant, D. H. Mosley, J. Delhalle, J. M. André, and J. G. Fripiat. RHF ab initio electronic and molecular structures of a $(-\mathrm{Be}_2 -)_\infty$ chain. *International Journal of Quantum Chemistry*, 57(5):871–879, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60441.

Flamant:1994:DES

[FMDA94] I. Flamant, D. H. Mosley, M. Deleuze, and J.-M. André. Dependence of the electronic structure on the chain geometry in stereoregular polypropylene: An exploratory theoretical study. *International Journal of Quantum Chemistry. Symposium*, 28: 469–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Fabian:1994:AAL

[FMPJ94] E. San Fabian, F. Moscardo, and J. M. Perez-Jorda. Applicability to atoms of a large set of correlation energy functionals. *International Journal of Quantum Chemistry*, 52(4):1027–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fanelli:1999:TSR

[FMS+99] Francesca Fanelli, Cristina Menziani, Alexander Scheer, Susanna Cotecchia, and Pier G. De Benedetti. Theoretical study on receptor-G protein recognition: New insights into the mechanism of the α1b-adrenergic receptor activation. *International Journal of Quantum Chemistry*, 73 (2):71–83, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003507; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003507&PLACEBO=IE.pdf`. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998*. Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Fritsche:1993:MMA

[FMT93] L. Fritsche, H. Monkhorst, and S. Trickey. In memoriam: Michael Andreas Schluter, 1945–1992. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27: 91–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Ferenczy:1999:QMS

[FNSV99] György G. Ferenczy, Gábor Náray-Szabó, and Péter Várnai. Quantum mechanical study of the hydride shift step in the xylose isomerase catalytic reaction with the fragment self-consistent field method. *International Journal of Quantum Chemistry*, 75(3):215–222, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/65000663/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000663&PLACEBO=IE.pdf`.

Fortunelli:1994:ICI

[For94] A. Fortunelli. Ab initio calculations of isotropic hyperfine coupling constants in -ketoenolyl radicals. *International Journal* *of Quantum Chemistry*, 52(1):97–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Forner:1997:DSP

[För97] Wolfgang Förner. Davydov solitons in proteins. *International Journal of Quantum Chemistry*, 64(3):351–377, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42692; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42692&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Fournier:1994:BAC

[Fou94] R. Fournier. Bonding of acetylene to copper atom, dimer, and trimer. *International Journal of Quantum Chemistry*, 52(4):973–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fantucci:1994:DME

[FP94] P. Fantucci and S. Polezzo. Direct minimization of the energy in density functional theory. *International Journal of Quantum Chemistry*, 52(4):817–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ferrari:1996:SSD

[FP96] Anna Maria Ferrari and Gianfranco Pacchioni. Size and shape dependence of the electrostatic potential in cluster models of the MgO (100) surface. *International Journal of Quantum Chemistry*, 58(3):241–250, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60479.

Flock:1992:ISI

[FR92] M. Flock and M. Ramek. Ab-initio SCF investigation of glycolic acid. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:505–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Flock:1993:BSD

[FR93a] M. Flock and M. Ramek. Basis set dependence of ab-initio calculated vibration frequencies. *International Journal of Quan-*

tum Chemistry. Quantum Chemistry Symposium, 27:331–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Flores:1993:ASO

[FR93b] J. R. Flores and P. Redondo. Accurate second-order correlation energies for Mg and Ar. *International Journal of Quantum Chemistry*, 45(6):563–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Flores-Riveros:1998:GHG

[FR98] A. Flores-Riveros. Generalized Hylleraas–Gaussian basis sets applied to the variational treatment of two-electron atoms. *International Journal of Quantum Chemistry*, 66 (4):287–300, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29865; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29865&PLACEBO=IE.pdf`.

Francisco:1999:ISS

[Fra99] Joseph S. Francisco. An ab initio study of the structures and energetics of CH_3 OCl and CH_3 ClO. *International Journal of Quantum Chemistry*, 73(1):29–35, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55001578; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55001578&PLACEBO=IE.pdf`.

Fritsche:1993:FPAa

[Fri93a] L. Fritsche. A first-principles approach to high-T_c superconductivity I. A consistent one-electron theory of the N-electron problem. *International Journal of Quantum Chemistry*, 48(3): 185–??, November 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fritsche:1993:FPAb

[Fri93b] L. Fritsche. A first-principles approach to High-T_c superconductivity II. the superconducting ground state. *International Journal of Quantum Chemistry*, 48(3):210–??, November 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fortunelli:1993:NIS

[FS93a] A. Fortunelli and O. Salvetti. A numerical integration scheme for the evaluation of correlation energy functionals. *International Journal of Quantum Chemistry*, 47(2):135–??, July 15, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fortunelli:1993:RRE

[FS93b] A. Fortunelli and O. Salvetti. Recurrence relations for the evaluation of electron repulsion integrals over spherical Gaussian functions. *International Journal of Quantum Chemistry*, 48(4): 257–??, November 10, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fortunelli:1994:AIO

[FS94] A. Fortunelli and O. Salvetti. An analysis of the integrand occurring in correlation energy functionals. *International Journal of Quantum Chemistry*, 52(4):705–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fazzio:1995:ESP

[FS95a] A. Fazzio and T. M. Schmidt. Electronic structure of periodically Si-d-doped GaAs. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:203–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Fortunelli:1995:EAI

[FS95b] A. Fortunelli and O. Salvetti. Erratum — an analysis of the integrand occurring in correlation energy functionals. *International Journal of Quantum Chemistry*, 55(6):493–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Frolov:1995:BST

[FS95c] A. M. Frolov and V. H. Smith. On bound states in two-body systems. *International Journal of Quantum Chemistry*, 53(1): 9–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Frolov:1997:EFS

[FS97] Alexei M. Frolov and Vedene H. Smith Jr. Exact finite series for the few-body auxiliary functions. *International Journal of Quantum Chemistry*, 63(1):269–278, May 15, 1997. CODEN

IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42572; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42572&PLACEBO=IE.pdf.

Fujimoto:1999:QTO

[FS99] Hiroshi Fujimoto and Tomohiro Suzuki. Quantum theory in organic chemistry: Electronic structure and chemical reactivity of (π-allyl)palladium complexes. *International Journal of Quantum Chemistry*, 74(6):735–744, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001789; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001789&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Fernandez-Serra:1995:GSS

[FSBS+95] P. Fernandez-Serra, V. Botella, Y. G. Smeyers, A. Galano, and G. Delgado-Barrio. Ground-state and some excited states of Li_2 by the half-projected Hartree–Fock method. *International Journal of Quantum Chemistry*, 54(5):305–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fujimoto:1996:TBC

[FSF96] Hiroshi Fujimoto, Ken Sakata, and Kenichi Fukui. Transient bonds and chemical reactivity of molecules. *International Journal of Quantum Chemistry*, 60(1):401–408, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60602.

Fender:1999:VAI

[FSHC99] Bruce J. Fender, Kurt W. Short, David K. Hahn, and Patrik R. Callis. Vibrational assignments for indole with the aid of ultrasharp phosphorescence spectra. *International Journal of Quantum Chemistry*, 72(4):347–356, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006311; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006311&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Filippetti:1997:HCN

[FSVZ97] A. Filippetti, A. Satta, David Vanderbilt, and W. Zhong. Hardness conservation as a new transferability criterion: Application to fully nonlocal pseudopotentials. *International Journal of Quantum Chemistry*, 61(3):421–427, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42437; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42437&PLACEBO=IE.pdf.

Fang:1995:HBE

[FT95] J.-Y. Fang and C. Thomson. Hydrogen-bonding effects, electrostatic potential, and the antitumor activity of flavone acetic acid and related compounds. I. ab initio studies on the first stable conformations. *International Journal of Quantum Chemistry*, 54(5):313–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fang:1996:HBE

[FT96] Jian-Yun Fang and Colin Thomson. Hydrogen-bonding effects, electrostatic potential, and the antitumor activity of flavone acetic acid and related compounds. II. Ab initio studies on the second stable conformations. *International Journal of Quantum Chemistry*, 60(4):897–909, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60649.

Fang:1997:HBE

[FT97a] Jian-Yun Fang and Colin Thomson. Hydrogen-bonding effects, electrostatic potential, and the antitumor activity of flavone acetic acid and related compounds. III. Ab initio studies on the conformation space. *International Journal of Quantum Chemistry*, 62(1):97–113, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42483; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42483&PLACEBO=IE.pdf.

Filatov:1997:NCE

[FT97b] Michael Filatov and Walter Thiel. A nonlocal correlation energy density functional from a Coulomb hole model. *International Journal of Quantum Chemistry*, 62(6):603–616,

???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42545; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42545&PLACEBO=IE.pdf.

Fuentealba:1994:CEF

[Fue94] P. Fuentealba. A correlation-energy functional from a correlation-factor model. *International Journal of Quantum Chemistry*, 49(4):549–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuentealba:1998:MVE

[Fue98] P. Fuentealba. A modified version of the electron localization function (ELF). *International Journal of Quantum Chemistry*, 69(4):559–565, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30010; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30010&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Fulde:1997:SDI

[FUI97] Peter Fulde, Patrick Unger, and Jun-Ichi Igarashi. Spectral densities of infinite systems with strong electron correlations. *International Journal of Quantum Chemistry*, 63(3):645–653, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42626; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42626&PLACEBO=IE.pdf.

Fukui:1995:UNH

[Fuk95] K. Fukui. The uniqueness of nature and human beings. *International Journal of Quantum Chemistry*, 53(1):119–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fisier:1996:CSR

[FV96] Jirîí Fisîer and Jan Vojtík. CI study of rovibrational dependence of nuclear quadrupole coupling constants of all isotopic variants of OH^+ in the $X^3\Sigma^-$ state. *International Journal of Quantum*

Chemistry, 57(3):441–448, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60381.

Ford:1992:PCCa

[FW92a] G. P. Ford and B. Wang. Prototropic changes in cationic base-pair adducts. I guanine protonation. *International Journal of Quantum Chemistry*, 44(4):587–??, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ford:1992:PCCb

[FW92b] G. P. Ford and B. Wang. Prototropic changes in cationic Base-Pair adducts. II. guanine methylation. *International Journal of Quantum Chemistry*, 44(4):605–??, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Forni:1994:CHC

[FWBT94] A. Forni, G. Wiesenekker, E. J. Baerends, and G. F. Tantardini. The chemisorption of hydrogen on cu(111): A dynamical study. *International Journal of Quantum Chemistry*, 52(4):1067–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fluekiger:1993:CSD

[FWC+93] P. Fluekiger, J. Weber, R. Chiarelli, A. Rassat, and Y. Ellinger. Chirality and spin density: Ab initio and density functional approaches. *International Journal of Quantum Chemistry*, 45 (6):649–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fink:1997:ICM

[FWS97] K. Fink, C. Wang, and V. Staemmler. Ab initio calculations of the magnetic exchange coupling in sulfur-bridged binuclear Ni(II) complexes. *International Journal of Quantum Chemistry*, 65(5):633–641, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42794; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42794&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Fushman:1996:BDP

[FWT+96] David Fushman, Rüdiger Weisemann, Harald Thüring, Oliver Ohlenschläger, and Heinz Rüterjans. Backbone dynamics of proteins studied by two-dimensional heteronuclear NMR spectroscopy and molecular dynamics simulations. *International Journal of Quantum Chemistry*, 59(4):291–300, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60549`.

Feng:1997:TSP

[FWZ97] Wenlin Feng, Yan Wang, and Shaowen Zhang. Theoretical study on the pyrolysis mechanism and kinetics of β-hydroxyketones. *International Journal of Quantum Chemistry*, 62(3):297–302, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42515; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42515&PLACEBO=IE.pdf`.

Fang:1995:TSP

[FY95] W-H Fang and X.-Z. You. Theoretical study on the photodecarboxylation reaction of methacrylic acid in the gas phase. *International Journal of Quantum Chemistry*, 56(1):43–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Filatov:1992:NMN

[FZZ92] M. J. Filatov, I. L. Zilberberg, and G. M. Zhidomirov. NDDO/MC: A new semiempirical SCF MO method for transition metal complexes. *International Journal of Quantum Chemistry*, 44(4):565–585, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gonzalez:1997:CRA

[GAdAC97] J. A. González, G. A. Aucar, M. C. Ruiz de Azúa, and R. H. Contreras. Cloppa RPA-AM1 analysis of the anisotropy of NMR ^{1}J(XY) coupling tensors in Me_3XY compounds (X = ^{13}C, ^{29}Si, ^{119}Sn, ^{207}Pb; Y = ^{19}F, ^{35}Cl). *International Journal of Quantum Chemistry*, 61(5):823–833, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL

http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42466; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42466&PLACEBO=IE.pdf.

Gallup:1972:EPM

[Gal72a] G. A. Gallup. The N-electron problem and matrices representing the symmetric groups. *International Journal of Quantum Chemistry*, 6(??):761–778, ?? 1972. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gallup:1972:VBC

[Gal72b] G. A. Gallup. Valence-bond calculations and matrix elements between two tableau functions of non-orthogonal orbitals. *International Journal of Quantum Chemistry*, 6(??):899–910, ?? 1972. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Galasso:1996:TSS

[Gal96] V. Galasso. Theoretical study of spectroscopic properties of bicyclobutane, tricyclopentane, tricyclohexane, and octabisvalene. *International Journal of Quantum Chemistry*, 57(4):587–594, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60423.

Galasso:1998:TSS

[Gal98] V. Galasso. Theoretical study of structure and NMR properties of the μ-hydrido-bridged cyclodecyl cation and related systems. *International Journal of Quantum Chemistry*, 70(2):313–320, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74999; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74999&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Gao:1993:SEP

[Gao93] J. Gao. Solvent effect on the potential surface of the proton transfer in $[H_3\,N–H–NH_3]^+$. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:491–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Goscinski:1971:PAP

[GB71] O. Goscinski and E. Brändas. Padé approximants to physical properties via inner projections. *International Journal of Quantum Chemistry*, 5(??):131–156, ?? 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Graovac:1990:EQI

[GB90] A. Graovac and D. Babić. The evaluation of quantum indices by the method of moments. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:251–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Gauntes:1994:OCC

[GBJMA94] R. Gauntes, F. Borondo, C. Jaffe, and S. Miret-Artes. The onset of classical chaos in atom-surface scattering. *International Journal of Quantum Chemistry*, 52(2):515–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Glukhovtsev:1997:HLC

[GBL97] Mikhail N. Glukhovtsev, Robert D. Bach, and Sergei Laiter. High-level computational study on the thermochemistry of saturated and unsaturated three- and four-membered nitrogen and phosphorus rings. *International Journal of Quantum Chemistry*, 62(4):373–384, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42524; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42524&PLACEBO=IE.pdf`.

Glossman:1994:NEK

[GBRA94] M. D. Glossman, L. C. Balbas, A. Rubio, and J. A. Alonso. Nonlocal exchange and kinetic energy density functionals with correct asymptotic behavior for electronic systems. *International Journal of Quantum Chemistry*, 49(3):171–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gianturco:1993:SDE

[GBS93a] F. A. Gianturco, E. Buonomo, and S. Serna. Selective dynamic energy transfers in proton collisions with hydrogen fluoride. *International Journal of Quantum Chemistry*, 47(5):375–??, 1993.

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

Giaturco:1993:IPE

[GBS+93b] F. A. Giaturco, E. Buonomo, E. Semprini, F. Stefani, and A. Palma. Ab initio potential energy function for the dynamics of the fluoronium ion. *International Journal of Quantum Chemistry*, 47(5):335–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grozema:1999:SDC

[GBS99] Ferdinand C. Grozema, Yuri A. Berlin, and Laurens D. A. Siebbeles. Sequence-dependent charge transfer in donor-DNA-acceptor systems: A theoretical study. *International Journal of Quantum Chemistry*, 75(6):1009–1016, December 20, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004789/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004789&PLACEBO=IE.pdf.

Gantchev:1993:SEM

[GBVM93] T. G. Gantchev, F. Beaudry, J. E. Van Lierg, and A. G. Michel. Semi-empirical molecular orbital studies of porphine and phthalocyanine derivatives, to simulate their intermolecular interactions. *International Journal of Quantum Chemistry*, 46(1):191–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:1994:ILD

[GD94] S. K. Ghosh and B. M. Deb. Improved local density functional approach for atomic systems. *International Journal of Quantum Chemistry*, 51(2):79–??, July 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gianturco:1996:SSR

[GD96] F. A. Gianturco and M. P. De Lara-Castells. Stability and structure of rare-gas ionic clusters using density functional methods: A study of helium clusters. *International Journal of Quantum Chemistry*, 60(1):593–608, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60622.

Galabov:1998:CIT

[GDID98] Boris Galabov, Todor Dudev, Sonia Ilieva, and James R. Durig. Creation of intensity theory in vibrational spectroscopy: Key role of ab initio quantum mechanical calculations. *International Journal of Quantum Chemistry*, 70 (2):331–339, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75001; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75001&PLACEBO=IE.pdf`. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Guan:1997:LAA

[GDYY97] Daren Guan, Shiliang Ding, Benhui Yang, and Xizhang Yi. Lie algebraic approach to the collinear collisions between two diatomic molecules. *International Journal of Quantum Chemistry*, 65(2):159–165, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42753; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42753&PLACEBO=IE.pdf`.

GarciadelaVega:1994:SBI

[GF94] J. M. Garcia de la Vega and E. San Fabian. Symmetry breaking and its influence on the correlation energy for CF0+4 and CF020-3 ions. *International Journal of Quantum Chemistry*, 52(4):947–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gioia:1999:IIS

[GFGB99] L. De Gioia, P. Fantucci, B. Guigliarelli, and P. Bertrand. Ab initio investigation of the structural and electronic differences between active-site models of [NiFe] and [NiFeSe] hydrogenases. *International Journal of Quantum Chemistry*, 73(2):187–195, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003516; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003516&PLACEBO=IE.pdf`. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba*

(Italy), September 8-11, 1998. Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Grosch:1994:GSP

[GFRR94] G. H. Grosch, B. Freytag, K.-J. Range, and U. Roessler. Ground-state properties of $\mathrm{Cd}_x\mathrm{Sn}1-x\mathrm{Te}$: The role of d-electrons. *International Journal of Quantum Chemistry*, 52(4): 919–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ge:1999:DST

[GFY+99] Maofa Ge, Jikang Feng, Cheng Yang, Zhiru Li, and Chi-achung Sun. DFT studies on $\mathrm{Ti}_n\mathrm{C}_{2n}$ ($n = 1--6$) clusters. *International Journal of Quantum Chemistry*, 71(4): 313–318, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10049345; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10049345&PLACEBO=IE.pdf.

Ghanty:1997:DFS

[GG97a] Tapan K. Ghanty and Swapan K. Ghosh. Density functional study of the relationship between energy, hardness, and polarizability of molecules in nonequilibrium situations. *International Journal of Quantum Chemistry*, 63 (5):917–926, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42642; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42642&PLACEBO=IE.pdf.

Grabo:1997:OEP

[GG97b] T. Grabo and E. K. U. Gross. The optimized effective potential method of density functional theory: Applications to atomic and molecular systems. *International Journal of Quantum Chemistry*, 64(1):95–110, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42658; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42658&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Grigera:1994:MDS

[GGHP94] J. R. Grigera, T. S. Grigera, E. I. Howard, and A. Podjarny. Molecular dynamics simulation of crystal water with X-ray constraints. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21: 109–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Goh:1998:TLS

[GGSA98] Sor Koon Goh, Roger T. Gallant, and Alain St-Amant. Toward linear scaling with fitted exchange-correlation terms in the LCGTO-DF method via a divide-and-conquer approach. *International Journal of Quantum Chemistry*, 69 (3):405–421, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29995; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29995&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Goscinski:1996:MEM

[GH96a] Osvaldo Goscinski and Lotten Hägg. The maximum entropy method and relaxation for multiple collisions involving highly charged ions. *International Journal of Quantum Chemistry*, 58(6):689–698, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60509.

Grein:1996:SFTa

[GH96b] F. Grein and M. R. J. Hachey. The a, a^* state in formaldehyde and thioformaldehyde. *International Journal of Quantum Chemistry*, 60(7):449–??, 1996. CODEN IJQCB2.

Grein:1996:SFTb

[GH96c] F. Grein and M. R. J. Hachey. The π, π^* state in formaldehyde and thioformaldehyde. *International Journal of Quantum Chemistry*, 60(7):1661–1671, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60727.

Grein:1996:SFTc

[GH96d] F. Grein and M. R. J. Hachey. The π, π^* state in formaldehyde and thioformaldehyde. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):449–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Gnanakaran:1999:EVC

[GH99] S. Gnanakaran and R. M. Hochstrasser. Effect of vibrational coherence on rotational dynamics in solution. *International Journal of Quantum Chemistry*, 72(4):451–462, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006322; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006322&PLACEBO=IE.pdf`. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Gkoutos:1999:EDA

[GHB+99] George V. Gkoutos, Christopher Higgs, Robert P. Bywater, Paul R. Gouldson, and Christopher A. Reynolds. Evidence for dimerization in the β_2-adrenergic receptor from the evolutionary trace method. *International Journal of Quantum Chemistry*, 74(3):371–379, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62004767; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62004767&PLACEBO=IE.pdf`. Special Issue: *Biophysics Quarterly*.

Ghosh:1994:EHS

[Gho94] S. K. Ghosh. Electronegativity, hardness, and a semiempirical density functional theory of chemical binding. *International Journal of Quantum Chemistry*, 49(3):239–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghose:1995:SRE

[Gho95] K. B. Ghose. Stationary response with exponential transformation: A perturbative analysis for molecular static properties. *International Journal of Quantum Chemistry*, 53(3):275–??, February 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guseinov:1996:EOI

[GİA96] I. I. Guseinov, Aslan İli·k, and S. I. Allahverdiyev. On the evaluation of overlap integrals with the same screening parameters of Slater-type orbitals using binomial coefficients. *International Journal of Quantum Chemistry*, 60(2):637–640, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60630`.

Gineityte:1995:IHE

[Gin95] V. Gineityte. Interpretation of the high-energy band within the photoelectron spectra of alkanes both in terms of appropriate orbitals and on the basis of chemical structure. *International Journal of Quantum Chemistry*, 53(2):245–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gineityte:1996:AWS

[Gin96a] V. Gineityte. An alternative way of solving secular equations for the Hamiltonian matrices of regular quasi-one-dimensional systems. *International Journal of Quantum Chemistry*, 60(3):717–729, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60639`.

Gineityte:1996:SPC

[Gin96b] V. Gineityte. Secular polynomials for chemical graphs of alkanes in terms of atoms and bonds and their spectral properties. *International Journal of Quantum Chemistry*, 60(3):743–752, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60641`.

Gineityte:1997:IEB

[Gin97] V. Gineityte. Interpretation of energy bands of polyethylene in terms of effective interactions between first- and second-neighboring CH_2 groups. *International Journal of Quantum Chemistry*, 64(4):481–494, September 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42697`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42697&PLACEBO=IE.pdf`.

Gineityte:1998:BDP

[Gin98] V. Gineityte. Block diagonalization problem for a Fockian matrix of molecule and its solution by means of noncommutative Rayleigh–Schrödinger perturbation theory. *International Journal of Quantum Chemistry*, 68(2):119–127, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29931; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29931&PLACEBO=IE.pdf.

Gineityte:1999:MFN

[Gin99] V. Gineityte. The matrix form of the noncanonical theory of molecular orbitals. *International Journal of Quantum Chemistry*, 72(6):559–570, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=50000014; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=50000014&PLACEBO=IE.pdf.

Gerwens:1995:MMM

[GJ95] H. Gerwens and K. Jug. Modeling of the mutual molecular polarization with an electronegativity equalization approach. *International Journal of Quantum Chemistry*, 56(5):563–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grand:1997:CSD

[GJDD97] A. Grand, F. Jolibois, J. P. Denis, and J. Delhalle. Comparative study of DFT (LSD-CGA) and RHF molecular structures of quinoid and aromatic model systems for head-to-tail electroactive polymers. *International Journal of Quantum Chemistry*, 61(4):689–697, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42441; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42441&PLACEBO=IE.pdf.

Gomez-Jeria:1999:QCS

[GJLA99] Juan Sebastian Gómez-Jeria and Luis Lagos-Arancibia. Quantum-chemical structure-affinity studies on kynurenic acid derivatives as gly/NMDA receptor ligands. *International Journal of Quantum Chemistry*, 71(6):505–511, ???? 1999. CODEN

IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=15000349; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=15000349&PLACEBO=IE.pdf.

Gomez-Jeria:1997:EME

[GJOV97] Juan Sebastián Gómez-Jeria and Mario Ojeda-Vergara. Electrostatic medium effects and formal quantum structure-activity relationships in apomorphines interacting with D_1 and D_2 dopamine receptors. *International Journal of Quantum Chemistry*, 61(6):997–1002, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42472; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42472&PLACEBO=IE.pdf.

Gill:1992:IPH

[GJPF92] P. M. W. Gill, B. G. Johnson, J. A. Pople, and M. J. Frisch. An investigation of the performance of a hybrid of Hartree–Fock and density functional theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:319–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Gersdorf:1997:CEH

[GJPZ97] Peter Gersdorf, Walter John, John P. Perdew, and Paul Ziesche. Correlation entropy of the H_2 molecule. *International Journal of Quantum Chemistry*, 61(6):935–941, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42477; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42477&PLACEBO=IE.pdf.

Gross:1991:DFT

[GK91] E. K. U. Gross and Stefan Kurth. Density-functional theory of the superconducting state. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:289–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Gilmore:1997:AFD

[GKKA97] D. W. Gilmore, P. M. Kozlowski, D. B. Kinghorn, and L. Adamowicz. Analytic first derivatives for explicitly correlated, multicenter, Gaussian geminals. *International Journal* *of Quantum Chemistry*, 63(5):991–999, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42648; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42648&PLACEBO=IE.pdf.

Gal:1996:PSC

[GKKM96] Jean-François Gal, Ilmar Koppel, Riho Kurg, and Pierre-Charles Maria. PM3 semiempirical calculations of lithium-cation and proton affinities for XYZPO and $XYSO_2$ compounds. *International Journal of Quantum Chemistry*, 59(5): 409–420, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60559.

Gurskii:1999:GSP

[GKS99] L. I. Gurskiĭ, L. I. Komarov, and A. M. Solodukhin. Group of symmetry of the periodic system of chemical elements. *International Journal of Quantum Chemistry*, 72 (5):499–508, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006352; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006352&PLACEBO=IE.pdf.

Godin:1992:CMT

[GL92] T. J. Godin and J. P. LaFemina. Comparison of MNDO to tight-binding, total energy methods for surface atomic structure determination: Aluminum phosphide (110). *International Journal of Quantum Chemistry*, 44(4):533–542, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gadomski:1994:SRC

[GL94] A. Gadomski and J. Luczka. Some remarks concerning spherulitic growth. *International Journal of Quantum Chemistry*, 52(2):301–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gorling:1995:DIF

[GL95] A. Gorling and M. Levy. DFT ionization formulas and a DFT perturbation theory for exchange and correlation, through adiabatic connection. *International Journal of Quantum Chem-*

istry. Quantum Chemistry Symposium, 29:93–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Guo:1996:HQCa

[GL96a] H. Guo and L. Liu. Hybrid quantum/classical studies of photodissociation and recombination of I_2(A) in rare gas matrices: A linear chain model. *International Journal of Quantum Chemistry*, 60(7):267–??, 1996. CODEN IJQCB2.

Guo:1996:HQCc

[GL96b] H. Guo and L. Liu. Hybrid quantum/classical studies of photodissociation and recombination of I_2(A) in rare gas matrices: A linear chain model. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):267–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Guo:1996:HQCb

[GL96c] Hua Guo and Li Liu. Hybrid quantum/classical studies of photodissociation and recombination of $I_2(A)$ in rare gas matrices: A linear chain model. *International Journal of Quantum Chemistry*, 60(7):1479–1486, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60706`.

Gorb:1997:IPG

[GL97] Leonid Gorb and Jerzy Leszczynski. Ab initio prediction of the geometry and IR frequencies of the mono- and dihydrated complexes of the oxo-amino-tautomers of guanine. *International Journal of Quantum Chemistry*, 65(5): 759–765, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42809; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42809&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Gorb:1998:IPT

[GL98] Leonid Gorb and Jerzy Leszczynski. Intramolecular proton transfer in monohydrated tautomers of cytosine: An ab initio post-Hartree–Fock study. *International Journal of*

Quantum Chemistry, 70(4-5):855–862, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75063; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75063&PLACEBO=IE.pdf.

Gerratt:1999:SCW

[GL99] J. Gerratt and W. N. Lipscomb. Spin-coupled wave functions for atoms and molecules. *International Journal of Quantum Chemistry*, 74(2):83–85, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003353; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003353&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Grochowski:1996:DFB

[GLBM96] P. Grochowski, B. Lesyng, P. Bala, and J. A. McCammon. Density functional based parametrization of a valence bond method and its applications in quantum-classical molecular dynamics simulations of enzymatic reactions. *International Journal of Quantum Chemistry*, 60(6):1143–1164, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60680.

Gutman:1994:NSM

[GLLY94] I. Gutman, S.-L. Lee, Y.-L. Luo, and Y.-N. Yeh. Net signs of molecular graphs: Dependence of molecular structure. *International Journal of Quantum Chemistry*, 49(2):87–??, January 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grassi:1998:ECE

[GLMP98] A. Grassi, G. M. Lombardo, N. H. March, and R. Pucci. $1/Z$ expansion, correlation energy, and Shannon entropy of heavy atoms in nonrelativistic limit. *International Journal of Quantum Chemistry*, 69(6):721–726, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74989; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74989&PLACEBO=IE.pdf.

GarciadelaVega:1994:OES

[GM94] J. M. Garcia de la Vega and B. Miguel. Orbitals expanded in Slater functions with single-exponent by shell and by subshell. *International Journal of Quantum Chemistry*, 51(6):397–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gotoh:1995:MCA

[GMI95] M. Gotoh, K. Mori, and R. Itoh. Method of computer algebraic calculation of the matrix elements in the second quantization language. *International Journal of Quantum Chemistry*, 56(3): 163–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guihery:1997:UCB

[GMMH97] Nathalie Guihery, Jean-Paul Malrieu, Daniel Maynau, and Klaus Handrick. Unexpected CASSCF bistability phenomenon. *International Journal of Quantum Chemistry*, 61 (1):45–54, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42384; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42384&PLACEBO=IE.pdf`.

Goursot:1993:GSM

[GMR+93] A. Goursot, F. Mele, N. Russo, D. R. Salahub, and M. Toscano. Geometrical, spectroscopic, and magnetic properties of an oxygen atom adsorbed on the Ni(100) surface. *International Journal of Quantum Chemistry*, 48(5):277–??, December 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

GarciadelaVega:1997:DFC

[GMS97] J. M. Garcia De La Vega, B. Miguel, and E. San Fabian. Density functional calculations on Jahn–Teller effect of tetrachloromethane cation. *International Journal of Quantum Chemistry*, 61(3):533–540, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42423; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42423&PLACEBO=IE.pdf`.

Graovac:1973:SOM

[GMZ73] A. Graovac, H. J. Monkhorst, and T. Zivkovic. Slater orbital molecular integrals with numerical Fourier transform methods. I. (coplanar) multicenter exchange integrals over 1s orbitals. *International Journal of Quantum Chemistry*, 7(??):233–251, ?? 1973. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guimaraes:1998:PSN

[GNA98] Cristiano Ruch Werneck Guimarães, Joaquim Delphino Da Motta Neto, and Ricardo Bicca De Alencastro. Phytochrome structure: A new methodological approach. *International Journal of Quantum Chemistry*, 70(6):1145–1157, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75082; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75082&PLACEBO=IE.pdf.

Godby:1990:ECD

[GNF90] R. W. Godby, R. J. Needs, and B. Farid. Exchange and correlation in density-functional theory and quasiparticle theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:681–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Goscinski:1968:CEP

[GÖ68] O. Goscinski and Y. Öhrn. Coupling of equivalent particles in A field of given symmetry. *International Journal of Quantum Chemistry*, 2(??):845–??, ?? 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guseinov:1998:COI

[GOAY98] I. I. Guseinov, A. Ozmen, U. Atav, and H. Yuksel. Computation of overlap integrals over Slater-type orbitals using auxiliary functions. *International Journal of Quantum Chemistry*, 67(4):199–204, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29900; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29900&PLACEBO=IE.pdf.

Gorling:1998:EEK

[Gör98] Andreas Görling. Exact exchange kernel for time-dependent density-functional theory. *International Journal of Quantum Chemistry*, 69(3):265–277, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30001; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30001&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Galvez:1995:PAF

[GP95] F. J. Galvez and I. Porras. Properties of the atomic form factor: Applications and shell structure. *International Journal of Quantum Chemistry*, 56(3):157–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:1997:ESD

[GP97] H. Guo and J. Paldus. Estimates of the structure and dimerization energy of polyacetylene from ab initio calculations on finite polyenes. *International Journal of Quantum Chemistry*, 63(2):345–360, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42606; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42606&PLACEBO=IE.pdf.

Gould:1994:QSP

[GPC94] M. D. Gould, J. Paldus, and J. Cizek. Quasi-spin and the pseudo-orthogonal group in the Hubbard model. *International Journal of Quantum Chemistry*, 50(3):207–??, April 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goursot:1994:NGD

[GPD94] A. Goursot, I. Papai, and C. A. Daul. Numerical grids for density functional calculations of molecular properties. *International Journal of Quantum Chemistry*, 52(4):799–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garza:1994:LHR

[GR94] J. Garza and J. Robles. Local hardness revisited: Definition and the spin-polarized Kohn–Sham formulation of density functional theory. *International Journal of Quantum Chemistry*, 49 (3):159–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gauss:1995:CMC

[GR95a] J. Gauss and K. Ruud. On the convergence of MBPT and cc nuclear magnetic shielding constants of BH towards the full CI limit. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:437–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Gdanitz:1995:FMR

[GR95b] R. J. Gdanitz and R. Rohse. A formulation of multiple-reference CI with terms linear in the interelectronic distances. II. an alternative Ansatz. *International Journal of Quantum Chemistry*, 55(2):147–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gazquez:1996:CGC

[GR96a] José L. Gázquez and Juvencio Robles. On the conjoint gradient correction to the Hartree–Fock kinetic and exchange energy density functionals. *International Journal of Quantum Chemistry*, 57(1):3–6, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60346`.

Gdanitz:1996:FMR

[GR96b] R. J. Gdanitz and R. Rohse. A formulation of multiple-reference CI with terms linear in the interelectronic distances. II. an alternative ansatz. *International Journal of Quantum Chemistry*, 59(6):505–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Graves:1997:GDE

[Gra97a] John L. Graves. Generalized double exponential potential functions for diatomic molecules. *International Journal of Quantum Chemistry*, 65(1):1–8, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42735;`

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42735&PLACEBO=IE.pdf.

Grayson:1997:SES

[Gra97b] Martin Grayson. Substitution effects by SCF and Hückel theory. *International Journal of Quantum Chemistry*, 61(6): 919–927, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42475; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42475&PLACEBO=IE.pdf.

Glossman:1993:NAE

[GRB+93] M. D. Glossman, A. Rubio, L. C. Balbas, J. A. Alonso, and Ll Serra. Nonclonal approximation to the exchange and kinetic energy functionals: Application to metallic clusters. *International Journal of Quantum Chemistry*, 45(4):333–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Glossman:1992:NEK

[GRBA92] M. D. Glossman, A. Rubio, L. C. Balbas, and J. A. Alonso. Nonlocal exchange and kinetic-energy density functionals for electronic systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:347–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Green:1994:PCK

[Gre94] W. H. Green. Predictive chemical kinetics: Density functional and Hartree–Fock calculations on free-radical reaction transition states. *International Journal of Quantum Chemistry*, 52 (4):837–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gregory:1998:BRC

[Gre98] Frederick Gregory. Book review: *The conscious mind: In search of a fundamental theory*, by David J. Chalmers. *International Journal of Quantum Chemistry*, 66(1):107–108, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29842; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29842&PLACEBO=IE.pdf.

Guo:1996:AEC

[GRK96] Xiaofeng Guo, M. Randić, and D. J. Klein. Analytical expressions for the count of LM-Conjugated circuits of benzenoid hydrocarbons. *International Journal of Quantum Chemistry*, 60(5):943–958, December 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60661.

Gianinetti:1996:MRE

[GRT96] E. Gianinetti, M. Raimondi, and E. Tornaghi. Modification of the Roothaan equations to exclude BSSE from molecular interaction calculations. *International Journal of Quantum Chemistry*, 60(1):157–166, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60578.

Gorb:1996:MLSa

[GRTR96a] L. G. Gorb, J.-L. Rivail, V. Thery, and D. Rinaldi. Modification of the local self-consistent field method for modeling surface reactivity of covalent solids. *International Journal of Quantum Chemistry*, 60(7):313–??, 1996. CODEN IJQCB2.

Gorb:1996:MLSb

[GRTR96b] L. G. Gorb, J.-L. Rivail, V. Thery, and D. Rinaldi. Modification of the local self-consistent field method for modeling surface reactivity of covalent solids. *International Journal of Quantum Chemistry*, 60(7):1525–1536, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60712.

Gorb:1996:MLSc

[GRTR96c] L. G. Gorb, J.-L. Rivail, V. Thery, and D. Rinaldi. Modification of the local self-consistent field method for modeling surface reactivity of covalent solids. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??): 313–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Gershgorn:1968:APT

[GS68] Z. Gershgorn and I. Shavitt. An application of perturbation theory ideas in configuration interaction calculations. *International Journal of Quantum Chemistry*, 2(??):751–??, ?? 1968.

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

Garcia-Sucre:1992:CRV

[GS92] M. Garcia-Sucre. Complex regional virial relations in molecules. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:207–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Glukhovtsev:1993:MOC

[GS93] M. N. Glukhovtsev and P. Von Rague Schleyer. The N_4 molecule has an open-chain triplet C_2h structure. *International Journal of Quantum Chemistry*, 46(1):119–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Glyde:1997:ELS

[GS97a] H. R. Glyde and M. S. Sullivan. Excitations in liquid and solid helium. *International Journal of Quantum Chemistry*, 62(3): 329–??, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gonzales:1997:CCC

[GS97b] Nick Gonzales and Jack Simons. ^{13}C carbonyl chemical shielding tensors: Comparing SCF, MBPT (2), and DFT predictions to experiment. *International Journal of Quantum Chemistry*, 63(4):875–894, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42638; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42638&PLACEBO=IE.pdf`.

Ghosh:1997:UDF

[GSD97] Swapan K. Ghosh, Alok Samanta, and B. M. Deb. Universal density functional approach to the calculation of correlation energies of atoms. *International Journal of Quantum Chemistry*, 62(5):461–465, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42533; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42533&PLACEBO=IE.pdf`.

Gutowski:1997:EDB

[GSJS97] Maciej Gutowski, Piotr Skurski, Kenneth D. Jordan, and Jack Simons. Energies of dipole-bound anionic states. *International Journal of Quantum Chemistry*, 64(2):183–191, August 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42680; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42680&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Gutle:1999:CEC

[GSKC99] Claudine Gutle, Andreas Savin, Joseph B. Krieger, and Jiqiang Chen. Correlation energy contributions from low-lying states to density functionals based on an electron gas with a gap. *International Journal of Quantum Chemistry*, 75(4–5):885–888, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004984/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004984&PLACEBO=IE.pdf.

Garcia-Sucre:1990:RVR

[GSM90] M. Garcia-Sucre and V. Mujica. Regional virial relations for arbitrary subsystems of particles of a molecule with nuclear motion quantum mechanically described. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24: 375–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Guarnieri:1998:SCP

[GSM98] F. Guarnieri, A. B. Schmidt, and E. L. Mehler. Screened Coulomb potential based implicit solvent model: Formulation and parameter development. *International Journal of Quantum Chemistry*, 69(1):57–64, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29973; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29973&PLACEBO=IE.pdf.

Garcia-Sucre:1993:ICE

[GSPSM93] M. Garcia-Sucre, J. L. Paz, E. Squitieri, and V. Mujica. Intramolecular coupling effect in the refractive index for a simple three-level model of molecules diluted in water. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:699–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Gilch:1996:CSF

[GSSD+96] H. Gilch, R. Schweitzer-Stenner, W. Dreybrodt, M. Leone, A. Cupane, and L. Cordone. Conformational substates of the Fe_2^+-His F_8 linkage in deoxymyoglobin and hemoglobin probed in parallel by the Raman band of the Fe-His stretching vibration and the near-infrared absorption band III. *International Journal of Quantum Chemistry*, 59(4):301–313, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60550.

Goodfriend:1993:MCU

[GT93] P. L. Goodfriend and S. I. Tsonchev. Molecular calculations using space-restricted basis functions. *International Journal of Quantum Chemistry*, 48(6):367–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grebneva:1997:CLV

[GT97] H. A. Grebneva and K. B. Tolpygo. Crystalline and local vibrations of paired bases in poly(dG)-poly(dC) interacting with the $h-b-1$ hydrogen bond. *International Journal of Quantum Chemistry*, 62(1):115–124, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42484; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42484&PLACEBO=IE.pdf.

Guiasu:1998:TWF

[Gui98] Silviu Guiasu. Trial wave functions induced by the minimum mean deviation from statistical equilibrium. *International Journal of Quantum Chemistry*, 68(3):175–190, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29938; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29938&PLACEBO=IE.pdf.

Gurin:1999:QCQ

[Gur99] V. S. Gurin. Quantum chemistry of quantum size-effects in semiconductors: Small clusters electronic structure calculations. *International Journal of Quantum Chemistry*, 71 (4):337–341, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10049348; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10049348&PLACEBO=IE.pdf.

Guseinov:1998:AEM

[Gus98] I. I. Guseinov. Analytical evaluation of molecular electric and magnetic multipole moment integrals over Slater-type orbitals. *International Journal of Quantum Chemistry*, 68 (3):145–150, June 5, 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29935; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29935&PLACEBO=IE.pdf.

Gutman:1999:HRT

[Gut99a] Ivan Gutman. On the Hall rule in the theory of benzenoid hydrocarbons. *International Journal of Quantum Chemistry*, 74(6):627–632, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001779; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001779&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Gutowski:1999:FPD

[Gut99b] Maciej Gutowski. Favorable performance of the DFT methods in predicting the minimum-energy structure of the lowest triplet state of WF_4. *International Journal of Quantum Chemistry*, 73(4):369–375, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61000533; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61000533&PLACEBO=IE.pdf.

Gritsenko:1996:OMEa

[GVB96a] O. V. Gritsenko, R. Van Leeuwen, and E. J. Baerends. On the optimal mixing of the exchange energy and the electron-electron interaction part of the exchange-correlation energy. *International Journal of Quantum Chemistry*, 60(7):163–??, 1996. CODEN IJQCB2.

Gritsenko:1996:OMEc

[GVB96b] O. V. Gritsenko, R. Van Leeuwen, and E. J. Baerends. On the optimal mixing of the exchange energy and the electron-electron interaction part of the exchange-correlation energy. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):163–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Gritsenko:1996:OMEb

[GVB96c] Oleg V. Gritsenko, Robert Van Leeuwen, and Evert Jan Baerends. On the optimal mixing of the exchange energy and the electron-electron interaction part of the exchange-correlation energy. *International Journal of Quantum Chemistry*, 60(7):1375–1384, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60695`.

Gritsenko:1997:DAL

[GVB97] Oleg V. Gritsenko, Robert Van Leeuwen, and Evert Jan Baerends. Direct approximation of the long- and short-range components of the exchange-correlation Kohn–Sham potential. *International Journal of Quantum Chemistry*, 61 (2):231–243, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42404; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42404&PLACEBO=IE.pdf`.

Gianinetti:1996:OSC

[GVC96] Ermanno Gianinetti, Ida Vandoni, and Sergio Colombo. Optimization of a spin-coupled wave function built with partially orthogonalized orbitals. *International Journal of Quantum Chemistry*, 57(3):369–375, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60374`.

Garcia-Viloca:1999:MDS

[GVK99] Mireia Garcia-Viloca and Peter A. Kollman. Molecular dynamics simulations can reproduce the subtle differences in NADP and NHDP binding to isocitrate dehydrogenase. *International Journal of Quantum Chemistry*, 75(3):231–243, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000665/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000665&PLACEBO=IE.pdf.

Gritsenko:1996:SOE

[GvLB96] Oleg Gritsenko, Robert van Leeuwen, and Evert Jan Baerends. Structure of the optimized effective Kohn–Sham exchange potential and its gradient approximations. *International Journal of Quantum Chemistry*, 57(1):17–33, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60353.

Georges:1990:SEA

[GVV+90] G. Georges, D. P. Vercauteren, D. J. Vanderveken, R. Horion, G. Evrard, J. G. Fripiat, J.-M. André, and F. Durant. Structural and electronic analysis of peripheral benzodiazepine ligands: Description of the pharmacophoric elements for their receptors. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17: 1–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Guiang:1998:QDL

[GW98a] Chona S. Guiang and Robert E. Wyatt. Quantum dynamics with Lanczos subspace propagation: Application to a laser-driven molecular system. *International Journal of Quantum Chemistry*, 67(5):273–285, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29906; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29906&PLACEBO=IE.pdf.

Guiang:1998:TEW

[GW98b] Chona S. Guiang and Robert E. Wyatt. Torsional eigenvalues of the water trimer on several ab initio potential surfaces. *International Journal of Quantum Chemistry*, 68 (4):233–252, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29944; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29944&PLACEBO=IE.pdf.

Gilardoni:1997:DFI

[GWB97] F. Gilardoni, J. Weber, and A. Baiker. Density functional investigation of the mechanism of the selective catalytic reduction of NO by NH_3 over vanadium oxide model clusters. *International Journal of Quantum Chemistry*, 61 (4):683–688, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42440; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42440&PLACEBO=IE.pdf.

Grigorov:1997:NEI

[GWCT97] Martin Grigorov, Jacques Weber, Henry Chermette, and Jean M. J. Tronchet. Numerical evaluation of the internal orbitally resolved chemical hardness tensor in density functional theory. *International Journal of Quantum Chemistry*, 61(3): 551–562, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42426; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42426&PLACEBO=IE.pdf.

Green:1995:KMS

[GX95] A. E. S. Green and H. Xue. Kinetic modeling of spectra of flames with suppressants. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:703–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Gong:1998:ISI

[GX98] Xuedong Gong and Heming Xiao. Ab initio study on the internal rotation of five π-conjugated hydrocarbons at MP2 level. *International Journal of Quantum Chemistry*, 69 (5):659–667, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30030;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30030&PLACEBO=IE.pdf.

Guseinov:1995:UTT

[GY95] I. I. Guseinov and R. F. Yassen. Unified treatment of two-center Coulomb, hybrid, and exchange integrals over Slater-type orbitals. *International Journal of Quantum Chemistry*, 54 (4):197–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guan:1997:ALA

[GYDY97] Daren Guan, Xizhang Yi, Shiliang Ding, and Benhui Yang. Application of the Lie algebraic approach to diffractionally and rotationally inelastic molecule-surface scattering. *International Journal of Quantum Chemistry*, 63(5): 981–989, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42647; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42647&PLACEBO=IE.pdf.

Green:1998:CPQ

[GZ98] Alex E. S. Green and Mauricio Zanardi. Cellulose pyrolysis and quantum chemistry. *International Journal of Quantum Chemistry*, 66(3):219–227, January 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29855; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29855&PLACEBO=IE.pdf.

Guan:1997:TPD

[GZDZ97] Daren Guan, Xian Zhao, Conghao Deng, and John Z. H. Zhang. Total and partial decay widths in vibrational predissociation of the HeI_2 van der Waals complex for lower initial vibrational excitations. *International Journal of Quantum Chemistry*, 62(1):89–96, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42492; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42492&PLACEBO=IE.pdf.

Grozema:1999:IBC

[GZSvD99] Ferdinand C. Grozema, Robert W. J. Zijlstra, Marcel Swart, and Piet Th. van Duijnen. Iodine-benzene charge-transfer complex: Potential energy surface and transition probabilities studied at several levels of theory. *International Journal of Quantum Chemistry*, 75(4–5):709–723, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004968/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004968&PLACEBO=IE.pdf`.

Hall:1993:EDA

[HA93] G. G. Hall and S. Arimoto. Eigenvalue distributions and asymptotic lines of the energy in alternant hydrocarbons. *International Journal of Quantum Chemistry*, 45(3):303–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hamed:1992:MOT

[HAEMA92] M. M. Hamed, R. H. Abu-Eittah, Z. Mobark, and M. M. Abdou. A molecular orbital treatment of the electronic spectra of some tryptamines. *International Journal of Quantum Chemistry*, 44 (3):379–??, September 30, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hagmann:1992:QTT

[Hag92] M. J. Hagmann. Quantum tunneling times: A new solution compared to 12 other methods. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:299–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Hagmann:1994:EFD

[Hag94] M. J. Hagmann. Effects of the finite duration of quantum tunneling in laser-assisted scanning tunneling microscopy. *International Journal of Quantum Chemistry. Symposium*, 28:271–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Hagmann:1995:ENM

[Hag95] M. J. Hagmann. Efficient numerical methods for solving the Schrödinger equation with a potential varying sinusoidally with time. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:289–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Hagmann:1996:ENMa

[Hag96a] M. J. Hagmann. Efficient numerical method for finding the initial response of quantum processes to changes in the potential. *International Journal of Quantum Chemistry*, 60(7):19–??, 1996. CODEN IJQCB2.

Hagmann:1996:ENMc

[Hag96b] M. J. Hagmann. Efficient numerical method for finding the initial response of quantum processes to changes in the potential. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):19–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Hagmann:1996:ENMb

[Hag96c] Mark J. Hagmann. Efficient numerical method for finding the initial response of quantum processes to changes in the potential. *International Journal of Quantum Chemistry*, 60(7):1231–1239, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60707`.

Hagmann:1997:SLA

[Hag97] Mark J. Hagmann. Simulations of laser-assisted field emission within the local density approximation of Kohn–Sham density-functional theory. *International Journal of Quantum Chemistry*, 65(5):857–865, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42816`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42816&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Hagmann:1998:SEN

[Hag98] Mark J. Hagmann. Stable and efficient numerical method for solving the Schrödinger equation to determine the response of tunneling electrons to a laser pulse. *International Journal of Quantum Chemistry*, 70(4-5):703–710, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?`

ID=75048; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75048&PLACEBO=IE.pdf.

Hagelberg:1999:END

[Hag99a] F. Hagelberg. Electron nuclear dynamics studies of H_3 and H_3^+. *International Journal of Quantum Chemistry*, 75(4–5):367–383, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004937/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004937&PLACEBO=IE.pdf.

Hagmann:1999:SPM

[Hag99b] Mark J. Hagmann. Single-photon and multiphoton processes causing resonance in the transmission of electrons by a single potential barrier in a radiation field. *International Journal of Quantum Chemistry*, 75(4–5):417–427, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004940/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004940&PLACEBO=IE.pdf.

Hall:1999:RR

[Hal99] George G. Hall. Recollections and reflections. *International Journal of Quantum Chemistry*, 74(5):439–453, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62502997; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62502997&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Harriman:1971:DMA

[Har71] J. E. Harriman. A density matrix approach to multiconfiguration calculations. *International Journal of Quantum Chemistry*, 4(??):363–??, ?? 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harriman:1990:RPS

[Har90] J. E. Harriman. N-representability of phase space functions for electrons. *International Journal of Quantum Chemistry. Quan-*

tum Chemistry Symposium, 24:119–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Harcourt:1996:IVS

[Har96] Richard D. Harcourt. Increased-valence structures and hypervalent molecules. *International Journal of Quantum Chemistry*, 60(1):553–566, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60619.

Harcourt:1997:VBS

[Har97a] Richard D. Harcourt. Valence bond studies of the D_{2h} isomer of O_4: An interim report. *International Journal of Quantum Chemistry*, 63(2):547–555, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42598; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42598&PLACEBO=IE.pdf.

Harris:1997:NAC

[Har97b] Frank E. Harris. New approach to calculation of the leaky aquifer function. *International Journal of Quantum Chemistry*, 63(5):913–916, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42641; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42641&PLACEBO=IE.pdf.

Harris:1998:ESS

[Har98a] Frank E. Harris. Ewald summations in systems with two-dimensional periodicity. *International Journal of Quantum Chemistry*, 68(6):385–404, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29957; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29957&PLACEBO=IE.pdf.

Harris:1998:MAL

[Har98b] Frank E. Harris. More about the leaky aquifer function. *International Journal of Quantum Chemistry*, 70(4–5):623–626, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75040;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75040&PLACEBO=IE.pdf.

Harris:1999:CGC

[Har99] Frank E. Harris. Computer generation of coupled-cluster equations. *International Journal of Quantum Chemistry*, 75(4–5):593–597, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004954/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004954&PLACEBO=IE.pdf.

Huang:1994:QSI

[HB94] M.-J. Huang and N. S. Bodor. Quantitative structure-inhibitory activity relationships of substituted phenols on *Bacillus Subtilis* spore germination. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21:181–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Holmen:1995:TIS

[HB95] A. Holmen and A. Broo. A theoretical investigation of the solution N(7)H¡-¿N(9)H tautomerism of adenine. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):113–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Henriques:1999:CAS

[HBGR99] Elsa S. Henriques, Margarida Bastos, Carlos F. G. C. Geraldes, and Maria João Ramos. Computational approaches to the study of some lanthanide (III)-polyazamacrocyclic chelates for magnetic resonance imaging. *International Journal of Quantum Chemistry*, 73(2):237–248, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003521; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003521&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998.* Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Hu:1998:IDF

[HBH98] Ching-Han Hu, Tore Brinck, and Karl Hult. Ab initio and density functional theory studies of the catalytic mechanism for ester hydrolysis in serine hydrolases. *International Journal of Quantum Chemistry*, 69(1):89–103, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29964; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29964&PLACEBO=IE.pdf.

Han:1999:TCC

[HBL99] Young-Kyu Han, Cheolbeom Bae, and Yoon Sup Lee. Two-component calculations of spin-orbit effects for a van der Waals molecule Rn_2. *International Journal of Quantum Chemistry*, 72(2):139–143, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002780; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002780&PLACEBO=IE.pdf.

Harriman:1993:HRS

[HC93] J. E. Harriman and M. E. Casida. Husimi representation for stationary states. *International Journal of Quantum Chemistry*, 45(3):263–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

He:1996:SOMa

[HC96a] Zhi He and Dieter Cremer. Sixth-order many-body perturbation theory. I. Basic theory and derivation of the energy formula. *International Journal of Quantum Chemistry*, 59(1):15–29, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60524.

He:1996:SOMb

[HC96b] Zhi He and Dieter Cremer. Sixth-order many-body perturbation theory. II. Implementation and application. *International Journal of Quantum Chemistry*, 59(1):31–55, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60525.

He:1996:SOMc

[HC96c] Zhi He and Dieter Cremer. Sixth-order many-body perturbation theory. III. Correlation energies of size-extensive MP6 methods. *International Journal of Quantum Chemistry*, 59(1): 57–69, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60526`.

He:1996:SOMd

[HC96d] Zhi He and Dieter Cremer. Sixth-order many-body perturbation theory. IV. Improvement of the Møller–Plesset correlation energy series by using Padé, Feenberg, and other approximations up to sixth order. *International Journal of Quantum Chemistry*, 59(1):71–95, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60527`.

Ho:1996:EFG

[HC96e] Tse-Ming Ho and Tse-Chiang Chang. Electric-field gradient calculations for atoms with axial symmetry. *International Journal of Quantum Chemistry*, 57(2):229–233, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60371`.

Haeberlen:1994:RDF

[HCR94] O. D. Haeberlen, S.-C. Chung, and N. Roesch. Relativistic density-functional studies of naked and ligated gold clusters. *International Journal of Quantum Chemistry. Symposium*, 28: 595–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Huang:1995:NRC

[HDB+95] M.-J. Huang, D. Doerge, M. Bodor, E. Pop, and M. E. Brewster. Nitrogen radical cations as intermediates in enzymatically mediated oxidative deaminations-application of molecular parametric models. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):171–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Hennico:1991:PTS

[HDY+91] G. Hennico, J. Delhalle, E. Younang, M. Defranceschi, G. Lecayon, and C. Boiziau. Preliminary theoretical study of acrylonitrile and its methyl derivatives as monomers for cathodic electropolymerization. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:507–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Head:1997:CVF

[Hea97] John D. Head. Computation of vibrational frequencies for adsorbates on surfaces. *International Journal of Quantum Chemistry*, 65(5):827–838, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42814; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42814&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Hedin:1995:ECK

[Hed95] L. Hedin. Electron correlation: Keeping close to an orbital description. *International Journal of Quantum Chemistry*, 56 (5):445–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hermansson:1993:ERB

[Her93a] K. Hermansson. Erratum: Redshifts and blueshifts of OH vibrations. *International Journal of Quantum Chemistry*, 47(2):175–??, July 15, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hermansson:1993:RBO

[Her93b] K. Hermansson. Redshifts and blueshifts of OH vibrations. *International Journal of Quantum Chemistry*, 45(6):747–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Herschbach:1996:DSR

[Her96] Dudley R. Herschbach. Dimensional scaling and renormalization. *International Journal of Quantum Chemistry*, 57(3):295–308, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60391`.

Herman:1997:UCP

[Her97] Zelek S. Herman. On the use of the character projection operator in the determination of the symmetry of molecular orbitals and in the construction of hybrid bond orbitals. *International Journal of Quantum Chemistry*, 63 (1):49–56, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42580; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42580&PLACEBO=IE.pdf.

Herman:1998:DSD

[Her98] Michael F. Herman. The development of semiclassical dynamical methods and their application to vibrational relaxation in condensed-phase systems. *International Journal of Quantum Chemistry*, 70(4-5):897–907, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75067; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75067&PLACEBO=IE.pdf.

Hartke:1993:MTS

[HGC93] B. Hartke, D. A. Gibson, and E. A. Carter. Multiple time scale Hartree–Fock molecular dynamics. *International Journal of Quantum Chemistry*, 45(1):59–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hovorun:1999:NAG

[HGL99] Dmytro M. Hovorun, Leonid Gorb, and Jerzy Leszczynski. From the nonplanarity of the amino group to the structural nonrigidity of the molecule: A post-Hartree–Fock ab initio study of 2-aminoimidazole. *International Journal of Quantum Chemistry*, 75(3):245–253, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000666/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000666&PLACEBO=IE.pdf.

Hui:1991:ESC

[HGP91] X. Hui, N. Gresh, and B. Pullman. Effect of side chains on the groove-binding specificity of anthraquinone intercalators.

International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology., 18:205–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Horvat:1992:ITI

[HGP+92] D. Horvat, A. Graovac, D. Plavšić, N. Trinajstić, and M. Strunje. On the intercorrelation of topological indices in benzenoid hydrocarbons. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:401–408, 1992. CODEN IJQSDI. ISSN 0161-3642.

Hargittai:1992:ECB

[HH92] M. Hargittai and I. Hargittai. Experimental and computed bond lengths: The importance of their differences. *International Journal of Quantum Chemistry*, 44(6):1057–??, December 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harriman:1997:LEM

[HH97] John E. Harriman and Douglas E. Hoch. Locality of exchange matrices for common Gaussian basis sets. *International Journal of Quantum Chemistry*, 63(1):111–119, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42558; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42558&PLACEBO=IE.pdf.

Hu:1999:CRS

[HHHP99] Wan-Ping Hu, Sean A. Harris, Peter W. Harland, and Leon F. Phillips. Collisional reorientation of symmetric-top molecules in Stark fields. *International Journal of Quantum Chemistry*, 71(1):75–82, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000015; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000015&PLACEBO=IE.pdf.

Hertwig:1995:IMA

[HHKM95] R. H. Hertwig, M. C. Holthausen, W. Koch, and Z. B. Maksic. Ab initio MO and approximate density functional theory studies on the lowest singlet and triplet states of *s*- and *as*-indacene. *International Journal of Quantum Chemistry*, 54(3):

147–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hill:1998:CGO

[Hil98] Robert Nyden Hill. Completeness of Gaussian orbital and geminal basis sets for linear molecules in L^2 and in the first and second Sobolev spaces. *International Journal of Quantum Chemistry*, 68(6):357–384, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29956; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29956&PLACEBO=IE.pdf`.

Hirschfelder:1969:CWD

[Hir69a] J. O. Hirschfelder. Coordinates which diagonalize the kinetic energy of relative motion. *International Journal of Quantum Chemistry*, 3S(??):17–??, ?? 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hirschfelder:1969:FRS

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

Hirao:1992:MMP

[Hir92] K. Hirao. Multireference Møller–Plesset perturbation treatment of potential energy curve of N_2. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26: 517–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Hameka:1994:TPI

[HJ94] H. F. Hameka and J. O. Jensen. Theoretical prediction of the infrared and Raman spectra of O-ethyl S-2-diisopropylaminoethylmethylphosphonothiolate. *International Journal of Quantum Chemistry*, 50(2):161–??, April 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jeung:1997:MCM

[hJH97] Gwang hi Jeung and Stéphane Haettel. Are metal-CO molecules linear? ScCO, TiCO, VCO, and CrCO cases studied in MRCI method compared with DFT method. *International Journal of Quantum Chemistry*, 61(3):547–550, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42425; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42425&PLACEBO=IE.pdf.

Harris:1995:CSP

[HK95a] F. E. Harris and A. G. Koures. Critical study of plane-wave density-functional methods for extended systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:235–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Hughes:1995:CCM

[HK95b] S. R. Hughes and U. Kaldor. The coupled-cluster method in high sectors of the Fock space. *International Journal of Quantum Chemistry*, 55(2):127–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:1997:MES

[HK97] Siqun Huang and Jonathan E. Kenny. A method to evaluate the Sachs formula. *International Journal of Quantum Chemistry*, 65(1):19–36, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42738; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42738&PLACEBO=IE.pdf.

He:1996:AQC

[HKC96] Zhi He, Elfi Kraka, and Dieter Cremer. Application of quadratic CI with singles, doubles, and triples (QCISDT): An attractive alternative to CCSDT. *International Journal of Quantum Chemistry*, 57(2):157–172, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60364.

Halkjaer:1979:PCN

[HL79] O. Halkjaer and J. Linderberg. Potential curves and nonadiabatic coupling matrix elements for the O^+–Ne system. *International Journal of Quantum Chemistry*, S13(??):475–484, ?? 1979. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hedman:1993:DPL

[HL93a] F. Hedman and A. Laaksonen. Data parallel large-scale molecular dynamics for liquids. *International Journal of Quantum Chemistry*, 46(1):27–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hutter:1993:SFN

[HL93b] J. Hutter and H. P. Luthi. The structure of n-fold negatively charged C_{60} ($n = 1, 2, \ldots, 6$). *International Journal of Quantum Chemistry*, 46(1):81–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Heinonen:1996:EDFa

[HLJ96a] O. Heinonen, M. I. Lubin, and M. D. Johnson. Ensemble density functional theory for inhomogeneous fractional quantum Hall systems. *International Journal of Quantum Chemistry*, 60(7): 231–??, 1996. CODEN IJQCB2.

Heinonen:1996:EDFb

[HLJ96b] O. Heinonen, M. I. Lubin, and M. D. Johnson. Ensemble density functional theory for inhomogeneous fractional quantum Hall systems. *International Journal of Quantum Chemistry*, 60(7):1443–1455, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60703`.

Heinonen:1996:EDFc

[HLJ96c] O. Heinonen, M. I. Lubin, and M. D. Johnson. Ensemble density functional theory for inhomogeneous fractional quantum Hall systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):231–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Hagfeldt:1994:ELS

[HLS94] A. Hagfeldt, S. Lunell, and H. O. G. Siegbahn. Energy levels of small titanium oxide clusters obtained from SCF calculations. *International Journal of Quantum Chemistry*, 49(2): 97–??, January 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Holas:1995:ETC

[HM95] A. Holas and N. H. March. Exact theorems concerning non-interacting kinetic energy density functional in D dimensions and their implications for gradient expansions. *International Journal of Quantum Chemistry*, 56(4):371–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harary:1997:CST

[HM97a] Frank Harary and Paul G. Mezey. Cell-shedding transformations, equivalence relations, and similarity measures for square-cell configurations. *International Journal of Quantum Chemistry*, 62(4):353–361, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42522; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42522&PLACEBO=IE.pdf.

Holas:1997:EEC

[HM97b] A. Holas and N. H. March. Exact exchange-correlation potential from low-order density matrices. *International Journal of Quantum Chemistry*, 61(2):263–272, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42407; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42407&PLACEBO=IE.pdf.

Holas:1997:FBE

[HM97c] A. Holas and N. H. March. Force balance equations in inhomogeneous classical and quantal liquids. *International Journal of Quantum Chemistry*, 64(1):21–29, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42661; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42661&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Hadfield:1999:ASD

[HM99] Andrea T. Hadfield and Adrian J. Mulholland. Active-site dynamics of ASADH-A bacterial biosynthetic enzyme. *International Journal of Quantum Chemistry*, 73(2):137–146, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003512; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003512&PLACEBO=IE.pdf.

Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998*. Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Habibollahzadeh:1993:XNR

[HMGP93] D. Habibollahzadeh, J. S. Murray, M. E. Grice, and P. Politzer. X-NO_2 rotational energy barriers: Local density functional calculations. *International Journal of Quantum Chemistry*, 45(1): 15–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:1996:KPMa

[HMK96a] L. Huang, L. Massa, and J. Karle. Kernel projector matrices for leu^1-zervamicin. *International Journal of Quantum Chemistry*, 60(7):479–??, 1996. CODEN IJQCB2.

Huang:1996:KPMc

[HMK96b] L. Huang, L. Massa, and J. Karle. Kernel projector matrices for leu^1-zervamicin. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):479–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Huang:1996:KPMb

[HMK96c] L. Huang, L. Massa, and J. Karle. Kernel projector matrices for leu^1 — zervamicin. *International Journal of Quantum Chemistry*, 60(7):1691–1700, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60732`.

Huang:1999:QCA

[HMK99] L. Huang, L. Massa, and J. Karle. Quantum crystallography applied to crystalline maleic anhydride. *International Journal of Quantum Chemistry*, 73(5):439–450, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61004335`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61004335&PLACEBO=IE.pdf`.

Hilger:1998:ULB

[HMLK98] Ralf Hilger, Hans-Peter Merckens, Arne Lüchow, and Heinz Kleindienst. Upper- and lower-bound Hylleraas-CI calculations for the nonrelativistic P^o states of the ^{4}He isotope. *International Journal of Quantum Chemistry*, 66 (1):25–30, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29836; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29836&PLACEBO=IE.pdf.

Havlas:1992:MCV

[HNB92] Z. Havlas, S. Nick, and H. Bock. MNDO calculations as a valuable tool for structure evaluation of contact ion pairs. *International Journal of Quantum Chemistry*, 44(4):449–467, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hierse:1994:FSA

[HO94] W. Hierse and P. M. Oppeneer. Fast and stable algorithm for the analytical computation of two-center Coulomb and overlap integrals over Slater-type orbitals. *International Journal of Quantum Chemistry*, 52(6):1249–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:1997:MTD

[HOF+97] Yuanhe Huang, Mayumi Okada, Kenichi Fukui, Kazuyoshi Tanaka, Hiroo Aoki, and Tokio Yamabe. Mixing of triply degenerated molecular orbitals in C_{60}^{2-} and C_{60}^{3-}. *International Journal of Quantum Chemistry*, 63(2):361–366, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42607; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42607&PLACEBO=IE.pdf.

Holas:1998:EMH

[Hol98] A. Holas. Exact modified-Hartree–Fock scheme through perturbation expansion of density matrices. *International Journal of Quantum Chemistry*, 69(4):469–483, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30020; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30020&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Homeier:1993:SAN

[Hom93] H. H. H. Homeier. Some applications of nonlinear convergence accelerators. *International Journal of Quantum Chemistry*, 45 (6):545–562, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hoor:1994:TSO

[Hoo94] M. J. Ten Hoor. Three stages of optimization and simple correlated wave functions. *International Journal of Quantum Chemistry*, 49(1):45–??, January 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hopfield:1990:DNN

[Hop90] J. J. Hopfield. Dynamics and neural network computation. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:633–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Hosoya:1997:BED

[Hos97] Haruo Hosoya. Back-of-envelope derivation of the analytical formulas of the atomic wave functions of a D-dimensional atom. *International Journal of Quantum Chemistry*, 64 (1):35–42, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42663; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42663&PLACEBO=IE.pdf`. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Hermansson:1997:CBI

[HP97] Kersti Hermansson and Michael Probst. Correlation between intramolecular bond distances and stretching vibrations for polar molecules: An ab initio study. *International Journal of Quantum Chemistry*, 63(2):537–546, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42597; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42597&PLACEBO=IE.pdf`.

Harcourt:1998:CTD

[HP98] Richard D. Harcourt and Nicholas Pyper. Charge transfer and dispersion interaction stabilization of the D_2h isomer of O_4. *International Journal of Quantum Chemistry*, 68(2):129–134, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29932; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29932&PLACEBO=IE.pdf.

Hemery:1997:TDR

[HPSC97] A. Hemery, G. Picard, M. Sibony, and B. Champin. Thermochemical data relative to the complex formation in gas phase derived from computational chemistry. *International Journal of Quantum Chemistry*, 61(3):483–489, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42416; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42416&PLACEBO=IE.pdf.

Hall:1995:DLL

[HR95] G. G. Hall and D. Rees. A discrete look at localization. *International Journal of Quantum Chemistry*, 53(2):189–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hall:1997:SH

[HR97] G. G. Hall and D. Rees. Spherical hybrids. *International Journal of Quantum Chemistry*, 63(1):197–214, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42565; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42565&PLACEBO=IE.pdf.

Hall:1999:TSP

[HR99] G. G. Hall and D. Rees. A theory of special points in two-dimensional solid-state calculations. *International Journal of Quantum Chemistry*, 74(6):601–615, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001793; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001793&PLACEBO=IE.pdf. Special Issue:

The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II). Issue Edited by Don Rees, Hiroshi Fujimotoi.

Henseler:1999:IHC

[HRH99] Debora Henseler, Rupert Rebentisch, and Georg Hohlneicher. Interconversions of Z-1,3,5-hexatriene conformers: A theoretical study. *International Journal of Quantum Chemistry*, 72(4):295–305, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006305; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006305&PLACEBO=IE.pdf`. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Hernandez-Rojas:1997:FHR

[HRRBL97] J. Hernández-Rojas, A. Ruiz, J. Bretón, and J. M. Gomez Llorente. Free and hindered rotations in endohedral C_{60} fullerene complexes. *International Journal of Quantum Chemistry*, 65(5):655–663, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42798; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42798&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Homeier:1991:IQM

[HS91] Herbert H. H. Homeier and E. Otto Steinborn. Improved quadrature methods for three-center nuclear attraction integrals with exponential-type basis functions. *International Journal of Quantum Chemistry*, 39(4):625–645, April 1991. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hariharan:1992:CSI

[HS92a] S. Hariharan and W. H. Shelver. Conformational studies of (S)idazoxan and (S)methoxyidazoxan using am7 and pm3 semiempirical molecular orbital methods. *International Journal of Quantum Chemistry*, 44(2):181–??, September 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Head:1992:LWE

[HS92b] J. D. Head and S. J. Silva. Localization of wavefunctions from extended systems using orbital occupation numbers. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:229–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Homeier:1992:IQM

[HS92c] Herbert H. H. Homeier and E. Otto Steinborn. Improved quadrature methods for the Fourier transform of a two-center product of exponential-type basis functions. *International Journal of Quantum Chemistry*, 41(3):399–411, February 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Homeier:1992:EOI

[HS92d] Herbert H. H. Homeier and E. Otto Steinborn. On the evaluation of overlap integrals with exponential-type basis functions. *International Journal of Quantum Chemistry*, 42(4):761–778, May 20, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harbola:1993:ASK

[HS93] M. K. Harbola and V. Sahni. Asymptotic structure of the Kohn–Sham effective potential at metal surfaces. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:101–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Hess:1995:CIS

[HS95] B. A. Hess, Jr. and L. Smentek. Calculated infrared spectra of unstable organic molecules and reactive intermediates. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:647–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Head:1999:CFR

[HS99] John D. Head and Yu Shi. Characterization of Fermi resonances in adsorbate vibrational spectra using cluster calculations: Methoxy adsorption on Al(111) and Cu(111). *International Journal of Quantum Chemistry*, 75(4–5):815–820, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004976/START`; `http://www3.`

interscience.wiley.com/cgi-bin/fulltext?ID=66004976&PLACEBO=IE.pdf.

Ho:1994:TAV

[HSES94] M. Ho, H. Schmider, K. E. Edgecombe, and V. H. Smith. Topological analysis of valence electron charge distributions from semiempirical and ab initio methods. *International Journal of Quantum Chemistry. Symposium*, 28:215–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Hagfeldt:1992:SCR

[HSLL92] A. Hagfeldt, H. Siegbahn, S.-E. Lindquist, and S. Lunell. Semiempirical calculations of TiO_2 (rutile) clusters. *International Journal of Quantum Chemistry*, 44(4):477–495, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ho:1995:MDA

[HSSW95] M. Ho, R. P. Sagar, H. Schmider, and D. F. Weaver. Measures of distance for atomic charge and momentum densities and their relationship to physical properties. *International Journal of Quantum Chemistry*, 53(6):627–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ho:1995:IDS

[HSWS95] M. Ho, R. P. Sagar, D. F. Weaver, and V. H. Smith, Jr. An investigation of the dependence of Shannon information entropies and distances measures on molecular geometry. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:109–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Huang:1997:DFO

[HT97] Fu Qiang Huang and Au Chin Tang. Dihedral fullerenes: Open, closed, and pseudoclosed shell. *International Journal of Quantum Chemistry*, 62(4):437–446, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42520; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42520&PLACEBO=IE.pdf.

Hirao:1994:FPC

[HU94] M. Hirao and T. Uda. First principles calculation of the optical properties and stability of hydrogenated silicon clusters.

International Journal of Quantum Chemistry, 52(4):1113–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:1992:VCW

[Hua92] M.-J. Huang. Vibrational calculations on water with improved force fields. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:427–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Hudson:1999:SPR

[Hud99] R. L. Hudson. Some properties of reduced density operators. *International Journal of Quantum Chemistry*, 74 (5):595–599, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62503010; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62503010&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Huzinaga:1996:IMP

[Huz96] S. Huzinaga. The ab initio model potential method and the optimized orbitals for the multiconfiguration self-consistent-field – configuration interaction approach. *International Journal of Quantum Chemistry*, 60(1):83–90, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60628.

Halasz:1998:BFS

[HVS98] G. Halász, Á. Vibók, and S. Suhai. A BSSE-free SCF algorithm for intermolecular interactions. IV. Generalization for open-shell systems. *International Journal of Quantum Chemistry*, 68(3):151–158, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29936; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29936&PLACEBO=IE.pdf.

Huang:1991:VCA

[HW91] Ming-Ju Huang and Max Wolfsberg. Variational calculations on ammonia using two symmetrical normal modes. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:441–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Haken:1995:PAQ

[HWB95] H. Haken, H. C. Wolf, and E. J. Brändas. The physics of atoms and quanta. *International Journal of Quantum Chemistry*, 54 (5):325–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:1997:TSIb

[HWB97a] Ming-Ju Huang, John D. Watts, and Nicholas Bodor. Theoretical studies of inclusion complexes of α- and β-cyclodextrin with benzoic acid and phenol. *International Journal of Quantum Chemistry*, 65(6):1135–1152, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42839`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42839&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on the Application of Fundamental Theory to Problems of Biology and Pharmocolgy*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Huang:1997:TSIa

[HWB97b] Ming-Ju Huang, John D. Watts, and Nicholas Bodor. Theoretical studies of inclusion complexes of β-cyclodextrin with methylated benzoic acids. *International Journal of Quantum Chemistry*, 64(6):711–719, September 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42732`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42732&PLACEBO=IE.pdf`.

Homeier:1992:SDO

[HWS92] Herbert H. H. Homeier, E. Joachim Weniger, and E. Otto Steinborn. Simplified derivation of a one-range addition theorem of the Yukawa potential. *International Journal of Quantum Chemistry*, 44(3):405–411, September 30, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hagmann:1993:EPD

[HZ93] M. J. Hagmann and L. Zhao. Experiments pursuant to determining the barrier traversal time for quantum tunneling. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:807–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Hu:1994:MCC

[HZ94] Z.-M. Hu and C.-G. Zhan. MBOHO calculations of C-H stretching frequencies in hydrocarbons and heterosubstituted hydrocarbons. *International Journal of Quantum Chemistry*, 52(1): 109–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hsiao:1999:CEG

[HZ99] Ya-Wen Hsiao and Michael C. Zerner. Calculating ESR G tensors of doublet radicals by the semiempirical INDO/S method. *International Journal of Quantum Chemistry*, 75(4–5):577–584, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004952/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004952&PLACEBO=IE.pdf`.

Imamura:1994:CES

[IANK94] A. Imamura, Y. Aoki, K. Nishimoto, and Y. Kurihara. Calculations of the electronic structure of various aperiodic polymers by an elongation method. *International Journal of Quantum Chemistry*, 52(2):309–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ishikawa:1995:SSH

[IBS95] Y. Ishikawa, R. C. Binning, Jr., and H. Sekino. Stable structures of $Na(H_2O)_n$ ($n = 1 \ldots 3$) clusters by ab initio simulated annealing. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:669–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Igawa:1995:MCM

[Iga95] A. Igawa. A method of calculation of the matrix elements between the spin-projected nonorthogonal Slater determinants. *International Journal of Quantum Chemistry*, 54(4):235–??,

1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ishikawa:1995:AGC

[IHG95] N. Ishikawa and M. Head-Gordon. Analytical gradient of the CIS(D) perturbative correction to single-excitation configuration interaction excited states. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:421–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Ikegami:1994:TSN

[II94] T. Ikegami and S. Iwata. Theoretical study on the non-adiabatic photodissociation process of argon cluster ions Ar0+7. *International Journal of Quantum Chemistry. Symposium*, 28:529–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Ichikawa:1994:ACP

[IK94] H. Ichikawa and H. Kagawa. Analysis of chemical phenomena by solving constrained Hartree–Fock equation. I. method and application to resonance energy in linear polyenes. *International Journal of Quantum Chemistry*, 52(3):575–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ishikawa:1997:RMB

[IK97] Yasuyuki Ishikawa and Konrad Koc. Relativistic many-body perturbation calculations for Zn and Cd and their singly ionized ions. *International Journal of Quantum Chemistry*, 65 (5):545–554, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42783; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42783&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods.* Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Ikegami:1999:CPM

[Ike99] Hidetsugu Ikegami. Coherent positronium molecule Ps_n and scanning clustering microscopy. *International Journal of Quantum Chemistry*, 71(1):83–99, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL

http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000016; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000016&PLACEBO=IE.pdf.

Iachello:1996:ATM

[ILL96] F. Iachello, R. D. Levine, and J. Linderberg. Algebraic theory of molecules. *International Journal of Quantum Chemistry*, 59(6): 503–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Inokuti:1996:RSP

[Ino96] Mitio Inokuti. Remarks on stopping power: Its connections with particle transport and with the electronic structure of matter. *International Journal of Quantum Chemistry*, 57(2):173–182, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60365.

Ischtwan:1993:GAE

[IP93] J. Ischtwan and S. D. Peyerimhoff. General algebraic expressions of totally symmetric potential functions for AX_n (n = 3,4) molecules. *International Journal of Quantum Chemistry*, 45(5):471–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Iyakutti:1994:ECT

[IP94] K. Iyakutti and R. R. Palanichamy. Electron crystallization in two dimensions. *International Journal of Quantum Chemistry*, 51(4 (or 5??)):329–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ishikawa:1990:ADF

[Ish90] Y. Ishikawa. Atomic Dirac–Fock–Breit self-consistent field calculations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:383–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Ishikawa:1991:EBS

[Ish91] Yasuyuki Ishikawa. Effects of basis set contraction on relativistic and breit interaction energies. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:113–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Ishikawa:1992:RMB

[Ish92] Y. Ishikawa. Relativistic many-body perturbation theory using the discrete basis expansion method: Analysis of relativistic pair correlation energies of the Xe atom. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26: 127–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Ishida:1996:AAR

[Ish96] Kazuhiro Ishida. ACE algorithm for the rapid evaluation of the electron-repulsion integral over Gaussian-Type orbitals. *International Journal of Quantum Chemistry*, 59(3):209–218, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60540`.

Imamura:1999:ITS

[ISOA99] Akira Imamura, Hiroyuki Sugiyama, Yuuichi Orimoto, and Yuriko Aoki. Ab initio through space/bond interaction analysis on the stereoelectronic effect by modifying the exponents of the basis set. *International Journal of Quantum Chemistry*, 74(6):761–768, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001792; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001792&PLACEBO=IE.pdf`. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Ivanov:1996:SMLa

[Iva96a] S. Ivanov. Simple modification of the Lee–Yang–Parr correlation functional to satisfy exact nonuniform scaling requirements. *International Journal of Quantum Chemistry*, 60(7): 191–??, 1996. CODEN IJQCB2.

Ivanov:1996:SMLc

[Iva96b] S. Ivanov. Simple modification of the Lee–Yang–Parr correlation functional to satisfy exact nonuniform scaling requirements. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):191–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Ivanov:1996:SMLb

[Iva96c] Stanislav Ivanov. Simple modification of the Lee–Yang–Parr correlation functional to satisfy exact nonuniform scaling requirements. *International Journal of Quantum Chemistry*, 60 (7):1403–1407, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60699. See erratum [Iva97].

Ivanov:1997:ESM

[Iva97] Stanislav Ivanov. Erratum: Simple modification of the Lee–Yang–Parr correlation functional to satisfy exact nonuniform scaling requirements. *International Journal of Quantum Chemistry*, 65(2):195, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42747; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42747&PLACEBO=IE.pdf. See [Iva96c].

Ichikawa:1999:COT

[IY99] Hiroshi Ichikawa and Atsushi Yoshida. Complete one- and two-center partitioning scheme for the total energy in the Hartree–Fock theory. *International Journal of Quantum Chemistry*, 71(1):35–46, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000011; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000011&PLACEBO=IE.pdf.

Ishikawa:1999:ANM

[IYFI99] Hideaki Ishikawa, Kazuo Yamamoto, Kazumi Fujima, and Misako Iwasawa. An accurate numerical multicenter integration for molecular orbital theory. *International Journal of Quantum Chemistry*, 72(5):509–523, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006353; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006353&PLACEBO=IE.pdf.

Jacchieri:1992:EBH

[Jac92] S. G. Jacchieri. An examination of the basic hypothesis of Zimm–Bragg theory based on energy distributions of peptide chains. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19: 255–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Jacchieri:1997:CAP

[Jac97] Saul G. Jacchieri. Conformational analysis of polypeptide chains with the aid of density of states calculations. *International Journal of Quantum Chemistry*, 65(6): 1115–1124, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42837; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42837&PLACEBO=IE.pdf`. See erratum [Jac98]. Special Issue: *Proceedings of the International Symposium on the Application of Fundamental Theory to Problems of Biology and Pharmocolgy.* Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Jacchieri:1998:ECA

[Jac98] Saul G. Jacchieri. Erratum: Conformational analysis of polypeptide chains with the aid of density of states calculations. *International Journal of Quantum Chemistry*, 67(5):341, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29913; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29913&PLACEBO=IE.pdf`. See [Jac97].

Jug:1995:SCV

[JAG95] K. Jug, B. Ahlswede, and G. Geudtner. SINDO1 calculations of vibrational frequencies of adsorbed molecules. *International Journal of Quantum Chemistry*, 55(5):411–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jain:1970:SSP

[Jai70] D. C. Jain. A study of some potential energy functions for diatomic molecules. *International Journal of Quantum Chemistry*, 4(??):579–586, ?? 1970. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jakobsson:1993:HSM

[Jak93] E. Jakobsson. Hierarchies of simulation methods in understanding biomolecular function. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:25–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Jaszunski:1994:LRC

[Jas94] M. Jaszunski. Linear response calculation of potential energy curves of BH. *International Journal of Quantum Chemistry*, 51 (4 (or 5??)):307–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jayasuriya:1992:SEP

[Jay92] K. Jayasuriya. Substituents effects in phospha alkynes: A computational investigation. *International Journal of Quantum Chemistry*, 44(3):327–??, September 30, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jeziorski:1997:CCE

[JBS97] Bogumił Jeziorski, Robert Bukowski, and Krzysztof Szalewicz. Completeness criteria for explicitly correlated Gaussian geminal bases of axial symmetry. *International Journal of Quantum Chemistry*, 61(5):769–776, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42462; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42462&PLACEBO=IE.pdf`.

Janssens:1995:RBE

[JBT+95] G. O. A. Janssens, B. G. Baekelandt, H. Toufar, W. J. Mortier, and R. A. Schoonheydt. On the relation between electronic and nuclear vibrations via the response matrix derived from semiempirical density functional-based sensitivity analysis. *International Journal of Quantum Chemistry*, 56(4):317–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jansen:1996:MQC

[JCÁ96] Georg Jansen, François Colonna, and János G. Ángyán. Mixed quantum-classical calculations on the water molecule in liquid phase: Influence of a polarizable environment on electronic properties. *International Journal of Quantum Chemistry*, 58(3):251–265, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60480`.

Jacquemin:1997:ECE

[JCA97] Denis Jacquemin, Benoît Champagne, and Jean-Marie André. Electron correlation effects upon the static (hyper)polarizabilities of push-pull conjugated polyenes and polyynes. *International Journal of Quantum Chemistry*, 65(5):679–688, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42800`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42800&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Judson:1992:DIC

[JCM+92] R. S. Judson, M. E. Colvin, J. C. Meza, A. Huffer, and D. Gutierrez. Do intelligent configuration search techniques outperform random search for large molecules? *International Journal of Quantum Chemistry*, 44(2):277–??, September 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jernigan:1999:RSF

[JDB99] R. L. Jernigan, M. C. Demirel, and I. Bahar. Relating structure to function through the dominant slow modes of motion of DNA topoisomerase II. *International Journal of Quantum Chemistry*, 75(3):301–312, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/65000671/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000671&PLACEBO=IE.pdf`.

Jarzecki:1999:SQM

[JDJP99] Andrzej A. Jarzecki, Ernest R. Davidson, Quan Ju, and Charles S. Parmenter. Scaled quantum mechanical study of vibrational force field for *p*-difluorobenzene and *p*-fluorotoluene.

International Journal of Quantum Chemistry, 72(4):249–260, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006328; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006328&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Jones:1990:MMI

[JE90] H. W. Jones and B. Etemadi. Multicenter molecular integrals using harmonic expansions of Slater-type orbitals and numerical integrations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:405–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Jones:1992:RBF

[JEB92] H. W. Jones, B. Etemadi, and F. B. Brown. Restricted basis functions for H_2^+ with use of overlap integrals of Slater-type orbitals. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:265–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Jenichen:1994:ICR

[Jen94] A. Jenichen. Ab initio calculations to the reactions of HF and HCl with $Si(OH)_4$ and $(HO)_3$ $SiOSi(OH)_3$: Modeling of SiO_2 etching reactions. *International Journal of Quantum Chemistry*, 52(1):117–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jensen:1999:BRT

[Jen99] Frank Jensen. Book review: *Theoretical Organic Chemistry*, by C. Parkanyi. *International Journal of Quantum Chemistry*, 72(5):535, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006356; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006356&PLACEBO=IE.pdf.

Jankowski:1995:PVU

[JG95] K. Jankowski and I. Grabowski. Performance of valence-universal multireference coupled-cluster theory for quasi-degenerate states: The H_8 and DZP H_4 models. *International Journal of Quantum Chemistry*, 55(2):205–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jacchieri:1996:CECa

[JGCJ96a] S. G. Jacchieri, M. Gomes, A. C. M. Camargo, and L. Juliano. Cross examination of the conformational spaces of a set of peptide chains: Study of oligopeptidase action. *International Journal of Quantum Chemistry*, 60(8):91–??, 1996. CODEN IJQCB2.

Jacchieri:1996:CECb

[JGCJ96b] S. G. Jacchieri, M. Gomes, A. C. M. Camargo, and L. Juliano. Cross examination of the conformational spaces of a set of peptide chains: Study of oligopeptidase action. *International Journal of Quantum Chemistry*, 60(8):1815–1827, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60753`.

Jacchieri:1996:CECc

[JGCJ96c] S. G. Jacchieri, M. Gomes, A. C. M. Camargo, and L. Juliano. Cross examination of the conformational spaces of a set of peptide chains: Study of oligopeptidase action. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 23(??):91–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

Jankowski:1998:MSIb

[JGR98] K. Jankowski, J. Gryniaków, and K. Rubiniec. Model study of the impact of orbital choice on the accuracy of coupled-cluster energies. II. valence-universal coupled-cluster method. *International Journal of Quantum Chemistry*, 67 (4):221–237, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29902; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29902&PLACEBO=IE.pdf`.

Jones:1990:DFC

[JH90] R. O. Jones and D. Hohl. Density functional calculations with simulated annealing — isomers of ssub 7 X [X = O, S, se], sesub 8, osub 8. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:141–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Jacchieri:1995:CST

[JI95] S. G. Jacchieri and A. S. Ito. Characterization of structural transitions from aqueous solution to a lipid phase for α-MSH. *International Journal of Quantum Chemistry*, 53(3):335–341, February 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jones:1996:EAFa

[JJ96a] H. W. Jones and J. L. Jain. Evaluation of the alpha-function for large parameter values. *International Journal of Quantum Chemistry*, 60(7):45–??, 1996. CODEN IJQCB2.

Jones:1996:EAFb

[JJ96b] H. W. Jones and J. L. Jain. Evaluation of the alpha-function for large parameter values. *International Journal of Quantum Chemistry*, 60(7):1257–1260, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60736`.

Jones:1996:EAFc

[JJ96c] H. W. Jones and J. L. Jain. Evaluation of the alpha-function for large parameter values. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):45–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Ju:1997:IIE

[JJ97] Guan-Zhi Ju and Ning Ju. On intra- and interpair electron correlation in LiF_2. *International Journal of Quantum Chemistry*, 64(2):171–174, August 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42678; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42678&PLACEBO=IE.pdf`. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Jug:1992:CPS

[JK92] K. Jug and M. Krack. Consistent parametrization of semiempirical MO methods. *International Journal of Quantum Chemistry*, 44(4):517–531, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jankowski:1999:CBP

[JKGM99] K. Jankowski, K. Kowalski, I. Grabowski, and H. J. Monkhorst. Correspondence between physical states and solutions to the coupled-cluster equations. *International Journal of Quantum Chemistry*, 75(4–5):483–496, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004944/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004944&PLACEBO=IE.pdf`.

Jankowski:1994:MSS

[JKJ94] K. Jankowski, K. Kowalski, and P. Jankowski. Multiple solutions of the single-reference coupled-cluster equations. I. H_4 model revisited. *International Journal of Quantum Chemistry*, 50(5):353–??, May 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jankowski:1995:MSS

[JKJ95] K. Jankowski, K. Kowalski, and P. Jankowski. Multiple solutions of the single-reference coupled-cluster equations. II. alternative reference states. *International Journal of Quantum Chemistry*, 53(5):501–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jahns:1992:AIL

[JKK+92] V. Jahns, S. Kostlmeier, M. Kotzian, N. Rosch, and P. L. Watson. On the agostic interaction in lanthanide phenylene complexes: An INDO study of $[(Cp^{*}over_2M)_2C_6H_4](M = Sc, Lu)$ employing an energy-partitioning analysis. *International Journal of Quantum Chemistry*, 44(5):853–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jankowski:1998:MSIa

[JKRW98] K. Jankowski, K. Kowalski, K. Rubiniec, and J. Wasilewski. Model study of the impact of orbital choice on the accuracy of coupled-cluster energies. I. single-reference-state formulation. *International Journal of Quantum Chemistry*, 67 (4):205–219, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29901`;

`http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29901&PLACEBO=IE.pdf`.

Jorgensen:1970:TDH

[JL70] P. Jørgensen and J. Linderberg. Time-dependent Hartree–Fock calculations in the Pariser–Parr–Pople model applications to aniline, azulene and pyridine. *International Journal of Quantum Chemistry*, 4(??):587–602, ?? 1970. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jankowski:1993:MSV

[JM93a] K. Jankowski and P. Malinowski. Multiple solutions of the valence-universal coupled-cluster equations for Be, B^{+}, and C^{2+}. *International Journal of Quantum Chemistry*, 48(1):59–??, October 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jeziorski:1993:ECE

[JM93b] B. Jeziorski and R. Moszynski. Explicitly connected expansion for the average value of an observable in the coupled-cluster theory. *International Journal of Quantum Chemistry*, 48(3):161–??, November 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jug:1994:CSS

[JM94] K. Jug and M. Matuschewski. Classification of substituents by sigma and pi electron energy separation. *International Journal of Quantum Chemistry*, 49(3):197–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jankowski:1995:AVU

[JM95] K. Jankowski and P. Malinowski. Application of the valence-universal coupled-cluster method based on various model spaces to 1S states of be. *International Journal of Quantum Chemistry*, 55(3):269–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jankowski:1996:AVU

[JM96a] K. Jankowski and P. Malinowski. Application of the valence-universal coupled-cluster method based on various model spaces. II. Nonstandard solutions for Be. *International Journal of Quantum Chemistry*, 59(3):239–249, ???? 1996. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60543.

John:1996:CNS

[JM96b] P. E. John and R. B. Mallion. Calculating the number of spanning trees in a labeled planar molecular graph whose inner dual is a tree. *International Journal of Quantum Chemistry*, 60(1):59–66, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60625.

Jursic:1996:CBD

[JM96c] Branko S. Jursic and Robin M. Martin. Calculation of bond dissociation energies for oxygen containing molecules by ab initio and density functional theory methods. *International Journal of Quantum Chemistry*, 59(6):495–501, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60568.

Jorge:1999:AAG

[JM99] F. E. Jorge and E. P. Muniz. Accurate adapted Gaussian basis sets for the atoms from H through Xe. *International Journal of Quantum Chemistry*, 71(4):307–312, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10049344; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10049344&PLACEBO=IE.pdf.

Ju:1995:ECN

[JMD95] G.-Z. Ju, F. B. C. Machado, and E. R. Davidson. On electron correlation in $NaCl_2$. *International Journal of Quantum Chemistry*, 54(5):299–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jagielska:1999:LSP

[JMP99] Anna Jagielska, Robert Moszynski, and Lucjan Piela. A large structural polarization by intermolecular forces: Ab initio theoretical investigation of the H_3 N$\cdots H_2$CN and $H_3N\cdots B(CN)_3$ interactions. *International Journal of Quantum Chemistry*, 75(3):177–185, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000659/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000659&PLACEBO=IE.pdf.

Jankowski:1998:MSIc

[JMR98] K. Jankowski, L. Meissner, and K. Rubiniec. Model study of the impact of orbital choice on the accuracy of coupled-cluster energies. III. state-universal coupled-cluster method. *International Journal of Quantum Chemistry*, 67 (4):239–250, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29903; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29903&PLACEBO=IE.pdf.

Jin:1995:CSE

[JMS95] Q. Jin, C. Mei, and V. H. Smith, Jr. Comparison study of the electronic structure of high-T_c superconductors. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:189–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Janezic:1994:IMM

[JO94] D. Janezic and B. Orel. Improvement of methods for molecular dynamics intergration. *International Journal of Quantum Chemistry*, 51(6):407–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jones:1997:MBA

[JOC97] Matthew D. Jones, Gerardo Ortiz, and David M. Ceperley. Many-body approaches to atoms and molecules in external magnetic fields. *International Journal of Quantum Chemistry*, 64(5):523–552, September 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42717; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42717&PLACEBO=IE.pdf. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

Johnson:1967:MSG

[Joh67] K. H. Johnson. Multiple scattering (Green's function) model for polyatomic molecules II. theory. *International Journal of Quantum Chemistry*, 1S(??):361–??, ?? 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jones:1992:LAF

[Jon92] H. W. Jones. Löwdin alpha-function, overlap integral, and computer algebra. *International Journal of Quantum Chemistry*, 41 (5):749–754, March 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jones:1993:BVT

[Jon93] H. W. Jones. Benchmark values for two-center Coulomb integrals over Slater-type orbitals. *International Journal of Quantum Chemistry*, 45(1):21–30, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jones:1994:DMM

[Jon94] H. W. Jones. Developments in multicenter molecular integrals over STOs using expansions in spherical harmonics. *International Journal of Quantum Chemistry*, 51(6):417–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jones:1997:CSC

[Jon97] Herbert W. Jones. Comprehensive strategy for the calculation of overlap integrals with Slater-type orbitals. *International Journal of Quantum Chemistry*, 61(6):881–889, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42469; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42469&PLACEBO=IE.pdf`.

Jorgensen:1992:BRB

[Jør92] Poul Jørgensen. Book review: Review of algebraic and diagrammatic methods in many-fermion theory. By Frank E. Harris, Hendrik J. Monkhorst, and David L. Freeman, Oxford University Press, Inc., New York, 1992. *International Journal of Quantum Chemistry*, 44(6):1069, December 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [**?**].

Jost:1997:MFC

[Jos97] Remy Jost. Magnetic field control of molecular dissociation energies. *International Journal of Quantum Chemistry*, 64 (5):571–580, September 15, 1997. CODEN IJQCB2. ISSN

0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42720; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42720&PLACEBO=IE.pdf. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

Joubert:1997:TRI

[Jou97] Daniel P. Joubert. Translational and rotational invariance requisites for density functional derivatives. *International Journal of Quantum Chemistry*, 61(2):355–360, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42400; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42400&PLACEBO=IE.pdf.

Janoschek:1967:WAM

[JPD67] R. Janoschek, H. Preuss, and G. Diercksen. Wellenmechanische Absolutrechnungen an Molekulen und Atomsystemen mit der SCF-MO-LC(LCGO) Methode XI. Das Hydroxylanion $(OH)^{-}$. *International Journal of Quantum Chemistry*, 1(??):649–652, ?? 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jeziorski:1995:UGA

[JPJ95] B. Jeziorski, J. Paldus, and P. Jankowski. Unitary group approach to spin-adapted open-shell coupled cluster theory. *International Journal of Quantum Chemistry*, 56(3):129–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jaszunski:1996:MCF

[JR96] Michał Jaszuński and Antonio Rizzo. MCSCF calculation of the frequency-dependent hyperpolarizability of the lithium atom. *International Journal of Quantum Chemistry*, 60(1):487–492, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60611.

Jansen:1999:ESO

[JRS+99] Thomas La Cour Jansen, Sten Rettrup, C. R. Sarma, Jaap G. Snijders, and Paolo Palmieri. On the evaluation of spin-orbit coupling matrix elements in a spin-adapted basis. *International Journal of Quantum Chemistry*, 73

(1):23–27, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55001577; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55001577&PLACEBO=IE.pdf.

Jug:1997:EMC

[JSG97] Karl Jug, André M. Schmidt, and Heiko Gerwens. Electrostatic model calculations on multiple adsorption at NaCl surfaces. *International Journal of Quantum Chemistry*, 63 (3):685–693, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42612; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42612&PLACEBO=IE.pdf.

Jurimae:1995:SSH

[JSKC95] T. Jurimae, M. Strandberg, M. Karelson, and J-L Calais. A semiempirical study of heterocycle oligomers and polymers in different dielectric media. *International Journal of Quantum Chemistry*, 54(6):369–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jamin:1996:PII

[JTZ+96] Nadège Jamin, Véronique Le Tilly, Loussinee Zargarian, Anne Bostad, Iris Besançon-Yoshpe, Pierre-Noël Lirsac, Odd S. Gabrielsen, and Flavio Toma. Preliminary investigation of the interaction between the R2R3 DNA binding domain of the oncoprotein c-Myb and DNA fragments. *International Journal of Quantum Chemistry*, 59(4):333–341, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60552.

Jug:1996:ESM

[Jug96] Karl Jug. Extension of semiempirical methods to simulation of surfaces. *International Journal of Quantum Chemistry*, 58(3): 283–295, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60482.

Jursic:1996:DFC

[Jur96a] Branko S. Jursic. Density functional calculations of difluorodiazete structures with Gaussian-Orbital-Type approach. *International Journal of Quantum Chemistry*, 57(2):213–217, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60369.

Jursic:1996:SNO

[Jur96b] Branko S. Jursic. A study of nitrogen oxides by using density functional theory and their comparison with ab initio and experimental data. *International Journal of Quantum Chemistry*, 58(1):41–46, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60462.

Jursic:1997:AEA

[Jur97a] Branko S. Jursic. An accurate evaluation of activation barriers for hydrogen abstraction reactions with Becke's 88 density functional theory and high-level G1 and G2 ab initio methods. *International Journal of Quantum Chemistry*, 65(1):75–82, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42743; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42743&PLACEBO=IE.pdf.

Jursic:1997:CBD

[Jur97b] Branko S. Jursic. Computation of bond dissociation energy for sulfides and disulfides with ab initio and density functional theory methods. *International Journal of Quantum Chemistry*, 62(3):291–296, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42514; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42514&PLACEBO=IE.pdf.

Jursic:1997:CGF

[Jur97c] Branko S. Jursic. Computation of geometries and frequencies of singlet and triplet nitromethane with density functional theory using Gaussian-type orbitals. *International Journal of Quantum Chemistry*, 64(2):263–269, August 5, 1997. CODEN

IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42676; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42676&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Jursic:1997:CSI

[Jur97d] Branko S. Jursic. Computation of some ionization potentials for second-row elements by ab initio and density functional theory methods. *International Journal of Quantum Chemistry*, 64(2):255–261, August 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42675; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42675&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Jursic:1997:CPE

[Jur97e] Branko S. Jursic. The computation of the potential energy surface for H_2 + OH → H_2O + H using ab initio and density functional theory methods. *International Journal of Quantum Chemistry*, 62(6):639–644, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42547; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42547&PLACEBO=IE.pdf.

Jursic:1997:DFT

[Jur97f] Branko S. Jursic. Density functional theory study of difluorovinylidene isomerization to difluoroacetylene. *International Journal of Quantum Chemistry*, 62(5):515–520, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42539; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42539&PLACEBO=IE.pdf.

Jursic:1997:EAM

[Jur97g] Branko S. Jursic. Electron affinities of metals computed by density functional theory and ab initio methods. *Inter-*

national Journal of Quantum Chemistry, 61(1):93–100, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42374`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42374&PLACEBO=IE.pdf`.

Jursic:1998:CBSa

[Jur98a] Branko S. Jursic. Complete basis set ab initio and hybrid density functional theory exploration of the potential energy surface in the reaction between an amino radical and nitrogen oxide. *International Journal of Quantum Chemistry*, 66 (6):409–414, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29876`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29876&PLACEBO=IE.pdf`.

Jursic:1998:CBSb

[Jur98b] Branko S. Jursic. Complete basis set and Gaussian-2 ab initio computational studies of planar Hückel and Möbius aromatic hydrogen clusters. *International Journal of Quantum Chemistry*, 69(5):679–687, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30032`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30032&PLACEBO=IE.pdf`.

Jursic:1999:HLIb

[Jur99a] Branko S. Jursic. High-level ab initio computational study of acetylene radical cation and anion decomposition process. *International Journal of Quantum Chemistry*, 72(6): 571–579, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=50000015`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=50000015&PLACEBO=IE.pdf`.

Jursic:1999:HLIa

[Jur99b] Branko S. Jursic. High-level ab initio computational study of doublet and quartet nitrogen reaction with methane. *International Journal of Quantum Chemistry*, 71(6):481–490, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=15000346`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=15000346&PLACEBO=IE.pdf`.

Jursic:1999:HLIc

[Jur99c] Branko S. Jursic. High level of ab initio and density functional theory evaluation of the C — O bond dissociation energies in the dimethyl ether anion. *International Journal of Quantum Chemistry*, 73(3):299–306, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003697`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003697&PLACEBO=IE.pdf`.

Jursic:1999:HDF

[Jur99d] Branko S. Jursic. Hybrid density functional theory study of hydrogen cluster aromaticity by computing their relative energies and magnetic properties. *International Journal of Quantum Chemistry*, 73(5):451–458, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61004336`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61004336&PLACEBO=IE.pdf`.

Jiang:1994:ARQ

[JY94] T.-F. Jiang and J.-M. Yuan. Aspects related to quantum studies of multiphoton excitation and dissociation of diatomic molecules. *International Journal of Quantum Chemistry. Symposium*, 28:65–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Jursic:1995:TICa

[JZ95a] B. S. Jursic and Z. Zdravkovski. Theoretical investigation of *cis*- and *trans*-nitric oxide dimers with ab initio and density functional Gaussian-type orbital approach. *International Journal of Quantum Chemistry*, 54(3):161–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jursic:1995:TICb

[JZ95b] B. S. Jursic and Z. Zdravkovski. Theoretical investigation of the conrotatory ring opening of cyclobutene and 1,2-Dihydro-1,2-diazacyclobutadienes with ab initio and density functional Gaussian-type-orbital approach. *International Jour-*

nal of Quantum Chemistry, 56(2):115–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kozlowski:1995:ENC

[KA95a] P. M. Kozlowski and L. Adamowicz. Effective nonadiabatic calculations on the ground state of the HD^+ molecule. *International Journal of Quantum Chemistry*, 55(3):245–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kozlowski:1995:MEO

[KA95b] P. M. Kozlowski and L. Adamowicz. Matrix elements for J_2 and J_z operators over explicitly correlated Cartesian Gaussian functions. *International Journal of Quantum Chemistry*, 55(5): 367–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khait:1996:TSE

[KA96] Yu. G. Khait and A. S. Averyanov. Theoretical study of the external electric field effect on the HeH_2 ($2^1A\prime$) metastable state. *International Journal of Quantum Chemistry*, 58(5):461–469, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60501`.

Kolmodin:1999:CMC

[KÅ99] Karin Kolmodin and Johan Åqvist. Computational modeling of catalysis and binding in low-molecular-weight protein tyrosine phosphatase. *International Journal of Quantum Chemistry*, 73(2):147–159, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003513; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003513&PLACEBO=IE.pdf`. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998.* Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Kaldor:1990:VFG

[Kal90] U. Kaldor. Vibrational frequencies and geometry of N_3 and $N_3{}^{---}$ the coupled-cluster method. *International Journal of*

Quantum Chemistry. Quantum Chemistry Symposium, 24:291–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Kanev:1993:ESH

[Kan93] I. Kanev. Electronic structure and hyperpolarizability of some conjugated molecules in excited states. *International Journal of Quantum Chemistry*, 48(5):333–??, December 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaplan:1999:NBS

[Kap99] I. G. Kaplan. Nature of binding in small metal clusters. *International Journal of Quantum Chemistry*, 74(2): 241–247, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003368; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003368&PLACEBO=IE.pdf`. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Karpfen:1990:ISH

[Kar90] A. Karpfen. Ab initio studies on hydrogen-bonded clusters: Structure and vibrational spectra of cyclic $(HF)_n$ complexes. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:129–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Karwowski:1994:STS

[Kar94] J. Karwowski. Statistical theory of spectra. *International Journal of Quantum Chemistry*, 51(6):425–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karlsson:1996:FCD

[Kar96] H. O. Karlsson. *Frontiers of Chemical Dynamics*. edited by E. Yurtsever. *International Journal of Quantum Chemistry*, 60(3): 789–??, 1996. CODEN IJQCB2.

Karna:1998:TCE

[Kar98] Shashi P. Karna. Theory and calculations of electric field effects on hyperfine interactions. *International Journal of Quantum Chemistry*, 70(4-5):771–778, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL

http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75055; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75055&PLACEBO=IE.pdf.

Kashiwagi:1976:IAB

[Kas76] H. Kashiwagi. Integral approximations on the basis of semiorthogonalized orbitals. *International Journal of Quantum Chemistry*, 10(??):135–141, ?? 1976. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kasha:1999:ILG

[Kas99] Michael Kasha. Introduction: Lionel Goodman's research career. *International Journal of Quantum Chemistry*, 72 (4):237, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006313; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006313&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Katriel:1993:PCS

[Kat93] J. Katriel. Products of class-sums of the symmetric group: Generalizing the recurrence relations. *International Journal of Quantum Chemistry*, 47(4):243–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Katriel:1997:PCS

[Kat97] Jacob Katriel. Products of class sums of the symmetric group: Rules of partial elimination. *International Journal of Quantum Chemistry*, 63(5):961–979, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42646; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42646&PLACEBO=IE.pdf.

Katriel:1998:CSP

[Kat98a] Jacob Katriel. Class-sum products in the symmetric group: Combinatorial interpretation of the reduced class coefficients. *International Journal of Quantum Chemistry*, 68 (2):103–118, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29930;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29930&PLACEBO=IE.pdf.

Katriel:1998:PAC

[Kat98b] Jacob Katriel. Products of arbitrary class-sums in the symmetric group. *International Journal of Quantum Chemistry*, 70(3):429–440, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75013; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75013&PLACEBO=IE.pdf.

Kucharski:1992:CCM

[KB92] S. A. Kucharski and R. J. Bartlett. Coupled-cluster method for an incomplete model space. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:107–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Kumicak:1993:CSL

[KB93] J. Kumicak and E. Brändas. Complex scaling and Lyapunov converters. *International Journal of Quantum Chemistry*, 46 (3):391–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Keith:1996:SHB

[KBA96] T. A. Keith, R. F. W. Bader, and Y. Aray. Structural homeomorphism between the electron density and the virial field. *International Journal of Quantum Chemistry*, 57(2):183–198, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60366.

Karlsson:1997:DSA

[KBGE97] H. O. Karlsson, G. L. Bendazzoli, O. Goscinski, and S. Evangelisti. Density of states of alternant cyclic polyenes (CH)N by a direct Lanczos method. *International Journal of Quantum Chemistry*, 63(3):719–728, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42615; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42615&PLACEBO=IE.pdf.

Kapuy:1993:ICE

[KBKT93] E. Kapuy, F. Bogar, C. Kozmutza, and E. Tfirst. Investigation of the correlation energy component of the intermolecular interaction energy. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:43–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Kleindienst:1995:AIH

[KBL95] H. Kleindienst, G. Buesse, and A. Luechow. Atomic integrals in Hylleraas-CI calculations with double-linked correlation terms. *International Journal of Quantum Chemistry*, 53 (5):575–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kapuy:1994:AMB

[KBT94] E. Kapuy, F. Bogar, and E. Tfirst. Application of many-body perturbation theory in the localized representation for the all-trans conjugated polyenes. *International Journal of Quantum Chemistry*, 52(1):127–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karwowski:1996:EMH

[KBWJ96] Jacek Karwowski, Dorota Bielínska-Waż, and Jacek Jurkowski. Eigenvalues of model Hamiltonian matrices from spectral density distribution moments: The Heisenberg spin Hamiltonian. *International Journal of Quantum Chemistry*, 60(1):185–193, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60582`.

Kovacs:1997:VAT

[KC97] Attila Kovács and Gábor I. Csonka. Vibrational analysis of $TeCl_4$. II. A Hartree–Fock, MP2, and density functional study. *International Journal of Quantum Chemistry*, 65(5): 817–826, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42813; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42813&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Konkoli:1998:NWAa

[KC98a] Zoran Konkoli and Dieter Cremer. A new way of analyzing vibrational spectra. I. derivation of adiabatic internal modes. *International Journal of Quantum Chemistry*, 67(1):1–9, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29881; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29881&PLACEBO=IE.pdf.

Konkoli:1998:NWAc

[KC98b] Zoran Konkoli and Dieter Cremer. A new way of analyzing vibrational spectra. III characterization of normal vibrational modes in terms of internal vibrational modes. *International Journal of Quantum Chemistry*, 67(1):29–40, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29883; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29883&PLACEBO=IE.pdf.

Krieger:1998:TDE

[KCI98] J. B. Krieger, J. Chen, and G. J. Iafrate. Theoretical determination of exact-exchange-mixing parameter employing the ionization energy theorem. *International Journal of Quantum Chemistry*, 69(3):255–264, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30000; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30000&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Krieger:1995:KST

[KCLI95] J. B. Krieger, J. Chen, Y. Li, and G. J. Iafrate. Kohn–Sham theory for orbital dependent exchange-correlation energy functionals: Application to the calculation of ionization potentials and electron affinities. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:79–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Krakauer:1990:ESE

[KCP90] H. Krakauer, R. E. Cohen, and W. E. Pickett. Evidence of strong electron-phonon coupling in the high T_c copper oxide superconductors. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:693–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Kozlowski:1995:OEP

[KD95] P. M. Kozlowski and E. R. Davidson. One-electron properties of molecules calculated using second-order multireference perturbation theory. *International Journal of Quantum Chemistry*, 53(2):149–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kessi:1998:DFC

[KD98] A. Kessi and B. Delley. Density functional crystal vs. cluster models as applied to zeolites. *International Journal of Quantum Chemistry*, 68(2):135–144, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29933; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29933&PLACEBO=IE.pdf`.

Karo:1990:SDS

[KDHW90] A. M. Karo, T. M. Deboni, J. R. Hardy, and G. A. Weiss. Shock dynamics in the sub-nanometer femtosecond domain. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:277–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Konschin:1991:MMP

[KE91] H. Konschin and M. Ekholm. Molecular modeling of pilocarpine prodrugs: A theoretical investigation of pilocarpic acid esters. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:247–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Kurasov:1993:CSS

[KE93] P. B. Kurasov and N. Elander. Complex scaling and self-adjoint dilations. *International Journal of Quantum Chemistry*, 46(3):415–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karadakov:1997:ESB

[KEG+97] Peter B. Karadakov, Michaela Ellis, Joseph Gerratt, David L. Cooper, and Mario Raimondi. The electronic structure of borabenzene: Combination of an aromatic π-sextet and a reactive σ-framework. *International Journal of Quantum Chemistry*, 63(2):441–449, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42588; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42588&PLACEBO=IE.pdf.

Kellman:1997:NSC

[Kel97] Michael E. Kellman. Nonrigid systems in chemistry: A unified view. *International Journal of Quantum Chemistry*, 65 (5):399–409, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42806; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42806&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Koch:1993:FES

[KEMM93] W. Koch, M. Eckert-Maksic, and Z. B. Maksic. Fluorination effect on the structural properties in benzocyclobutenes and benzocyclobutadienes. *International Journal of Quantum Chemistry*, 48(5):319–??, December 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kendall:1993:HPC

[Ken93] R. A. Kendall. High performance computing in chemistry and massively parallel computers: A simple transition? *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:769–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Kendrick:1997:EPF

[Ken97] Brian Kendrick. The effects of pseudomagnetic fields in molecular spectra and scattering. *International Journal of Quantum Chemistry*, 64(5):581–597, September 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42721; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42721&PLACEBO=IE.pdf. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

Kendrick:1998:EPF

[Ken98] Brian Kendrick. The effects of pseudomagnetic fields in molecular spectra and scattering. *International Journal of Quantum Chemistry*, 66(1):111, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29834; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29834&PLACEBO=IE.pdf.

Kurasov:1993:RIS

[KEP93] P. B. Kurasov, N. Elander, and B. Pavlov. Resonances and irreversibility for Schrödinger evolution. *International Journal of Quantum Chemistry*, 46(3):401–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koizumi:1996:FMCa

[KF96a] H. Koizumi and Y. Fukumoto. Fission of metal clusters: A comparison of jellium model calculations and shell correction method calculations. *International Journal of Quantum Chemistry*, 60(7):489–??, 1996. CODEN IJQCB2.

Koizumi:1996:FMCc

[KF96b] H. Koizumi and Y. Fukumoto. Fission of metal clusters: A comparison of jellium model calculations and shell correction method calculations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):489–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Koizumi:1996:FMCb

[KF96c] Hiroyasu Koizumi and Yuji Fukumoto. Fission of metal clusters: A comparison of jellium model calculations and shell correction method calculations. *International Journal of Quantum Chemistry*, 60(7):1701–1707, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60733.

Kladko:1998:PCE

[KF98] K. Kladko and P. Fulde. On the properties of cumulant expansions. *International Journal of Quantum Chemistry*, 66 (5):377–389, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29872; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29872&PLACEBO=IE.pdf.

Kanzler:1992:SIT

[KFS92] A. W. Kanzler, K. F. Freed, and M. G. Sheppard. Spin-independent three-body effective valence-shell operators: Application to molecular oxygen. *International Journal of Quantum Chemistry*, 44(4):643–??, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kubli-Garfias:1997:EST

[KG97] Carlos Kubli-Garfias. Electronic structure of testosterone: A semiempirical and ab initio assessment. *International Journal of Quantum Chemistry*, 62(3):279–289, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42513; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42513&PLACEBO=IE.pdf.

Kubli-Garfias:1998:IAE

[KG98] Carlos Kubli-Garfias. Ab initio assessment of the electronic structure of 5α-reduced progestins. *International Journal of Quantum Chemistry*, 67(5):329–338, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29911; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29911&PLACEBO=IE.pdf.

Kubli-Garfias:1999:CSE

[KG99] Carlos Kubli-Garfias. Comparative study of the electronic structure of pregnanolones by ab initio theory. *International Journal of Quantum Chemistry*, 71(5):433–440, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10050252; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10050252&PLACEBO=IE.pdf.

Karadakov:1996:MVB

[KGC+96] Peter B. Karadakov, Joseph Gerratt, David L. Cooper, Mario Raimondi, and Maurizio Sironi. Modern valence-bond description of the electronic structure of benzocyclobutadiene. *International Journal of Quantum Chemistry*, 60(1):545–552, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60618.

Korkin:1993:PAA

[KGS93] A. Korkin, M. Glukhovtsev, and P. Von Rague Schleyer. Polysila analogs of aromatic hydrocarbon ions: Structures and energies of $Si_3H_3{}^+$, $Si_4H_4{}^{2+}$, and $Si_5H_5{}^-$. *International Journal of Quantum Chemistry*, 46(1):137–144, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kubli-Garfias:1997:CAS

[KGVM97] Carlos Kubli-Garfias, Ricardo Vazquez, and Jesús Mendieta. Comparative AM1 study of the electronic structure of etiocholanes. *International Journal of Quantum Chemistry*, 64 (2):249–254, August 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42674; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42674&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Kim:1990:ENS

[KH90] H. J. Kim and J. T. Hynes. Equilibrium and nonequilibrium solvation and solute electronic structure. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24: 821–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Koures:1995:LCH

[KH95] V. G. Koures and F. E. Harris. Light cone Hamiltonian in quantum chemistry: Gaussian basis representation for quantum electrodynamics. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:277–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Kirby:1996:SLD

[KH96a] Robert A. Kirby and Aage E. Hansen. Study of locally dense and locally saturated basis sets in localized molecular orbital calculations of nuclear shielding: Ab initio LORG calculations for ^{13}C and ^{17}O in norbornenone. *International Journal of Quantum Chemistry*, 57(2):199–205, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60367.

Koures:1996:ICE

[KH96b] Antonios G. Koures and Frank E. Harris. Improved correlation energy functional. *International Journal of Quantum Chemistry*, 59(1):3–6, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60522.

Koures:1996:SCQa

[KH96c] V. G. Koures and F. E. Harris. Sinc collocation in quantum chemistry: Solving the planar Coulomb Schrödinger equation. *International Journal of Quantum Chemistry*, 60(7):99–??, 1996. CODEN IJQCB2.

Koures:1996:SCQc

[KH96d] V. G. Koures and F. E. Harris. Sinc collocation in quantum chemistry: Solving the planar Coulomb Schrödinger equation. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):99–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Koures:1996:SCQb

[KH96e] Vasilios G. Koures and Frank E. Harris. Sinc collocation in quantum chemistry: Solving the planar Coulomb Schrödinger equation. *International Journal of Quantum Chemistry*, 60 (7):1311–1318, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60688.

Kovacs:1997:HBI

[KH97] Attila Kovács and István Hargittai. Hydrogen-bonding interactions of the trifluoromethyl group: 2-Trifluoromethylvinyl alcohol. *International Journal of Quantum Chemistry*, 62

(6):645–652, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42548; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42548&PLACEBO=IE.pdf.

Khutorsky:1992:SAR

[Khu92] V. E. Khutorsky. Structure-activity relationships of ion transport compounds. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:187–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Keshari:1994:FPM

[KI94] V. Keshari and Y. Ishikawa. First-principles Monte Carlo simulated annealing study of the structures and properties of hydrogenated lithium clusters. *International Journal of Quantum Chemistry. Symposium*, 28:541–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Kidera:1999:SMC

[Kid99] Akinori Kidera. Smart Monte Carlo simulation of a globular protein. *International Journal of Quantum Chemistry*, 75(3):207–214, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000662/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000662&PLACEBO=IE.pdf.

Kiejna:1997:NRA

[Kie97] A. Kiejna. Nonlinear response of aluminum surface to electric field. *International Journal of Quantum Chemistry*, 61(4):699–703, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42442; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42442&PLACEBO=IE.pdf.

King:1993:IMT

[Kin93] J. W. King. The inverse molecular transform index: A descriptor for molecular similarity analysis. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and*

Quantum Pharmacology., 20:139–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

King:1994:CPC

[Kin94] J. W. King. Correlation of the partition coefficient with the molecular transform index in series of organophosphorus compounds. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21: 209–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Kinghorn:1996:IDC

[Kin96] Donald B. Kinghorn. Integrals and derivatives for correlated Gaussian functions using matrix differential calculus. *International Journal of Quantum Chemistry*, 57(2):141–155, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60361`.

King:1999:CAA

[Kin99] Frederick W. King. Convergence accelerator approach for the evaluation of some three-electron integrals containing explicit r_{ij} factors. *International Journal of Quantum Chemistry*, 72(2):93–99, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002776; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002776&PLACEBO=IE.pdf`.

Kirtman:1995:LQC

[Kir95] B. Kirtman. Local quantum chemistry: The local space approximation for Møller–Plesset perturbation theory. *International Journal of Quantum Chemistry*, 55(2):103–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koster:1993:MMA

[KJ93] A. M. Koster and K. Jug. Multipole moment analysis for hydrides, fluorides, and lithium compounds of first- and second-row elements. *International Journal of Quantum Chemistry*, 48 (5):295–??, December 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kar:1995:TTC

[KJ95] T. Kar and K. Jug. Is there any three-center CBC bond in 1,5-$C_2B_3H_5$ and 1,5-$C_2B_3H_3$? *International Journal of Quantum Chemistry*, 53(4):407–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Krissinel:1997:ANA

[KJ97] E. B. Krissinel and J. Jellinek. 13-atom Ni-Al alloy clusters: Structures and dynamics. *International Journal of Quantum Chemistry*, 62(2):185–197, March 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42502; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42502&PLACEBO=IE.pdf`.

Kalia:1993:ASP

[KJdL+93] R. K. Kalia, W. Jin, S. W. de Leeuw, A. Nakano, and P. Vashishta. Atomistic simulations on parallel architectures. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:781–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Kim:1996:UPIc

[KJL96a] M. S. Kim, Q. Jiang, and P. R. LeBreton. UV photoelectron and ab initio quantum mechanical characterization of nucleotides: The valence electronic structure of anionic 2'-deoxyadenosine-5'-phosphate. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 23(??):11–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

Kim:1996:UPIa

[KJL96b] N. S. Kim, Q. Jiang, and P. R. Lebreton. UV photoelectron and ab initio quantum mechanical characterization of nucleotides: The valence electronic structure of anionic 2'-deoxyadenosine-5'-phosphate. *International Journal of Quantum Chemistry*, 60 (8):11–??, 1996. CODEN IJQCB2.

Kim:1996:UPIb

[KJL96c] Nancy S. Kim, Qing Jiang, and Pierre R. Lebreton. UV photoelectron and ab initio quantum mechanical characterization of nucleotides: The valence electronic structure of anionic 2′-deoxyadenosine-5′-phosphate. *International Journal* of *Quantum Chemistry*, 60(8):1735–1743, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60746.

King:1991:DRI

[KK91] J. W. King and R. J. Kassel. Dimensional response of the integrated molecular transform. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:289–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

King:1992:MTQ

[KK92] J. W. King and R. J. Kassel. Molecular transform quantization of enzyme surface probes. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:179–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Koppenol:1993:ICO

[KK93] W. H. Koppenol and L. Klasinc. Ab initio calculations on ONOOH and $ONOO^-$. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:1–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Kafafi:1999:IDS

[KK99a] Sherif A. Kafafi and Morris Krauss. Ab initio determination of the structure of the active site of a metalloenzyme: Metal substitution in phosphotriesterase using density functional methods. *International Journal of Quantum Chemistry*, 75(3):289–299, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000670/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000670&PLACEBO=IE.pdf.

Kakkar:1999:ASP

[KK99b] Rita Kakkar and Vandana Katoch. AM1 study of proton-transfer reactions of barbituric acid. *International Journal of Quantum Chemistry*, 74(3):327–336, ???? 1999. CODEN

IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62004762; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62004762&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly*.

Kozmutza:1996:ALR

[KKE+96] C. Kozmutza, E. Kapuy, E. M. Evleth, J. Pipek, and L. Trezl. Application of the localized representation for studying interaction energies. *International Journal of Quantum Chemistry*, 57(4):775–780, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60416.

Koch:1994:BCC

[KKJ94] H. Koch, R. Kobayashi, and P. Jorgensen. Brueckner coupled cluster response functions. *International Journal of Quantum Chemistry*, 49(6):835–??, March 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

King:1990:IMT

[KKK90] J. W. King, R. J. Kassell, and B. B. King. The integrated molecular transform as a correlation parameter. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17:27–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Kofranek:1990:SFF

[KKL90] M. Kofranek, A. Karpfen, and H. Lischka. A scaled force field for polyenes derived from ab initio calculations including electron correlation effects. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:721–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Kushwaha:1999:CDM

[KKM99] P. S. Kushwaha, Anil Kumar, and P. C. Mishra. Charge distributions and molecular electrostatic potentials around amino acids: Usefulness of hybridization displacement charge. *International Journal of Quantum Chemistry*, 74(3):271–289, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62004768; http://www3.interscience.

wiley.com/cgi-bin/fulltext?ID=62004768&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly*.

Kawabe:1997:FTI

[KKNN97] H. Kawabe, K. Kodama, H. Nagao, and K. Nishikawa. Finite temperature ab initio calculation by path integral Monte Carlo method. *International Journal of Quantum Chemistry*, 65(5):471–476, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42775; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42775&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Kiribayashi:1999:SCF

[KKNY99] Shinji Kiribayashi, Takao Kobayashi, Masayoshi Nakano, and Kizashi Yamaguchi. Self-consistent-field calculations of molecular magnetic properties using gauge-invariant atomic orbitals. *International Journal of Quantum Chemistry*, 75(4–5):637–643, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004960/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004960&PLACEBO=IE.pdf.

Keseru:1999:ICP

[KKS99] György M. Keserü, István Kolossváry, and István Székely. Inhibitors of cytochrome P450 catalyzed insecticide metabolism: A rational approach. *International Journal of Quantum Chemistry*, 73(2):123–135, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003511; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003511&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998*. Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Koga:1993:AAD

[KKT93] T. Koga, Y. Kasai, and A. J. Thakkar. Accurate algebraic densities and intracules for heliumlike ions. *International Journal of Quantum Chemistry*, 46(6):689–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koga:1997:NPQ

[KKT97] Toshikatsu Koga, Katsutoshi Kanayama, and Ajit J. Thakkar. Noninteger principal quantum numbers increase the efficiency of Slater-type basis sets. *International Journal of Quantum Chemistry*, 62(1):1–11, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42482; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42482&PLACEBO=IE.pdf`.

Koga:1999:AHF

[KKWT99] Toshikatsu Koga, Katsutoshi Kanayama, Shinya Watanabe, and Ajit J. Thakkar. Analytical Hartree–Fock wave functions subject to cusp and asymptotic constraints: He to Xe, Li^+ to Cs^+, H^- to I^-. *International Journal of Quantum Chemistry*, 71(6):491–497, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=15000347; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=15000347&PLACEBO=IE.pdf`.

Kwiatkowski:1992:IPH

[KL92] J. S. Kwiatkowski and J. Leszczynski. Ab initio post-Hartree–Fock studies on molecular structure and vibrational IR spectrum of formaldehyde. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:421–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Kim:1993:PER

[KL93a] H. S. Kim and P. R. LeBreton. Polarization effects on the reversible and covalent DNA binding of bay- and K-region metabolites of benzo[a]pyrene and benz[a]anthracene. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:127–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Kleindienst:1993:MTO

[KL93b] H. Kleindienst and A. Luchow. Multiplication theorems for orthogonal polynomials. *International Journal of Quantum Chemistry*, 48(4):239–??, November 10, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

H:1993:HCL

[KL93c] Kleindienst, H. and A. Luchow. Hylleraas-CI with linked correlation terms. *International Journal of Quantum Chemistry*, 45(1):87–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Klein:1994:ECI

[KL94] D. J. Klein and X. Liu. Elemental carbon isomerism. *International Journal of Quantum Chemistry. Symposium*, 28:501–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Kravchenko:1997:AGT

[KL97a] Yu. P. Kravchenko and M. A. Liberman. Application of Gaussian-type basis sets to ab initio calculations in strong magnetic fields. *International Journal of Quantum Chemistry*, 64 (5):513–522, September 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42716; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42716&PLACEBO=IE.pdf`. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

Kravchenko:1997:AEP

[KL97b] Yu. P. Kravchenko and M. A. Liberman. On the application of extended precision arithmetic to quantum mechanical calculations. *International Journal of Quantum Chemistry*, 62(6):593–601, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42544; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42544&PLACEBO=IE.pdf`.

Kwiatkowski:1997:DFT

[KL97c] Józef S. Kwiatkowski and Jerzy Leszczynski. Density functional theory study on molecular structure and vibrational IR spectra of isocytosine. *International Journal of Quantum Chemistry*, 61(3):453–465, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42413; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42413&PLACEBO=IE.pdf.

Klauder:1993:QFT

[Kla93] J. R. Klauder. Quantum field theory: A modern introduction. by Michio Kaku. *International Journal of Quantum Chemistry*, 48(2):147–??, October 15, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Konkoli:1998:NWAb

[KLC98a] Zoran Konkoli, J. Andreas Larsson, and Dieter Cremer. A new way of analyzing vibrational spectra. II. comparison of internal mode frequencies. *International Journal of Quantum Chemistry*, 67(1):11–27, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29882; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29882&PLACEBO=IE.pdf.

Konkoli:1998:NWAd

[KLC98b] Zoran Konkoli, J. Andreas Larsson, and Dieter Cremer. A new way of analyzing vibrational spectra. IV. Application and testing of adiabatic modes within the concept of the characterization of normal modes. *International Journal of Quantum Chemistry*, 67(1):41–55, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29884; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29884&PLACEBO=IE.pdf.

Karasiev:1998:SCD

[KLLB98] V. Karasiev, E. V. Ludeña, and R. López-Boada. SCF calculations with density-dependent local-exchange potential. *International Journal of Quantum Chemistry*, 70(4-5):591–600, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75037; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75037&PLACEBO=IE.pdf.

Krieger:1997:SAA

[KLLI97] J. B. Krieger, Yan Li, Yili Liu, and G. J. Iafrate. Simplified accurate approximation for the Kohn–Sham potential using the KLI method. *International Journal of Quantum Chemistry*, 61(2):273–279, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42408; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42408&PLACEBO=IE.pdf`.

Klotz:1990:HBF

[Klo90] I. M. Klotz. How to become famous by being wrong in science. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:881–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Kim:1998:KUH

[KLO+98] Yong Suk Kim, Sang Yeon Lee, Won Seok Oh, Bo Hyun Park, Young Kyu Han, Su Jin Park, and Yoon Sup Lee. Kramers' unrestricted Hartree–Fock and second-order Møller–Plesset perturbation methods using relativistic effective core potentials with spin-orbit operators: Test calculations for HI and CH_3 I. *International Journal of Quantum Chemistry*, 66(1):91–98, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29840; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29840&PLACEBO=IE.pdf`.

Kotochigova:1997:CRC

[KLT97] S. Kotochigova, H. Levine, and I. Tupitsyn. Correlated relativistic calculation of the giant resonance in the Gd_3^+ absorption spectrum. *International Journal of Quantum Chemistry*, 65(5):575–584, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42787; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42787&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Klasinc:1990:PSB

[KM90] L. Klasinc and S. P. McGlynn. Photoelectron spectroscopy of biologically active molecules 21. thiooxamides. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:813–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Karafiloglou:1992:IPS

[KM92] P. Karafiloglou and E. Sanchez Marcos. Investigating the possibility of simultaneously finding an electron-hole and an electron-pair in a molecule: Delocalization competition of ionic vs. covalent character, and related effects in push-pull ethylenes. *International Journal of Quantum Chemistry*, 44(3):337–??, September 30, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

King:1997:COD

[KM97] James W. King and Stephen P. Molnar. Correlation of organic diamagnetic susceptibility with structure via the integrated molecular transform. *International Journal of Quantum Chemistry*, 64(5):635–645, September 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42713; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42713&PLACEBO=IE.pdf`. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

King:1999:SAM

[KM99a] James W. King and Stephen P. Molnar. Surface area minimization in small peptide folding. *International Journal of Quantum Chemistry*, 75(6):1043–1047, December 20, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004791/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004791&PLACEBO=IE.pdf`.

Koga:1999:ECE

[KM99b] Toshikatsu Koga and Hisashi Matsuyama. Explicitly correlated extracule densities for two-electron atoms. *International Journal of Quantum Chemistry*, 74(5):455–465, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62502998; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62502998&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Kumar:1995:HDC

[KMM95] A. Kumar, C. G. Mohan, and P. C. Mishra. Hybridization displacement charge in molecules and its effects on electrostatic potentials and fields. *International Journal of Quantum Chemistry*, 55(1):53–??, July 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kuhn:1996:TDD

[KMM96] O. Kühn, D. Malzahn, and V. May. Theoretical description of dissipative vibrational dynamics using the density matrix in the state representation. *International Journal of Quantum Chemistry*, 57(3):343–353, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60395.

Kibler:1994:GKC

[KMP94] M. Kibler, L. G. Mardoyan, and G. S. Pogosyan. On a generalized Kepler–Coulomb system: Interbasis expansions. *International Journal of Quantum Chemistry*, 52(6):1301–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kibler:1997:GOS

[KMP97] Maurice Kibler, Levon G. Mardoyan, and George S. Pogosyan. On a generalized oscillator system: Interbasis expansions. *International Journal of Quantum Chemistry*, 63(1):133–148, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42560; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42560&PLACEBO=IE.pdf.

Knuts:1995:SOC

[KMVA95] S. Knuts, B. F. Minaev, O. Vahtras, and H. Agren. Spin-orbit coupling in the intersystem crossing of the ring-opened oxirane biradical. *International Journal of Quantum Chemistry*, 55(1):

23–??, July 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Korchowiec:1992:GEF

[KN92] J. Korchowiec and R. F. Nalewajski. Group electronegativity and Fukui function studies of the substituent effects in aromatic and inorganic systems. *International Journal of Quantum Chemistry*, 44(6):1027–??, December 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Komninos:1999:EMS

[KN99a] Yannis Komninos and Cleanthes A. Nicolaides. Erratum: Molecular shape, shape of the geometrically active atomic states, and hybridization. *International Journal of Quantum Chemistry*, 74(4):435, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62502087; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62502087&PLACEBO=IE.pdf. See [KN99b].

Komninos:1999:MSS

[KN99b] Yannis Komninos and Cleanthes A. Nicolaides. Molecular shape, shape of the geometrically active atomic states, and hybridization. *International Journal of Quantum Chemistry*, 71(1):25–34, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000010; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000010&PLACEBO=IE.pdf. See erratum [KN99a].

Kawabe:1994:PIA

[KNA94] H. Kawabe, K. Nishikawa, and S. Aono. Path integral approach to correlation energy. *International Journal of Quantum Chemistry*, 51(4 (or 5??)):265–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kawabe:1996:PIF

[KNN96a] H. Kawabe, H. Nagao, and K. Nishikawa. Path integral formulation for many-electron system. *International Journal of Quantum Chemistry*, 59(6):457–469, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60564.

Kawabe:1996:PIMa

[KNN96b] H. Kawabe, H. Nagao, and K. Nishikawa. Path integral Monte Carlo method for ab initio calculation. *International Journal of Quantum Chemistry*, 60(7):11–??, 1996. CODEN IJQCB2.

Kawabe:1996:PIMb

[KNN96c] H. Kawabe, H. Nagao, and K. Nishikawa. Path integral Monte Carlo method for ab initio calculation. *International Journal of Quantum Chemistry*, 60(7):1223–1230, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60696`.

Kawabe:1996:PIMc

[KNN96d] H. Kawabe, H. Nagao, and K. Nishikawa. Path integral Monte Carlo method for ab initio calculation. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??): 11–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Kouba:1969:PME

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

Kristyan:1995:CEN

[KO95] S. Kristyan and J. A. Olson. Charge-exchange in the nonadiabatic Na/W gas-surface reaction using a diabatic representation. *International Journal of Quantum Chemistry*, 56(1):51–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kohn:1995:DFT

[Koh95] W. Kohn. Density functional theory for systems of very many atoms. *International Journal of Quantum Chemistry*, 56(4): 229–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kollmar:1997:COR

[Kol97] Christian Kollmar. Convergence optimization of restricted open-shell self-consistent field calculations. *International Journal of Quantum Chemistry*, 62(6):617–637, ???? 1997. CODEN

IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42546; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42546&PLACEBO=IE.pdf.

Konarski:1994:NMM

[Kon94] J. Konarski. A new model of a molecule based on the soft body. *International Journal of Quantum Chemistry*, 51(6):439–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kornberg:1995:ULC

[Kor95] A. Kornberg. Understanding life as chemistry. *International Journal of Quantum Chemistry*, 53(1):125–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kovalenko:1998:ESS

[Kov98a] Andriy Kovalenko. Extended states of a shallow donor located near a semiconductor-insulator interface. *International Journal of Quantum Chemistry*, 66(6):435–456, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29879; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29879&PLACEBO=IE.pdf.

Kovarsky:1998:MPE

[Kov98b] Victor A. Kovarsky. Multiquantum processes in the enzyme molecules immobilized on biological membranes. *International Journal of Quantum Chemistry*, 66(3):255–260, January 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29859; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29859&PLACEBO=IE.pdf.

Kaufman:1975:TCC

[KP75] J. J. Kaufman and H. E. Popkie. Test of charge-conserving integral approximations for A variable retention of diatomic differential overlap (VRDO) procedure for semi-ab initio molecular orbital calculations on large molecules. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology* *and Quantum Pharmacology.*, 2(??):279–288, ?? 1975. CODEN IJQBDZ. ISSN 0360-8832.

Katriel:1993:ESC

[KP93] J. Katriel and R. Pauncz. Eigenvalues of single-cycle class-sums in the symmetric group II. *International Journal of Quantum Chemistry*, 48(2):125–??, October 15, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kakkar:1996:CHT

[KP96] Rita Kakkar and Bhabani S. Padhi. C_3 H_4: Theoretical study of structures and stabilities of isomers. *International Journal of Quantum Chemistry*, 58(4):389–398, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60495.

Kinghorn:1997:IGF

[KP97] Donald B. Kinghorn and R. D. Poshusta. Implementation of gradient formulas for correlated Gaussians: He, $^{\infty}$He, Ps_2, $_9$Be, and $^{\infty}$Be test results. *International Journal of Quantum Chemistry*, 62(2):223–235, March 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42495; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42495&PLACEBO=IE.pdf.

Khait:1995:SSP

[KPA95] Yu G. Khait, A. I. Panin, and A. S. Averyanov. Search for stationary points of arbitrary index by augmented Hessian method. *International Journal of Quantum Chemistry*, 54(6):329–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kurth:1999:MSS

[KPB99] Stefan Kurth, John P. Perdew, and Peter Blaha. Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs. *International Journal of Quantum Chemistry*, 75(4–5):889–909, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004985/START; http://www3.

interscience.wiley.com/cgi-bin/fulltext?ID=66004985&PLACEBO=IE.pdf.

Kasha:1993:CCQ

[KPD93] M. Kasha, D. Parthenopoulos, and B. Dellinger. Challenges to computational quantum chemistry from contemporary advances in polyatomic molecular electronic spectroscopy. *International Journal of Quantum Chemistry*, 45(6):689–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Krishna:1990:TAD

[KPM+90] K. M. Krishna, V. A. Pai, V. R. Marathe, M. Sharon, and M. K. Mishra. A theoretical approach to the design of reduced band gap noncorrosive electrodes for photoelectrochemical solar cells. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:419–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Karwowski:1997:AEE

[KPR97] J. Karwowski, J. Planelles, and F. Rajadell. Average energy of an N-electron system in a finite-dimensional and spin-adapted model space. *International Journal of Quantum Chemistry*, 61(1):63–65, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42386; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42386&PLACEBO=IE.pdf.

Klasinc:1993:LRI

[KPTS+93] L. Klasinc, L. J. Pasa-Tolic, H. Spiegl, J. V. Knop, and S. P. McGlynn. Long-range interactions of substituents in steroidal molecules. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:191–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Kolezynski:1994:ECF

[KPTS94] A. Kolezynski, W. S. Ptak, and K. Tkacz-Smiech. Effective crystal field approach to the binding energy calculation of alkaline metals. *International Journal of Quantum Chemistry*, 52(2):321–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kolezynski:1997:OSM

[KPTS97] Andrzej Koleżyński, Wiesław S. Ptak, and Katarzyna Tkacz-Śmiech. Overlapping shells model applied to diamondlike crystals. *International Journal of Quantum Chemistry*, 61 (5):741–746, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42456; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42456&PLACEBO=IE.pdf`.

Klasinc:1997:LRE

[KPTVT+97] Leo Klasinc, Ljiljana Paša-Tolić, Dražen Vikić-Topić, Jan V. Knop, and Sean P. McGlynn. Long-range electronic interactions in androstanediones. *International Journal of Quantum Chemistry*, 63(3):797–803, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42621; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42621&PLACEBO=IE.pdf`.

Kelterer:1993:ISI

[KR93] A.-M. Kelterer and M. Ramek. Ab initio SCF investigation of the potential energy surface of 4-aminobutanol. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:479–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Klein:1997:HOD

[KRB+97] Douglas J. Klein, Milan Randić, Darko Babić, Bono Lučić, Sonja Nikolić, and Nenad Trinajstić. Hierarchical orthogonalization of descriptors. *International Journal of Quantum Chemistry*, 63(1):215–222, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42566; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42566&PLACEBO=IE.pdf`.

Klein:1994:CCP

[KRBT94] D. J. Klein, M. Randić, D. Babić, and N. Trinajstić. On conjugated-circuit polynomials. *International Journal of Quantum Chemistry*, 50(5):369–384, May 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kombo:1999:CAV

[KRRB99] David C. Kombo, G. Ravishanker, S. Rackovsky, and David L. Beveridge. Computational analysis of variants of the operator binding domain of the bacteriophage λ repressor. *International Journal of Quantum Chemistry*, 75(3):313–325, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/65000672/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000672&PLACEBO=IE.pdf`.

Kruglevsky:1992:EHD

[Kru92] V. Kruglevsky. Electronic Hamiltonian of diatomic molecules in the basis of coupled momenta eigenfunctions. *International Journal of Quantum Chemistry*, 44(3):393–??, September 30, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kruger:1997:ECM

[Krü97] Thomas Krüger. EPR correlations in the molecular domain. *International Journal of Quantum Chemistry*, 64(6):679–687, September 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42729`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42729&PLACEBO=IE.pdf`.

Kryachko:1993:CPC

[Kry93] E. S. Kryachko. On the Car–Parrinello computational scheme: Rigouous treatment. *International Journal of Quantum Chemistry*, 48(2):109–??, October 15, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:1995:WFC

[Kry95] E. S. Kryachko. On wave-function correction to Hellmann–Feynman force: Hartree–Fock method. *International Journal of Quantum Chemistry*, 56(1):3–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:1996:LME

[Kry96] Eugene S. Kryachko. Lagrangian many-electron molecular dynamics — A modern tool for attacking the chemical bond:

The physics behind the equations. *International Journal of Quantum Chemistry*, 60(1):331–346, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60596`.

Kryachko:1998:WCA

[Kry98] Eugene S. Kryachko. Water cluster approach to study hydrogen-bonded pattern in liquid water: Ab initio orientational defects in water hexamers and octamers. *International Journal of Quantum Chemistry*, 70(4-5):831–853, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75062`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75062&PLACEBO=IE.pdf`.

Kotzian:1991:ICT

[KRZ91] M. Kotzian, N. Rosch, and M. C. Zerner. An INDO/ S-CI treatment including spin-orbit interaction based on Rumer spin functions. application to the hydrated cerium ion. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:545–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Kashiwagi:1973:GLO

[KS73] H. Kashiwagi and F. Sasaki. A generalization of the Löwdin orthogonalization. *International Journal of Quantum Chemistry*, S7(??):515–520, ?? 1973. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaschner:1994:IHB

[KS94a] R. Kaschner and G. Seifert. Investigations of hydrogen-bonded systems: Local density approximation and gradient corrections. *International Journal of Quantum Chemistry*, 52(4):957–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kieninger:1994:DFS

[KS94b] M. Kieninger and S. Suhai. Density functional studies on hydrogen-bonded complexes. *International Journal of Quantum Chemistry*, 52(2):465–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kirschner:1994:QMI

[KS94c] K. N. Kirschner and G. C. Shields. Quantum-mechanical investigation of large water clusters. *International Journal of Quantum Chemistry. Symposium*, 28:349–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Kar:1995:PTE

[KS95a] T. Kar and S. Scheiner. Proton transfer in $H_5O_2^+$ and $H_3O_2{}^-$ with an external restraining force. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:567–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Kibler:1995:CEA

[KS95b] M. Kibler and Y. Smirnov. Coulomb energy averaged over the nl^N-atomic states with a definite spin. *International Journal of Quantum Chemistry*, 53(5):495–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kohout:1996:ASS

[KS96] M. Kohout and A. Savin. Atomic shell structure and electron numbers. *International Journal of Quantum Chemistry*, 60(4): 875–882, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60647`.

Kello:1998:PCC

[KS98] Vladimir Kellö and Andrzej J. Sadlej. Picture change and calculations of expectation values in approximate relativistic theories. *International Journal of Quantum Chemistry*, 68(3):159–174, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29937; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29937&PLACEBO=IE.pdf`.

Kadolkar:1993:SRM

[KSG93] C. Kadolkar, C. R. Sarma, and D. K. Ghosh. A scheme for representation matrices of a permutation group using spin-paired functions. *International Journal of Quantum Chemistry*, 47(3): 185–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kais:1994:LDA

[KSH94] S. Kais, S. M. Sung, and D. R. Herschbach. Large-Z and -N dependence of atomic energies from renormalization of the large-dimension limit. *International Journal of Quantum Chemistry*, 49(5):657–??, February 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kulander:1991:SAE

[KSK91] Kenneth C. Kulander, Kenneth J. Schafer, and Jeffrey L. Krause. Single-active electron calculation of multiphoton process in krypton. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:415–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Kumar:1999:DLR

[KSK+99] Anil Kumar, Bidhan C. Saha, Ali A. Khan, Vijay Kumar, Sunil K. Verma, and Krishna K. Prasad. Depopulation of low-Rydberg Na atom in collisions with rare gases: A molecular-state treatment. *International Journal of Quantum Chemistry*, 73(3):307–316, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003698; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003698&PLACEBO=IE.pdf`.

Kantorovich:1994:QCS

[KSKJ94] L. Kantorovich, A. Stashans, E. Kotomin, and P. W. M. Jacobs. Quantum chemical simulations of hole self-trapping in semi-ionic crystals. *International Journal of Quantum Chemistry*, 52 (5):1177–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaplan:1993:TSG

[KSN93] I. G. Kaplan, R. Santamaria, and O. Novaro. Theoretical study of the geometric structures and energetic properties of anionic clusters. ag_n^- (n = 2to6). *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:743–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Kaplan:1995:NIR

[KSN95] I. G. Kaplan, R. Santamaria, and O. Novaro. Nonadditive interactions and the relative stability of neutral and anionic silver clusters. *International Journal of Quantum Chemistry*, 55(3): 237–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kadolkar:1995:CIS

[KSR95] C. Kadolkar, C. R. Sarma, and S. Rettrup. Configuration interaction studies using biorthogonal approach to VB basis. *International Journal of Quantum Chemistry*, 53(2):183–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kumar:1998:SEC

[KSW98] Anil Kumar, Bidhan C. Saha, and Charles A. Weatherford. Single-electron-capture cross sections by alpha-particles from ground state K(4*s*) and Rb(5*s*): A molecular-state approach. *International Journal of Quantum Chemistry*, 70 (4-5):909–917, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75068; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75068&PLACEBO=IE.pdf.

Kobayashi:1997:CFD

[KSY97] Takao Kobayashi, Kotoku Sasagane, and Kizashi Yamaguchi. Calculation of frequency-dependent polarizabilities for open-shell systems at the second-order Møller–Plesset perturbation theory level based on the quasi-energy derivative method. *International Journal of Quantum Chemistry*, 65(5):665–677, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42799; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42799&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Kotochigova:1995:ESM

[KT95] S. Kotochigova and I. Tupitsyn. Electronic structure of molecules by the numerical generalized-valence-bond wave functions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:307–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Koga:1996:KEA

[KT96] Toshikatsu Koga and Ajit J. Thakkar. Kinetic energy analysis of atomic multiplets. *International Journal of Quantum Chemistry*, 57(1):89–94, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60347`.

Komninos:1993:PTE

[KTCN93] Y. Komninos, S. Themelis, M. Chrysos, and C. A. Nicolaides. Properties of the two-electron ionization ladder and related good quantum numbers. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:399–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Koga:1997:RLL

[KTT97] Toshikatsu Koga, Tomomi Tanabe, and Ajit J. Thakkar. Radial limit of lithium revisited. *International Journal of Quantum Chemistry*, 63(2):287–290, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42582; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42582&PLACEBO=IE.pdf`.

Kumar:1993:QFT

[Kum93a] P. Kumar. *Quantum Field Theory and Critical Phenomena*, by J. Zinn-Justin. *International Journal of Quantum Chemistry*, 46(6):745–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kumar:1993:TCP

[Kum93b] P. Kumar. The theory of critical phenomena: An introduction to the renormalization group. by J. J. Binney, N. J. Dowrickm, A. J. Fisher, and M. E. J. Newman. *International Journal of Quantum Chemistry*, 46(5):671–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kunz:1990:CMS

[Kun90] A. B. Kunz. Cluster modeling of solid state defects and adsorbates: Beyond the Hartree–Fock level. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24: 607–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Kamada:1998:EHA

[KUN+98] Kenji Kamada, Minoru Ueda, Hidemi Nagao, Keiko Tawa, Takushi Sugino, Yo Shimizu, and Koji Ohta. Effect of heavy atom on the second hyperpolarizability of tetrahydrofuran homologs investigated by ab initio molecular orbital method. *International Journal of Quantum Chemistry*, 70 (4-5):737–743, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75051; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75051&PLACEBO=IE.pdf`.

Kunne:1999:RBD

[Kün99] L. Künne. Relations between DFT and CI approximation. *International Journal of Quantum Chemistry*, 74 (1):55–58, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62000138; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62000138&PLACEBO=IE.pdf`.

Kuprievich:1994:ACD

[Kup94] V. A. Kuprievich. Alternating charge densities, Peierls distortion, and charge-conjugation symmetry in correlated one-dimensional diatomic systems. *International Journal of Quantum Chemistry*, 52(2):329–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kuprievich:1998:MSA

[Kup98] Victor A. Kuprievich. Multiconfigurational SCF approach for high-symmetry molecules and its applications to fullerene trianion. *International Journal of Quantum Chemistry*, 68 (5):293–304, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29950; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29950&PLACEBO=IE.pdf`.

Kurtz:1990:SCH

[Kur90] H. A. Kurtz. Semiempirical calculation of the hyperpolarizabilities of polyenes. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:791–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Kutzelnigg:1994:TEW

[Kut94] W. Kutzelnigg. Theory of the expansion of wave functions in a Gaussian basis. *International Journal of Quantum Chemistry*, 51(6):447–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kutzelnigg:1996:EEP

[KV96] Werner Kutzelnigg and Stefan Vogtner. Extremal electron pairs. *International Journal of Quantum Chemistry*, 60(1): 235–248, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60587.

Karwowski:1997:DLV

[KVB97] Jacek Karwowski, Oscar N. Ventura, and Małgorzata Bancewicz. Density of levels in vibrational spectra of molecules. *International Journal of Quantum Chemistry*, 63(4):835–842, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42634; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42634&PLACEBO=IE.pdf.

Kieninger:1998:DFI

[KVS98] Martina Kieninger, Oscar N. Ventura, and Sandor Suhai. Density functional investigations of carboxyl free radicals: Formyloxyl, acetyloxyl, and benzoyloxyl radicals. *International Journal of Quantum Chemistry*, 70(2):253–267, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74994; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74994&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Kakkar:1992:TST

[KW92] R. Kakkar and V. Walia. Theoretical study of the thermal unimolecular rearrangement of fluoroethylidenes. *International Journal of Quantum Chemistry*, 44(3):363–??, September 30, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Krauss:1998:VCS

[KW98] M. Krauss and B. D. Wladkowski. Vanadate complex spectroscopy at the RNase A active site. *International Journal of Quantum Chemistry*, 69(1):11–19, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29968; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29968&PLACEBO=IE.pdf.

Koga:1995:NHF

[KWT95] T. Koga, S. Watanabe, and A. J. Thakkar. Numerical Hartree–Fock results for atoms Cs through Lr. *International Journal of Quantum Chemistry*, 54(4):261–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kollman:1998:ITC

[KWZ98] Peter Kollman, Harel Weinstein, and Michael Zerner. Introduction: Theoretical chemistry in biology: From molecular structure to functional mechanisms. *International Journal of Quantum Chemistry*, 69(1):1, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29962; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29962&PLACEBO=IE.pdf.

Kong:1993:EAM

[KY93] J. Kong and J.-M. Yan. The effects of atomic multipole moments obtained by the potential-derived method on hydrogen bonding. *International Journal of Quantum Chemistry*, 46(2):239–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Krakauer:1995:ILR

[KYW95] H. Krakauer, R. Yu, and C.-Z. Wang. Ab initio linear response calculations of lattice dynamics using an LAPW basis. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:131–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Kneisler:1994:SEC

[KZ94] J. Kneisler and Z. Zhou. Substituent effects on chemical hardness. *International Journal of Quantum Chemistry*, 49(3):309–

??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kennedy:1999:EIS

[KZ99] H. L. Kennedy and Y. Zhao. Evaluation of integrals over STOs on different centers and the complementary convergence characteristics of ellipsoidal-coordinate and zeta-function expansions. *International Journal of Quantum Chemistry*, 71(1):1–13, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000006; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000006&PLACEBO=IE.pdf.

Klein:1997:MBV

[KZVGB97] D. J. Klein, H. Zhu, R. Valenti, and M. A. Garcia-Bach. Many-body valence-bond theory. *International Journal of Quantum Chemistry*, 65(5):421–438, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42832; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42832&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Lefebvre:1997:GFM

[LA97] R. Lefebvre and O. Atabek. Gauges and fluxes in multiphoton absorption by H_2^+. *International Journal of Quantum Chemistry*, 63(2):403–414, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42584; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42584&PLACEBO=IE.pdf.

Ladik:1997:OGF

[Lad97a] Janos Ladik. Outlines of a general framework of cancer initiation in the cell. *International Journal of Quantum Chemistry*, 64(3):379–385, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42693;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42693&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Ladik:1997:CCE

[Lad97b] Janos J. Ladik. Correlation-corrected energy band (level) structures of low-dimensional systems. *International Journal of Quantum Chemistry*, 63(3):631–635, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42624; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42624&PLACEBO=IE.pdf.

Lahti:1992:SII

[Lah92] P. M. Lahti. A semiempirical investigation of interelectronic exchange coupling in bisected poly(1,4-phenylene) polycation model systems. *International Journal of Quantum Chemistry*, 44(5):785–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lai:1994:CAF

[Lai94] S.-T. Lai. Computation of algebraic formulas for Wigner 3-j, 6-j, and 9-j symbols by Maple. *International Journal of Quantum Chemistry*, 52(3):593–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Laszlo:1993:SEE

[Las93] I. Laszlo. Stable electronic energy level in the presence of off-diagonal disorder. *International Journal of Quantum Chemistry*, 48(2):135–??, October 15, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lundqvist:1995:DFT

[LAS+95] B. I. Lundqvist, Y. Andersson, H. Shao, S. Chan, and D. C. Langreth. Density functional theory including van der Waals forces. *International Journal of Quantum Chemistry*, 56(4):247–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larsson:1993:PMP

[LB93] S. Larsson and M. Braga. Pathways and mobile pi electrons in biological electron transfer. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:65–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Loegdlund:1994:SSI

[LB94] M. Loegdlund and J. L. Brédas. Semiempirical studies of the interaction between metals and — conjugated polymers: Sodium on diphenylpolyenes and aluminum on poly(p-phenylenevinylene) and derivatives. *International Journal of Quantum Chemistry. Symposium*, 28:481–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Lohr:1995:DMH

[LB95] L. L. Lohr and S. M. Blinder. Deltafunction model for the helium dimer. *International Journal of Quantum Chemistry*, 53(4):413–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

LaManna:1996:MSH

[LB96a] Gianfranco La Manna and Giampaolo Barone. The molecular structure of *N*-hydroxyurea. *International Journal of Quantum Chemistry*, 57(5):971–974, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60435`.

Levitina:1996:PWNa

[LB96b] T. Levitina and E. J. Brändas. Partial waves in the nonspherical case. *International Journal of Quantum Chemistry*, 60(7):5–??, 1996. CODEN IJQCB2.

Levitina:1996:PWNb

[LB96c] T. Levitina and E. J. Brändas. Partial waves in the nonspherical case. *International Journal of Quantum Chemistry*, 60(7):1217–1221, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60685`.

Levitina:1996:PWNc

[LB96d] T. Levitina and E. J. Brandas. Partial waves in the nonspherical case. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):5–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Levitina:1997:SPS

[LB97] T. Levitina and E. J. Brändas. Scattering by a potential separable in ellipsoidal coordinates. *International Journal of Quantum Chemistry*, 65(5):601–608, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42790; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42790&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Levitina:1998:PEW

[LB98] T. Levitina and E. J. Brändas. Perturbed ellipsoidal wave functions for quantum scattering. *International Journal of Quantum Chemistry*, 70(4-5):1017–1022, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75023; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75023&PLACEBO=IE.pdf.

Lorenzini:1998:TAP

[LBBE98] M. L. Lorenzini, L. Bruno-Blanch, and G. L. Estiú. Theoretical approach to the pharmacophoric pattern of GABAB analogs. *International Journal of Quantum Chemistry*, 70 (6):1195–1208, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75087; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75087&PLACEBO=IE.pdf.

Larsson:1991:EFB

[LBBK91] S. Larsson, M. Braga, A. Broo, and B. Kallebring. Electronic factor in biological electron transfer systems role of aromatic side groups. *International Journal of Quantum Chemistry.*

Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology., 18:99–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Lushington:1995:ISM

[LBG95] G. H. Lushington, P. Bundgen, and F. Grein. Ab initio study of molecular g-tensors. *International Journal of Quantum Chemistry*, 55(5):377–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lushington:1997:ESM

[LBG97] Gerald H. Lushington, Pablo J. Bruna, and Friedrich Grein. Electron-spin magnetic moments of the $^2\Sigma^+$ ions Li_2^+, Li_2^-, and Be_2^+: An ab initio ROHF study. *International Journal of Quantum Chemistry*, 63(2):511–521, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42594; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42594&PLACEBO=IE.pdf.

Lopez-Boada:1998:AKE

[LBKLC98] R. Lopez-Boada, V. Karasiev, E. V. Ludena, and R. Colle. Atomic kinetic- and exchange-energy functionals by means of local-scaling transformations. *International Journal of Quantum Chemistry*, 69(4):503–512, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30023; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30023&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Lopez-Boada:1998:HFC

[LBL98] R. López-Boada and E. V. Ludeña. Hartree–Fock calculations in the context of the local-scaling transformation version of density functional theory. Applications to the Lithium and Beryllium atoms. *International Journal of Quantum Chemistry*, 69(4):485–496, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30021; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30021&PLACEBO=IE.pdf. Special Issue: *Symposium on Den-*

sity Functional Theory and Applications (Part II of II). Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Lopez-Boada:1998:GEE

[LBLKC98] R. López-Boada, E. V. Ludeña, V. Karasiev, and R. Colle. Generation of explicit electron correlation functional by means of local scaling transformations. *International Journal of Quantum Chemistry*, 69(4):439–450, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30006; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30006&PLACEBO=IE.pdf`. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Lavin:1994:RQD

[LBM94] C. Lavin, C. Barrientos, and I. Martin. Relativistic quantum defect calculations on the copper isoelectronic sequence. *International Journal of Quantum Chemistry*, 50(6):411–??, June 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lopez-Bonilla:1995:HTM

[LBMR95] J. L. López-Bonilla, J. Morales, and M. A. Rosales. Hypervirial theorem and matrix elements for the Coulomb potential. *International Journal of Quantum Chemistry*, 53(1):3–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lopez-Boada:1997:EEM

[LBPL97] R. López-Boada, R. Pino, and E. V. Ludeña. Explicit expressions for $T_s[\rho]$ and $E_x[\rho]$ by means of Padé approximants to local-scaling transformations. *International Journal of Quantum Chemistry*, 63(6):1025–??, July 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Loew:1993:TSO

[LC93] G. H. Loew and Y.-T. Chang. Theoretical studies of the oxidation of N- and S-containing compounds by cytochrome P450. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:815–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Lam:1998:VEC

[LCB98] Kin-Chung Lam, Federico G. Cruz, and Kieron Burke. Virial exchange-correlation energy density in Hooke's atom. *International Journal of Quantum Chemistry*, 69(4):533–540, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30007; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30007&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Liu:1995:NBT

[LCLO95] H.-L. Liu, N.-Y. Chen, J. J. Ladik, and P. Otto. A new boundary treatment: HF surface potential model applied to solid-state cluster calculations. *International Journal of Quantum Chemistry*, 54(2):89–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luan:1991:BSC

[LCP+91] C. H. Luan, D. K. Chang, T. M. Parker, N. Rama Krishna, and D. W. Urry. beta-Spiral conformations of the elastomeric polytetrapeptides, $(VPGG)_n$ and $(IPGG)_n$, by 2D NMR and molecular mechanics studies. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:183–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Lu:1998:TSFb

[LCS98] Li-Hwa Lu, Cheng Chen, and Kuang-Chung Sun. Theoretical study of fullerene derivatives: C_{40} H_4 and C_{40} X_4 cluster molecules. *International Journal of Quantum Chemistry*, 68(4):273–284, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29947; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29947&PLACEBO=IE.pdf.

Lisini:1994:CEP

[LD94] A. Lisini and P. Decleva. Calculation of excitation and photoionization spectra by quasi-degenerate perturbation theory.

International Journal of Quantum Chemistry, 52(2):549–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lisini:1995:QCA

[LD95] A. Lisini and P. Decleva. The QDPT CI approach for excitation and ionization spectra: A test on the CO molecule. *International Journal of Quantum Chemistry*, 55(3):281–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lamanna:1996:GOS

[LDGA96] Ugo T. Lamanna, Nicola Durante, Carla Guidotti, and Giovanni P. Arrighini. Generalized oscillator strengths of polyatomic molecules. II. NH_3. *International Journal of Quantum Chemistry*, 60(1):475–486, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60610`.

Li:1993:CAF

[LDP93] Y. Li, X. Dong, and S. Pan. Computation of auxiliary functions in STO molecular integrals up to arbitrary accuracy. I. evaluation of incomplete gamma function $E_n(X)$ by forward recursion. *International Journal of Quantum Chemistry*, 45(1): 3–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

LeRouzo:1997:MEC

[Le 97] H. Le Rouzo. Multipole expansion of Cartesian Gaussian orbitals about a new origin. *International Journal of Quantum Chemistry*, 64(6):647–653, September 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42723`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42723&PLACEBO=IE.pdf`.

Lunell:1992:ISE

[LE92] S. Lunell and L. A. Eriksson. Isotope substitution effects on preferred conformations of some hydrocarbon radical cations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:575–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Lunell:1994:CPS

[LEAS94] S. Lunell, C. Enkvist, M. Agback, and S. Svensson. Core photoionization satellites in fullerene and related model systems. *International Journal of Quantum Chemistry*, 52(1):135–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lefebvre:1997:AGT

[Lef97] R. Lefebvre. Adiabaticity and gauge transformations for an oscillator coupled to a single-mode field. *International Journal of Quantum Chemistry*, 64(1):111–119, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42659; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42659&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Lefebvre:1999:HFF

[Lef99] R. Lefebvre. High-frequency Floquet theory: Test of the applicability of the Golden Rule. *International Journal of Quantum Chemistry*, 72(4):261–267, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006329; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006329&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Liang:1994:ESO

[LEGH94] X. L. Liang, D. E. Ellis, O. V. Gubanova, and B. M. Hoffman. Electronic structure and optical properties of a tin-encapsulated nickel porphyrazine compound. *International Journal of Quantum Chemistry*, 52(3):657–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leitner:1999:IQE

[Lei99] David M. Leitner. Influence of quantum energy flow and localization on molecular isomerization in gas and condensed phases. *International Journal of Quantum Chemistry*, 75(4–5):523–531, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004947/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004947&PLACEBO=IE.pdf.

Leszczynski:1991:SPU

[Les91] J. Leszczynski. Structure and properties of uracil and its sulfur analogs: A systematic study of basis set effects in ab initio SCF calculations. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:9–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Leszczynski:1992:AGN

[Les92] J. Leszczynski. Are the amino groups in the nucleic acid bases coplanar with the molecular rings? ab initio HF/ 6-31Gsup * and MP2/ 6-21Gsup * studies. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:43–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Levine:1994:COS

[Lev94] Z. H. Levine. Calculation of optical second-harmonic susceptibilities and optical activity for crystals. *International Journal of Quantum Chemistry. Symposium*, 28:411–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Levy:1997:ADF

[Lev97] Mel Levy. Additive density functional correlation corrections to single particle theories. *International Journal of Quantum Chemistry*, 61(2):281–285, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42391; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42391&PLACEBO=IE.pdf.

Levine:1999:ICE

[Lev99] R. D. Levine. On the independence of correlated events. *International Journal of Quantum Chemistry*, 74(5):467–478, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62502999; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62502999&PLACEBO=IE.pdf.

Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Longo:1990:ATP

[LF90] R. L. Longo and L. C. G. Freitas. Adenine-Thymine proton relay: Electric field and environmental effects on point mutation DNA. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17: 35–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Li:1995:ESY

[LF95] M. Li and W. Fu. Electronic structures of $YBa_2Cu_3O_y$ doped by La. *International Journal of Quantum Chemistry*, 56(3): 187–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lemus:1999:GAL

[LF99] R. Lemus and A. Frank. General anharmonic local mode approach to molecular vibrations. *International Journal of Quantum Chemistry*, 75(4–5):465–481, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004962/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004962&PLACEBO=IE.pdf`.

Ladik:1996:BCC

[LFB96] Janos Ladik, Wolfgang Forner, and E. J. Brandas. The beginnings of cancer in the cell. *International Journal of Quantum Chemistry*, 57(2):261–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lisini:1994:TSM

[LFD94] A. Lisini, G. Fronzoni, and P. Decleva. Theoretical study of many-body effects in the photoelectron spectra of unsaturated hydrocarbons. *International Journal of Quantum Chemistry*, 52(2):527–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liubich:1999:IBT

[LFD99] Vlad Liubich, David Fuks, and Simon Dorfman. Interstitial boron in tungsten: Electronic structure, ordering tendencies, and total energy calculations. *International Journal of Quantum Chemistry*, 75(4–5):917–926, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004986/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004986&PLACEBO=IE.pdf`.

Li:1994:CSN

[LFS94] J. Li, J. Feng, and C. Sun. Calculations on the spectra and nonlinear third-order optical susceptibility of C_{70}. *International Journal of Quantum Chemistry*, 52(3):673–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1969:EPS

[LG69] P. O. Löwdin and O. Goscinski. The exchange phenomenon, the symmetric group, and the spin degeneracy problem. *International Journal of Quantum Chemistry*, 3S(??):533–??, ?? 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1971:SPT

[LG71] P. O. Löwdin and O. Goscinski. Studies in perturbation theory. XIV. treatment of constants of motion, degeneracies and symmetry properties by means of multidimensional partitioning. *International Journal of Quantum Chemistry*, 5(??):685–??, ?? 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Levy:1995:NER

[LG95a] M. Levy and A. Gorling. New exact relations for improving the exchange and correlation potentials. *International Journal of Quantum Chemistry*, 56(4):385–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luders:1995:FDL

[LG95b] M. Luders and E. K. U. Gross. Frequency-dependent linear response of superconducting systems. *International Journal of*

Quantum Chemistry, 56(5):521–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lushington:1996:ETMb

[LG96a] G. H. Lushington and F. Grein. The electronic *g*-tensor of MgF: A comparison of ROHF and MRD–CI level results. *International Journal of Quantum Chemistry*, 60(7):1679–1684, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60730`.

Lushington:1996:ETMa

[LG96b] G. H. Lushington and F. Grein. The electronic *g*-tensor of MgF: A comparison of ROHF and MRD-CI level results. *International Journal of Quantum Chemistry*, 60(7):467–??, 1996. CODEN IJQCB2.

Lushington:1996:ETMc

[LG96c] G. H. Lushington and F. Grein. The electronic *g*-tensor of MgF: A comparison of ROHF and MRD-CI level results. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):467–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Lagana:1994:PDC

[LGBL94] A. Lagana, O. Gervasi, R. Baraglia, and D. Laforenza. From parallel to distributed computing for reactive scattering calculations. *International Journal of Quantum Chemistry. Symposium*, 28:85–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Li:1994:QCS

[LGT94] Q. S. Li, F. L. Gu, and A. C. Tang. Quantum chemistry study on B_14, $B_1^{2-}4$, and $B_14H_1^{2-}4$. *International Journal of Quantum Chemistry*, 50(3):173–??, April 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:1994:SIA

[LH94] L.-M. Li and G.-Y. Hong. Study of improving the accuracy of the total energy calculated by the DV-Xalpha method. *International Journal of Quantum Chemistry*, 49(4):343–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leszczynski:1991:TES

[LHL91] Jerzy Leszczynski, Brian Hale, and Danuta Leszczynska. Theoretical and experimental study on small molecular ions. I ab initio calculations on CSe, CSesup +, and HCSesup + species. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:451–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Lahti:1999:CSL

[LHNK99] Ari Lahti, Matti Hotokka, Kari Neuvonen, and Gunnar Karlström. A CASSCF study on the lowest $\pi \rightarrow \pi*$ excitation of urocanic acid. *International Journal of Quantum Chemistry*, 72(1):25–37, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002300; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002300&PLACEBO=IE.pdf`.

Li:1993:ESH

[Li93] M. Li. Electronic structures of High-T_c superconductors $LnBa_2Cu_3O_7$ (ln=pr, nd, gd, dy). *International Journal of Quantum Chemistry*, 48(1):49–??, October 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:1997:ROC

[Li97] Ming Li. Role of oxygen content in electronic structures of $Ba_{0.6}$ $K_{0.4}$ $BiO_{3-\delta}$. *International Journal of Quantum Chemistry*, 64 (6):703–710, September 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42731; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42731&PLACEBO=IE.pdf`.

Linderberg:1981:ARR

[Lin81] J. Linderberg. Algebraic reduction of the real symmetric 4×4 secular problem. *International Journal of Quantum Chemistry*, 19(??):237–249, ?? 1981. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Linderberg:1992:FEP

[Lin92] J. Linderberg. Finite elements and partial waves in scattering calculations. *International Journal of Quantum Chemistry.*

Quantum Chemistry Symposium, 26:717–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Linderberg:1994:CPT

[Lin94] J. Linderberg. Correlation and propagation in time. *International Journal of Quantum Chemistry. Symposium*, 28:7–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Lindgren:1996:RMB

[Lin96] Ingvar Lindgren. Relativistic many-body and QED calculations on atomic systems. *International Journal of Quantum Chemistry*, 57(4):683–695, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60405`.

Linderberg:1997:HAT

[Lin97] Jan Linderberg. Hybrids and atomic theory. *International Journal of Quantum Chemistry*, 63(1):15–22, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42575; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42575&PLACEBO=IE.pdf`.

Liotard:1992:ATS

[Lio92] D. A. Liotard. Algorithmic tools in the study of semiempirical potential surfaces. *International Journal of Quantum Chemistry*, 44(5):723–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lipscomb:1991:MSFa

[Lip91a] William N. Lipscomb. Molecular structure and function. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:1–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Lipscomb:1991:MSFb

[Lip91b] William N. Lipscomb. Molecular structure and function. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:1–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Lagowski:1995:ISS

[LJ95] J. B. Lagowski and R. Jaeger. Ab initio study of the structures of polythionylphosphazene molecular mimics with H, Cl, and CH_3 side groups: 3-21G* and 6-31G* basis sets comparison. *International Journal of Quantum Chemistry*, 53(3):321–??, February 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luo:1998:SRD

[LJN+98] Y. Luo, D. Jonsson, P. Norman, K. Ruud, O. Vahtras, B. Minaev, H. Ågren, A. Rizzo, and K. V. Mikkelsen. Some recent developments of high-order response theory. *International Journal of Quantum Chemistry*, 70(1):219–239, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74367; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74367&PLACEBO=IE.pdf`. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Lively:1994:HBN

[LJS94] T. N. Lively, M. W. Jurema, and G. C. Shields. Hydrogen bonding of nucleotide base pairs: Application of the PM3 method. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21:95–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Larsson:1990:CSD

[LK90] S. Larsson and B. Kallbring. Charge separation in 9,9'-Dianthryl and a special pair treated by a semi-empirical reaction field method. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17:189–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Luchow:1993:AIC

[LK93] A. Luchow and H. Kleindienst. Atomic integrals containing $r_2^{\lambda} 3 r_1^{\mu} 3 r_1^{\nu} 2$ with $\lambda, \mu, \nu > -2$. *International Journal of Quantum Chemistry*, 45(5):445–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larsson:1999:SCM

[LK99] Sven Larsson and Agris Klimkäns. Superconducting currents from molecular theory. *International Journal of Quantum Chemistry*, 75(4–5):543–548, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004949/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004949&PLACEBO=IE.pdf.

Ley-Koo:1997:ERA

[LKBJ97] E. Ley-Koo, C. F. Bunge, and R. Jáuregui. Evaluation of relativistic atomic integrals using perimetric coordinates. *International Journal of Quantum Chemistry*, 63 (1):93–97, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42555; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42555&PLACEBO=IE.pdf.

Ley-Koo:1998:HAI

[LKFF98] E. Ley-Koo and A. Flores-Flores. Helium atom inside boxes with paraboloidal walls. *International Journal of Quantum Chemistry*, 66(2):123–130, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29846; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29846&PLACEBO=IE.pdf.

Liu:1998:PPR

[LKLBP98] Shubin Liu, Valentin Karasiev, Roberto López-Boada, and Frank De Proft. Polynomial and Padé representations for the kinetic component $T_c[\rho]$ of the correlation energy density functional. *International Journal of Quantum Chemistry*, 69(4):513–522, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30024; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30024&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Larsson:1999:SHP

[LKM99] Per-Erik Larsson, Lars M. Kristensen, and Kurt V. Mikkelsen. Studies of hyperpolarizabilities for *para*-nitroaniline in the charge-transfer state: Application of a reaction-field response method. *International Journal of Quantum Chemistry*, 75(4–5):449–456, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004942/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004942&PLACEBO=IE.pdf`.

Ley-Koo:1993:HAS

[LKMC93] E. Ley-Koo and S. Mateos-Cortes. The hydrogen atom in a semi-infinite space limited by a hyperboloidal boundary. *International Journal of Quantum Chemistry*, 46(5):609–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ley-Koo:1995:VLF

[LKMCVT95] E. Ley-Koo, S. Mateos-Cortes, and G. Villa-Torres. Vibrational levels and Franck–Condon factors of diatomic molecules via Morse potentials in a box. *International Journal of Quantum Chemistry*, 56(3):175–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ley-Koo:1996:VRL

[LKMCVT96] E. Ley-Koo, S. Mateos-Cortés, and G. Villa-Torres. Vibrational-rotational levels and Franck–Condon factors of diatomic molecules via Morse potentials in a box. *International Journal of Quantum Chemistry*, 58(1):23–28, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60460`.

Luan:1990:CAP

[LKU90] C.-H. Luan, N. R. Krishna, and D. W. Urry. Cyclododecapeptide analog of the polyhexapeptide of elastin: 2-D NMR and molecular dynamics studies. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17:145–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Ley-Koo:1997:HAS

[LKVS97] E. Ley-Koo and K. P. Volke-Sepúlveda. The helium atom in a semi-infinite space limited by a paraboloidal boundary. *International Journal of Quantum Chemistry*, 65(3): 269–275, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42763; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42763&PLACEBO=IE.pdf.

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] P. Lindner and P. O. Löwdin. Upper and lower bounds in second-order perturbation theory and the Unsöld approximation. *International Journal of Quantum Chemistry*, 2S(??): 161–??, ?? 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1970:CLB

[LL70] P. O. Löwdin and T. K. Lim. Calculation of lower bounds to energy eigenvalues by reduced density matrices and the representability problem. *International Journal of Quantum Chemistry*, 3S(??):697–??, ?? 1970. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:1992:SCM

[LL92] Y.-L. Lu and S.-L. Lee. Semiempirical calculations of molecular polarizabilities and hyperpolarizabilities of polycyclic aromatic compounds. *International Journal of Quantum Chemistry*, 44 (5):773–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lee:1994:SDL

[LL94a] S.-L. Lee and C.-K. Lee. Simulation of diffusion-limited aggregation and reactions over its surfaces. *International Journal of Quantum Chemistry*, 52(2):339–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lee:1994:CSG

[LL94b] S.-L. Lee and C. Li. Chemical signed graph theory. *International Journal of Quantum Chemistry*, 49(5):639–??, February 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lee:1997:HRF

[LL97] Shyi-Long Lee and Chung-Kung Lee. Heterogeneous reactions over fractal surfaces: A multifractal scaling analysis. *International Journal of Quantum Chemistry*, 64(3): 337–350, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42691; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42691&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Lin:1999:SEL

[LL99] Ying-Ting Lin and Shyi-Long Lee. Structural effects on the low cubic hyperpolarizability of C_{60}: A scaling of conjugation in three-dimensional curvature ofπ-conjugation systems. *International Journal of Quantum Chemistry*, 75(4–5):457–463, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004991/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004991&PLACEBO=IE.pdf.

Lukes:1999:PCH

[LLB99] Vladimír Lukeš, Viliam Laurinc, and Stanislav Biskupič. Perturbative calculation of the Hartree–Fock interaction energy using orthogonalized orbitals. *International Journal of Quantum Chemistry*, 75(2):81–88, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=64000653; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=64000653&PLACEBO=IE.pdf.

Ludena:1995:LST

[LLBM+95] E. V. Ludena, R. Lopez-Boada, J. E. Maldonado, E. Valderrama, E. S. Kryachko, T. Koga, and J. Hinze. Local-scaling transformation version of density functional theory. *International Journal of Quantum Chemistry*, 56(4):285–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lee:1994:AMD

[LLC+94] C. Lee, X. Long, I. Carpenter, S. Smithline, and G. Fitzgerald. Applications of molecular dynamics simulations coupled with Harris functional approximation to argon. *International Journal of Quantum Chemistry*, 49(4):527–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larson:1992:SCE

[LLL92] E. G. Larson, M. Li, and G. C. Larson. Some comments on the electrostatic potential of a molecule. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26: 181–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Lepetit:1997:BOE

[LLL97] Marie-Bernadette Lepetit, Lilian Lafon, and Xavier Lafage. Box orbitals for extended systems. *International Journal of Quantum Chemistry*, 64(4):411–420, September 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42699; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42699&PLACEBO=IE.pdf.

Liao:1998:CAC

[LLZ98] Meng-Sheng Liao, Xin Lü, and Qian-Er Zhang. Cyanide adsorbed on coinage metal electrodes: A relativistic density functional investigation. *International Journal of Quantum Chemistry*, 67(3):175–185, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29897; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29897&PLACEBO=IE.pdf.

Lavrik:1991:TRM

[LM91] N. L. Lavrik and Yu. N. Molin. Time-resolved magnetic field effects in the recombination products of geminate triplet pairs for electron phototransfer reactions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:387–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Lino:1993:PGU

[LMAK93] A. T. Lino, N. Meskini, H. W. L. Alves, and K. Kunc. TO(Γ) phonons in GaAs under uniaxial strain. *International Journal of Quantum Chemistry*, 45(1):43–49, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lamare:1997:LES

[LMC97a] L. Lamare and F. Michel-Calendini. LDA electronic structure calculations on Au_{13} cluster. *International Journal of Quantum Chemistry*, 61(4):635–639, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42449; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42449&PLACEBO=IE.pdf`.

Lamare:1997:STT

[LMC97b] L. Lamare and F. Michel-Calendini. Simulation of tungsten tip-Al(100) surface electronic structure through LCAO-LSD calculations. *International Journal of Quantum Chemistry*, 61(4):711–717, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42444; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42444&PLACEBO=IE.pdf`.

Lippert:1996:DDS

[LMD96] E. Lippert, J. D. Macomber, and L. J. Dunne. Dynamics during spectroscopic transitions-basic concepts. *International Journal of Quantum Chemistry*, 60(2):709–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lavin:1993:RQD

[LMMK93] C. Lavin, P. Martin, I. Martin, and J. Karwowski. Relativistic quantum defect orbital calculations of singlet-singlet transitions in the zinc and cadmium isoelectronic sequences. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:385–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Lefebvre:1994:TRR

[LMR94] R. Lefebvre, N. Moiseyev, and V. Ryaboy. Thermal reaction rates with a two-point flux-flux correlation function. *International Journal of Quantum Chemistry*, 51(6):465–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lavin:1992:SDS

[LMV92] C. Lavin, I. Martin, and M. J. Vallejo. Study of the diffuse spectral series of boron-like atomic systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26: 455–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Lieb:1996:BAR

[LN96] Elliott H. Lieb and Bruno Nachtergaele. Bond alternation in ring-shaped molecules: The stability of the Peierls instability. *International Journal of Quantum Chemistry*, 58(6):699–706, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60510`.

Lukovits:1999:RDR

[LNT99] I. Lukovits, S. Nikolić, and N. Trinajstić. Resistance distance in regular graphs. *International Journal of Quantum Chemistry*, 71(3):217–225, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10016708`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10016708&PLACEBO=IE.pdf`.

Lin:1990:EPT

[LO90] J. S. Lin and J. V. Ortiz. Electron propagator test of atomic natural orbital basis sets. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:585–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Ladik:1993:CCB

[LO93] J. Ladik and P. Otto. Correlation corrected band structures of quasi 1D and 2D periodic systems and level distributions of disordered chains; new method with correlation for dynamic nonlinear optical properties of periodic polymers. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:111–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Lohr:1991:RPE

[Loh91] Lawrence L. Lohr. Relativistically parameterized extended huckel calculations 13. energy bands for uranium compounds UBsub 2, UBsub 4, UC, UBC, and UPtsub 3. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:121–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Lohr:1996:ESR

[Loh96] Lawrence L. Lohr. Energies and structures of rotating argon clusters: Analytic descriptions and numerical simulations. *International Journal of Quantum Chemistry*, 57(4):707–714, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60407.

Longo:1999:CDB

[Lon99] Ricardo L. Longo. Charge-dependent basis sets. I. First row elements. *International Journal of Quantum Chemistry*, 75(4–5):585–591, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004953/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004953&PLACEBO=IE.pdf.

Lowdin:1967:EPL

[Löw67a] P. O. Löwdin. Eigenvalue problem in A linearly dependent basis and the super secular equation. *International Journal of Quantum Chemistry*, 1S(??):811–??, ?? 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1967:NQC

[Löw67b] P. O. Löwdin. Nature of quantum chemistry. *International Journal of Quantum Chemistry*, 1(??):1–??, ?? 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1968:SCT

[Löw68a] P. O. Löwdin. Some comments on the treatment of symmetry properties in perturbation theory. *International Journal of Quantum Chemistry*, 2S(??):137–??, ?? 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1968:SPT

[Löw68b] P. 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(??):867–??, ?? 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1971:SPI

[Löw71] P. O. Löwdin. Some properties of inner projections. *International Journal of Quantum Chemistry*, 4(??):231–237, ?? 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1990:Ea

[Löw90a] P. O. Löwdin. Editorial. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17:v, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Lowdin:1990:Eb

[Löw90b] P. O. Löwdin. Editorial. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:xi, 1990. CODEN IJQSDI. ISSN 0161-3642.

Lowdin:1991:E

[Löw91] P. O. Löwdin. Editorial. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:ix, 1991. CODEN IJQSDI. ISSN 0161-3642.

Lowdin:1992:E

[Löw92] P.-O. Löwdin. Editorial. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:v, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Lowdin:1993:Ea

[Löw93a] P.-O. Löwdin. Editorial. *International Journal of Quantum Chemistry*, 45(1):1–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1993:Eb

[Löw93b] P.-O. Löwdin. Editorial. *International Journal of Quantum Chemistry*, 47(1):1–??, July 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1993:SPG

[Löw93c] P.-O. Löwdin. On some properties of general linear operators. *International Journal of Quantum Chemistry*, 46(3):505–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1993:SRR

[Löw93d] P.-O. Löwdin. Some remarks on the resemblance theorems associated with various orthonormalization procedures. *International Journal of Quantum Chemistry*, 48(4):225–??, November 10, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1994:SCP

[Löw94] P.-O. Löwdin. Some current problems in theoretical chemical physics to be solved. *International Journal of Quantum Chemistry*, 51(6):473–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1995:HDE

[Löw95a] P.-O. Löwdin. The historical development of the electron correlation problem. *International Journal of Quantum Chemistry*, 55(2):77–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1995:FLC

[Löw95b] P.-O. Löwdin. On fundamentals, logic, and the connection between the natural sciences. *International Journal of Quantum Chemistry*, 53(1):97–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1996:MJL

[Löw96a] P. O. Löwdin. In memory of Jean-Louis Calais. *International Journal of Quantum Chemistry*, 57(1):1–??, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lowdin:1996:SCP

[Löw96b] Per-Olov Löwdin. Some comments on the properties of unitary transformations on linear spaces having an indefinite metric and the connection with the theory of spin. *International Journal of Quantum Chemistry*, 58(6):549–568, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60513`.

Lowdin:1997:I

[Löw97a] Per-Olov Löwdin. Introduction. *International Journal of Quantum Chemistry*, 63(1):1–2, ???? 1997. CODEN IJQCB2. ISSN

0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42552; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42552&PLACEBO=IE.pdf.

Lowdin:1997:SAD

[Löw97b] Per-Olov Löwdin. Some aspects on the development of the natural sciences and their importance for modern society and for our global environment. *International Journal of Quantum Chemistry*, 64(2):157–169, August 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42677; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42677&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Lowdin:1999:CBS

[Löw99] Per-Olov Löwdin. Connection between semi-empirical and ab initio methods in the quantum theory of molecular electronic spectra. *International Journal of Quantum Chemistry*, 72(4):379–391, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006316; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006316&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Linderberg:1974:DPH

[LP74] J. Linderberg and D. Prato. Dynamic polarizability of helium: A random phase approximation calculation. *International Journal of Quantum Chemistry*, 8(??):901–913, ?? 1974. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:1993:MSA

[LP93] X. Li and J. Paldus. Multiconfigurational spin-adapted single-reference coupled cluster formalism. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:269–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Levy:1994:DFE

[LP94] M. Levy and J. P. Perdew. Density functionals for exchange and correlation energies: Exact conditions and comparison of approximations. *International Journal of Quantum Chemistry*, 49(4):539–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:1996:BLA

[LP96] Xiangzhu Li and Josef Paldus. Bond length alternation in cyclic polyenes. VII. valence bond theory approach. *International Journal of Quantum Chemistry*, 60(1):513–527, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60615`.

Lamm:1997:LDC

[LP97a] Gene Lamm and George R. Pack. Local dielectric constants and Poisson–Boltzmann calculations of DNA counterion distributions. *International Journal of Quantum Chemistry*, 65 (6):1087–1093, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42845; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42845&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on the Application of Fundamental Theory to Problems of Biology and Pharmocolgy*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Leao:1997:MOA

[LP97b] M. B. C. Leão and A. C. Pavão. Molecular orbital analysis of chemical carcinogens. *International Journal of Quantum Chemistry*, 62(3):323–328, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42508; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42508&PLACEBO=IE.pdf`.

Lefebvre:1997:FQE

[LP97c] R. Lefebvre and A. Palma. Floquet quasi-energies and eigenfunctions of the parabolic barrier. *International Journal of Quantum Chemistry*, 65(5):487–497, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42777; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42777&PLACEBO=IE.pdf`. Special

Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Li:1997:EEA

[LP97d] Jiabo Li and Ruben Pauncz. Efficient evaluation of the algebrants of VB wave functions using the successive expansion method. I. Spin $S = 0, 1/2$. *International Journal of Quantum Chemistry*, 62(3):245–259, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42509; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42509&PLACEBO=IE.pdf.

Li:1998:UGB

[LP98] Xiangzhu Li and Josef Paldus. Unitary-group-based open-shell coupled-cluster method with corrections for connected triexcited clusters. I. Theory. *International Journal of Quantum Chemistry*, 70(1):65–75, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74370; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74370&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Li:1999:SDE

[LP99] Xiangzhu Li and Josef Paldus. Size dependence of the $X^1A_g \to 1^1B_u$ excitation energy in linear polyenes. *International Journal of Quantum Chemistry*, 74(2):177–192, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003363; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003363&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Lopez:1994:CTC

[LR94] R. Lopez and G. Ramirez. Calculation of two-center exchange integrals with STOs using Möbius transformations. *International Journal of Quantum Chemistry*, 49(1):11–??, January 5,

1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larsson:1993:CPI

[LRM93] S. Larsson and L. Rodriguez-Monge. Correlation and pairing in $C_{60}2n$-ions superconductivity of alkali and alkaline earth compounds of C_{60}. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:655–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Larsson:1996:CPI

[LRM96] Sven Larsson and Lucia Rodriguez-Monge. Conductivity in polyacetylene. II. ab initio and tight-binding calculations of soliton structure and reorganization energy in ordered and disordered structures. *International Journal of Quantum Chemistry*, 58(5):517–532, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60505`.

Larsson:1997:CPV

[LRM97] Sven Larsson and Lucia Rodriguez-Monge. Conductivity in polyacetylene. VI. semiconductor-metal transition of alkali-doped polymer. *International Journal of Quantum Chemistry*, 63(3):655–665, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42627; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42627&PLACEBO=IE.pdf`.

Larsson:1998:RSC

[LRM98] Sven Larsson and Lucía Rodríguez-Monge. Role of π stabilization in cyclic polyenes. *International Journal of Quantum Chemistry*, 67(2):107–113, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29891; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29891&PLACEBO=IE.pdf`.

Lefebvre:1967:EHF

[LS67] R. Lefebvre and Y. G. Smeyers. Extended Hartree–Fock calculations for the helium ground state. *International Journal of Quantum Chemistry*, 1(??):403–??, ?? 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larson:1971:DMA

[LS71] E. G. Larson and D. W. Smith. A density matrix analysis of Slater's hyper-Hartree–Fock method. *International Journal of Quantum Chemistry*, 4(??):87–??, ?? 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leszczynski:1992:BSA

[LS92a] J. Leszczynski and R. H. Sullivan. Biuret and its sulfur analogs: Structures and energies. *International Journal of Quantum Chemistry*, 44(2):301–??, September 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luth:1992:CBP

[LS92b] K. Luth and S. Scheiner. Calculation of barriers to proton transfer using a variety of electron correlation methods. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:817–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Lambin:1993:ESM

[LS93a] Ph. Lambin and P. Senet. Ewald summation of multipolar interactions at an arbitrary order on a two-dimensional lattice. *International Journal of Quantum Chemistry*, 46(1):101–107, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luth:1993:CGT

[LS93b] K. Luth and S. Scheiner. Comparison of ground and triplet state geometries of malonaldehyde. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:419–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Liebman:1996:ESH

[LS96] Joel F. Liebman and Per N. Skancke. Evaluation of strain in heterosiliranes: Systematics, surprises, and problems. *International Journal of Quantum Chemistry*, 58(6):707–715, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60511`.

Lee:1999:CSA

[LS99] Jooyoung Lee and Harold A. Scheraga. Conformational space annealing by parallel computations: Extensive conformational search of Met-enkephalin and of the 20-residue membrane-bound portion of melittin. *International Journal of Quantum Chemistry*, 75(3):255–265, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000667/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000667&PLACEBO=IE.pdf.

Lu:1998:TSFa

[LSC98] Li-Hwa Lu, Kuang-Chung Sun, and Cheng Chen. Theoretical study of fullerene derivatives: C 28H4 and $C_{28}X_4$ cluster molecules. *International Journal of Quantum Chemistry*, 67(3):187–197, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29898; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29898&PLACEBO=IE.pdf.

Luo:1991:DBS

[LSGS91] J. Luo, M. H. Sarma, G. Gupta, and R. H. Sarma. DNA bending studied by MD and 2D NMR NOESY simulations: Role of the junction sequence between the A/T tracts. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:213–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Lee:1996:CSLa

[LSS96a] S.-L. Lee, M.-L. Sun, and Z. Slanina. Computational studies of less common fullerene-related species. *International Journal of Quantum Chemistry*, 60(7):355–??, 1996. CODEN IJQCB2.

Lee:1996:CSLc

[LSS96b] S.-L. Lee, M.-L. Sun, and Z. Slanina. Computational studies of less common fullerene-related species. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):355–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Lee:1996:CSLb

[LSS96c] Shyi-Long Lee, Mei-Ling Sun, and Zdeněk Slanina. Computational studies of less common fullerene-related species. *International Journal of Quantum Chemistry*, 60(7):1567–1576,

???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60716.

Li:1999:VSN

[LT99] Qian Shu Li and Au Chin Tang. Vibration spectra and NMR spectra of octahedral (O_h and O) fullerenes. *International Journal of Quantum Chemistry*, 72(3):199–205, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40003032; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40003032&PLACEBO=IE.pdf.

Li:1996:CBD

[LTP96] Zhiru Li, Fu-Ming Tao, and Yuh-Kang Pan. Calculation of bond dissociation energies of diatomic molecules using bond function basis sets with counterpoise corrections. *International Journal of Quantum Chemistry*, 57(2):207–212, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60368.

Lino:1996:BCDc

[LTSL96a] A. T. Lino, E. K. Takahashi, L. M. R. Scolfaro, and J. R. Leite. Behavior of carriers in d-doped quantum wells under in-plane magnetic fields. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):347–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Lino:1996:BCDb

[LTSL96b] A. T. Lino, E. K. Takahashi, L. M. R. Scolfaro, and J. R. Leite. Behavior of carriers in δ-doped quantum wells under in-plane magnetic fields. *International Journal of Quantum Chemistry*, 60(7):1559–1566, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60715.

Lino:1996:BCDa

[LTSL96c] A. T. Lino, E. K. Takahashi, L. M. R. Scolfaro, and J. R. Leite. Behavior of carriers in e-doped quantum wells under in-plane magnetic fields. *International Journal of Quantum Chemistry*, 60(7):347–??, 1996. CODEN IJQCB2.

Lu:1999:DFS

[Lu99] Li-Hwa Lu. Density functional study of tricyclo(3,3,1,13,7)decane and tricyclo(3,3,1,13,7)decsilane and their halogen derivatives. *International Journal of Quantum Chemistry*, 72 (3):189–198, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40003031; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40003031&PLACEBO=IE.pdf.

Lukovits:1992:CBC

[Luk92] I. Lukovits. Correlation between components of the weiner index and partition coefficients of hydrocarbons. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:217–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Luo:1995:CTR

[Luo95] L. Luo. Conformation-Transitional rate in protein folding. *International Journal of Quantum Chemistry*, 54(4):243–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:1971:ESN

[LV71] H. P. D. Liu and G. Verhaegen. Electronic states of NH and OH+. *International Journal of Quantum Chemistry*, 5S(??): 103–??, ?? 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lagowski:1993:PMI

[LV93] J. B. Lagowski and G. J. Vancso. Polystyrene models. III. modeling backbone/side-group interactions by an ab initio study of 2,4-diphenylpentane. *International Journal of Quantum Chemistry*, 46(2):271–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lievin:1997:USA

[LV97] Jacques Liévin and Nathalie Vaeck. Use of symmetry-adapted Brillouin theorem to analyze the variational content of molecular wave functions along potential energy surfaces: Application to BH_2 and PO_2. *International Journal of Quantum*

Chemistry, 62(5):521–541, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42540; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42540&PLACEBO=IE.pdf.

Larin:1998:AMC

[LV98] A. V. Larin and D. P. Vercauteren. Approximations of the Mulliken charges for the oxygen and silicon atoms of zeolite frameworks calculated with a periodic Hartree–Fock scheme. *International Journal of Quantum Chemistry*, 70 (4-5):993–1001, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75077; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75077&PLACEBO=IE.pdf.

Loew:1991:CEP

[LVCP91] G. H. Loew, H. O. Villar, C. Cometta, and J. J. Perez. Conformational and electronic properties of met-enkephalin. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:165–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Laloyaux:1993:RSE

[LVL+93] Th. Laloyaux, J.-P. Vigneron, Ph. Lambin, I. Derycke, and A. A. Lucas. Resolution of Schrödinger's equation for a scattering problem by a finite-element method. *International Journal of Quantum Chemistry*, 45(6):637–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lewandowski:1992:ISC

[LW92] A. C. Lewandowski and T. M. Wilson. Ab initio SCF calculations on Mn-related defects in CaFsub 2. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26: 673–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Li:1995:SMM

[LX95] Y. M. Li and H. M. Xiao. Studies on the mechanism of Mannich reaction involving iminium salt as potential Mannich reagent. III. furan as pseudo acid component. *International Journal of*

Quantum Chemistry, 54(5):293–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:1999:CCB

[LXWZ99] Xin Lü, Xin Xu, Nanqin Wang, and Qianer Zhang. Convergence from clusters to the bulk solid: Ab initio calculations of $(MgO)_x$ ($x = 2--16$) clusters. *International Journal of Quantum Chemistry*, 73(4):377–386, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61000534; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61000534&PLACEBO=IE.pdf.

Lee:1998:FDM

[LY98] Tai-Sung Lee and Weitao Yang. Frozen density matrix approach for electronic structure calculations. *International Journal of Quantum Chemistry*, 69(3):397–404, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29994; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29994&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Lee:1995:TSM

[LYSL95] S-L Lee, K-C Yang, J-H Sheu, and Y.-J. Lu. Theoretical studies of the molecular second-order hyperpolarizabilities of polycyclic aromatics. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:509–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Lowdin:1992:IPS

[LZ92] P. Löwdin and M. C. Zerner. Introduction to the paper symposium on semiempirical methods in quantum chemistry and solid-state theory. *International Journal of Quantum Chemistry*, 44(4):421–??, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lazzeretti:1996:MMP

[LZ96] Paolo Lazzeretti and Riccardo Zanasi. Molecular magnetic properties via formal annihilation of paramagnetic contribution to electronic current density. *International Journal of*

Quantum Chemistry, 60(1):249–259, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60588.

Minaev:1996:SCP

[MÅ96] Boris F. Minaev and Hans Ågren. Spin-catalysis phenomena. *International Journal of Quantum Chemistry*, 57(3):519–532, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60390.

McWeeny:1999:LNQ

[MA99a] Roy McWeeny and Claudio Amovilli. Locality and non-locality in quantum mechanics: A two-proton EPR experiment. *International Journal of Quantum Chemistry*, 74 (5):573–584, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62503008; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62503008&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Minaev:1999:SUE

[MÅ99b] Boris Minaev and Hans Ågren. Spin uncoupling in ethylene activation by palladium and platinum atoms. *International Journal of Quantum Chemistry*, 72(6):581–596, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=50000016; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=50000016&PLACEBO=IE.pdf.

Murray:1998:MSE

[MAAP+98] Jane S. Murray, Fakher Abu-Awwad, Peter Politzer, Leslie C. Wilson, Allan S. Troupin, and Ryan E. Wall. Molecular surface electrostatic potentials of anticonvulsant drugs. *International Journal of Quantum Chemistry*, 70(6):1137–1143, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75081; http://www3.

interscience.wiley.com/cgi-bin/fulltext?ID=75081&PLACEBO=IE.pdf.

Measures:1996:MSE

[MAC96] Peter T. Measures, Neil L. Allan, and David L. Cooper. Momentum-space electron densities — localized orbitals in hydrocarbons, boranes, and transition metal complexes. *International Journal of Quantum Chemistry*, 60(1):579–592, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60621.

Mirabella:1998:EOB

[MAD98] D. A. Mirabella, C. M. Aldao, and R. R. Deza. Exact one-band model calculation using the tight-binding method. *International Journal of Quantum Chemistry*, 68(4):285–291, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29948; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29948&PLACEBO=IE.pdf.

Mitani:1995:ESL

[MAI95] M. Mitani, Y. Aoki, and A. Imamura. Electronic structures of large, extended, nonperiodic systems by using the elongation method: Model calculations for the cluster series of a polymer and the molecular stacking on a surface. *International Journal of Quantum Chemistry*, 54(3):167–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mitani:1997:GOP

[MAI97] Masaki Mitani, Yuriko Aoki, and Akira Imamura. Geometry optimization of polymers by the elongation method. *International Journal of Quantum Chemistry*, 64(3):301–323, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42689; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42689&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Martins:1996:HHI

[MALT96] João B. L. Martins, Juan Andrés, Elson Longo, and C. A. Taft. H2O and H2 interaction with ZnO surfaces: A MNDO, AM1, and PM3 theoretical study with large cluster models. *International Journal of Quantum Chemistry*, 57(5):861–870, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60440`.

Manaa:1995:FSA

[Man95] M. R. Manaa. The fragmentation of SH(A_2S+): Ab initio calculations of spin-orbit and Coriolis interactions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:577–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Manaa:1999:PNI

[Man99] M. Riad Manaa. Photodissociation of NaK: Ab initio spin-orbit interactions of the Na (3^2S) K (4^2P_J) manifold. *International Journal of Quantum Chemistry*, 75(4–5):693–697, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004966/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004966&PLACEBO=IE.pdf`.

Morales:1992:AAF

[MAPLB92] J. Morales, G. Arreaga, J. J. Pena, and J. Lopez-Bonilla. Alternative approach to the factorization method. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:171–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

March:1990:MBF

[Mar90] N. H. March. Molecular binding in free space and in cold dense plasmas. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:621–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

March:1991:AII

[Mar91] N. H. March. Atoms and ions in intense magnetic and electric fields. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:401–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

March:1992:EDT

[Mar92] N. H. March. Electron density theory in extreme homogeneous and heterogeneous environments and in intense external fields. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:377–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Maranon:1993:NRE

[Mar93a] J. Maranon. Nonlinear Roothaan's equations. *International Journal of Quantum Chemistry*, 48(3):151–??, November 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:1993:LPI

[Mar93b] N. H. March. Light particles interacting with organic molecules. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:607–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Marathon:1994:PIS

[Mar94a] J. Marathon. Path integral's semiclassical quantification. *International Journal of Quantum Chemistry*, 52(3):609–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:1994:BBE

[Mar94b] N. H. March. Building blocks for electron density in free molecules and in condensed matter phases. *International Journal of Quantum Chemistry*, 49(3):321–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:1994:RBMc

[Mar94c] N. H. March. The relation between magnetism and electronic transport properties in strongly correlated electron liquids, including high T_c materials. *International Journal of Quantum Chemistry. Symposium*, 28:421–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

March:1994:RBMa

[Mar94d] N. H. March. The role of the bond midpoint electron density in homonuclear molecular binding. *International Journal* of *Quantum Chemistry*, 52(1):247–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:1995:SED

[Mar95a] M. H. March. Subtle energies in density functional theory, correlation and molecular dissociation. *International Journal of Quantum Chemistry*, 56(4):257–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:1995:DFT

[Mar95b] N. H. March. Density functional theory via density matrices. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:137–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Maroulis:1995:EPC

[Mar95c] G. Maroulis. Evaluating the performance of correlated methods in molecular property calculations: Pattern recognition and clustering in spaces of theoretical descriptions. *International Journal of Quantum Chemistry*, 55(2):173–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:1996:MPS

[Mar96] N. H. March. Momentum and position space densities in many-electron systems. *International Journal of Quantum Chemistry*, 60(1):307–320, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60594`.

March:1997:FBA

[Mar97a] N. H. March. Forces between atoms and atomic planes in condensed metallic phases and in semiconducting silicon. *International Journal of Quantum Chemistry*, 65(5):907–917, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42822; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42822&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

March:1997:SCC

[Mar97b] N. H. March. Some cluster and condensed-phase properties of light elements: B to P. *International Journal of Quantum Chemistry*, 63(3):695–707, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42613; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42613&PLACEBO=IE.pdf.

March:1998:DFT

[Mar98a] N. H. March. Density functional theory in relation to X-ray and neutron scattering experiments. *International Journal of Quantum Chemistry*, 69(4):551–557, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30009; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30009&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

March:1998:DEG

[Mar98b] N. H. March. Differential equations for ground-state electron density and Slater sum in atoms and molecules with and without external fields. *International Journal of Quantum Chemistry*, 70(4-5):779–788, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75056; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75056&PLACEBO=IE.pdf.

March:1999:MET

[Mar99a] N. H. March. Many-electron theory: Density functional approach generalized to treat spin eigenfunctions and relation to spinless low-order density matrices. *International Journal of Quantum Chemistry*, 74(2):163–176, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003362; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003362&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Martin:1999:QDT

[Mar99b] Inmaculada Martin. Quantum defect and transition probabilities. *International Journal of Quantum Chemistry*, 74 (5):479–489, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62503000; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62503000&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Matsen:1996:SFQ

[Mat96] F. A. Matsen. Spin-free quantum chemistry. XXVI. The Ising, small-bipolaron theory of cuprate superconductivity. *International Journal of Quantum Chemistry*, 57(6):1057–1066, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60450.

Matsson:1997:BRR

[Mat97] Olle Matsson. Book review: *The reaction path in chemistry: current approaches and perspectives*, D. Heidrich, Editor. *International Journal of Quantum Chemistry*, 65 (4):375, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42771; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42771&PLACEBO=IE.pdf.

Matsen:1999:FTM

[Mat99] F. A. Matsen. The freeon theory of molecular magnets. III. the linear polyene model. *International Journal of Quantum Chemistry*, 72(4):325–329, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006308; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006308&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Mavri:1998:IIH

[Mav98] Janez Mavri. Irreversible inhibition of the HIV-1 protease: A theoretical study. *International Journal of Quantum Chem-*

istry, 69(6):753–759, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74991; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74991&PLACEBO=IE.pdf`.

Mayer:1992:AII

[May92] I. Mayer. On the additivity and interference of interactions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:773–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Mayer:1997:SPP

[May97] I. Mayer. Simple proof of the pairing theorem. *International Journal of Quantum Chemistry*, 63(1):31–33, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42577; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42577&PLACEBO=IE.pdf`.

Mayer:1998:CHA

[May98] I. Mayer. The chemical Hamiltonian approach for treating the BSSE problem of intermolecular interactions. *International Journal of Quantum Chemistry*, 70(1):41–63, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74369; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74369&PLACEBO=IE.pdf`. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Mazziotti:1998:CSE

[Maz98] David A. Mazziotti. 3,5-Contracted Schrödinger equation: Determining quantum energies and reduced density matrices without wave functions. *International Journal of Quantum Chemistry*, 70(4-5):557–570, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75034; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75034&PLACEBO=IE.pdf`.

Meissner:1993:EPT

[MB93] L. Meissner and R. J. Bartlett. Electron propagator theory with the ground state correlated by the coupled-cluster method. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:67–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Maverick:1997:CSE

[MB97a] Andrew W. Maverick and Leslie G. Butler. Chemical systems for exploration of high magnetic field effects. *International Journal of Quantum Chemistry*, 64(5):607–611, September 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42709; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42709&PLACEBO=IE.pdf`. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

Menchi:1997:DLP

[MB97b] M. Menchi and A. Bosin. DFT-LDA pseudopotentials in quantum Monte Carlo. *International Journal of Quantum Chemistry*, 61(2):295–302, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42393; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42393&PLACEBO=IE.pdf`.

Medhi:1998:MSP

[MB98] Chitrani Medhi and S. P. Bhattacharyya. Macroscopic solvent polarization-induced reorganization of the electron density in different excited states: A study on formaldehyde molecule by a multiconfiguration self-consistent reaction-field method. *International Journal of Quantum Chemistry*, 70(3):415–428, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75012; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75012&PLACEBO=IE.pdf`.

Moreno:1994:DUM

[MBA94] M. Moreno, M. T. Barriuso, and J. A. Aramburu. The dependence of 10Dq upon the metal-ligand distance, R. for transition-metal complexes. what is its microscopic origin? *International*

Journal of Quantum Chemistry, 52(4):829–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mekelleche:1997:COE

[MBA97] Sidi Mohamed Mekelleche and Abdellatif Baba-Ahmed. Calculation of the one-electron two-center integrals over Slater-type orbitals by means of the ellipsoidal coordinates method. *International Journal of Quantum Chemistry*, 63 (4):843–852, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42635; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42635&PLACEBO=IE.pdf`.

Morales:1991:TSA

[MBML91] J. Morales, M. Bonilla-Marin, and A. Langagne. Theoretical study on Al multiple substitutions in the MFI zeolite. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:659–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Murray:1991:SLI

[MBP91] J. S. Murray, T. Brinck, and P. Politzer. Surface local ionization energies and electrostatic potentials of the conjugate bases of a series of cyclic hydrocarbons in relation to their aqueous acidities. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18: 91–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Muinasmaa:1997:CBD

[MBP97] Urmas Muinasmaa, Peeter Burk, and Jaan Pentchuk. Complexes between divalent metals and carboxylic acids: Semiempirical study. *International Journal of Quantum Chemistry*, 62(6):653–658, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42549; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42549&PLACEBO=IE.pdf`.

Matyus:1998:DPI

[MBV+98] Péter Mátyus, András P. Borosy, András Varró, Julius G. Papp, Daniela Barlocco, and Giorgio Cignarella. Development of pharmacophores for inhibitors of the rapid component of the cardiac delayed rectifier potassium current. *International Journal of Quantum Chemistry*, 69(1):21–30, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29969; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29969&PLACEBO=IE.pdf.

Mitra:1994:PSC

[MC94] A. Mitra and J. F. Capitani. A PM3 study of the critical distance factor in the activation/cyclization of selected neocarzinostatin analogs. *International Journal of Quantum Chemistry*, 49(4):363–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morley:1995:TSS

[MC95] J. O. Morley and M. H. Charlton. Theoretical studies on the structure and electronic properties of 3-Isothiazolones. *International Journal of Quantum Chemistry*, 55(4):361–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matsen:1997:FTMa

[MC97a] F. A. Matsen and L. L. Campbell. The freeon theory of magnetism. I. the Heisenberg interaction. *International Journal of Quantum Chemistry*, 65(4):287–297, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42766; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42766&PLACEBO=IE.pdf.

Matsen:1997:FTMb

[MC97b] F. A. Matsen and L. L. Campbell. The freeon theory of magnetism. II. molecular magnets. *International Journal of Quantum Chemistry*, 65(4):299–304, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42767; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42767&PLACEBO=IE.pdf.

Mendizabal:1992:IEF

[MCA92] F. Mendizabal, R. R. Contreras, and A. J. Aizman. Introduction of external field effects in the frontier molecular orbital theory of chemical reactivity. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:751–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Mosley:1995:DFS

[MCA95] D. H. Mosley, B. Champagne, and J.-M. André. Density functional study of the static longitudinal polarizability of model polymeric chains. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:117–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Mondal:1999:MQD

[MCB99] Chandan Kumar Mondal, Pinaki Chaudhury, and S. P. Bhattacharyya. Modeling quantum dynamics of photodetachment from closed-shell anions: Static versus fluctuating well-depth models. *International Journal of Quantum Chemistry*, 73 (6):469–478, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61007364; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61007364&PLACEBO=IE.pdf`.

Mota:1995:MIT

[MCCF95] R. Mota, J. C. Cechin, S. Canuto, and A. Fazzio. Metal-insulator transition in fullerides: K_3C_{60} versus Na_3C_{60}. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:217–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

McDowell:1997:CGM

[McD97] Sean A. C. McDowell. Computation of general multipole moment expansions for N atoms by MAPLE. *International Journal of Quantum Chemistry*, 62(4):343–351, April 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42521; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42521&PLACEBO=IE.pdf`.

Mandix:1993:IIP

[MCE+93] K. Mandix, A. Colding, K. Elming, L. Sunesen, and L. Shim. Ab initio investigation of phloroglucinol. *International Journal of Quantum Chemistry*, 46(1):159–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

McHale:1991:IVR

[McH91] Jeanne L. McHale. Intermolecular vibrational resonance coupling: Intensity borrowing in polarized Raman spectroscopy. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:593–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Martin:1995:ETR

[MCL95] I. Martin, P. Campo, and C. Lavin. Electronic transitions in the Rydberg radical H_3O. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:631–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Miguel:1998:CCT

[MCM98] Beatriz Miguel, Maixent Cousy, and Jean-Paul Malrieu. Coupled cluster treatments of periodic systems from strongly localized reference functions: 1-D and 2-D spin and electron lattices. *International Journal of Quantum Chemistry*, 67(2):115–132, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29892; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29892&PLACEBO=IE.pdf`.

Marquez:1994:SPP

[MCOS94] A. Marquez, M. J. Capitan, J. A. Odriozola, and J. Fernandez Sanz. Spectroscopic properties and potential energy curves of some low-lying electronic states of AlO, AlO0+, LaO, and LaO0+: An ab initio CASSCF study. *International Journal of Quantum Chemistry*, 52(6):1329–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Miguel:1998:FPS

[MCS98] M. A. San Miguel, C. J. Calzado, and Javier Fernández Sanz. First principles study of Na adsorption on TiO_2 (110) surface. *International Journal of Quantum Chemistry*, 70(2):351–357, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75003; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75003&PLACEBO=IE.pdf`. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Mennucci:1999:MEP

[MCT99] B. Mennucci, R. Cammi, and J. Tomasi. Medium effects on the properties of chemical systems: Electric and magnetic response of donor-acceptor systems within the polarizable continuum model. *International Journal of Quantum Chemistry*, 75(4–5):767–781, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004973/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004973&PLACEBO=IE.pdf.

McWeeny:1990:VBT

[McW90] R. McWeeny. Valence bond theory: Progress and prospects. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:733–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

McWeeny:1996:ISS

[McW96] Roy McWeeny. Inside story — some scientific reminiscences. *International Journal of Quantum Chemistry*, 60(1):3–19, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60570.

McWeeny:1999:IFC

[McW99] Roy McWeeny. An ab initio form of classical valence-bond theory. *International Journal of Quantum Chemistry*, 74 (2):87–96, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003354; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003354&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Mowrey:1991:DAA

[MD91] R. C. Mowrey and B. I. Dunlap. Dissociative adsorption and associative desorption of H_2 on a flat surface. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:641–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Mestres:1993:IRC

[MD93a] J. Mestres and M. Duran. Intrinsic reaction coordinate of perturbed potential energy surfaces: Construction of perturbed energy profiles. *International Journal of Quantum Chemistry*, 47(4):307–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mujica:1993:GFC

[MD93b] V. Mujica and G. Doyen. A Green's function calculation of the zero-voltage STM resistance of a one-dimensional chain coupled to two jellium surfaces. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:687–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Mukherjee:1993:GFN

[MD93c] A. K. Mukherjee and D. K. Das. Graph factorization: A new mode of application of vertex-alternation scheme. *International Journal of Quantum Chemistry*, 46(4):519–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mallik:1994:SQR

[MD94] B. Mallik and S. N. Datta. Semiempirical quantum f reduction potentials of quinone and plastoquinone in water. *International Journal of Quantum Chemistry*, 52(3):629–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mallik:1995:SQC

[MD95] B. Mallik and S. N. Datta. Semiempirical quantum chemical treatment of the standard reduction potentials of quinone and plastoquinone in water. *International Journal of Quantum Chemistry*, 54(4):271–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meller:1999:SDM

[MD99] Jarosław Meller and Włodzisław Duch. SGA derivation of matrix elements between spin-adapted perturbative wave functions. *International Journal of Quantum Chemistry*, 74 (2):123–133, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003358; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003358&PLACEBO=IE.pdf`. Special Issue: *Quantum The-*

ory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Mathieu:1993:ISI

[MDD93] D. Mathieu, M. Defranceschi, and J. Delhalle. Ab initio study of the influence of aggregation on the infrared spectrum of acetonitrile. *International Journal of Quantum Chemistry*, 45(6): 735–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Michelini:1998:DFS

[MDJ98] M. C. Michelini, R. Pis Diez, and A. H. Jubert. A density functional study of small nickel clusters. *International Journal of Quantum Chemistry*, 70(4-5):693–701, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75047; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75047&PLACEBO=IE.pdf.

Morrison:1994:ELA

[MDM94] R. C. Morrison, C. M. Dixon, and J. R. Mizell. Examination of the limits of accuracy of the extended Koopmans' theorem ionization potentials into excited states of ions of LiH, He_2, and Li_2. *International Journal of Quantum Chemistry. Symposium*, 28:309–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Morokuma:1998:SIN

[MDS98] Keiji Morokuma, Ernest R. Davidson, and Henry F. Schaefer, III. Special issue: The Ninth International Congress of Quantum Chemistry (Part I of II). *International Journal of Quantum Chemistry*, 70(1):??, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matar:1997:LDF

[MECE97] S. F. Matar, V. Eyert, B. Chevalier, and J. Etourneau. Local density functional calculations of the electronic structures of the intermetallic systems U_2 Fe_2 Sn and UFe_2 Ge_2. *International Journal of Quantum Chemistry*, 61(4): 705–709, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42443; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42443&PLACEBO=IE.pdf.

Mendizabal:1999:TSA

[Men99] Fernando Mendizabal. Theoretical study of the Au-ethylene interaction. *International Journal of Quantum Chemistry*, 73(3):317–324, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003699; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003699&PLACEBO=IE.pdf`.

Mei:1993:TAC

[MESH93] C. Mei, K. E. Edgecombe, V. H. Smith, Jr., and A. Heilingbruner. Topological analysis of the charge density of solids: bcc sodiuum and lithium. *International Journal of Quantum Chemistry*, 48(5):287–??, December 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moustafa:1994:EGE

[METHH94] H. Moustafa, S. El-Taher, M. M. Hamed, and R. Hilal. Equilibrium geometry and electronic of benzylidene, arylethylidene, and heterocyclic arylidene malononitriles. *International Journal of Quantum Chemistry*, 49(6):805–??, March 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meyer:1994:CLI

[Mey94] J. Meyer. Construction of linearly independent relativistic symmetry orbitals for finite double-point groups including time reversal symmetry. *International Journal of Quantum Chemistry*, 52(6):1369–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meyer:1997:ACL

[Mey97] J. Meyer. Addendum to construction of linearly independent relativistic symmetry orbitals for finite double-point groups including time-reversal symmetry. *International Journal of Quantum Chemistry*, 61(6):929–933, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42476; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42476&PLACEBO=IE.pdf`.

Mezei:1994:IEC

[Mez94a] M. Mezei. Iso-energy cutoff for the calculation of interionic potential of mean force in water. *International Journal of Quan-*

tum Chemistry, 52(1):147–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mezey:1994:SMB

[Mez94b] P. G. Mezey. Semisimilarity of molecular bodies: Scaling-nesting similarity measures. *International Journal of Quantum Chemistry*, 51(4 (or 5??)):255–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mezey:1997:PMP

[Mez97a] Paul G. Mezey. A proof of the metric properties of the symmetric scaling-nesting dissimilarity measure and related symmetry deficiency measures. *International Journal of Quantum Chemistry*, 63(1):105–109, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42557; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42557&PLACEBO=IE.pdf`.

Mezey:1997:QSM

[Mez97b] Paul G. Mezey. Quantum similarity measures and Löwdin's transform for approximate density matrices and macromolecular forces. *International Journal of Quantum Chemistry*, 63 (1):39–48, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42579; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42579&PLACEBO=IE.pdf`.

Mann:1996:IMC

[MF96] Matthias Mann and Jürgen Fabian. Ab initio MO calculations on 1,2-dithietes and valence isomers. *International Journal of Quantum Chemistry*, 60(4):859–874, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60659`.

Mezey:1998:PSF

[MFAT98] Paul G. Mezey, Kenichi Fukui, Shigeru Arimoto, and Keith Taylor. Polyhedral shapes of functional group distributions in biomolecules and related similarity measures. *International Journal of Quantum Chemistry*, 66(1):99–105, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29841; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29841&PLACEBO=IE.pdf.

Mosley:1993:ECE

[MFCA93] D. H. Mosley, J. G. Fripiat, B. Champagne, and J.-M André. Efficient computation of electron-repulsion integrals in ab initio studies of polymeric systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:793–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Mosley:1994:IIS

[MFCA94] D. H. Mosley, J. G. Fripiat, B. Champagne, and J.-M André. Ab initio investigation of the static polarizability of planar and twisted infinite polythiophene chains. *International Journal of Quantum Chemistry. Symposium*, 28:451–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Marx:1996:SDD

[MFP96] D. Marx, E. S. Fois, and M. Parrinello. Static and dynamic density functional investigation of hydrated beryllium dications. *International Journal of Quantum Chemistry*, 57(4):655–662, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60402.

Mayer:1993:UEP

[MG93a] I. Mayer and A. Gomory. Use of energy partitioning for predicting primary mass spectrometric fragmentation steps: A preliminary account. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:599–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Melo:1993:TSI

[MG93b] A. Melo and J. A. N. F. Gomes. Theoretical study of ionization potentials in monosubstituted benzenes. *International Journal of Quantum Chemistry*, 46(5):651–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Magalhaes:1997:DFM

[MG97] A. L. Magalhães and J. A. N. F. Gomes. Density-functional methods for the study of the ground-state vibrations of the guanidinium ion. *International Journal of Quantum Chemistry*, 61(4):725–739, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42446; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42446&PLACEBO=IE.pdf.

Monaco:1999:SSR

[MGK99] Regina R. Monaco, William C. Gardiner, and Stephen Kirschner. Semiempirical studies of ring twisting in *cis*-stilbene and related biomolecules. *International Journal of Quantum Chemistry*, 71(1):57–62, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000013; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000013&PLACEBO=IE.pdf.

Morales:1995:IRF

[MGLBP95] J. Morales, V. Gaftoi, J. Lopez-Bonilla, and J. J. Pena. Improved recursion formulas for the calculation of two-center central potential integrals. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:339–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Medvedeva:1995:ODO

[MGNK95] N. I. Medvedeva, V. A. Gubanov, D. L. Novikov, and B. M. Klein. Oxygen defects ordering in d-Bi_2O_3: LMTO-ASA and FPLMTO calculations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:541–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Michels:1968:VCI

[MH68] H. H. Michels and F. E. Harris. Valence configuration interaction calculations for atomic scattering. *International Journal of Quantum Chemistry*, 2(??):21–27, ?? 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohamed:1998:ESP

[MH98] Adel A. Mohamed and Maher M. Hamed. Electronic spectra of phenyl-, 3-Pyridyl-, furfuryl-, and 2- theinyl-imino derivatives of thiazole: Molecular orbital treatment. *International Journal of Quantum Chemistry*, 66(6):415–423, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL

http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29877; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29877&PLACEBO=IE.pdf.

Marelius:1998:CLB

[MHÅ98] J. Marelius, T. Hansson, and J. Åqvist. Calculation of ligand binding free energies from molecular dynamics simulations. *International Journal of Quantum Chemistry*, 69 (1):77–88, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29963; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29963&PLACEBO=IE.pdf.

Maurice:1995:CIS

[MHG95] D. Maurice and M. Head-Gordon. Configuration interaction with single substitutions for excited states of open-shell molecules. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:361–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Massa:1995:QCU

[MHK95] L. Massa, L. Huang, and J. Karle. Quantum crystallography and the use of kernel projector matrices. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29: 371–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Magers:1994:DDD

[MHL94] D. H. Magers, R. B. Hood, and J. Leszczynski. Diborane, dialane, and digallane: Accurate geometries and vibrational frequencies. *International Journal of Quantum Chemistry. Symposium*, 28:579–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Masik:1995:AQDb

[MHM95a] J. Mášik, I. Hubac, and P. Mach. Applicability of quasi-degenerate many-body perturbation theory of the ground state of the F_2 molecule. *International Journal of Quantum Chemistry*, 53(3):297–??, February 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Masik:1995:AQDa

[MHM95b] J. Mášik, I. Hubac, and P. Mach. Applicability of quasi-degenerate many-body perturbation theory to quasi-degenerate electronic states: The H_4 model revisited. *International Journal of Quantum Chemistry*, 53(2):207–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:1998:SCT

[MHN98] N. H. March, A. Holas, and Á. Nagy. Self-consistent Thomas–Fermi–Dirac theory, extended by Gell-Mann and Brueckner correlation, in terms of density n and its two reduced gradients $\nabla^2 n/n$ and $\nabla n/n$. *International Journal of Quantum Chemistry*, 69(2):145–149, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29976; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29976&PLACEBO=IE.pdf`.

Maslov:1995:CME

[MHS95] I. V. Maslov, H. H. H. Homeier, and E. O. Steinborn. Calculation of multicenter electron repulsion integrals in Slater-type basis sets using the S-separation method. *International Journal of Quantum Chemistry*, 55(1):9–22, July 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

McKellar:1998:BCA

[MHY98] Alexander J. McKellar, Dodi Heryadi, and Danny L. Yeager. Balanced complete active space choices with the multiconfigurational spin tensor electron propagator method: The vertical ionization potentials of NH_2. *International Journal of Quantum Chemistry*, 70(4-5):729–736, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75050; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75050&PLACEBO=IE.pdf`.

Maekawa:1993:ESA

[MI93] K. Maekawa and A. Imamura. Electronic structures around the local defects in all-trans-polyacetylene: An analysis by the cluster-series model. *International Journal of Quantum Chemistry*, 47(6):449–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Michels:1992:MSH

[Mic92] H. H. Michels. Memorial session in honor of Arnold Karo. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:xxvii, 1992. CODEN IJQSDI. ISSN 0161-3642.

Micha:1994:TRE

[Mic94] D. A. Micha. Temporal rearrangement of electronic densities in slow atomic collisions. *International Journal of Quantum Chemistry*, 51(6):499–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Micha:1996:SMT

[Mic96a] D. A. Micha. *Statistical Mechanics and Thermodynamics*, Claude Garrod. *International Journal of Quantum Chemistry*, 60(2):711–??, 1996. CODEN IJQCB2.

Micha:1996:TEM

[Mic96b] David A. Micha. Time-evolution of multiconfiguration density functions driven by nuclear motions. *International Journal of Quantum Chemistry*, 60(1):109–118, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60573.

Michl:1997:BRM

[Mic97] Josef Michl. Book review: *Molecular and Biomolecular Electronics*, Robert R. Birge, Ed. *International Journal of Quantum Chemistry*, 62(2):237–238, March 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42496; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42496&PLACEBO=IE.pdf.

Micha:1999:BR

[Mic99] David A. Micha. Book review. *International Journal of Quantum Chemistry*, 73(4):387–388, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61000535; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61000535&PLACEBO=IE.pdf.

Mikami:1994:EEM

[Mik94] Y. Mikami. Evaluation of electronic matrix elements of long-range electron transfer in proteins by the recursive residue generation method. *International Journal of Quantum Chemistry*, 52(2):479–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Milman:1997:ISE

[Mil97] V. Milman. Ab initio study of epitaxial growth on stepped Si(100) surface. *International Journal of Quantum Chemistry*, 61(4):719–724, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42445; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42445&PLACEBO=IE.pdf.

Mintmire:1990:GOM

[Min90] J. W. Mintmire. Geometry optimization of molecules within an LCGTO local-density functional approach. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:851–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Ming:1994:BSD

[Min94a] L. Ming. Band structures of A_1 doped superconductors $YBa_2Cu_{3-x}Al_xO_{7+\delta}$. *International Journal of Quantum Chemistry*, 50(4):233–??, May 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Minyaev:1994:RPG

[Min94b] R. M. Minyaev. Reaction path as a gradient line on a potential energy surface. *International Journal of Quantum Chemistry*, 49(2):105–??, January 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ming:1996:ROC

[Min96] Li Ming. Role of the oxygen content in $TlBa_{1.2}La_{0.8}CuO_{5+\delta}$ superconductors. *International Journal of Quantum Chemistry*, 60(5):1057–1064, December 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60664.

Ming:1998:BSS

[Min98] Li Ming. Band structure study on $LiBeH_{3-y}$. *International Journal of Quantum Chemistry*, 68(6):415–419, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29959; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29959&PLACEBO=IE.pdf.

Munoz:1991:KDF

[MIW91] Luis A. Munoz, Yasuyuki Ishikawa, and Brad R. Weiner. Kinematic distribution function to calculate rotational populations of photofragments from photodissociation of triatomic molecules. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:359–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Moule:1999:TSD

[MJLL99] David C. Moule, Richard H. Judge, Haisheng Liu, and Edward C. Lim. Torsional symmetry dependence of S_1 dynamics in molecules that undergo methyl internal rotation. *International Journal of Quantum Chemistry*, 71(2):167–176, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000024; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000024&PLACEBO=IE.pdf.

Moszynski:1993:MPE

[MJS93] R. Moszynski, B. Jeziorski, and K. Szalewicz. Møller–Plesset expansion of the dispersion energy in the ring approximation. *International Journal of Quantum Chemistry*, 45(5):409–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meath:1990:RIA

[MK90] W. J. Meath and A. Kumar. Reliable isotropic and anisotropic dipolar dispersion energies, evaluated using constrained dipole oscillator strength techniques, with application to interactions involving H_2, N_2, and the rare gases. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:501–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Molnar:1995:SPC

[MK95] S. P. Molnar and J. W. King. Structure-pKa correlation via the integrated molecular transform. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):201–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Molnar:1996:CDTa

[MK96a] S. P. Molnar and J. W. King. Correlation of dermal transport with structure via the integrated molecular transform. *International Journal of Quantum Chemistry*, 60(8):121–??, 1996. CODEN IJQCB2.

Molnar:1996:CDTc

[MK96b] S. P. Molnar and J. W. King. Correlation of dermal transport with structure via the integrated molecular transform. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 23(??):121–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

Molnar:1996:CDTb

[MK96c] Stephen P. Molnar and James W. King. Correlation of dermal transport with structure via the integrated molecular transform. *International Journal of Quantum Chemistry*, 60 (8):1845–1849, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60744`.

March:1997:KEF

[MK97a] Norman H. March and Sabre Kais. Kinetic energy functional derivative for the Thomas–Fermi atom in D dimensions. *International Journal of Quantum Chemistry*, 65(5): 411–413, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42817`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42817&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Molnar:1997:CUS

[MK97b] Stephen P. Molnar and James W. King. Correlation of ultraviolet spectra with structure via the integrated molecular and electronic transforms. *International Journal of Quantum Chemistry*, 65(6):1047–1056, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42841; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42841&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on the Application of Fundamental Theory to Problems of Biology and Pharmocolgy*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Molnar:1998:CTD

[MK98a] Stephen P. Molnar and James W. King. Correlation of di- and tripeptide distribution coefficients with structure via unitary molecular indices. *International Journal of Quantum Chemistry*, 69(1):49–56, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29972; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29972&PLACEBO=IE.pdf.

Molnar:1998:PTM

[MK98b] Stephen P. Molnar and James W. King. Parametric transform and moment indices in the molecular dynamics of n-alkanes. *International Journal of Quantum Chemistry*, 70 (6):1185–1194, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75086; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75086&PLACEBO=IE.pdf.

Mishra:1999:MHD

[MK99] P. C. Mishra and Anil Kumar. Modified hybridization displacement charge scheme for π-electron systems: Study of molecular electrostatic potential maps. *International Journal of Quantum Chemistry*, 71(2):191–200, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000027; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000027&PLACEBO=IE.pdf.

Molder:1997:PSM

[MKBP97] U. Mölder, I. Koppel, P. Burk, and R. Pikver. Photoelectron spectra of molecules. II. Carboxylic acids and their esters. *International Journal of Quantum Chemistry*, 62 (3):303–314, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42516; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42516&PLACEBO=IE.pdf.

Martin:1993:QDO

[MKDL93] I. Martin, J. Karwowski, G. H. F. Diercksen, and C. Lavin. Quantum defect orbital study of electron transitions in Rydberg molecules. I. triatomic hydrogen. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27: 723–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Maran:1996:CAIa

[MKK96a] U. Maran, M. Karelson, and A. R. Katritzky. A comparative AM1 and ab initio study of the intramolecular proton transfer in tautomeric organic compounds. *International Journal of Quantum Chemistry*, 60(8):41–??, 1996. CODEN IJQCB2.

Maran:1996:CAIc

[MKK96b] U. Maran, M. Karelson, and A. R. Katritzky. A comparative AM1 and ab initio study of the intramolecular proton transfer in tautomeric organic compounds. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 23(??):41–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

Maran:1996:CAIb

[MKK96c] Uko Maran, Mati Karelson, and Alan R. Katritzky. A comparative AM1 and ab initio study of the intramolecular proton transfer in tautomeric organic compounds. *International Journal of Quantum Chemistry*, 60(8):1765–1773, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60748.

Maran:1998:TSA

[MKK98] Uko Maran, Alan R. Katritzky, and Mati Karelson. Theoretical study of aminoalkylation in the Mannich reaction of furan with methyleneimminium salt. *International Journal of Quantum Chemistry*, 67(6):359–366, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29916; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29916&PLACEBO=IE.pdf.

Mareschal:1993:MSA

[MKM93a] M. Mareschal, E. Kestemont, and M. M. Mansour. The molecular simulation approach to complex hydrodynamics. *International Journal of Quantum Chemistry*, 46(1):39–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohan:1993:EFM

[MKM93b] C. G. Mohan, A. Kumar, and P. C. Mishra. Electric-field mapping of some anions and cations of adenine and guanine. *International Journal of Quantum Chemistry*, 48(4):233–??, November 10, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohan:1996:OAC

[MKM96] C. Gopi Mohan, Anil Kumar, and P. C. Mishra. An optimized approach to compute hybridization displacement charge and a study of its effects on electrostatic potentials of some biologically important molecules. *International Journal of Quantum Chemistry*, 60(2):699–708, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60637.

Mohan:1997:IHD

[MKM97] C. Gopi Mohan, Anil Kumar, and P. C. Mishra. Influence of hybridization displacement charge on the description of electrostatic potentials of molecules with multiple electrophilic sites. *International Journal of Quantum Chemistry*, 62(1):67–76, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42490; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42490&PLACEBO=IE.pdf.

March:1999:SCS

[MKRW99] N. H. March, D. J. Klein, A. K. Ray, and X. Wu. Si_n clusters: Surface energy considerations for large n and all-electron Hartree–Fock calculations for $n = 45$. *International Journal of Quantum Chemistry*, 75(4–5):829–838, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004979/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004979&PLACEBO=IE.pdf.

McGlynn:1997:DPA

[ML97] Seán E. McGlynn and Robert J. Livingston. The distribution of polynuclear aromatic hydrocarbons between aquatic plants and sediments. *International Journal of Quantum Chemistry*, 64(3):271–283, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42686; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42686&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Mishra:1999:CEL

[ML99] Rama K. Mishra and Shyi-Long Lee. Conversion of edge-to-loop and loop-to-edge technique used to study $[\pi^2 + \pi^2]$ and $[\pi^2 + \pi^4]$ chemical reactions. *International Journal of Quantum Chemistry*, 75(4–5):821–827, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004977/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004977&PLACEBO=IE.pdf.

Martins:1993:ZCM

[MLA93] J. B. L. Martins, E. Longo, and J. Andrés. ZnO clusters models: An AM1 and MNDO study. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:643–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Martin:1992:FSO

[MLB92] I. Martin, C. Lavin, and C. Barrientos. Fine-structure oscillator strengths for excited-state transitions in Cu-Like ions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:465–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Minaev:1994:CII

[MLK94] B. F. Minaev, S. Lunell, and G. I. Kobzev. Collision-induced intensity of the $b^1\Sigma_g^+ - a^1\Delta_g$ transition in molecular oxygen: Model calculations for the collision complex $O_2 + H_2$. *International Journal of Quantum Chemistry*, 50(4):279–??, May 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mebel:1999:IMO

[MLL99] A. M. Mebel, H. L. Lin, and S. H. Lin. Ab initio molecular orbital and density functional study of the C_6 $H_6{\cdot}I_2$ complex in the ground and excited electronic states. *International Journal of Quantum Chemistry*, 72 (4):307–318, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006306; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006306&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Molina:1998:MLA

[MLR+98] L. M. Molina, M. J. López, A. Rubio, J. A. Alonso, and M. J. Stott. Mixed lead-alkali clusters in the gas phase and in liquid alloys. *International Journal of Quantum Chemistry*, 69(3):341–348, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29989; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29989&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Monard:1996:HCQ

[MLT+96] Gérald Monard, Michel Loos, Vincent Théry, Kristofor Baka, and Jean-Louis Rivail. Hybrid classical quantum force field for modeling very large molecules. *International Journal of Quantum Chemistry*, 58(2):153–159, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60471`.

Martins:1998:CNI

[MLT98] João B. L. Martins, Elson Longo, and Carlton A. Taft. CO_2 and NH_3 interaction with ZnO surface: An AM1 study. *International Journal of Quantum Chemistry*, 70 (2):367–374, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75005; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75005&PLACEBO=IE.pdf`. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Malinsky:1991:ETM

[MM91] J. Malinsky and Y. Magarshak. Electron transfer in macromolecules: Green's function and diagrammatic techniques (continued fraction representation). *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:183–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Medikeri:1994:TMR

[MM94] M. N. Medikeri and M. K. Mishra. Treatment of molecular resonances using the bi-orthogonal dilated electron propagator with application to the $^2\Pi_g$ shape resonance in e-N_2 scattering. *International Journal of Quantum Chemistry. Symposium*, 28: 29–37, 1994. CODEN IJQSAF. ISSN 0538-821X.

Mrozek:1995:CRT

[MM95] J. Mrozek and A. Michalak. Chemical reactivity trends of ergotamine and butenolide from electrostatic potentials and charge sensitivities. *International Journal of Quantum Chemistry*, 56 (5):633–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohan:1998:EPM

[MM98] C. Gopi Mohan and P. C. Mishra. Electrostatic potential mapping using hybridization displacement charge:

Atomic parameters and transferability of charge and potential. *International Journal of Quantum Chemistry*, 66 (2):149–156, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29849; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29849&PLACEBO=IE.pdf.

Maggiora:1999:FSA

[MM99a] Gerald M. Maggiora and Paul G. Mezey. A fuzzy-set approach to functional-group comparisons based on an asymmetric similarity measure. *International Journal of Quantum Chemistry*, 74(5):503–514, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62503002; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62503002&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

McNicholas:1999:SSC

[MM99b] S. J. McNicholas and F. R. Manby. State-selective core-optimized spin-coupled theory. *International Journal of Quantum Chemistry*, 74(2):97–102, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003355; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003355&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Maloteau:1992:ACE

[MMA+92] M. Maloteau, D. H. Mosley, J.-M. André, J. Delhalle, and B. T. Pickup. Attempts to calculate the electron affinity of acrylonitrile. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:563–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Martinez-Magadan:1999:TSH

[MMCC99] J. M. Martínez-Magadán, A. Cuán, and M. Castro. Theoretical study of the n-heptane-HZSM-5 ring structure model interaction. *International Journal of Quantum Chemistry*, 75(4–5):725–740, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004969/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004969&PLACEBO=IE.pdf.

Morrison:1996:GOA

[MMD96] Robert C. Morrison, Jerry R. Mizell Jr., and Orville W. Day Jr. Generalized overlap amplitudes for the lithium atom. *International Journal of Quantum Chemistry*, 57(3):355–360, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60396.

Malrieu:1995:MCC

[MMP95] J.-P. Malrieu, B. Miguel, and A. Pelegatti. Modified coupled cluster amplitudes. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:245–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Mathanes:1994:MFE

[MMPS94] A. Mathanes, M. Membrado, A. F. Pacheco, and J. Sathudo. A mass formula for the energy of metal clusters. *International Journal of Quantum Chemistry*, 52(4):767–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martinez-Magadan:1992:TSI

[MMRSN92] J. M. Martinez-Magadan, A. Ramirez-Solis, and O. Novaro. Theoretical study of the interaction of Ga, Ga^{+}, and Ga^{2+} with the hydrogen molecule. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:781–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Mouesca:1995:DFC

[MNC95] J.-M. Mouesca, L. Noodleman, and D. A. Case. Density-functional calculations of spin coupling in $(Fe_4S_4)^{3+}$ clusters. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):95–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

March:1996:FERa

[MNT96a] N. H. March, A. M. L. Nip, and J. A. Tuszynski. Free energy in relation to order parameter in magnets and pyroelectrics. *International Journal of Quantum Chemistry*, 60(7):337–??, 1996. CODEN IJQCB2.

March:1996:FERb

[MNT96b] N. H. March, A. M. L. Nip, and J. A. Tuszyński. Free energy in relation to order parameter in magnets and pyroelectrics. *International Journal of Quantum Chemistry*, 60(7):1549–1558, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60714.

March:1996:FERc

[MNT96c] N. H. March, A. M. L. Nip, and J. A. Tuszynski. Free energy in relation to order parameter in magnets and pyroelectrics. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):337–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Martin:1998:MFT

[MO98] Richard M. Martin and Gerardo Ortiz. Microscopic functional theory of dielectrics. *International Journal of Quantum Chemistry*, 69(4):567–572, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30011; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30011&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Moc:1999:KSS

[Moc99] Jerzy Moc. On the kinetic stability of the SH_3 X species with X = F, Cl. *International Journal of Quantum Chemistry*, 73(1):37–43, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55001579; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55001579&PLACEBO=IE.pdf.

Moiseyev:1997:LMI

[Moi97] Nimrod Moiseyev. Localization of multiphoton ionization/dissociation resonance wave functions in AC fields. *International Journal of Quantum Chemistry*, 63(1):279–285, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42573; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42573&PLACEBO=IE.pdf.

Monkhorst:1993:CGT

[Mon93] H. J. Monkhorst. *Chemical Graph Theory: Reactivity and Kinetics*, Vol. 2, Edited by D. Bonchev and D. H. Rouvray. *International Journal of Quantum Chemistry*, 46(6):747–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monkhorst:1994:LRC

[Mon94] H. Monkhorst. Long-range Casimir forces — theory and recent experiments on atomic systems. Edited by Frank S. Levin and David A. Micha. *International Journal of Quantum Chemistry*, 49(6):877–??, March 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monaco:1998:DAC

[Mon98] Guglielmo Monaco. On the definition of the atomic charge. relationship between 13C NMR chemical shifts, dipole moments, and charges in saturated hydrocarbons. *International Journal of Quantum Chemistry*, 68(3):201–210, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29940; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29940&PLACEBO=IE.pdf.

Monkhorst:1999:BRa

[Mon99a] Hendrik J. Monkhorst. Book review. *International Journal of Quantum Chemistry*, 71(4):357–358, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10049351; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10049351&PLACEBO=IE.pdf.

Monkhorst:1999:BRb

[Mon99b] Hendrik J. Monkhorst. Book review. *International Journal of Quantum Chemistry*, 71(5):441–442, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10050253; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10050253&PLACEBO=IE.pdf.

Monkhorst:1999:VMC

[Mon99c] Hendrik J. Monkhorst. Views of a molecule by chemists and physicists. *International Journal of Quantum Chemistry*, 72(4):281–285, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006303; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006303&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman.* Issue Edited by Michael Kasha.

Morley:1993:NOP

[Mor93a] J. O. Morley. Nonlinear optical properties of organic molecules. XII. calculations of the hyperpolarizabilities of donor-acceptor polyynes. *International Journal of Quantum Chemistry*, 46(1):19–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morrison:1993:NRC

[Mor93b] R. C. Morrison. The non-N-representability of the Colle–Salvetti second-order reduced density matrix. *International Journal of Quantum Chemistry*, 46(4):583–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morrison:1994:EKT

[Mor94] R. C. Morrison. Extended Koopmans' theorem ionization potentials for beryllium atom shake-up transitions. *International Journal of Quantum Chemistry*, 49(5):649–??, February 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morales:1996:AFE

[Mor96a] Daniel A. Morales. Analytical formulas for the eigenvalues and eigenfunctions of a d-Dimensional hydrogen atom with a potential defined by Gauss' law. *International Journal of Quantum*

Chemistry, 57(1):7–15, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60352.

Morley:1996:CFD

[Mor96b] John O. Morley. Calculation of the frequency-dependent hyperpolarizability of donor-acceptor azabutadienes. *International Journal of Quantum Chemistry*, 59(5):401–407, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60558.

Morley:1996:TAS

[Mor96c] John O. Morley. A theoretical analysis of the structure and electronic properties of 2-nitrophenylcyanate and 2-nitrophenylthiocyanate. *International Journal of Quantum Chemistry*, 59(2):167–172, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60535.

Mora:1997:MOS

[Mor97a] M. A. Mora. A molecular orbital study of the dimerization process of vinyl monomers. *International Journal of Quantum Chemistry*, 65(5):767–785, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42810; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42810&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Morley:1997:CSE

[Mor97b] John O. Morley. Calculations of the structure and electronic properties of extended polar hydrocarbons. *International Journal of Quantum Chemistry*, 61(6):991–996, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42471; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42471&PLACEBO=IE.pdf.

Morley:1998:TSS

[Mor98a] John O. Morley. Theoretical studies on the structure and electronic properties of aryl sulfides and sulfones. *International Journal of Quantum Chemistry*, 66(2):141–147, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29848; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29848&PLACEBO=IE.pdf.

Morokuma:1998:I

[Mor98b] Keiji Morokuma. Introduction. *International Journal of Quantum Chemistry*, 70(1):1, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74365; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74365&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Mosley:1998:PJB

[Mos98] David H. Mosley. Perspectives for Java-based computational quantum chemistry. *International Journal of Quantum Chemistry*, 70(1):159–165, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74360; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74360&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Mosley:1993:EAH

[MP93] D. H. Mosley and B. T. Pickup. Electron attachment to homonuclear diatomic molecules. *International Journal of Quantum Chemistry*, 45(6):719–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Murray:1999:CDM

[MPIP99] Jane S. Murray, Zenaida Peralta-Inga, and Peter Politzer. Conformational dependence of molecular surface electrostatic potentials. *International Journal of Quantum Chem-*

istry, 75(3):267–273, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000668/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000668&PLACEBO=IE.pdf.

Moscardo:1997:NFC

[MPJ97] F. Moscardó and A. J. Pérez-Jiménez. New functionals for correlation energy deduced in the framework of the correlation factor approach. *International Journal of Quantum Chemistry*, 61(2):313–323, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42395; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42395&PLACEBO=IE.pdf.

Moscardo:1998:CPA

[MPJ98] Federico Moscardó and Angel J. Pérez-Jiménez. Correlation potentials for the He atom and the hydrogen molecule: A comparison between the correlation factor approach and DFT correlation energy functionals. *International Journal of Quantum Chemistry*, 67(3):143–156, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29895; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29895&PLACEBO=IE.pdf.

Mas:1994:SPS

[MPKR94] V. Mas, J. Planelles, J. Karwowski, and R. Rajadell. Statistical properties of spin-adapted reduced Hamiltonians. *International Journal of Quantum Chemistry*, 51(6):487–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morales:1999:TCD

[MPOG99] J. Morales, J. J. Peña, G. Ovando, and V. Gaftoi. Theoretical and computational development — generalized potentials: Free particle, harmonic, and Morse partner potentials. *International Journal of Quantum Chemistry*, 71(6):465–472, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=15000344; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=15000344&PLACEBO=IE.pdf.

Morales:1997:GBR

[MPP+97] J. Morales, J. J. Peña, P. Portillo, G. Ovando, and V. Gaftoi. Generalization of the Blanchard's rule. *International Journal of Quantum Chemistry*, 65(3):205–211, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42758`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42758&PLACEBO=IE.pdf`.

Mishra:1997:AOI

[MPR97] Manoj K. Mishra, D. A. Padmavathi, and Herschel A. Rabitz. Assessing the options for identifying critically important potential surface regions: Applications to nonadiabatic transitions. *International Journal of Quantum Chemistry*, 63 (1):121–131, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42559`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42559&PLACEBO=IE.pdf`.

Mota:1997:ESP

[MPSF97] R. Mota, P. Piquini, T. M. Schmidt, and A. Fazzio. Electronic and structural properties of defects in c-BN. *International Journal of Quantum Chemistry*, 65(5):941–946, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42825`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42825&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Morales:1991:LOC

[MPSLB91] J. Morales, J. J. Pena, M. Sanchez, and J. Lopez-Bonilla. Ladder operators for central potential wave functions from the algebraic representation of orthogonal polynomials. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:155–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Mola:1994:PBM

[MPV94] E. E. Mola, C. A. Paola, and J. L. Vicente. Potential-barrier model at metal surfaces: Thin films and its dependence on the film thickness. *International Journal of Quantum Chemistry*, 52(3):617–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mogensen:1992:AVO

[MR92] B. J. Mogensen and S. Rettrup. Average virtual orbitals in configuration interaction studies with application to the low-lying singlet states of the carbon monoxide and acetone molecules. *International Journal of Quantum Chemistry*, 44(6):1045–??, December 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mulholland:1994:CSI

[MR94] A. J. Mulholland and W. G. Richards. A comparison of semiempirical and ab initio transition states for HF elimination in unimolecular decompositions. *International Journal of Quantum Chemistry*, 51(3):161–??, July 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mineva:1997:SEC

[MR97] T. Mineva and N. Russo. Solvent effects computed with the Gaussian density functional method. *International Journal of Quantum Chemistry*, 61(4):665–671, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42453; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42453&PLACEBO=IE.pdf.

Melo:1999:NPS

[MR99] André Melo and Maria João Ramos. A new partitioning scheme for molecular interacting systems within a multiconfigurational or monoconfigurational Hartree–Fock formalism. *International Journal of Quantum Chemistry*, 72 (3):157–176, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40003029; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40003029&PLACEBO=IE.pdf.

McGill:1996:UTDc

[MRB+96a] R. A. McGill, J. K. Rice, A. P. Baronavski, J. C. Owrutsky, A. H. Lowrey, K. K. Stavrev, T. Tamm, and M. C. Zerner. Using theoretical descriptors to model solvent effects in the isomerization of cis-stilbene. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):383–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

McGill:1996:UTDb

[MRB+96b] R. Andrew McGill, Jane K. Rice, A. P. Baronavski, J. C. Owrutsky, Alfred H. Lowrey, Krassimir K. Stavrev, Toomas Tamm, and Michael C. Zerner. Using theoretical descriptors to model solvent effects in the isomerization of *cis*-stilbene. *International Journal of Quantum Chemistry*, 60(7):1595–1606, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60720`.

McGill:1996:UTDa

[MRBO96] R. A. McGill, J. K. Rice, A. R. Baronavski, and J. C. Owrutsky. Using theoretical descriptors to model solvent effects in the isomerization of cis-stilbene. *International Journal of Quantum Chemistry*, 60(7):383–??, 1996. CODEN IJQCB2.

Magnasco:1999:NTM

[MRC99] Valerio Magnasco, Arnaldo Rapallo, and Massimo Casanova. New translation method for STOs and its application to calculation of overlap integrals. *International Journal of Quantum Chemistry*, 73(4):333–340, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61000529; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61000529&PLACEBO=IE.pdf`.

Merawa:1999:CPP

[MRL99] Mohammadou Mérawa, Michel Rérat, and Albert Lichanot. Compton profiles and polarizability as two similar probes of the electronic structure of 14 electron diatomic molecules: An ab initio study. *International Journal of Quantum Chemistry*, 71(1):63–74, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000014;`

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000014&PLACEBO=IE.pdf.

Marino:1997:DFS

[MRT97] Tiziana Marino, Nino Russo, and Marirosa Toscano. Density functional study of oxo-hydroxy tautomerism of 5-fluorouracil. *International Journal of Quantum Chemistry*, 62(5):489–494, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42536; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42536&PLACEBO=IE.pdf.

Mota:1990:TSP

[MS90] F. De Brito Mota and A. Ferreira Da Silva. A theoretical study to a polarization catastrophe in doped semiconductors. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:411–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Mei:1993:TUE

[MS93a] C. Mei and V. H. Smith. Towards an understanding of the electronic structure of Mott-insulating transition metal oxides. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:187–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Montagnani:1993:CMC

[MS93b] R. Montagnani and O. Salvetti. Computation of many-center exchange integrals over Slater orbitals up to 4d by means of optimized Gaussian expansions. *International Journal of Quantum Chemistry*, 47(3):225–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mei:1994:RDH

[MS94] C. Mei and V. H. Smith. On the role of doping in high-T_c superconductors. *International Journal of Quantum Chemistry. Symposium*, 28:687–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Meissner:1997:IDE

[MS97a] Holger Meißner and E. Otto Steinborn. Iterative determination of eigenvalues of the time-independent Schrödinger equation by the use of the generalized Bloch equation. *International Journal of Quantum Chemistry*, 63(1):257–268, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42571; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42571&PLACEBO=IE.pdf.

Meissner:1997:NIM

[MS97b] Holger Meißner and E. Otto Steinborn. A new iterative method for solving the time-independent Schrödinger equation based on the generalized Bloch equation. I. Boson systems: The quartic anharmonic oscillator. *International Journal of Quantum Chemistry*, 61(5):777–795, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42463; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42463&PLACEBO=IE.pdf.

Mathieu:1998:HIS

[MS98] Didier Mathieu and Philippe Simonetti. Harmonic IR spectra from empirical force fields and ab initio dipole-moment derivatives. *International Journal of Quantum Chemistry*, 69(6):705–711, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74987; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74987&PLACEBO=IE.pdf.

Murray:1992:AME

[MSCP92] J. S. Murray, J. M. Seminario, M. C. Concha, and P. Politzer. An analysis of molecular electrostatic potentials obtained by a local density functional approach. *International Journal of Quantum Chemistry*, 44(2):113–??, September 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohandas:1995:IMO

[MSCS95] P. Mohandas, M. C. Shivaglal, J. Chandrasekhar, and S. Singh. Ab initio molecular orbital calculations on the associated complexes of lithium cyanide with ammonia. *International Journal of Quantum Chemistry*, 55(6):477–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matsubara:1996:TNI

[MSM96] Toshiaki Matsubara, Stefan Sieber, and Keiji Morokuma. A test of the new "integrated MO + MM" (IMOMM) method for the conformational energy of ethane and n-butane. *International Journal of Quantum Chemistry*, 60(6):1101–1109, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60677`.

Matveev:1999:DFS

[MSMR99] Alexei Matveev, Markus Staufer, Markus Mayer, and Notker Rösch. Density functional study of small molecules and transition-metal carbonyls using revised PBE functionals. *International Journal of Quantum Chemistry*, 75(4–5):863–873, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004982/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004982&PLACEBO=IE.pdf`.

Murray:1994:DAI

[MSP94] J. S. Murray, J. M. Seminario, and P. Politzer. Does antiaromaticity imply net destabilization? *International Journal of Quantum Chemistry*, 49(5):575–??, February 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Murray:1990:ALI

[MSPS90] J. S. Murray, J. M. Seminario, P. Politzer, and P. Sjoberg. Average local ionization energies computed on the surfaces of some strained molecules. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:645–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Martin:1993:ASS

[MSRSP93] M. Martin, L. Sandoval, J. F. Rivas-Silva, and A. Palma. Amplitude squared squeezed states in the Fock–Bargmann space. *International Journal of Quantum Chemistry*, 46(4):515–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malli:1995:ICR

[MSS95] G. L. Malli, J. Styszynski, and A. B. F. Da Silva. Ab initio calculations of relativistic and electron correlation effects in polyatomics using the universal Gaussian basis set: XeF_2. *International Journal of Quantum Chemistry*, 55(3):213–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mizobe:1999:PIP

[MSS99a] Hideki Mizobe, Hiroko Shimada, and Ryoichi Shimada. Pressure-induced phase transitions of 1,2,4,5- tetrafluorobenzene crystal. *International Journal of Quantum Chemistry*, 72(4):287–293, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006304; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006304&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Mukherjee:1999:HPH

[MSS99b] Prasanta K. Mukherjee, M. Luisa Senent, and Yves G. Smeyers. Half-projected Hartree–Fock calculations for the spectroscopic parameters, frequencies, and intensities of the torsional mode of the lowest lying singlet excited states of hydrogen peroxide. *International Journal of Quantum Chemistry*, 75(4–5):631–636, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004959/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004959&PLACEBO=IE.pdf.

Mundim:1996:GOC

[MT96] Kleber C. Mundim and Constantino Tsallis. Geometry optimization and conformational analysis through generalized simulated annealing. *International Journal of Quantum Chemistry*, 58(4):373–381, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60493.

Michel:1993:ISE

[MTD93] A. G. Michel, Y. Trudel, and C. Dion. Ab initio study of the electronic properties of potential antagonists of the glycine receptor: 1. transition state of the 2-Pyridone H_2O/ 2-Hydroxypyridine . H_2O tautomeric equilibrium. *International Journal of Quantum Chemistry*, 46(1):183–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morrison:1996:CBH

[MTD96] Robert C. Morrison, Wei Tong, and Orville W. Day Jr. Chemical bonding in the hydrogen molecule. *International Journal of Quantum Chemistry*, 60(1):421–431, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60605.

Mosyagin:1997:GRE

[MTL97] N. S. Mosyagin, A. V. Titov, and Z. Latajka. Generalized relativistic effective core potential: Gaussian expansions of potentials and pseudospinors for atoms Hg through Rn. *International Journal of Quantum Chemistry*, 63(6): 1107–1122, July 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42654; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42654&PLACEBO=IE.pdf.

Manmoto:1999:DCD

[MTNF99] Yoshinori Manmoto, Minaru Tei, Junichi Nogami, and Masakuni Furuyama. Determination of off-center displacements in NaBr:F^- by nuclear magnetic double resonance. *International Journal of Quantum Chemistry*, 75(4–5):961–965, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004990/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004990&PLACEBO=IE.pdf.

Martins:1998:TSM

[MTP+98] João B. L. Martins, Carlton A. Taft, Marco A. Perez, Fulvia M. L. G. Stamato, and Elson Longo. Theoretical study of metiamide, A histamine H2 antagonist. *International Journal of Quantum Chemistry*, 69(1):117–128, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29966; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29966&PLACEBO=IE.pdf.

Mielke:1993:PWF

[MTTS93] S. L. Mielke, G. J. Tawa, D. G. Truhlar, and D. W. Schwenke. Partial widths of Feshbach funnel resonances in the na(3p)b· H_2

exciplex. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:621–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Mukhopadhyay:1996:GSP

[Muk96] Atri Mukhopadhyay. On a general system-partitioning in the many-electron correlation problem. *International Journal of Quantum Chemistry*, 60(1):261–271, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60589.

Mach:1999:QCS

[MUL99] Pavel Mach, Jan Urban, and Jerzy Leszczynski. Quantum chemical study of ground-state merocyanine 540 model compounds. *International Journal of Quantum Chemistry*, 75(4–5):741–750, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004970/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004970&PLACEBO=IE.pdf.

Masik:1997:AMM

[MUMH97] Jozef Mášik, Ján Urban, Pavel Mach, and Ivan Hubač. Applicability of multireference many-body perturbation theory to the Ne_2^+ molecule. *International Journal of Quantum Chemistry*, 63(2):333–343, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42605; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42605&PLACEBO=IE.pdf.

Mola:1990:IST

[MV90] E. E. Mola and J. L. Vicente. Image states in thin metal films: I. beryllium films. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:311–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Moyano:1992:FSA

[MV92] G. E. Moyano and J. L. Villaveces. A fibered space approach to chemical reaction mechanisms. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:761–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Manoharan:1998:TIR

[MV98a] M. Manoharan and P. Venuvanalingam. Theoretical investigation on the reactivity of sulfur-centered heterocumulenes as dienophiles in Diels–Alder reactions and endo-lone-pair effect. *International Journal of Quantum Chemistry*, 66(4):309–322, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29867; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29867&PLACEBO=IE.pdf`.

Matamala-Vasquez:1998:LOC

[MV98b] Adelio Matamala-Vásquez. Ladder operators in commutator perturbation method. *International Journal of Quantum Chemistry*, 68(2):79–90, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29928; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29928&PLACEBO=IE.pdf`.

Moyano:1999:AWF

[MV99] Gloria E. Moyano and José L. Villaveces. Approximation to wave functions, energies, and energy derivatives for molecular systems based on distribution theory. *International Journal of Quantum Chemistry*, 71(2):121–132, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000018; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000018&PLACEBO=IE.pdf`.

Mola:1992:OOA

[MVB92] E. E. Mola, J. L. Vicente, and L. Blum. Orientational ordering of adsorbed monolayers. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:621–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Mayer:1996:BFS

[MVHV96] I. Mayer, Á. Vibók, G. Halász, and P. Valiron. A BSSE-free SCF algorithm for intermolecular interactions. III. Generalization for three-body systems and for using bond functions. *International Journal of Quantum Chemistry*, 57(6):1049–1055,

???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60449.

Mesquita:1996:NDC

[MVL96] Marcus V. Mesquita, Áurea R. Vasconcellos, and Roberto Luzzi. Near dissipationless coherent excitations in biosystems. *International Journal of Quantum Chemistry*, 60(2):689–697, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60636.

Mesquita:1998:PFE

[MVL98] Marcus V. Mesquita, Áurea R. Vasconcellos, and Roberto Luzzi. Positive-feedback-enhanced Fröhlich's Bose–Einstein-like condensation in biosystems. *International Journal of Quantum Chemistry*, 66(2):177–187, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29851; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29851&PLACEBO=IE.pdf.

Mikusik:1996:HCP

[MvPC+96] Peter Mikušík, Šteěpán Pick, Norberto J. Castellani, Pierre Légaré, and Claude Demangeat. Hydrogen chemisorption on Pt/Ni (111) systems. *International Journal of Quantum Chemistry*, 57(5):887–896, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60443.

Martinez:1997:ARC

[MVS97] Ana Martínez, Alberto Vela, and Dennis R. Salahub. Achieving reliability of calculations for flat potential surfaces in density functional theory: The case of Al_4 and Al_4^{+1}. *International Journal of Quantum Chemistry*, 63(2):301–311, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42603; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42603&PLACEBO=IE.pdf.

Miao:1997:LCC

[MVV+97] M. S. Miao, P. E. Van Camp, V. E. Van Doren, J. J. Ladik, and J. W. Mintmire. An LDA calculation of the conformation and electronic structure of polytetrafluoroethylene. *International Journal of Quantum Chemistry*, 64(2): 243–246, August 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42672; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42672&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Marron:1968:VPE

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

Michels:1990:SSM

[MW90] H. H. Michels and J. M. Wadehra. Structure and stability of Li_xH_y molecules and anions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:521–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Marshall:1992:IFL

[MW92] T. S. Marshall and T. M. Wilson. Ab initio factorized LCAO calculations of the electronic band structure of ZnSe, ZnS, and the $(ZnSe)_1$ $(ZnS)_1$ strained-layer superlattice. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:687–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Mishima:1999:TSQ

[MY99] Kenji Mishima and Koichi Yamashita. A theoretical study on quantum control of photodissociation dynamics by ultrashort chirped laser pulses. *International Journal of Quantum Chemistry*, 72(5):525–532, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006354; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006354&PLACEBO=IE.pdf.

Maki:1996:NLO

[MYN+96] Jun Maki, Hiroya Yamagishi, Takeshi Noro, Fukashi Sasaki, and Yuicihi Yamamoto. New "localized orbitals" appropriate for Post-Hartree–Fock calculations. *International Journal of Quantum Chemistry*, 60(3):731–742, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60640.

Monaco:1993:CSP

[MZ93] R. R. Monaco and M. Zhao. Computational studies of peripheral ring twisting in meso-N-methyl pyridyl-substituted porphyrins. *International Journal of Quantum Chemistry*, 46(6): 701–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mo:1995:WCW

[MZ95] Y. Mo and Q. Zhang. Why N_2O_2 is *cis* while (CHO_2) is *trans*: MO and VB studies. *International Journal of Quantum Chemistry*, 56(1):19–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mancini:1994:APC

[MZM94] J. D. Mancini, Y. Zhou, and P. F. Meier. Analytic properties of connected moments expansions. *International Journal of Quantum Chemistry*, 50(2):101–??, April 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:1994:SVT

[Nag94] A. Nagy. Spin virial theorem in the density functional theory. *International Journal of Quantum Chemistry*, 49(4):353–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:1995:CSA

[Nag95a] A. Nagy. Coordinate scaling and adiabatic connection formula for ensembles of fractionally occupied excited states. *International Journal of Quantum Chemistry*, 56(4):225–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:1995:EEE

[Nag95b] A. Nagy. Exact ensemble exchange potentials for multiplets. *International Journal of Quantum Chemistry. Quantum Chem-*

istry Symposium, 29:297–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Nagaoka:1996:SPIa

[Nag96a] M. Nagaoka. Stochastic path-integral method for chemical reaction dynamics: Application to the full 3D H_3 system. *International Journal of Quantum Chemistry*, 60(7):91–??, 1996. CODEN IJQCB2.

Nagaoka:1996:SPIc

[Nag96b] M. Nagaoka. Stochastic path-integral method for chemical reaction dynamics: Application to the full 3D H_3 system. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):91–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Nagaoka:1996:SPIb

[Nag96c] Masataka Nagaoka. Stochastic path-integral method for chemical reaction dynamics: Application to the full 3D H_3 system. *International Journal of Quantum Chemistry*, 60(7):1303–1310, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60687.

Nagy:1998:ESD

[Nag98a] Á. Nagy. Excited states in density functional theory. *International Journal of Quantum Chemistry*, 70(4-5):681–691, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75046; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75046&PLACEBO=IE.pdf.

Nagy:1998:OPM

[Nag98b] Á. Nagy. Optimized potential method for ensembles of excited states. *International Journal of Quantum Chemistry*, 69(3):247–254, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29999; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29999&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Nakatsuji:1992:TMS

[Nak92] H. Nakatsuji. Theoretical model studies for surface-molecule interacting systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:725–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Nandel:1995:CSA

[NAK95] F. S. Nandel, A. Ahluwalia, and A. Kaur. Conformational structure of the amphipathic peptide insecticide L-KALA. *International Journal of Quantum Chemistry*, 55(1):61–??, July 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nalewajski:1992:CPE

[Nal92] R. F. Nalewajski. Chemical potential (electronegativity)-related quantities in a model multilevel system. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:253–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Nalewajski:1994:SAC

[Nal94] R. F. Nalewajski. Sensitivity analysis of charge transfer systems: In situ quantities, intersecting state model and its implications. *International Journal of Quantum Chemistry*, 49(5): 675–??, February 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nalewajski:1995:CRC

[Nal95] R. F. Nalewajski. Chemical reactivity concepts in charge sensitivity analysis. *International Journal of Quantum Chemistry*, 56(5):453–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nalewajski:1997:CRC

[Nal97] Roman F. Nalewajski. Charge response criteria of chemical reactivity: Fukui function indices and populational reference frames reflecting the interreactant charge coupling. *International Journal of Quantum Chemistry*, 61 (2):181–196, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42390; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42390&PLACEBO=IE.pdf.

Nalewajski:1998:KSD

[Nal98] Roman F. Nalewajski. Kohn–Sham description of equilibria and charge transfer in reactive systems. *International Journal of Quantum Chemistry*, 69(4):591–605, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30014`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30014&PLACEBO=IE.pdf`. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Nunez:1993:ACE

[NB93] M. A. Nunez and G. B. Izquierdo. Accurate computation of eigenfunctions for Schrödinger operators in one dimension. *International Journal of Quantum Chemistry*, 47(6):405–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nooijen:1997:ALR

[NB97] Marcel Nooijen and Rodney J. Bartlett. Analysis of long-range effects in many-body correlation approaches for one-dimensional periodic systems. *International Journal of Quantum Chemistry*, 63(3):601–614, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42611`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42611&PLACEBO=IE.pdf`.

Nefedova:1995:IET

[NBS95] V. V. Nefedova, A. I. Boldyrev, and J. Simons. Ab initio energies and tunneling lifetimes of the doubly charged ${AH_2}^+$ (A = Mg–Ar) diatomics. *International Journal of Quantum Chemistry*, 55(6):441–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nour:1995:BSS

[NC95] S. Nour and H. Chermette. Band structure of solids from clusters SCF potentials. *International Journal of Quantum Chemistry*, 53(1):83–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Neto:1993:SPT

[NdA93] J. D. Da Motta Neto and R. Bicca de Alencastro. On the spectral properties of tryptamine derivatives. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:107–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Neymeyr:1995:NDDc

[NE95] K. Neymeyr and K. Engel. "neglect of diatomic differential overlap" in nonempirical quantum chemical orbital theories. III. on the spectrum of the overlap matrix for diatomic molecules over locally orthogonalized basis functions. *International Journal of Quantum Chemistry*, 53(5):519–535, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nesbet:1971:EPC

[Nes71] R. K. Nesbet. Electronic pair correlation in atoms and molecules. *International Journal of Quantum Chemistry*, 4(??): 117–??, ?? 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nesbet:1994:ESM

[Nes94] R. K. Nesbet. Electron scattering mechanisms in giant magnetoresistance computed by the LACO full-potential method. *International Journal of Quantum Chemistry. Symposium*, 28: 77–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Newman:1997:VAG

[New97] F. T. Newman. A very accurate grid method for the solution of Schrödinger equations: The helium ground state. *International Journal of Quantum Chemistry*, 63(6):1065–1078, July 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42651; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42651&PLACEBO=IE.pdf`.

Neymeyr:1995:NDDd

[Ney95a] K. Neymeyr. "neglect of diatomic differential overlap" in nonempirical quantum chemical orbital theories. IV. an examination of the justification of the neglect of diatomic differential overlap (NDDO) approximation. *International Journal of*

Quantum Chemistry, 53(5):541–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Neymeyr:1995:NDDe

[Ney95b] K. Neymeyr. "neglect of diatomic differential overlap" in nonempirical quantum chemical orbital theories. V. A calculus of error concerning the justification of the neglect of diatomic differential overlap (NDDO) approximation. *International Journal of Quantum Chemistry*, 53(5):553–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nalewajski:1994:QMV

[NFVM94] R. F. Nalewajski, S. J. Formosinho, A. J. C. Varandas, and J. Mrozek. Quantum mechanical valence study of a bond-breaking-bond-forming process in triatomic systems. *International Journal of Quantum Chemistry*, 52(5):1153–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nogueira:1995:EFG

[NG95] S. R. Nogueira and D. Guenzburger. Electric-field gradients and magnetic hyperfine parameters of square-pyramidal $(M(CN)_5)^{3-}$ (M = Co, Rh, and Ir) complexes. *International Journal of Quantum Chemistry*, 54(6):381–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nogueira:1996:REE

[NG96] S. R. Nogueira and Diana Guenzburger. Relativistic effects on the electronic structure and bonding of $(Ir(CN)_5)^-_3$. *International Journal of Quantum Chemistry*, 57(3):471–479, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60386.

Nemukhin:1997:MPH

[NG97] A. V. Nemukhin and B. L. Grigorenko. Modeling properties of the HF dimer in argon clusters. *International Journal of Quantum Chemistry*, 62(1):55–65, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42489; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42489&PLACEBO=IE.pdf.

Nikitina:1995:CII

[NGM+95] E. A. Nikitina, T. A. Golubina, A. I. Malkin, V. S. Yushchenko, V. D. Khavryuthcenko, and E. F. Sheka. Computational investigation of the influence of the environment on mechanical properties of solids. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:161–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Northrup:1990:BSP

[NH90] S. H. Northrup and R. G. Herbert. Brownian simulation of protein association and reaction. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17:55–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Nakatsuji:1997:TSC

[NHN97] Hiroshi Nakatsuji, Zhen-Ming Hu, and Hiromi Nakai. Theoretical studies on the catalytic activity of Ag surface for the oxidation of olefins. *International Journal of Quantum Chemistry*, 65(5):839–855, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42815; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42815&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Nunez:1994:NAB

[NI94] M. A. Nuñez and G. B. Izquierdo. New approximation to the bound states of Schrödinger operators with Coulomb interaction. *International Journal of Quantum Chemistry. Symposium*, 28:241–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Nicolaides:1996:SSA

[Nic96] Cleanthes A. Nicolaides. The state-specific approach to the solution of problems of electronic structure and dynamics involving excited states. *International Journal of Quantum Chemistry*, 60(1):119–129, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60574`.

Nicolaides:1999:ACQ

[Nic99] Cleanthes A. Nicolaides. On the application of conventional quantum chemistry methods of computation to states perturbed by the continuous spectrum. *International Journal of Quantum Chemistry*, 71(2):209–213, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000019; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000019&PLACEBO=IE.pdf.

Nakajima:1996:AEH

[NK96a] Hideo Nakajima and Osamu Kikuchi. Analysis of electrostatic and hydrophobic complementarities between chymotrypsin and avian ovomucoid third domains using molecular electrostatic potential: Effect of residue replacements. *International Journal of Quantum Chemistry*, 60(5):1081–1091, December 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60667.

Negadi:1996:PTF

[NK96b] T. Negadi and M. Kibler. The periodic table in flatland. *International Journal of Quantum Chemistry*, 57(1):53–61, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60356.

Nicolaides:1998:GAA

[NK98] Cleanthes A. Nicolaides and Yannis Komninos. Geometrically active atomic states and the formation of molecules in their normal shapes. *International Journal of Quantum Chemistry*, 67(5):321–328, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29910; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29910&PLACEBO=IE.pdf.

Nagao:1996:NTMb

[NKS+96a] H. Nagao, K. Kodama, Y. Shigeta, K. Nishikawa, H. Kawabe, M. Nakano, and K. Yamaguchi. Nonadiabatic treatment of molecular systems by the wavepackets method. *International Journal of Quantum Chemistry*, 60(7):1261–1270, ???? 1996.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60737.

Nagao:1996:NTMc

[NKS+96b] H. Nagao, K. Kodama, Y. Shigeta, N. Nishikawa, H. Kawabe, M. Nakano, and K. Yamaguchi. Nonadiabatic treatment of molecular systems by the wavepackets method. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):49–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Nagao:1996:NTMa

[NKSN96] H. Nagao, K. Kodama, Y. Shigeta, and N. Nishikawa. Nonadiabatic treatment of molecular systems by the wavepackets method. *International Journal of Quantum Chemistry*, 60(7): 49–??, 1996. CODEN IJQCB2.

Neogrady:1997:IPE

[NKUS97] Pavel Neogrády, Vladimir Kellö, Miroslav Urban, and Andrzej J. Sadlej. Ionization potentials and electron affinities of Cu, Ag, and Au: Electron correlation and relativistic effects. *International Journal of Quantum Chemistry*, 63(2): 557–565, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42599; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42599&PLACEBO=IE.pdf.

Nowek:1996:ISH

[NL96a] Andrzej Nowek and Jerzy Leszczyński. An ab initio study on HXC(double bond)O ... HY molecular complexes (X, Y = F, Cl). *International Journal of Quantum Chemistry*, 57(4): 757–766 (or 757–765??), ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60414.

Nowek:1996:PHF

[NL96b] Andrzej Nowek and Jerzy Leszczýnski. Post-Hartree–Fock and DFT level studies on the Cl_2 CO ... Cl_2 complex: Accurate molecular parameters, harmonic vibrational frequencies, and interaction energies. *International Journal of Quantum Chemistry*, 60(5):1007–1013, December 5, 1996. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60673.

Nalewajski:1995:UCS

[NM95] R. F. Nalewajski and A. Michalak. Use of charge sensitivity analysis in diagnosing chemisorption clusters: Minimum-energy coordinate and Fukui function study of model toluene-(V_2O_5) systems. *International Journal of Quantum Chemistry*, 56(5): 603–613, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nalewajski:1996:HFD

[NM96] Roman F. Nalewajski and Janusz Mrozek. Hartree–Fock difference approach to chemical valence: Three-electron indices in UHF approximation. *International Journal of Quantum Chemistry*, 57(3):377–389, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60375.

Nicolaides:1994:MEM

[NMKP94] C. A. Nicolaides, T. Mercouris, Y. Komninos, and I. D. Petsalakis. Many-electron, many-photon theory of nonstationary states. *International Journal of Quantum Chemistry*, 51(6): 529–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nalewajski:1997:TEV

[NMM97] Roman F. Nalewajski, Janusz Mrozek, and Artur Michalak. Two-electron valence indices from the Kohn–Sham orbitals. *International Journal of Quantum Chemistry*, 61(3): 589–601, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42430; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42430&PLACEBO=IE.pdf.

Nagao:1997:PCS

[NMN+97] Hidemi Nagao, Masaki Mitani, Masamichi Nishino, Yasunori Yoshioka, and Kizashi Yamaguchi. Possibilities of charge- and/ or spin-mediated superconductors and photo-induced superconductors in the intermediate region of metal-insulator transitions. *International Journal of Quantum Chemistry*, 65(5):

947–964, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42826; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42826&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Nagao:1998:PCM

[NMN+98] Hidemi Nagao, Masaki Mitani, Masamichi Nishino, Yasuteru Shigeta, Yasunori Yoshioka, and Kizashi Yamaguchi. Possibility of charge-mediated superconductors in the intermediate region of metal-insulator transitions. *International Journal of Quantum Chemistry*, 70(4-5):1075–1084, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75030; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75030&PLACEBO=IE.pdf.

Nagao:1999:TSA

[NMN+99] Hidemi Nagao, Masaki Mitani, Masamichi Nishino, Yasuteru Shigeta, Yasunori Yoshioka, and Kizashi Yamaguchi. Theoretical studies on anomalous phases in molecular systems with external field: Possibility of photo-induced superconductivity. *International Journal of Quantum Chemistry*, 75(4–5):549–561, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004950/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004950&PLACEBO=IE.pdf.

Nandel:1999:CSP

[NMSJ99] Fateh S. Nandel, Nandita Malik, Balvinder Singh, and D. V. S. Jain. Conformational structure of peptides containing dehydroalanine: Formation of β-bend ribbon structure. *International Journal of Quantum Chemistry*, 72(1):15–23, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002299; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002299&PLACEBO=IE.pdf.

Nagy:1998:ESA

[NMvB+98] L. Turi Nagy, M. Micov, Ľ. Benco, M. Liška, P. Mach, and D. Tunega. Electronic structure of alumina surface. *International Journal of Quantum Chemistry*, 70(2): 341–350, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75002; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75002&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Nakatsuji:1994:TSM

[NN94] H. Nakatsuji and T. Nakao. Theoretical study on metal NMR chemical shifts: Germanium compounds. *International Journal of Quantum Chemistry*, 49(3):279–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakayama:1998:TSE

[NNH98] Kenichi Nakayama, Haruyuki Nakano, and Kimihiko Hirao. Theoretical study of the $\pi \to \pi^*$ excited states of linear polyenes: The energy gap between $1^1B_u^+$ and $2^1A_g^-$ states and their character. *International Journal of Quantum Chemistry*, 66(2):157–175, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29850; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29850&PLACEBO=IE.pdf.

Nada:1996:BSI

[NNMH96] Roberto Nada, John B. Nicholas, Maureen I. McCarthy, and Anthony C. Hess. Basis sets for ab initio periodic Hartree–Fock studies of zeolite/adsorbate interactions: He, Ne, and Ar in silica sodalite. *International Journal of Quantum Chemistry*, 60(4):809–820, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60653.

Nagao:1996:MEWb

[NNY+96a] H. Nagao, M. Nakano, S. Yamanaka, S. Yamada, D. Yamaki, I. Shigemoto, S. Kiribayashi, K. Yamaguchi, and Y. Shigeta.

Many-electron-wavepackets method. *International Journal of Quantum Chemistry*, 60(7):1291–1301, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60686.

Nagao:1996:MEWc

[NNY+96b] H. Nagao, M. Nakano, S. Yamanaka, S. Yamada, D. Yamaki, I. Shigemoto, S. Kiribayashi, K. Yamaguchi, and Y. Shigeta. Many-electron-wavepackets method. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??): 79–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Nagao:1996:MEWa

[NNYY96] H. Nagao, M. Nakano, S. Yamanaka, and S. Yamada. Many-electron-wavepackets method. *International Journal of Quantum Chemistry*, 60(7):79–??, 1996. CODEN IJQCB2.

Nobutoki:1999:BSO

[Nob99] Hideharu Nobutoki. Broken-symmetry orbitals for the quasidiabatic electronic states of polymers. *International Journal of Quantum Chemistry*, 74(6):745–752, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001790; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001790&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Nagao:1997:TSS

[NONY97] Hidemi Nagao, Koji Ohta, Masayoshi Nakano, and Kizashi Yamaguchi. Theoretical studies of second hyperpolarizability by path integral method: Effects of external magnetic field. *International Journal of Quantum Chemistry*, 65(5): 697–707, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42802; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42802&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue

Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Norman:1991:HSR

[Nor91] M. R. Norman. Hund's second rule and the electronic structure of transition-metal oxides. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:431–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Nagaoka:1998:SMU

[NOY98] Masataka Nagaoka, Yoshishige Okuno, and Tokio Yamabe. "statistical-mechanical" understanding of chemical reaction mechanism in solution: Energy fluctuations and heat capacities for isomerization of formamidine in aqueous solution. *International Journal of Quantum Chemistry*, 70 (1):133–145, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74358; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74358&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Nagaoka:1994:MTS

[NOYY94] M. Nagaoka, Y. Okuno, N. Yoshida, and T. Yamabe. A microscopic theory for solution chemical reactions: Introduction of reactant and medium structures into generalized Langevin equation formalism. *International Journal of Quantum Chemistry*, 51(6):519–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:1996:IEM

[NP96a] Á. Nagy and Robert G. Parr. Information entropy as a measure of the quality of an approximate electronic wave function. *International Journal of Quantum Chemistry*, 58(4):323–327, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60486.

Nordio:1996:CDA

[NP96b] P. L. Nordio and A. Polimeno. Classical description of activated conformational processes in molecular systems coupled to solvent degrees of freedom. *International Journal of*

Quantum Chemistry, 60(1):321–329, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60595`.

Neto:1990:TDF

[NPL90] J. J. Soares Neto, S. B. Padkjoer, and J. Linderberg. Two different finite element schemes applied to quantum mechanical calculations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:467–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Nooijen:1992:CCA

[NS92] M. Nooijen and J. G. Snijders. Coupled cluster approach to the single-particle Green's function. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:55–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Nooijen:1993:CCG

[NS93a] M. Nooijen and J. G. Snijders. Coupled cluster Green's function method: Working equations and applications. *International Journal of Quantum Chemistry*, 48(1):15–??, October 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nooijen:1993:DAA

[NS93b] M. Nooijen and J. G. Snijders. Diagrammatic analysis and application of the coupled cluster response approach to ground-state expectation values. *International Journal of Quantum Chemistry*, 47(1):3–??, July 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Neymeyr:1995:NDDa

[NS95a] K. Neymeyr and F. F. Seelig. "neglect of diatomic differential overlap" in nonempirical quantum chemical orbital theories. I. on the justification of the neglect of diatomic differential overlap approximation. *International Journal of Quantum Chemistry*, 53(5):515–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Neymeyr:1995:NDDb

[NS95b] K. Neymeyr and F. F. Seelig. "neglect of diatomic differential overlap" in nonempirical quantum chemical orbital theories. II. A polynomial expansion for $\Delta^{-1/2}$ in terms of Legendre and Chebyshev polynomials. *International Journal of Quantum Chemistry*, 53(5):519–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Novakovskaya:1997:PSN

[NS97a] Yulia V. Novakovskaya and Nikolai F. Stepanov. The problem of small negatively ionized water clusters. *International Journal of Quantum Chemistry*, 63(3):737–748, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42617`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42617&PLACEBO=IE.pdf`.

Novakovskaya:1997:SEP

[NS97b] Yulia V. Novakovskaya and Nikolai F. Stepanov. Structure and energy of the positively ionized water clusters. *International Journal of Quantum Chemistry*, 61(6):981–990, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42470`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42470&PLACEBO=IE.pdf`.

Nakajima:1995:PSI

[NSS+95] Y. Nakajima, Y. Sakagishi, M. Shiibashi, Y. Suzuki, and H. Kato. A PM3 study on intrinsic decarboxylation process of methyl-ethyl-α-pyridylacetic acid. *International Journal of Quantum Chemistry*, 54(1):51–59, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nobel:1994:TII

[NST94] J. A. Nobel, J. R. Sabin, and S. B. Trickey. Theoretical ion implantation profiles for low energy protons under channeling conditions. *International Journal of Quantum Chemistry. Symposium*, 28:283–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Naray-Szabo:1994:NDD

[NSTFC94] G. Naray-Szabo, G. Toth, G. G. Ferenczy, and G. Csonka. The neglect of diatomic differential overlap (NDDO) fragment self-consistent field method for the treatment of very large covalent systems. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Sym-*

posium on Quantum Biology and Quantum Pharmacology., 21: 227–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Nagy:1996:MIP

[NTL96] L. Turi Nagy, D. Tunega, and M. Liška. Modeling of interaction properties of surfaces of phyllosilicates: A theoretical forecast of adsorption isotherms of noble gases at the talc surface. *International Journal of Quantum Chemistry*, 57(5):843–849, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60438`.

Neogrady:1995:SAR

[NU95] P. Neogrady and M. Urban. Spin-adapted restricted Hartree–Fock reference coupled-cluster theory for open shell systems: Noniterative triples for noncanonical orbitals. *International Journal of Quantum Chemistry*, 55(2):187–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nunez:1994:ACE

[Nuñ94a] M. A. Nuñez. Accurate computation of eigenfunctions for screened Coulomb potentials. *International Journal of Quantum Chemistry*, 51(2):57–??, July 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nunez:1994:NCB

[Nun94b] M. A. Nunez. Numerical computation of bounded states for Schrödinger operators. *International Journal of Quantum Chemistry*, 50(2):113–??, April 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nunez:1995:CEV

[Nuñ95a] M. A. Nuñez. Computation of expectation values with Dirichlet one-dimensional wave functions. *International Journal of Quantum Chemistry*, 53(1):15–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nunez:1995:GCA

[Nuñ95b] M. A. Nuñez. General criteria for assessing the accuracy of approximate wave functions and their densities. *International Journal of Quantum Chemistry*, 53(1):27–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nunez:1996:ABE

[Núñ96] Marco A. Núñez. Asymptotic behavior of electron densities and computation of one-electron properties. *International Journal of Quantum Chemistry*, 57(6):1077–1096, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60452.

Nunez:1997:RCC

[Núñ97] Marco A. Núñez. Rate of convergence of calculations with one-dimensional Dirichlet wave functions. *International Journal of Quantum Chemistry*, 62(5):449–460, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42530; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42530&PLACEBO=IE.pdf.

Nolting:1994:ERSa

[NV94a] V. Nolting and W. S. Verwoerd. Extrapolation of real-space quantum chemical calculations from finite-size super cells to the ideal infinite system. I. theory. *International Journal of Quantum Chemistry*, 52(6):1273–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nolting:1994:ERSb

[NV94b] V. Nolting and W. S. Verwoerd. Extrapolation of real-space quantum chemical calculations from finite-size super cells to the ideal infinite system. II. application to one-dimensional polymers. *International Journal of Quantum Chemistry*, 52 (6):1287–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nolting:1997:ERS

[NV97a] V. Nolting and W. S. Verwoerd. Extrapolation of real-space quantum chemical calculations from finite-size supercells to the ideal infinite system. III. Application to two-dimensional systems. *International Journal of Quantum Chemistry*, 63 (4):895–911, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42639; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42639&PLACEBO=IE.pdf.

Nyulaszi:1997:APS

[NV97b] László Nyulászi and Tamás Veszprémi. Assignment of photoelectron spectra by the help of density functional calculations. *International Journal of Quantum Chemistry*, 61(3): 399–403, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42434; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42434&PLACEBO=IE.pdf`.

Nyulaszi:1991:PSH

[NVR+91] L. Nyulaszi, T. Veszpremi, J. Reffy, G. Zsombok, T. Cvitas, B. Kovac, L. Klasinc, and S. P. McGlynn. Photoelectron spectra of halogenofurans. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:479–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Nilsson:1999:CMH

[NWG+99] Anna M. Nilsson, Mihirinie Wijaywardene, George Gkoutos, Keith M. Wilson, Nelson Fernández, and Christopher A. Reynolds. Correlated mutations in the HLA class II molecule. *International Journal of Quantum Chemistry*, 73(2):85–96, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003508; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003508&PLACEBO=IE.pdf`. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998.* Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Nakano:1998:NCL

[NY98] M. Nakano and K. Yamaguchi. Numerical coupled Liouville approach: Quantum dynamics of linear molecular aggregates under intense electric fields. *International Journal of Quantum Chemistry*, 70(1):77–87, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74371; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74371&PLACEBO=IE.pdf`. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II).* Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Nakano:1998:HOD

[NYKY98] M. Nakano, S. Yamada, S. Kiribayashi, and K. Yamaguchi. Hyperpolarizabilities of one-dimensional H_n systems: Second hyperpolarizability density analyses for regular and charged solitonlike linear chains. *International Journal of Quantum Chemistry*, 70(2):269–282, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74995; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74995&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Nunez-Yepez:1997:OOT

[NYLBNSB97] H. N. Nuñez-Yepez, J. L. López-Bonilla, D. Navarrete, and A. L. Salas-Brito. Oscillators in one and two dimensions and ladder operators for the Morse and Coulomb problems. *International Journal of Quantum Chemistry*, 62(2): 177–183, March 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42501; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42501&PLACEBO=IE.pdf.

Nakano:1999:NCL

[NYNY99] M. Nakano, S. Yamada, H. Nagao, and K. Yamaguchi. Numerical coupled Liouville approach: Application to second hyperpolarizability of molecular aggregate. *International Journal of Quantum Chemistry*, 71(4):295–306, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10049343; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10049343&PLACEBO=IE.pdf.

Nagaoka:1996:EBM

[NYY96] Masataka Nagaoka, Naoto Yoshida, and Tokio Yamabe. On the equivalence between the microscopic frictional theory and transition-state theory. *International Journal of Quantum Chemistry*, 60(1):287–295, October 5, 1996. CODEN

IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60591`.

Neto:1992:ISA

[NZA92] J. D. Da Motta Neto, M. C. Zerner, and R. Bicca De Alencastro. On the implications of the structure of 3prime-azido-3prime-deoxythymidine and related compounds to antiviral activity. *International Journal of Quantum Chemistry*, 44(5): 743–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Osman:1999:I

[OAG99] Roman Osman, Giuliano Alagona, and Caterina Ghio. Introduction. *International Journal of Quantum Chemistry*, 73(2):59–60, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003524; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003524&PLACEBO=IE.pdf`. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998*. Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Olah:1995:KAP

[OB95] K. Oláh and J. Bódiss. Kinetics and atom-photon interactions. *International Journal of Quantum Chemistry*, 53(3): 265–??, February 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

OConnell:1996:DFP

[O'C96] R. F. O'Connell. Dissipative and fluctuation phenomena in quantum mechanics with applications. *International Journal of Quantum Chemistry*, 58(6):569–581, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60514`.

Ogliaro:1999:BBV

[OCK99] François Ogliaro, David L. Cooper, and Peter B. Karadakov. Bent-bond versus separated-bond models: A spin-coupled survey for a few organic and inorganic systems. *International Journal of Quantum Chemistry*, 74(2):223–229, ???? 1999. CODEN

IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003366; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003366&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Oliveira:1990:EDF

[OGK90] L. N. Oliveira, E. K. U. Gross, and W. Kohn. Ensemble-density functional theory for excited states. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:707–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Ohrn:1993:Ia

[Öhr93] N. Y. Öhrn. Introduction. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:v, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Ortiz-Henarejos:1997:DBI

[OHSF97] Ester Ortiz-Henarejos and Emilio San-Fabián. Differences between ab initio and density functional electron densities. *International Journal of Quantum Chemistry*, 61(2): 245–252, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42405; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42405&PLACEBO=IE.pdf.

Ohta:1998:NBE

[Oht98] Katsuhisa Ohta. New bosonic excitation operators in many-electron wave functions. *International Journal of Quantum Chemistry*, 67(2):71–75, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29887; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29887&PLACEBO=IE.pdf.

Oddershede:1977:DEE

[OJB77] Jens Oddershede, Poul Jørgensen, and Nelson H. F. Beebe. Determination of excitation energies and transition moments in a second order polarization propagator approach. application to the Be atom and the CH^+ molecule. *International Journal of Quantum Chemistry*, 12:655–670, 1977. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olszewski:1996:PNB

[OK96] S. Olszewski and T. Kwiatkowski. Properties of Non-Bloch LCAO wave functions for cubic crystals in the presence of an external electric field. *International Journal of Quantum Chemistry*, 57(1):113–121, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60350.

Ohwada:1998:EBM

[OKI98] Tomohiko Ohwada, Hirotaka Kagawa, and Hiroshi Ichikawa. Electrons-in-a-box model for conjugation in linear carbanions. *International Journal of Quantum Chemistry*, 68 (1):65–72, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29923; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29923&PLACEBO=IE.pdf.

Okuno:1998:ERP

[Oku98] Yoshishige Okuno. Effects of reaction path curvature on reaction dynamics and rates: Reaction path Hamiltonian calculations for gas-phase SN_2 reaction Cl^- + CH_3Cl. *International Journal of Quantum Chemistry*, 68(4):261–271, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29946; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29946&PLACEBO=IE.pdf.

Ohta:1999:OAA

[OKY+99] Y. Ohta, H. Kizu, A. Yamada, T. Yoshimoto, and K. Nishikawa. One approach to adiabatic population transfer by Hückel molecular orbital theory. *International Journal of Quantum Chemistry*, 75(4–5):511–522, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004946/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004946&PLACEBO=IE.pdf.

Ohrn:1978:CCG

[ÖL78] Y. Öhrn and J. Linderberg. Characteristics of the consistent ground state of the random phase of approximation. *International Journal of Quantum Chemistry*, ??(??):1–18, ?? 1978. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Orozco:1996:TRS

[OLC+96] Modesto Orozco, J. M. López, C. Colomines, C. Alhambra, M. A. Busquets, and F. J. Luque. Theoretical representation of solvation in biochemical systems: From discrete solute-solvent interactions to bulk solvation. *International Journal of Quantum Chemistry*, 60(6):1179–1187, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60682`.

Oliva:1999:BBM

[Oli99] Josep M. Oliva. Bonding in benzene methylene isomers: Modern VB study using spin-coupled theory. *International Journal of Quantum Chemistry*, 71(4):319–327, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10049346; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10049346&PLACEBO=IE.pdf`.

Olszewski:1996:DEO

[Ols96] S. Olszewski. Distribution of electron orbits having a definite angular momentum in a static magnetic field. *International Journal of Quantum Chemistry*, 57(1):35–41, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60354`.

Oberbrodhage:1997:MDS

[OMTS97] J. Oberbrodhage, H. Morgner, O. Tapia, and H. O. G. Siegbahn. Molecular dynamics simulation of the free surface of liquid formamide. *International Journal of Quantum Chemistry*, 63(6):1123–1131, July 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42655; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42655&PLACEBO=IE.pdf`.

Ohrn:1996:BMB

[ÖOD96] Yngve Öhrn, Juan Oreiro, and Erik Deumens. Bond making and bond breaking in molecular dynamics. *International Journal of Quantum Chemistry*, 58(6):583–591, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60515`.

Ortiz:1991:RGS

[Ort91] J. V. Ortiz. Renormalized ground states in electron propagator theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:35–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Ortiz:1992:TEE

[Ort92] J. V. Ortiz. Total energies and energy gradients in electron propagator theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:1–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Ortiz:1993:CGS

[Ort93] J. V. Ortiz. A comparison of ground-state averages in electron propagator theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:407–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Ortiz:1995:CIE

[Ort95] J. V. Ortiz. Contour integrals in electron propagator theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:331–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Ortiz:1997:PTO

[Ort97] J. V. Ortiz. Partial third-order quasiparticle theory: An application to the photoelectron spectrum of S-tetrazine. *International Journal of Quantum Chemistry*, 63(2):291–299, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42593; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42593&PLACEBO=IE.pdf`.

Ortiz:1998:ABO

[Ort98a] J. V. Ortiz. Approximate Brueckner orbitals and shakeup operators in electron propagator calculations: Applications to F^- And OH^-. *International Journal of Quantum Chemistry*, 70(4-5):651–658, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75043; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75043&PLACEBO=IE.pdf.

Ortiz:1998:SOS

[Ort98b] J. V. Ortiz. Second-order shakeup terms in electron propagator calculations on F_2 and H_2O_2. *International Journal of Quantum Chemistry*, 69(2):175–182, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29980; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29980&PLACEBO=IE.pdf.

Ortiz:1999:ABO

[Ort99] J. V. Ortiz. Approximate Brueckner orbitals in electron propagator calculations. *International Journal of Quantum Chemistry*, 75(4–5):615–621, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004957/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004957&PLACEBO=IE.pdf.

Olofson:1995:GQE

[OS95] A. E. S. Olofson and R. H. Squire. Is "$4n+2$" a general quantum electromagnetic topological invariant? *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:313–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Oliva:1997:UMA

[OSA+97] Mónica Oliva, Vicent S. Safont, Juan Andrés, Raquel Castillo, and Vicente Moliner. Understanding the mechanism of the addition of organomagnesium reagents to 2-Hydroxypropanal: An ab initio molecular orbital analysis. *International Journal of Quantum Chemistry*, 65(5):719–728, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42804;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42804&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Ojamae:1995:PES

[OSS95] L. Ojamae, I. Shavitt, and S. J. Singer. Potential energy surfaces and vibrational spectra of H_5O^{2+} and larger hydrated proton complexes. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:657–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Ohrn:1990:Ia

[ÖSZ90a] N. Y. Öhrn, J. R. Sabin, and M. C. Zerner. Introduction. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17:vii, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Ohrn:1990:Ib

[ÖSZ90b] N. Y. Öhrn, J. R. Sabin, and M. C. Zerner. Introduction. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:xiii, 1990. CODEN IJQSDI. ISSN 0161-3642.

Ohrn:1991:Ia

[ÖSZ91a] N. Y. Öhrn, J. R. Sabin, and M. C. Zerner. Introduction. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:vii, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Ohrn:1991:Ib

[ÖSZ91b] N. Y. Öhrn, J. R. Sabin, and M. C. Zerner. Introduction. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:xi, 1991. CODEN IJQSDI. ISSN 0161-3642.

Ohrn:1992:Ia

[ÖSZ92a] N. Y. Öhrn, J. R. Sabin, and M. C. Zerner. Introduction. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on*

Quantum Biology and Quantum Pharmacology., 19:vii, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Ohrn:1992:Ib

[ÖSZ92b] N. Y. Öhrn, J. R. Sabin, and M. C. Zerner. Introduction. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:ix, 1992. CODEN IJQSDI. ISSN 0161-3642.

Ohrn:1993:Ib

[ÖSZ93] N. Y. Öhrn, J. R. Sabin, and M. C. Zerner. Introduction. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:ix, 1993. CODEN IJQSDI. ISSN 0161-3642.

Ohrn:1995:I

[ÖSZ95] Y. Öhrn, J. R. Sabin, and M. C. Zerner. Introduction. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):1–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Ohrn:1996:I

[ÖSZ96] N. Öhrn, J. R. Sabin, and M. C. Zerner. Introduction. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):1–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Ohrn:1997:Ia

[ÖSZ97a] N. Y. Öhrn, J. R. Sabin, and M. C. Zerner. Introduction. *International Journal of Quantum Chemistry*, 65(5): 377, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42773; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42773&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods.* Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Ohrn:1997:Ib

[ÖSZ97b] N. Y. Öhrn, J. R. Sabin, and M. C. Zerner. Introduction. *International Journal of Quantum Chemistry*, 65

(6):1031, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42836; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42836&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on the Application of Fundamental Theory to Problems of Biology and Pharmocolgy*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Ohrn:1999:Ia

[ÖSZ99a] N. Y. Öhrn, J. R. Sabin, and M. C. Zerner. Introduction. *International Journal of Quantum Chemistry*, 75(4–5):333, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004992/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004992&PLACEBO=IE.pdf.

Ohrn:1999:Ib

[ÖSZ99b] N. Y. Öhrn, J. R. Sabin, and M. C. Zerner. Introduction. *International Journal of Quantum Chemistry*, 75(6):967, December 20, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004792/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004792&PLACEBO=IE.pdf.

OLeary:1995:SSS

[OTS+95] P. O'Leary, J. R. Thomas, H. F. Schaefer, III, B. J. Duke, and B. O'Leary. A study of the silagermylyne ($SiGeH_2$) molecule: A new monobridged structure. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:593–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Otto:1994:RDT

[Ott94] P. Otto. Recent developments in the theoretical design of low-gap polymers and their nonlinear optical properties. *International Journal of Quantum Chemistry*, 52(2):353–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Okuyama-Yoshida:1998:TSO

[OYNY98] Naoto Okuyama-Yoshida, Masataka Nagaoka, and Tokio Yamabe. Transition-state optimization on free energy surface: Toward solution chemical reaction ergodography. *International Journal of Quantum Chemistry*, 70(1):95–103, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74373; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74373&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Politzer:1998:CDF

[PAAM98] Peter Politzer, Fakher Abu-Awwad, and Jane S. Murray. Comparison of density functional and Hartree–Fock average local ionization energies on molecular surfaces. *International Journal of Quantum Chemistry*, 69(4):607–613, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30015; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30015&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Peralta:1998:EEP

[PAC98] Juan E. Peralta, Martín C. Ruiz De Azúa, and Rubén H. Contreras. Electrostatic effect of the polar bond-polarizable bond interaction on 13C chemical shifts. *International Journal of Quantum Chemistry*, 70(1):105–112, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74355; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74355&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Pahl:1998:ACA

[Pah98] Felix A. Pahl. Atomic calculations with an augmented Fourier basis. *International Journal of Quantum Chemistry*,

70(1):189–197, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74363; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74363&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Paikeday:1991:EAI

[Pai91] Joseph M. Paikeday. Electron-atom interaction potential by DCS minimization. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:569–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Paikeday:1997:EPA

[Pai97] Joseph M. Paikeday. Effective potential for *e*-atom scattering by DCS minimization at intermediate energies. *International Journal of Quantum Chemistry*, 65(5):585–590, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42788; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42788&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Paikeday:1999:EPA

[Pai99] Joseph M. Paikeday. Effective potential for *e*-argon and *e*-krypton scattering by DCS minimization at intermediate energies. *International Journal of Quantum Chemistry*, 75(4–5):399–407, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004994/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004994&PLACEBO=IE.pdf.

Palma:1992:ETA

[Pal92] R. Palma. Energy transfer along alpha-helical proteins. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:167–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Palma:1993:TIC

[Pal93a] R. Palma. Temperature-induced changes in protein heat capacity. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20: 117–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Palting:1993:HOT

[Pal93b] P. Palting. Harmonic oscillator tensors. II. angular momentum expressions of matrix elements of vibrational operators. *International Journal of Quantum Chemistry*, 46(2):257–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palafox:1994:ESC

[Pal94] M. A. Palafox. Eclipsed and staggered conformations of $(\mathrm{SiH}_3)_2F^+$: An ab initio study. *International Journal of Quantum Chemistry*, 50(1):69–90, March 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palting:1995:WSC

[Pal95] P. Palting. On weak and strong conjugacy in the antisymmetry principle. *International Journal of Quantum Chemistry*, 54(1): 19–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palma:1997:RRC

[Pal97a] Alejandro Palma. Recurrence relations and closed formulas connecting Franck–Condon factors and squeezed states. *International Journal of Quantum Chemistry*, 63(1):229–232, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42568; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42568&PLACEBO=IE.pdf`.

Palting:1997:HOT

[Pal97b] Pancracio Palting. Harmonic oscillator tensors. IV. A tensorial approach to internal rotations in molecules. *International Journal of Quantum Chemistry*, 65(4):305–315, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL

http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42768; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42768&PLACEBO=IE.pdf.

Palting:1998:HOT

[Pal98] Pancracio Palting. Harmonic oscillator tensors. V. the doubly degenerate harmonic oscillator. *International Journal of Quantum Chemistry*, 67(6):343–357, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29915; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29915&PLACEBO=IE.pdf.

Panas:1993:SSH

[Pan93] I. Panas. On the solid state of hydrogen fluoride: A self-consistent crystal field study. *International Journal of Quantum Chemistry*, 46(1):109–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Panas:1995:PET

[Pan95] Itai Panas. Practical expressions for the two-center multipole expansion of $r \pm 1_{12}$. *International Journal of Quantum Chemistry*, 53(3):255–263, February 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Parkinson:1992:CDP

[Par92] W. A. Parkinson. A comparison of dipole polarizability obtained from linear and quadratic response functions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:487–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Pariser:1994:BPT

[Par94a] R. Pariser. Bob parr, teacher, collaborator, friend: A personal view. *International Journal of Quantum Chemistry*, 49 (3):145–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Parr:1994:CS

[Par94b] R. G. Parr. Companions in the search. *International Journal of Quantum Chemistry*, 49(5):739–??, February 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Parr:1994:PL

[Par94c] R. G. Parr. Publication list. *International Journal of Quantum Chemistry*, 49(3):135–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Parry:1997:IPA

[Par97] David E. Parry. Ab initio propagator analysis of the valence double-ionization spectra of propyne. *International Journal of Quantum Chemistry*, 64(2):175–182, August 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42679; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42679&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Parry:1999:SRC

[Par99] David E. Parry. A$\Sigma^+ \not\leftrightarrow \Sigma^-$ selection rule for the collisions of some atomic ions with diatomic molecules. *International Journal of Quantum Chemistry*, 74(2):103–108, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003356; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003356&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Pettersson:1997:ADB

[PÅS+97] Lars G. M. Pettersson, Hans Ågren, Britta L. Schürmann, Andreas Lippitz, and Wolfgang E. S. Unger. Assembly and decomposition of building blocks to analyze polymer NEXAFS spectra. *International Journal of Quantum Chemistry*, 63(3):749–765, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42618; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42618&PLACEBO=IE.pdf.

Plakhutin:1993:CCS

[PAT93] B. N. Plakhutin, A. V. Arbuznikov, and A. B. Trofimov. Coupling coefficients for systems with two open electronic shells:

Transition metal ions with $p^M d^N$ configuration. *International Journal of Quantum Chemistry*, 45(4):363–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pauncz:1992:SPO

[Pau92] R. Pauncz. Studies in the paired orbital method. IV. orthogonal transformations in the virtual space. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:161–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Pauncz:1997:RAJ

[Pau97] Ruben Pauncz. Reminiscences about Jean-Louis Calais. *International Journal of Quantum Chemistry*, 63(1):3, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42563; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42563&PLACEBO=IE.pdf.

Pauncz:1999:BR

[Pau99] Ruben Pauncz. Book review. *International Journal of Quantum Chemistry*, 75(2):133, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=64000658; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=64000658&PLACEBO=IE.pdf.

Pathak:1995:EDW

[PB95a] R. K. Pathak and K. Bhattacharyya. Eigenstates of double wells at varying well depths. *International Journal of Quantum Chemistry*, 54(1):13–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pisani:1995:ECA

[PB95b] C. Pisani and U. Birkenheuer. Embedded-cluster approach to the study of catalytic reactions in zeolite cavities. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:221–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Ponec:1995:NPA

[PB95c] R. Ponec and R. C. Bochicchio. Nonlinear population analysis from geminal expansion of pair densities. *International Journal* of *Quantum Chemistry*, 54(2):99–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perdew:1996:CSG

[PB96] John P. Perdew and Kieron Burke. Comparison shopping for a gradient-corrected density functional. *International Journal of Quantum Chemistry*, 57(3):309–319, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60392.

Pohl:1997:ISA

[PB97a] Anna Pohl and Jean-Luc Brédas. Influence of silicon atoms on the π-conjugation in electroluminescent polymers. *International Journal of Quantum Chemistry*, 63(2): 437–440, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42587; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42587&PLACEBO=IE.pdf.

Pop:1997:DDH

[PB97b] Emil Pop and Marcus E. Brewster. Dimerization of dexanabinol by hydrogen bonding accounts for its hydrophobic character. *International Journal of Quantum Chemistry*, 65 (6):1057–1064, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42842; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42842&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on the Application of Fundamental Theory to Problems of Biology and Pharmocolgy.* Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Ponec:1999:NPP

[PB99] Robert Ponec and Roberto C. Bochicchio. Nonlinear pair population analysis: The study of basis-set dependence. *International Journal of Quantum Chemistry*, 72 (2):127–137, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002779; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002779&PLACEBO=IE.pdf.

Pierini:1992:ASC

[PBB92] A. B. Pierini, G. L. Borosky, and M. T. Baumgartner. An am1 study of the coupling reaction of radicals with the acetone enolate ion and some related nucleophiles. *International Journal of Quantum Chemistry*, 44(5):759–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perera:1994:LHP

[PBB94a] S. A. Perera, D. E. Bernholdt, and R. J. Bartlett. Localized Hartree product orbitals in correlated studies of molecules. *International Journal of Quantum Chemistry*, 49(5):559–??, February 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Polavieja:1994:QPS

[PBB94b] G. G. De Polavieja, F. Borondo, and R. M. Benito. Quantum phase-space densities for a quartic oscillator. *International Journal of Quantum Chemistry*, 51(6):555–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pop:1993:TSD

[PBBH93] E. Pop, M. E. Brewster, N. Bodor, and M.-J Huang. A theoretical study of the dithionite reduction of pyridinium salts. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:17–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Priyadarshy:1996:DDHc

[PBR96a] S. Priyadarshy, D. N. Beratan, and S. M. Risser. DNA double-helix-mediated long-range electron transfer. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 23(??):65–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

Priyadarshy:1996:DDHa

[PBR96b] S. Priyadarshy, D. N. Betatan, and S. M. Risser. DNA double-helix-mediated long-range electron transfer. *International Journal of Quantum Chemistry*, 60(8):65–??, 1996. CODEN IJQCB2.

Priyadarshy:1996:DDHb

[PBR96c] Satyam Priyadarshy, David N. Beratan, and Steven M. Risser. DNA double-helix-mediated long-range electron transfer. *International Journal of Quantum Chemistry*, 60(8):1789–1795, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60750`.

Pavlov:1999:NAH

[PBS99] Maria Pavlov, Margareta R. A. Blomberg, and Per E. M. Siegbahn. New aspects of H_2 activation by nickel-iron hydrogenase. *International Journal of Quantum Chemistry*, 73 (2):197–207, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003517; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003517&PLACEBO=IE.pdf`. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998*. Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Piris:1995:BAM

[PC95] M. Piris and R. Cruz. A BCS approach to molecular correlation. *International Journal of Quantum Chemistry*, 53(4):353–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ping:1999:SCS

[PC99] Jia-Lun Ping and Jin-Quan Chen. Subgroup-chain symmetry-adapted irreducible matrices and CG coefficients of point groups. *International Journal of Quantum Chemistry*, 75 (2):67–80, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=64000659; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=64000659&PLACEBO=IE.pdf`.

Perez:1994:EIA

[PCCO94] J. E. Perez, H. H. Cuenya, R. H. Contreras, and F. S. Ortiz. Evaluation of integrals appearing in the Hylleraas CI method by expanding $1/r_y$ in terms of a complete basis set. *International*

Journal of Quantum Chemistry. Symposium, 28:39–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Ponec:1999:CBC

[PCD99] Robert Ponec and Ramon Carbó-Dorca. Chemical bonds from the condition of minimal pair fluctuation: Correlated case. *International Journal of Quantum Chemistry*, 72(2):85–91, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002775; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002775&PLACEBO=IE.pdf.

Paglieri:1995:SED

[PCE95] L. Paglieri, G. Corongiu, and D. A. Estrin. Solvent effects in density functional calculations of uracil and cytosine tautomerism. *International Journal of Quantum Chemistry*, 56 (5):615–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Piquini:1994:SES

[PCF94] P. Piquini, S. Canuto, and A. Fazzio. Structural and electronic studies of Ga_3As_3, Ga_4As_3, and Ga_3As_4. *International Journal of Quantum Chemistry. Symposium*, 28:571–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Pavao:1993:GFE

[PCN93] A. C. Pavao, J. S. Craw, and M. A. C. Nascimento. Ground and first excited states of fractionally charged sodium atoms. *International Journal of Quantum Chemistry*, 48(4):219–??, November 10, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pierini:1993:SEP

[PD93] A. B. Pierini and J. S. Duca, Jr. Semiempirical evaluation for proton affinities of phosphorus compounds. *International Journal of Quantum Chemistry*, 48(6):343–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pinheiro:1997:GCH

[PDT97] J. C. Pinheiro, A. B. F. Da Silva, and M. Trsic. Generator coordinate Hartree–Fock method applied to the choice of a contracted Gaussian basis for the second-row atoms. *International Journal of Quantum Chemistry*, 63(5):927–934, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42643; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42643&PLACEBO=IE.pdf.

Pearson:1995:PMP

[Pea95] R. G. Pearson. The principle of maximum physical hardness. *International Journal of Quantum Chemistry*, 56(4):211–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perdew:1997:TPD

[PEBS97] John P. Perdew, Matthias Ernzerhof, Kieron Burke, and Andreas Savin. On-top pair-density interpretation of spin density functional theory, with applications to magnetism. *International Journal of Quantum Chemistry*, 61(2):197–205, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42401; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42401&PLACEBO=IE.pdf.

Pecul:1993:DIS

[Pec93] K. Pecul. Decomposition and interpretation of the SCF interaction and deformation energies by the modified Pauli blockade method. *International Journal of Quantum Chemistry*, 47 (2):145–??, July 15, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Penotti:1993:OBS

[Pen93] F. E. Penotti. The optimized-basis-set multiconfiguration spin-coupled method for the ab initio calculation of atomic and molecular electronic wave functions. *International Journal of Quantum Chemistry*, 46(4):535–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Penotti:1996:GOB

[Pen96] Fabio E. Penotti. Generalization of the optimized-basis-set multi-configuration spin-coupled method for the ab initio calculation of atomic and molecular electronic wave functions.

International Journal of Quantum Chemistry, 59(5):349–378, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60555.

Perdew:1993:LDG

[Per93] J. P. Perdew. Local density and gradient-corrected functionals for short-range correlation: Antiparallel-spin and Non-RPA contributions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:93–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Percus:1998:ODF

[Per98] J. K. Percus. Overcomplete density functional description. *International Journal of Quantum Chemistry*, 69(4):573–580, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30012; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30012&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Porras:1999:NPA

[PFK99] I. Porras, D. Matthew Feldmann, and Frederick W. King. A nonlinear programming approach to lower bounds for the ground-state energy of helium. *International Journal of Quantum Chemistry*, 71(6):455–463, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=15000343; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=15000343&PLACEBO=IE.pdf.

Perczel:1997:PMX

[PFMC97] András Perczel, Ödön Farkas, John F. Marcoccia, and Imre G. Csizmadia. Peptide models. XIV. ab initio study on the role of side-chain backbone interaction stabilizing the building unit of right- and left-handed helices in peptides and proteins. *International Journal of Quantum Chemistry*, 61(5):797–814, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42464;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42464&PLACEBO=IE.pdf.

Pacios:1994:OTZ

[PG94] L. F. Pacios and P. C. Gomez. Optimized triple-zeta Gaussian basis sets for use with relativistic effective potentials. *International Journal of Quantum Chemistry*, 49(6):817–??, March 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Petersilka:1996:SMEa

[PG96a] M. Petersilka and E. K. U. Gross. Spin-multiplet energies from time-dependent density functional theory. *International Journal of Quantum Chemistry*, 60(7):1393–1401, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60698.

Petersilka:1996:SMEb

[PG96b] M. Petersilka and E. K. U. Gross. Spin-multiplet energies from time-dependent density functional theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):181–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Peterslika:1996:SME

[PG96c] M. Peterslika and E. K. U. Gross. Spin-multiplet energies from time-dependent density functional theory. *International Journal of Quantum Chemistry*, 60(7):181–??, 1996. CODEN IJQCB2.

Pople:1995:SUC

[PGH95] J. A. Pople, P. M. W. Gill, and N. C. Handy. Spin-unrestricted character of Kohn–Sham orbitals for open-shell systems. *International Journal of Quantum Chemistry*, 56(4):303–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pal:1995:ECE

[PGM95] S. Pal, K. B. Ghose, and H.-D. Meyer. Electron correlation effects in target molecule in low-energy $e^- + \mathrm{N}_2$ scattering. *International Journal of Quantum Chemistry*, 55(3):291–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:1997:DFA

[PGS97] Peter Politzer, M. Edward Grice, and Jorge M. Seminario. Density functional analysis of a decomposition of 4-nitro-1,2,3-triazole through the evolution of N_2. *International Journal of Quantum Chemistry*, 61(3):389–392, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42432`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42432&PLACEBO=IE.pdf`.

Pop:1992:TSH

[PHBB92] E. Pop, M.-J. Huang, M. E. Brewster, and N. Bodor. A theoretical study of the hydrolysis of some sterically hindered phenolic esters. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19: 77–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Pop:1994:SSD

[PHBB94] E. Pop, M.-J. Huang, M. E. Brewster, and N. Bodor. Stability of the 1,3-substituted 1,4-dihydropyridines: Substituent effects on the acid catalyzed hydration and oxidation reactions. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21:173–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Pop:1995:HSA

[PHBB95] E. Pop, M.-J. Huang, M. Bodor, and M. E. Brewster. Hydrolytic stability of allylic and phenolic esters of some synthetic cannabinoids: A theoretical (AM1) study. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):137–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Pendergast:1994:CBS

[PHH94] P. Pendergast, J. M. Heck, and E. F. Hayes. A comparative basis-set study of NeH^+ using coupled-cluster techniques. *International Journal of Quantum Chemistry*, 49(4):495–509, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pickup:1992:PEP

[Pic92] B. T. Pickup. The perturbed electron propagator approach to molecular response properties. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:13–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Piecuch:1993:MSC

[Pie93] P. Piecuch. MAPLE symbolic computation of the long-range many-body intermolecular potentials: Three-body induction forces between two atoms and a linear molecule. *International Journal of Quantum Chemistry*, 47(4):261–305, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palafox:1994:DFD

[PIG94] M. A. Palafox, N. Iza, and M. Gil. Dimer form of 1,3-dimethyluracil studied by the AM1 semiempirical method. *International Journal of Quantum Chemistry*, 51(3):141–??, July 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ponec:1996:PAP

[PJ96] Robert Ponec and Karl Jug. Population analysis of pair densities: A new way of visualization of molecular structure. *International Journal of Quantum Chemistry*, 60(1):75–82, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60627`.

Popkie:1976:MCM

[PK76] H. E. Popkie and J. J. Kaufman. Molecular calculations with the MODPOT, VRDO, and MODPOT/VRDO procedures I. HF, F_2, HCl, Cl_2, formamide, pyrrole, pyridine, and nitrobenzene. *International Journal of Quantum Chemistry*, S10(??): 47–57, ?? 1976. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Popkie:1977:MCM

[PK77] H. E. Popkie and J. J. Kaufman. Molecular calculations with the MODPOT, VRDO and MODPOT/VRDO procedures. IV. boron hydrides and carboranes. *International Journal of Quantum Chemistry*, ??(??):??, ?? 1977. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Prasad:1994:NOE

[PK94] P. N. Prasad and S. P. Karna. Nonlinear optical effects in molecules and polymers: Issues and opportunities. *International Journal of Quantum Chemistry. Symposium*, 28:395–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Poshusta:1996:DMC

[PK96] R. D. Poshusta and D. B. Kinghorn. Density matrices for correlated Gaussians: Helium and dipositronium. *International Journal of Quantum Chemistry*, 60(1):213–224, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60585.

Philis:1999:SCB

[PK99] John G. Philis and Constantine Kosmidis. Searching for the conformers of n-butylbenzene. *International Journal of Quantum Chemistry*, 72(4):341–345, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006310; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006310&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Planelles:1999:AOE

[PKJ99] J. Planelles, J. Karwowski, and W. Jaskólski. Adaptation of one-electron basis sets to spatial confinements. *International Journal of Quantum Chemistry*, 73(4):341–347, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61000530; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61000530&PLACEBO=IE.pdf.

Parrondo:1993:EHR

[PKM93] R. Martin Parrondo, P. Karafiloglou, and E. Sanchez Marcos. Examination of the Hund rule in closed-shell systems: Investigation of spin correlation effects. *International Journal of Quantum Chemistry*, 47(3):191–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Parrondo:1994:NPP

[PKM94] R. M. Parrondo, P. Karafiloglou, and E. S. Marcos. Natural polyelectron population analysis. *International Journal of*

Quantum Chemistry, 52(5):1127–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pack:1993:CCT

[PL93] G. R. Pack and G. Lamm. Counterion condensation theory revisited: Limits on its applicability. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:213–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Paikeday:1998:EPN

[PL98] Joseph M. Paikeday and Amber Longstreet. Effective potential for *e*-neon and *e*-argon scattering by DCS minimization at intermediate energies. *International Journal of Quantum Chemistry*, 70(4-5):943–950, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75072; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75072&PLACEBO=IE.pdf`.

PerezDelValle:1998:DPE

[PLA98] C. Pérez Del Valle, R. Lefebvre, and O. Atabek. Dressed potential energy surface of the hydrogen molecule in high-frequency Floquet theory. *International Journal of Quantum Chemistry*, 70(1):199–203, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74364; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74364&PLACEBO=IE.pdf`. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Pogni:1999:LAH

[PLBB99] Rebecca Pogni, Giovanni Della Lunga, Elena Busi, and Riccardo Basosi. Lineshape analysis of heme-protein-derived radicals based on simulation of EPR spectra. *International Journal of Quantum Chemistry*, 73(2):249–254, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003522; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003522&PLACEBO=IE.pdf`. Special Issue:

Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998. Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Proft:1995:AFS

[PLG95] F. De Proft, W. Langenaeker, and P. Geerlings. Acidity of first- and second-row hydrides: Effects of electronegativity and hardness. *International Journal of Quantum Chemistry*, 55(6): 459–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palma:1999:CTF

[PLS99] A. Palma, V. M. León, and L. Sandoval. The convolution theorem and the Franck–Condon integral. *International Journal of Quantum Chemistry*, 75(1):11–15, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63003145; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63003145&PLACEBO=IE.pdf`.

Perez:1992:CSM

[PLV92] J. J. Perez, G. H. Loew, and H. O. Villar. Conformational study of met-enkephalin in its zwitterionic form. *International Journal of Quantum Chemistry*, 44(2):263–??, September 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Peskin:1993:CCS

[PM93] U. Peskin and N. Moiseyev. The complex coordinate scattering theory and its application to the study of the surface asymmetry effect in helium diffraction from copper. *International Journal of Quantum Chemistry*, 46(3):343–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Patra:1995:SCP

[PM95] S. M. Patra and R. K. Mishra. Splitting of the characteristic polynomial (CP) using a computational technique to obtain the factors of the mirror plane and two, three-, and n-fold symmetric graph. *International Journal of Quantum Chemistry*, 53 (4):361–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paniagua:1997:LCE

[PM97] Juan Carlos Paniagua and Albert Moyano. Localization-consistent electronic energy partitions. *International Journal of Quantum Chemistry*, 65(2):121–126, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42749; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42749&PLACEBO=IE.pdf.

Pavlov:1997:DFTa

[PMDM97] R. L. Pavlov, J. Maruani, Ya. I. Delchev, and R. McWeeny. Density functional theory for open-shell systems using a local-scaling transformation scheme. I. Single-density energy functional. *International Journal of Quantum Chemistry*, 65(3):241–256, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42761; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42761&PLACEBO=IE.pdf. See erratum [PMDM98].

Pavlov:1998:EDFa

[PMDM98] R. L. Pavlov, J. Maruani, Ya. I. Delchev, and R. McWeeny. Erratum: Density functional theory for open-shell systems using a local-scaling transformation scheme. I. Single-density energy functional. *International Journal of Quantum Chemistry*, 68(1):75, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29925; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29925&PLACEBO=IE.pdf. See [PMDM97].

Pop:1991:ESB

[PMJM+91] Emil Pop, Huang Ming-Ju, Simion Matei, Marcus E. Brewster, and Nicholas Bodor. Electrophilic substitution in the benzofuran series: A theoretical (AM1) study. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:325–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Patra:1997:GTS

[PMM97] Swarna M. Patra, Rama K. Mishra, and Bijaya K. Mishra. Graph-theoretic study of certain interstellar reactions. *International Journal of Quantum Chemistry*, 62(5):495–508,

???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42537; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42537&PLACEBO=IE.pdf.

Perevozchikov:1992:CTM

[PMN+92] V. I. Perevozchikov, I. V. Maslov, A. W. Niukkanen, Herbert H. Homeier, and E. Otto Steinborn. On the combination of two methods for the calculation of multicenter integrals using STO and B function basis sets. *International Journal of Quantum Chemistry*, 44(1):45–57, August 20, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Politzer:1994:ACS

[PMS94] P. Politzer, J. S. Murray, and J. M. Seminario. Antiaromaticity to 1,3,5,7-Cyclooctatetraene structures. *International Journal of Quantum Chemistry*, 50(4):273–??, May 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pluta:1994:DHE

[PNB94] Tadeusz Pluta, Jozef Noga, and Rodney J. Bartlett. Determination of higher electric polarizability tensors from unrelaxed coupled cluster density matrix calculations of electric multipole moments. *International Journal of Quantum Chemistry. Symposium*, 28:379–393, 1994. CODEN IJQSAF. ISSN 0538-821X.

Parkinson:1997:RFA

[PO97] William A. Parkinson and Jens Oddershede. Response function analysis of magnetic optical rotation. *International Journal of Quantum Chemistry*, 64(5):599–605, September 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42708; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42708&PLACEBO=IE.pdf. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

Ponec:1997:ERC

[Pon97] Robert Ponec. Electron reorganization in chemical reactions: Pair population analysis along concerted reaction path of allowed and forbidden pericyclic reactions.

International Journal of Quantum Chemistry, 62(2):171–176, March 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42500; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42500&PLACEBO=IE.pdf.

Ponec:1998:EPC

[Pon98] Robert Ponec. Electron pairing and chemical bonds: Chemical bonds from the condition of minimum fluctuation of electron pair. *International Journal of Quantum Chemistry*, 69 (2):193–200, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29982; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29982&PLACEBO=IE.pdf.

Popov:1998:EQV

[Pop98] Dušan Popov. Extension of the quantum virial and Hellmann–Feynman theorems to the quantum statistical averages. *International Journal of Quantum Chemistry*, 69(2):159–165, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29978; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29978&PLACEBO=IE.pdf.

Porter:1997:BBS

[Por97] L. E. Porter. Bethe–Bloch stopping power parameters for polystyrene, kapton, and mylar. *International Journal of Quantum Chemistry*, 65(5):997–1003, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42831; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42831&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Porter:1998:BBS

[Por98] L. E. Porter. Bethe–Bloch stopping-power parameters for GaAs and ZnSe. *International Journal of Quantum Chem-*

istry, 70(4-5):919–924, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75069; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75069&PLACEBO=IE.pdf.

Porter:1999:MBB

[Por99] L. E. Porter. Modified Bethe–Bloch stopping power parameters for kapton. *International Journal of Quantum Chemistry*, 75(4–5):943–950, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004988/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004988&PLACEBO=IE.pdf.

Poshusta:1991:AME

[Pos91] R. D. Poshusta. Algebrants in many electron quantum mechanics. II. new computational algorithms. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:225–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Piecuch:1991:SCC

[PP91] Piotr Piecuch and Josef Paldus. On the solution of coupled-cluster equations in the fully correlated limit of cyclic polyene model. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:9–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Packer:1995:ADL

[PP95] M. J. Packer and B. T. Pickup. An analysis of dynamic linear response properties at RPA level. *International Journal of Quantum Chemistry*, 54(4):223–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Patton:1998:TSR

[PP98a] David C. Patton and Mark R. Pederson. A theoretical study of rare-gas diatomic molecules with the generalized-gradient approximation to density functional theory. *International Journal of Quantum Chemistry*, 69(4):619–627, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30018; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30018&PLACEBO=IE.pdf. Special Issue:

Symposium on Density Functional Theory and Applications (Part II of II). Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Pollack:1998:ECC

[PP98b] L. Pollack and J. P. Perdew. Exchange-correlation corrections to lattice dynamics of simple metals, and a search for soft modes at normal and expanded volume. *International Journal of Quantum Chemistry*, 69(3):359–369, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29991; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29991&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Polak:1997:FDN

[PPK97] Rudolf Polák, Ivana Paidarová, and Philip J. Kuntz. On the fragmentation dynamics of $NH_3 \to NH_2 + H$. II diatomics-in-molecules potential energy surfaces. *International Journal of Quantum Chemistry*, 62(6):659–668, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42550; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42550&PLACEBO=IE.pdf.

Peris:1997:SRC

[PPP97] G. Peris, J. Planelles, and J. Paldus. Single-reference CCSD approach employing three- and four-body CAS SCF corrections: A preliminary study of a simple model. *International Journal of Quantum Chemistry*, 62(2):137–151, March 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42497; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42497&PLACEBO=IE.pdf.

Polak:1996:FDN

[PPSK96] Rudolf Polák, Ivana Paidarová, Vladimír Sîpirko, and Philip J. Kuntz. On the fragmentation dynamics of $NH_3 \to NH_2 +$ H. I. MRD CI potential energy surfaces. *International Journal of Quantum Chemistry*, 57(3):429–440, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60380.

Povill:1997:UFC

[PR97] Àngels Povill and Jaime Rubio. Using Full-CI algorithms in Bethe–Goldstone-Type expansions of the correlation energy. *International Journal of Quantum Chemistry*, 61(1): 35–43, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42383; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42383&PLACEBO=IE.pdf.

Pranata:1997:ERC

[Pra97] Julianto Pranata. The ene reaction: Comparison of results of Hartree–Fock, Møller–Plesset, CASSCF, and DFT calculations. *International Journal of Quantum Chemistry*, 62 (5):509–514, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42538; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42538&PLACEBO=IE.pdf.

Pop:1996:ARTa

[PRB96a] E. Pop, S. Rachwal, and M. E. Brewster. Allylic rearrangement of trans-pinocarveol esters. *International Journal of Quantum Chemistry*, 60(8):105–??, 1996. CODEN IJQCB2.

Pop:1996:ARTc

[PRB96b] E. Pop, S. Rachwal, and M. E. Brewster. Allylic rearrangement of trans-pinocarveol esters. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 23(??):105–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

Pop:1996:ARTb

[PRB96c] Emil Pop, Stanisław Rachwal, and Marcus E. Brewster. Allylic rearrangement of *trans*-pinocarveol esters. *International Journal of Quantum Chemistry*, 60(8):1829–1834, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60742.

Prigogine:1995:WIF

[Pri95] I. Prigogine. Why irreversibility? the formulation of classical and quantum mechanics for nonintegrable systems. *International Journal of Quantum Chemistry*, 53(1):105–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Primorac:1998:NEB

[Pri98] Miljenko Primorac. New expansion of the Boys function. *International Journal of Quantum Chemistry*, 68(5): 305–315, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29951; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29951&PLACEBO=IE.pdf.

Probst:1994:ICT

[Pro94] M. Probst. On the interaction of cyanate and thiocyanate anions with $Li0^+$ and $Mg0_20^+$. *International Journal of Quantum Chemistry. Symposium*, 28:553–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Probst:1995:IBN

[Pro95] M. Probst. The interaction between nitrate anion and the cations Li^+, Mg_2^+, and Ca_2^+: Frequencies and binding sites. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:559–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Perez-Romero:1997:TSA

[PRTV97] E. Pérez-Romero, L. M. Tel, and C. Valdemoro. Traces of spin-adapted reduced density matrices. *International Journal of Quantum Chemistry*, 61(1):55–61, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42385; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42385&PLACEBO=IE.pdf.

Proynov:1995:DED

[PRVS95] E. I. Proynov, E. Ruiz, A. Vela, and D. R. Salahub. Determining and extending the domain of exchange and correlation functionals. *International Journal of Quantum Chemistry. Quan-*

tum Chemistry Symposium, 29:61–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Pipano:1968:CSC

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

Park:1993:VES

[PS93] J. K. Park and H. Sun. Valence electronic states of NH^{2+} and PH^2+ dications. *International Journal of Quantum Chemistry*, 48(6):355–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ponec:1994:PAP

[PS94a] R. Ponec and M. Strnad. Population analysis of pair densities: A link between quantum chemical and classical picture of chemical structure. *International Journal of Quantum Chemistry*, 50 (1):43–??, March 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Proynov:1994:ASC

[PS94b] E. I. Proynov and D. R. Salahub. On the applicability of the screened-Coulomb exchange model in Kohn–Sham density functional studies. *International Journal of Quantum Chemistry*, 49 (2):67–??, January 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Panin:1996:CIS

[PS96] A. I. Panin and K. V. Simon. Configuration interaction spaces with arbitrary restrictions on orbital occupancies. *International Journal of Quantum Chemistry*, 59(6):471–475, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60565`.

Pan:1999:MBP

[PS99a] Baocheng Pan and Muttaiya Sundaralingam. Mismatched base pairing in RNA crystal structures. *International Journal of Quantum Chemistry*, 75(3):275–287, November 5,

1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000669/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000669&PLACEBO=IE.pdf.

Porras:1999:DCD

[PS99b] I. Porras and F. Arias De Saavedra. Description of correlated densities for few-electron atoms by simple functional forms. *International Journal of Quantum Chemistry*, 71 (6):443–454, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=15000342; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=15000342&PLACEBO=IE.pdf.

Papai:1990:CEG

[PSAUS90] I. Papai, A. St-Amant, J. Ushio, and D. Salahub. Calculation of equilibrium geometries and harmonic frequencies by the LCGTO-MCP-Local spin density method. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:29–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Persson:1998:PIC

[PSBL98] Petter Persson, Arvids Stashans, Robert Bergström, and Sten Lunell. Periodic INDO calculations of organic adsorbates on a TiO_2 surface. *International Journal of Quantum Chemistry*, 70(4-5):1055–1066, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75028; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75028&PLACEBO=IE.pdf.

Politzer:1997:DFI

[PSCZ97] Peter Politzer, Jorge M. Seminario, Monica C. Concha, and Angélica G. Zacariás. Density-functional investigation of some decomposition routes of methyl nitrate. *International Journal of Quantum Chemistry*, 64(2):205–210, August 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42682; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42682&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the Inter-*

national Society for Theoretical Chemical Physics. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Peluso:1997:VCE

[PSD97a] Andrea Peluso, Fabrizio Santoro, and Giuseppe Del Re. Vibronic coupling in electronic transitions with significant duschinsky effect. *International Journal of Quantum Chemistry*, 63(1):233–244, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42569; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42569&PLACEBO=IE.pdf.

Pike:1997:QTR

[PSD97b] E. R. Pike, S. Sarkar, and E. Deumens. The quantum theory of radiation. *International Journal of Quantum Chemistry*, 64(6):735, September 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42724; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42724&PLACEBO=IE.pdf.

Palma:1994:FCF

[PSM94] A. Palma, L. Sandoval, and M. Martin. Franck–Condon factors and squeezed states. *International Journal of Quantum Chemistry. Symposium*, 28:261–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Parkinson:1990:TPT

[PSO90] W. A. Parkinson, P. W. Sengelov, and J. Oddershede. Two-photon transition moments as determined from the quadratic response function. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:487–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Proynov:1997:ELF

[PSS97] E. I. Proynov, S. Sirois, and D. R. Salahub. Extension of the LAP functional to include parallel spin correlation. *International Journal of Quantum Chemistry*, 64(4):427–446, September 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42701; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42701&PLACEBO=IE.pdf.

Pohl:1994:EEN

[PTC94] A. Pohl, H. Taylor, and J.-L. Calais. END (electron nuclear dynamics) with the hydrogen molecule used as a model problem. *International Journal of Quantum Chemistry*, 50(5):333–??, May 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pratt:1997:BIM

[PTH+97] Lawrence R. Pratt, Gregory J. Tawa, Gerhard Hummer, Angel E. García, and Steven A. Corcelli. Boundary integral methods for the Poisson equation of continuum dielectric solvation models. *International Journal of Quantum Chemistry*, 64(1):121–141, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42660; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42660&PLACEBO=IE.pdf`. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Piecuch:1995:CCA

[PTP95] P. Piecuch, R. Tobola, and J. Paldus. Coupled-cluster approaches with an approximate account of triply and quadruply excited clusters: Implementation of the orthogonally spin-adapted CCD + ST(CCD),CCSD + T(CCSD), and ACPQ + ST(ACPQ) formalisms. *International Journal of Quantum Chemistry*, 55(2):133–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pullman:1990:YSS

[Pul90] B. Pullman. 30 years of Sanibel Symposia: Structure and activity of biomolecules. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17:81–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Pipek:1994:MCS

[PV94] J. Pipek and I. Varga. Mathematical characterization and shape analysis of localized, fractal, and complex distributions in extended systems. *International Journal of Quantum Chemistry*, 51(6):539–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pipek:1997:SED

[PV97] János Pipek and Imre Varga. Statistical electron densities. *International Journal of Quantum Chemistry*, 64 (1):85–93, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42668; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42668&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Pipek:1998:SBE

[PV98] János Pipek and Imre Varga. Scaling behavior of energy functionals of highly complex electron distributions. *International Journal of Quantum Chemistry*, 70(1):125–131, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74357; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74357&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Patra:1999:CPS

[PV99] S. M. Patra and S. Vishveshwara. Classification of polymer structures by graph theory. *International Journal of Quantum Chemistry*, 71(4):349–356, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10049350; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10049350&PLACEBO=IE.pdf.

Pasinszki:1992:PSM

[PVF+92] T. Pasinszki, T. Veszpremi, M. Feher, B. Kovac, L. Klasinc, and S. P. McGlynn. The photoelectron spectra of methyl pseudohalides. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:443–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Peeters:1993:ISC

[PVLG93] A. Peeters, C. Van Alsenoy, A. T. H. Lenstra, and H. J. Geise. Ab initio studies of crystal field effects. VII. structure of 2,3-

Diketopiperazine using a 13-molecule cluster, a calculation involving 1092 basis functions. *International Journal of Quantum Chemistry*, 46(1):73–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perez:1993:MDR

[PVU+93] J. J. Perez, H. O. Villar, E. Uyeno, L. Toll, and C. Olsen. Molecular determinants of recognition and activation at the mu-opioid receptor by met-enkephalin-like peptides. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:147–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Pardo:1997:SAM

[PW97] Leonardo Pardo and Harel Weinstein. On the structure and activity of membrane receptors: A computational simulation of ligand-triggered activation in a model 5-HT_{1A} receptor. *International Journal of Quantum Chemistry*, 63 (3):767–780, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42619; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42619&PLACEBO=IE.pdf`.

Pisani:1996:CTC

[PWC96] Lorenzo Pisani, Laurent De Windt, and Enrico Clementi. Comments on the topic "computation of large molecules". *International Journal of Quantum Chemistry*, 58(3):219–240, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60478`.

Pack:1995:TPF

[PWL95] G. R. Pack, L. Wong, and G. Lamm. Theoretical predictions of the functional interactions of DNA and mutagenic aziridines. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):29–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Pack:1998:PCT

[PWL98] George R. Pack, Linda Wong, and Gene Lamm. PK_a of cytosine on the third strand of triplex DNA: Preliminary Poisson–Boltzmann calculations. *International Journal of Quantum Chemistry*, 70(6):1177–1184, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75085; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75085&PLACEBO=IE.pdf`.

Parlant:1992:ASA

[PY92] G. Parlant and D. R. Yarkony. An adiabatic state approach to electronically nonadiabatic wave packet dynamics. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:737–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Polasek:1995:QCS

[PZ95] M. Polasek and R. Zahradnik. A quantum chemical study of small beryllium hydrides and their radical anions. *International Journal of Quantum Chemistry*, 54(2):93–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pavlov:1997:DFTb

[PZDM97] R. L. Pavlov, F. E. Zakhariev, A. I. Delchev, and J. Maruani. Density functional theory for open-shell systems using a local-scaling transformation scheme. II. Euler–Lagrange equation for $f(r)$ versus that for $\rho(r)$. *International Journal of Quantum Chemistry*, 65(3):257–268, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42762; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42762&PLACEBO=IE.pdf`. See erratum [PZDM98].

Pavlov:1998:EDFb

[PZDM98] R. L. Pavlov, F. E. Zakhariev, Ya. I. Delchev, and J. Maruani. Erratum: Density functional theory for open-shell systems using a local-scaling transformation scheme. II. Euler–Lagrange equation for $f(r)$ versus that for $\rho(r)$. *International Journal of Quantum Chemistry*, 68(1):77, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?`

ID=29926; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29926&PLACEBO=IE.pdf. See [PZDM97].

Perez:1999:BSE

[PZTPMC99] Patricia Pérez, Gerald Zapata-Torres, Julia Parra-Mouchet, and Renato Contreras. Basicity and solvent effects on hydrogen bonding in $NR_3 \cdots HCOOH$ (R = H, CH_3) model systems. *International Journal of Quantum Chemistry*, 74 (4):387–394, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62502082; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62502082&PLACEBO=IE.pdf.

Planelles:1993:SPF

[PZW93] J. Planelles and C. M. Zicovich-Wilson. A simple proof for the formula to get symmetrized powers of group representations. *International Journal of Quantum Chemistry*, 47(4):319–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Planelles:1996:SHS

[PZWJC96] J. Planelles, C. Zicovich-Wilson, W. Jaskólski, and A. Corma. Semiempirical Hamiltonians for spatially confined π-electron systems. *International Journal of Quantum Chemistry*, 60 (5):971–981, December 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60669.

Qian:1998:AAS

[QS98] Zhixin Qian and Viraht Sahni. Analytical asymptotic structure of the Pauli, Coulomb, and correlation-kinetic components of the Kohn–Sham theory exchange — correlation potential in atoms. *International Journal of Quantum Chemistry*, 70(4-5):671–680, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75045; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75045&PLACEBO=IE.pdf.

Reed:1991:CBH

[RA91] Lynne H. Reed and Leland C. Allen. 1,5-C_2 B_3 H_5 and C_5 H_8, 1,5- C_2 B_3 H_3 and C_5 H_6: Carborane-hydrocarbon structural analogs with unusual three-center bonds. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25: 489–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Roeggen:1996:IPS

[RA96] I. Røeggen and J. Almlöf. Interatomic potential for the $X^1\Sigma_g^+$ state of Be_2. *International Journal of Quantum Chemistry*, 60(1):453–466, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60608.

Rocha:1997:RPI

[RA97] William R. Rocha and Wagner B. De Almeida. Reaction path for the insertion reaction of $SnCl_2$ into the Pt — Cl bond: An ab initio study. *International Journal of Quantum Chemistry*, 65(5):643–650, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42796; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42796&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Ruiz:1994:ESP

[RAA94] E. Ruiz, S. Alvarez, and P. Alemany. Electronic structure and properties of hexagonal wurtzite-type SiC. *International Journal of Quantum Chemistry*, 52(2):365–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Requena:1994:VHM

[RABZ94] A. Requena, M. Alacid, A. Bastida, and J. Zuthiga. A vibrational Hamiltonian model for triatomic molecules based on the Kratzer and Poschl Teller potentials. *International Journal of Quantum Chemistry*, 52(1):165–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rather:1999:PEM

[RAI99] Gerd Räther, Yuriko Aoki, and Akira Imamura. Performance of the elongation method with larger basis sets. *International Journal of Quantum Chemistry*, 74(1):35–47, ???? 1999.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62000136; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62000136&PLACEBO=IE.pdf.

Ramek:1990:IHB

[Ram90] M. Ramek. Intramolecular hydrogen bonding in neutral glycine, beta-alanine, gamma-aminobutyric acid, and delta-aminopentane acid. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17:45–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Rozas:1991:IAD

[RAM91] I. Rozas, G. A. Arteca, and P. G. Mezey. On the inhibition of alcohol dehydrogenase: Shape group analysis of molecular electrostatic potential on van der Waals surfaces for some pyrazole derivatives. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:269–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Ramek:1994:ISI

[Ram94] M. Ramek. Ab initio SCF investigation of the intramolecular hydrogen bonding in -aminohexanoic acid. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21:79–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Ransil:1993:DMP

[Ran93] B. J. Ransil. The diatomic molecule project at LMSS 1956-1966: Broken bottlenecks. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:25–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Randic:1994:CFP

[Ran94] M. Randić. Curve-fitting paradox. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21:215–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Randic:1995:CCN

[Ran95] M. Randić. On characterization of the conformations of nine-membered rings. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):61–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Randic:1997:RCB

[Ran97] Milan Randić. Resonance in catacondensed benzenoid hydrocarbons. *International Journal of Quantum Chemistry*, 63 (2):585–600, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42602; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42602&PLACEBO=IE.pdf`.

Richman:1993:LLS

[RB93] K. W. Richman and A. Banerjee. Low-lying states of SF_6 and SF_6^-: Electron affinity of SF_6 and electron detachment of SF_6^-. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:759–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Rajagopal:1995:NTD

[RB95] A. K. Rajagopal and F. A. Buot. A nonequilibrium time-dependent functional theory based on Liouvillean quantum field dynamics. *International Journal of Quantum Chemistry*, 56(4): 389–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rubin:1994:IST

[RBBL94] Y. V. Rubin, Y. P. Blagoy, V. A. Bokovoy, and V. S. Leontiev. The investigation of structural transitions and energy transfer in DNA solution in range 4.2-273 K using 6-thioguanine. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21:187–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Raos:1999:RBA

[RBT99] Guido Raos, Pietro Bielli, and Elena Tornaghi. Rotational barriers of amides and polyisocyanates: A spin-coupled study. *International Journal of Quantum Chemistry*, 74 (2):249–258, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003369; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003369&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Ramek:1992:RPF

[RC92a] M. Ramek and V. K. W. Cheng. On the role of polarization functions in SCF calculations of glycine and related systems with intramolecular hydrogen bonding. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:15–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Richards:1992:CMD

[RC92b] N. G. J. Richards and M. Cory. Computational methods in the design of photocaged compounds I. spectroscopic calculations upon substituted isochromenes. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:65–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Rothlisberger:1999:IMD

[RC99] Ursula Rothlisberger and Paolo Carloni. Ab initio molecular dynamics studies of a synthetic biomimetic model of galactose oxidase. *International Journal of Quantum Chemistry*, 73(2):209–218, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003518; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003518&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998*. Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Rega:1999:TER

[RCB+99] Nadia Rega, Maurizio Cossi, Vincenzo Barone, Christian Silvio Pomelli, and Jacopo Tomasi. Toward an effective and reliable representation of solvent effects in the study of biochemical systems. *International Journal of Quantum Chemistry*, 73(2):219–227, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003519; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003519&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998.* Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Rovira:1994:TSS

[RCWN94] C. Rovira, P. Constans, M.-H. Whangbo, and J. J. Novoa. Theoretical study of the structure and vibrational spectra of the $(H_2O)_2$ HF and H_2O $(HF)_2$ molecular complexes. *International Journal of Quantum Chemistry*, 52(1):177–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ren:1990:CFE

[RD90] S. Y. Ren and J. D. Dow. Change of the frontier electronic orbitals due to substitutional impurities in large chemical or biological molecules. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17:73–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Randic:1998:OMC

[RD98] Milan Randić and Jan Cz. Dobrowolski. Optimal molecular connectivity descriptors for nitrogen-containing molecules. *International Journal of Quantum Chemistry*, 70(6):1209–1215, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75088; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75088&PLACEBO=IE.pdf.

Radicioni:1998:RPT

[RDF98] Marcelo D. Radicioni, Carlos G. Diaz, and Francisco M. Fernández. Renormalized perturbation theory by the moment method for degenerate states: Anharmonic oscillators. *International Journal of Quantum Chemistry*, 66(4):

261–272, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29861; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29861&PLACEBO=IE.pdf.

Romera:1997:ASD

[RDK97] E. Romera, J. S. Dehesa, and Toshikatsu Koga. Analytical Schwartz density applied to heavy two-electron ions. *International Journal of Quantum Chemistry*, 61(3):525–531, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42422; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42422&PLACEBO=IE.pdf. See erratum [RDK02].

Romera:2002:EAS

[RDK02] E. Romera, J. S. Dehesa, and T. Koga. Erratum: Analytical Schwartz density applied to heavy two-electron ions. *International Journal of Quantum Chemistry*, 87(5):322, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/91012971/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/91012971/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=91012971&PLACEBO=IE.pdf. See [RDK97].

Romera:1995:WFS

[RDY95] E. Romera, J. S. Dehesa, and R. J. Yáñez. The Weizsacker functional: Some rigorous results. *International Journal of Quantum Chemistry*, 56(5):627–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Recamier:1990:AMS

[Réc90] J. A. Récamier. An algebraic method for the study of collisions with an anharmonic oscillator. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:655–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Reggio:1992:SPW

[Reg92] P. H. Reggio. A search for properties which produce discrimination between cannabinoid psychoactivity and analgesic activity. *International Journal of Quantum Chemistry*, 44(2):165–??, September 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ross:1990:IMM

[REL+90] R. B. Ross, W. C. Ermler, V. Luana, R. M. Pitzer, and C. W. Kern. Ab initio models for be_{81} and be_{87} metal clusters. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:225–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Repyakh:1996:FET

[Rep96] Irina Repyakh. First π-electron transitions in finite polymethine chains. *International Journal of Quantum Chemistry*, 57(5):913–918, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60429.

Resta:1999:MPE

[Res99] Raffaele Resta. Macroscopic polarization from electronic wave functions. *International Journal of Quantum Chemistry*, 75(4–5):599–606, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004955/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004955&PLACEBO=IE.pdf.

Reynolds:1990:OLZ

[Rey90] P. J. Reynolds. Overcoming the large-Z problem in quantum Monte Carlo. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:679–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Rauk:1994:CTT

[RF94] A. Rauk and T. B. Freedman. Chiroptical techniques and their relationship to biological molecules, big or small. *International Journal of Quantum Chemistry. Symposium*, 28:315–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Raimondi:1999:SCS

[RFG99] M. Raimondi, A. Famulari, and E. Gianinetti. Spin-coupled study of hydrogen-bonded systems: The Nucleic Acid Pairs. *International Journal of Quantum Chemistry*,

74(2):259–269, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003370; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003370&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Reggio:1990:MRT

[RFM90] P. H. Reggio, V. Frecer, and A. P. Mazurek. A molecular reactivity template for cannabinoid analgesic activity. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17:119–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Randic:1994:GBO

[RG94] M. Randić and X. Guo. Generalized bond orders. *International Journal of Quantum Chemistry*, 49(3):215–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rudin:1996:RBC

[RG96] G. E. Rudin and M. Gadella. Resonant branch cuts in a generalized Friedrichs model. *International Journal of Quantum Chemistry*, 58(5):441–451, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60499.

Randic:1999:REG

[RG99] Milan Randić and Xiaofeng Guo. Resonance energy of giant benzenoid hydrocarbon $C_{78}H_{26}$. *International Journal of Quantum Chemistry*, 74(6):697–708, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001786; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001786&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Rioseras-Garcia:1994:TCS

[RGHH94] M. J. Rioseras-Garcia and J. M. Hernando-Huelmo. Theoretical conformational study of the stabilities and geometries of [2,2] (2,7) naphthalenophane-1,11-diene and related compounds. *International Journal of Quantum Chemistry*, 52(3):651–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raynes:1994:NSS

[RGO94] W. T. Raynes, J. Geertsen, and J. Oddershede. Nuclear spin-spin coupling and nuclear motion. *International Journal of Quantum Chemistry*, 52(1):153–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roeth:1995:AAC

[RGT95] M. Roeth, F. Gasser, and C. Tavard. Asymmetries and anisotropies in the Compton scattering from the hydrogen molecule. *International Journal of Quantum Chemistry*, 53(5):569–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rees:1995:LFC

[RH95a] D. Rees and G. G. Hall. Localized functions on a circle. *International Journal of Quantum Chemistry*, 54(6):351–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rees:1995:LPA

[RH95b] D. Rees and G. G. Hall. Localized planar atomic hybrids. *International Journal of Quantum Chemistry*, 54(6):361–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rees:1996:LFS

[RH96a] D. Rees and G. G. Hall. Localized functions on a sphere. *International Journal of Quantum Chemistry*, 60(1):99–108, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60572`.

Reinhardt:1996:EAS

[RH96b] W. P. Reinhardt and Seungsuk Han. Exploiting the analyticity of Schrödinger operators: Theory and the computation of partial cross sections. *International Journal of Quantum Chemistry*, 57(3):327–341, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60394`.

Reinhardt:1996:EGS

[RHC96] P. Reinhardt, B. A. Heß, and M. Causá. Electronic and geometrical structure of bulk rutile studied with Hartree–Fock and density functional methods. *International Journal of Quantum Chemistry*, 58(3):297–306, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60483`.

Rincon:1994:AMP

[Rin94] L. Rincon. Aromaticity in metallacyclobutadienes from the perspective of the valence bond theory. *International Journal of Quantum Chemistry*, 50(3):189–??, April 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rincon:1996:CCCa

[Rin96a] L. Rincon. Computation of curve-crossing diagrams by approximate valence bond method. *International Journal of Quantum Chemistry*, 60(7):37–??, 1996. CODEN IJQCB2.

Rincon:1996:CCCc

[Rin96b] L. Rincon. Computation of curve-crossing diagrams by approximate valence bond method. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):37–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Rincon:1996:CCCb

[Rin96c] Luis Rincón. Computation of curve-crossing diagrams by approximate valence bond method. *International Journal of Quantum Chemistry*, 60(7):1249–1256, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60729`.

Recamier:1992:ELQ

[RJ92] A. J. Récamier and R. R. Jauregui. Energy levels for a quartic oscillator using algebraic techniques. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:153–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

RecamierA:1997:TEO

[RJ97] José Récamier A. and Rocío Jáuregui. Time-evolution operator for a forced parametric oscillator. *International Journal of Quantum Chemistry*, 62(2):125–135, March 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42494; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42494&PLACEBO=IE.pdf`.

Roszak:1991:IHC

[RK91] S. Roszak and Joyce J. Kaufman. The ab-initio hybrid crystal orbital/molecular cluster approach to study the electronic structure of molecular crystals and reactions in the solid environment. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:619–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Roychoudhury:1995:CSC

[RK95] M. Roychoudhury and D. Kumar. A comparative study of crystal packing vs. conformational energy of N-Acetyl-2,3-Didehydroproline. *International Journal of Quantum Chemistry*, 55(1):71–??, July 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Randic:1996:BPCa

[RK96a] M. Randić and G. Krilov. Bond profiles for cuboctahedron and twist cuboctahedron. *International Journal of Quantum Chemistry*, 60(8):127–??, 1996. CODEN IJQCB2.

Randic:1996:BPCc

[RK96b] M. Randić and G. Krilov. Bond profiles for cuboctahedron and twist cuboctahedron. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 23(??):127–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

Randic:1996:BPCb

[RK96c] Milan Randić and Goran Krilov. Bond profiles for cuboctahedron and twist cuboctahedron. *International Journal of Quantum Chemistry*, 60(8):1851–1863, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60745.

Randic:1997:CMS

[RK97] Milan Randić and Goran Krilov. On characterization of molecular surfaces. *International Journal of Quantum Chemistry*, 65(6):1065–1076, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42843; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42843&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on the Application of Fundamental Theory to Problems of Biology and Pharmocolgy*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Randic:1999:CFP

[RK99] Milan Randić and Goran Krilov. On a characterization of the folding of proteins. *International Journal of Quantum Chemistry*, 75(6):1017–1026, December 20, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004794/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004794&PLACEBO=IE.pdf.

Rykova:1996:TSS

[RKG96] E. A. Rykova, N. M. Klimenko, and A. I. Grigorév. Theoretical studies of structure, stability, and chemical bonding in oxohydride OM_4H_6 complexes. *International Journal of Quantum Chemistry*, 57(4):697–705, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60406.

Rovira:1998:CSC

[RKH+98] Carme Rovira, Karel Kunc, Jürg Hutter, Pietro Ballone, and Michele Parrinello. A comparative study of O_2, CO, and NO binding to iron-porphyrin. *International Journal of Quantum*

Chemistry, 69(1):31–35, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29970; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29970&PLACEBO=IE.pdf.

Ramek:1997:IMM

[RKN97] Michael Ramek, Anne-Marie Kelterer, and Sonja Nikolić. Ab initio and molecular mechanics conformational analysis of neutral L-proline. *International Journal of Quantum Chemistry*, 65(6):1033–1045, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42840; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42840&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on the Application of Fundamental Theory to Problems of Biology and Pharmocolgy*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Ross:1995:ISE

[RKPE95] R. B. Ross, C. W. Kern, R. M. Pitzer, and W. C. Ermler. Ab initio studies of the electronic structure of Be_{93}, Be_{105}, Be_{111}, and Be_{123} clusters. *International Journal of Quantum Chemistry*, 55(5):393–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rienstra-Kiracofe:1999:BR

[RKS99] Jonathan C. Rienstra-Kiracofe and Henry F. Schaefer III. Book review. *International Journal of Quantum Chemistry*, 72(3):233–234, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40003035; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40003035&PLACEBO=IE.pdf.

Roszak:1992:MAV

[RL92] S. Roszak and J. Lipinski. The modified all-valence INDO method with the inclusion of spin-orbit coupling. *International Journal of Quantum Chemistry*, 44(5):831–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rabinowitz:1994:CQM

[RL94] J. R. Rabinowitz and S. B. Little. Comparison of quantum mechanical methods to compute the biologically relevant reactivities of cyclopenta-polycyclic aromatic hydrocarbons. *International Journal of Quantum Chemistry*, 52(3):681–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raja:1995:CSH

[RL95] A. V. Raja and J. B. Lagowski. Conformational study of halogen- and hydrogen-substituted polythionylphosphazenes using density functional theory method. *International Journal of Quantum Chemistry*, 54(2):117–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roothaan:1997:CJS

[RL97] Clemens C. J. Roothaan and Shan-Tao Lai. Calculation of 3n-j symbols by Labarthe's method. *International Journal of Quantum Chemistry*, 63(1):57–64, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42553; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42553&PLACEBO=IE.pdf`.

Remacle:1998:IBO

[RL98] F. Remacle and R. D. Levine. On the inverse Born–Oppenheimer separation for high Rydberg states of molecules. *International Journal of Quantum Chemistry*, 67(2):85–100, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29889; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29889&PLACEBO=IE.pdf`.

Ramusino:1996:ISL

[RM96] Marina Cotta Ramusino and Gianfranco La Manna. Ab initio study of lithiated N-methylpyridones. *International Journal of Quantum Chemistry*, 57(4):729–733, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60411`.

Raymond:1999:QCI

[RM99] Mary K. Raymond and Josef Michl. Quantum confinement induced collapse of a large to a small radius self-trapped exciton in a permethylated polysilane chain. *International Journal of Quantum Chemistry*, 72(4):361–367, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006314; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006314&PLACEBO=IE.pdf`. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Runge:1990:TDM

[RMF90] K. Runge, D. A. Micha, and E. Q. Feng. A time-dependent molecular orbital approach to electron transfer in ion-atom collisions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:781–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Ramos:1999:MEI

[RMH+99] Maria João Ramos, André Melo, Elsa S. Henriques, José A. N. F. Gomes, Nathalie Reuter, Bernard Maigret, Wely B. Floriano, and Marco A. C. Nascimento. Modeling enzyme-inhibitor interactions in serine proteases. *International Journal of Quantum Chemistry*, 74(3):299–314, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62004760; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62004760&PLACEBO=IE.pdf`. Special Issue: *Biophysics Quarterly*.

Rodriguez-Monge:1997:CPI

[RML97] Lucia Rodriguez-Monge and Sven Larsson. Conductivity in polyacetylene. IV. ab initio calculations for a two-site model for electron transfer between allyl anion and allyl. *International Journal of Quantum Chemistry*, 61(5):847–857, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42457; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42457&PLACEBO=IE.pdf`.

Reinhardt:1998:LON

[RMPR98] P. Reinhardt, J-P Malrieu, A. Povill, and J. Rubio. Localized orbitals in nonmetallic ring systems. *International Journal of Quantum Chemistry*, 70(1):167–180, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74361; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74361&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Raynes:1996:CCS

[RN96] W. T. Raynes and M. Nightingale. Calculation of ^{13}C shielding of the isotopomers CH_3Cl, CH_2DCl, CHD_2Cl, and CD_3Cl. *International Journal of Quantum Chemistry*, 60(1):529–534, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60616.

Rusho:1993:SOJ

[RNS93] J. Rusho, J. Nichols, and J. Simons. Second-order Jahn–Teller instability and the activation energy for $Al^+(^1S) + H_2 \rightarrow AlH^+(^2\Sigma^+) + H$. *International Journal of Quantum Chemistry*, 48(5):309–317, December 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roche:1999:NIK

[Roc99] Michel Roche. Numerical integration of the Kohn–Sham equations: Integral method for bound states. *International Journal of Quantum Chemistry*, 74(1):49–54, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62000137; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62000137&PLACEBO=IE.pdf.

Rodriguez:1991:STD

[Rod91] Wilfredo Rodriguez. Solution of the time-dependent Schrödinger equation using a continuous Fourier transform. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:107–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Ribbing:1990:SNC

[ROL+90] C. Ribbing, M. Odelius, A. Laaksonen, J. Kowalewski, and B. Roos. Simple nonempirical calculations of the zero-field splitting in transition metal systems: I. the Ni(II) — water complexes. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:295–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Roothaan:1993:MLP

[Roo93a] C. C. J. Roothaan. My life as a physicist: Memories and perspectives. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:1–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Roothaan:1993:NAC

[Roo93b] C. C. J. Roothaan. New algorithms for calculating 3n-j symbols. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:13–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Rosciszewski:1996:SEF

[Rość96] K. Rościszewski. Simple empirical formulas and good quality estimations for electron correlation energies of molecules and molecular clusters: First-row atom molecules. *International Journal of Quantum Chemistry*, 58(5):471–485, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60502`.

Rubio:1996:SCC

[ROSM96] Mercedes Rubio, Enrique Ortí, and José Sánchez-Marín. A study of coronene-coronene association using atom-atom pair potentials. *International Journal of Quantum Chemistry*, 57(4): 567–573, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60421`.

Rothstein:1996:VEV

[Rot96] Stuart M. Rothstein. Valence energy in variational Monte Carlo: CuH dissociation energy. *International Journal of Quantum Chemistry*, 60(4):803–808, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60652. See erratum [Rot97].

Rothstein:1997:EVE

[Rot97] Stuart M. Rothstein. Erratum: Valence energy in variational Monte Carlo: CuH dissociation energy. *International Journal of Quantum Chemistry*, 61(1):153, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42380; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42380&PLACEBO=IE.pdf. See [Rot96].

Rozas:1997:ACD

[Roz97] Isabel Rozas. Atomic charges derived from different methods: A comparative study applied to SO_2 heterocycles. *International Journal of Quantum Chemistry*, 62(5):477–487, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42535; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42535&PLACEBO=IE.pdf.

Rettrup:1996:RSG

[RP96] Sten Rettrup and Ruben Pauncz. Representations of the symmetric group generated by projected spin functions: A graphical approach. *International Journal of Quantum Chemistry*, 60(1):91–98, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60571.

Rovira:1998:OBI

[RP98a] Carme Rovira and Michele Parrinello. Oxygen binding to iron-porphyrin: A density functional study using both LSD and LSD + GC schemes. *International Journal of Quantum Chemistry*, 70(2):387–394, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75008; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75008&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Runeberg:1998:RPC

[RP98b] Nino Runeberg and Pekka Pyykkö. Relativistic pseudopotential calculations on Xe_2, RnXe, and Rn_2: The van der Waals properties of radon. *International Journal of Quantum Chemistry*, 66(2):131–140, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29847; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29847&PLACEBO=IE.pdf`.

Richardson:1997:ISE

[RPB+97] W. H. Richardson, C. Peng, D. Bashford, L. Noodleman, and D. A. Case. Incorporating solvation effects into density functional theory: Calculation of absolute acidities. *International Journal of Quantum Chemistry*, 61(2):207–217, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42402; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42402&PLACEBO=IE.pdf`.

Rajadell:1996:SBS

[RPJZW96] F. Rajadell, J. Planelles, W. Jaskólski, and C. Zicovich-Wilson. Selection of basis sets for atoms and molecules in cavities. *International Journal of Quantum Chemistry*, 60(5):993–999, December 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60671`.

Rajadell:1995:SDD

[RPKM95] F. Rajadell, J. Planelles, J. Karwowski, and V. Mas. Spectral density distribution of an N-electron Hamiltonian in a finite-dimensional and spin-adapted model space. *International Journal of Quantum Chemistry*, 56(2):71–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ray:1994:AHC

[RR94] N. K. Ray and R. C. Rastogi. Activation hardness and cycloadditions of even linear polyenes. *International Journal of Quantum Chemistry*, 51(2):99–??, July 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Razafinjanahary:1994:IMT

[RRC94] H. Razafinjanahary, R. Rogemond, and H. Chermette. Incidence of the muffin-tin approximation on the electronic structure of large clusters calculated by the MS-LSD method: The typical case of C_{60}. *International Journal of Quantum Chemistry*, 51(4 (or 5??)):319–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rubio:1997:DFP

[RRS97] J. Rubio, N. Russo, and E. Sicilia. Density functional potential energy hypersurface of protonated ozone: A comparison between different gradient-corrected nonlocal functionals. *International Journal of Quantum Chemistry*, 61(3): 415–420, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42436; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42436&PLACEBO=IE.pdf.

Rivas-Silva:1994:HAG

[RS94] J. F. Rivas-Silva. The helium atom in its ground state embedded in strong magnetic fields. *International Journal of Quantum Chemistry*, 51(3):135–??, July 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Runge:1997:IWP

[RS97a] K. Runge and J. R. Sabin. Introduction to the workshop on properties of molecules in strong magnetic fields. *International Journal of Quantum Chemistry*, 64(5):495–496, September 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42707; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42707&PLACEBO=IE.pdf. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

Runge:1997:EPH

[RS97b] Keith Runge and John R. Sabin. Electronic properties of H_2^+, H_2, and LiH in high magnetic fields. *International Journal of Quantum Chemistry*, 64(5):561–570, September 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42719;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42719&PLACEBO=IE.pdf. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

Rey:1998:VSL

[RS98] Jérôme Rey and Andreas Savin. Virtual space level shifting and correlation energies. *International Journal of Quantum Chemistry*, 69(4):581–590, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30013; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30013&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Roy:1997:DFC

[RSD97] Amlan K. Roy, Ranbir Singh, and B. M. Deb. Density functional calculations on triply excited states of lithium isoelectronic sequence. *International Journal of Quantum Chemistry*, 65(4):317–332, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42769; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42769&PLACEBO=IE.pdf.

Raimondi:1996:OSC

[RSGC96] M. Raimondi, M. Sironi, J. Gerratt, and D. L. Cooper. Optimized spin-coupled virtual orbitals. *International Journal of Quantum Chemistry*, 60(1):225–233, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60586.

Ramek:1998:RCA

[RT98] Michael Ramek and Sanja Tomic. RHF conformational analysis of the auxin phytohormones n-ethyl-Indole-3-Acetic acid ($n = 4, 5, 6$). *International Journal of Quantum Chemistry*, 70(6):1169–1175, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75084; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75084&PLACEBO=IE.pdf.

Ramek:1999:QCC

[RT99] Michael Ramek and Sanja Tomić. Quantum chemical conformational analysis of the auxin phytohormone 4-methyl-3-indole acetic acid. *International Journal of Quantum Chemistry*, 75(6):1003–1008, December 20, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004788/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004788&PLACEBO=IE.pdf.

Ramek:1995:SIS

[RTKP95] M. Ramek, S. Tomic, and B. Kojic-Prodic. Systematic ab initio SCF conformational analysis of indol-3-(??)ylacetic acid phytohormone (auxin): Comparison with experiment and molecular mechanics calculations. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):75–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Ramek:1996:CISa

[RTKP96a] M. Ramek, S. Tomic, and B. Kojic-Prodic. Comparative ab initio SCF conformational study of 4-chloro-indole-3-acetic acid and indole-3-acetic acid phytohormones (auxins). *International Journal of Quantum Chemistry*, 60(8):3–??, 1996. CODEN IJQCB2.

Ramek:1996:CISc

[RTKP96b] M. Ramek, S. Tomic, and B. Kojic-Prodic. Comparative ab initio SCF conformational study of 4-chloro-indole-3-acetic acid and indole-3-acetic acid phytohormones (auxins). *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 23(??):3–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

Ramek:1996:CISb

[RTKP96c] Michael Ramek, Sanja Tomić, and Biserka Kojić-Prodić. Comparative ab initio SCF conformational study of 4-chloro-indole-3-acetic acid and indole-3-acetic acid phytohormones (auxins). *International Journal of Quantum Chemistry*, 60(8):1727–1733, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-

461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60741.

Ramos:1997:PAI

[RVL97] J. G. Ramos, A. R. Vasconcellos, and Roberto Luzzi. Physicochemical aspects of an industrial process. *International Journal of Quantum Chemistry*, 65(3):277–285, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42764; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42764&PLACEBO=IE.pdf.

Rasolt:1992:CDF

[RVP92] M. Rasolt, G. Vignale, and F. Perrot. Current density functional theory in a continuum and lattice lagrangians: Application to spontaneously broken chiral ground states. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:359–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Rzepa:1992:TSS

[RW92] H. S. Rzepa and W. A. Wylie. Transition-state structures for the reaction between styrene and *t*-butyl cyanoketine: Theoretical evidence for antarafacial characteristics in a $\pi^2+\pi^2$ thermal cycloaddition. *International Journal of Quantum Chemistry*, 44(4):469–476, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ritchie:1998:UFF

[RW98] Burke Ritchie and Charles A. Weatherford. Use of a Fast Fourier Transform (FFT) 3D time-dependent Schrödinger equation solver in molecular electronic structure. *International Journal of Quantum Chemistry*, 70(4-5):627–635, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75041; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75041&PLACEBO=IE.pdf.

Ritchie:1999:QCC

[RW99] Burke Ritchie and Charles A. Weatherford. Quantum classical correspondence in nonrelativistic electrodynamics. *International Journal of Quantum Chemistry*, 75(4–5):655–658, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004943/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004943&PLACEBO=IE.pdf.

Richards:1991:EMC

[RWT91] N. G. J. Richards, P. B. Williams, and M. S. Tute. Empirical methods for computing molecular partition coefficients. I. upon the need to model the specific hydration of polar groups in fragment-based approaches. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:299–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Richards:1992:EMC

[RWT92] N. G. J. Richards, P. B. Williams, and M. S. Tute. Empirical methods for computing molecular partition coefficients: II. inclusion of comformational flexibility within fragment-based approaches. *International Journal of Quantum Chemistry*, 44(2):219–??, September 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rychlewski:1994:UEC

[Ryc94] J. Rychlewski. On the use of explicitly correlated functions in variational computations for small molecules. *International Journal of Quantum Chemistry*, 49(4):477–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ryde:1994:CCC

[Ryd94] U. Ryde. The coordination chemistry of the catalytic zinc ion in alcohol dehydrogenase studied by ab initio quantum chemical calculations. *International Journal of Quantum Chemistry*, 52(5):1229–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rylov:1999:CQC

[Ryl99] Yu. A. Rylov. Coupled quantum-classical description in the Schrödinger representation. *International Journal of Quantum Chemistry*, 72(5):483–498, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006351;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006351&PLACEBO=IE.pdf.

Rice:1996:NAC

[RZ96] Stuart A. Rice and Meishan Zhao. New approaches to a classical theory of unimolecular reaction rate. *International Journal of Quantum Chemistry*, 58(6):593–635, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60516.

Sarma:1996:ECS

[SA96] C. R. Sarma and M. A. H. Ahsan. Electron correlation studies: Rumer basis approach. *International Journal of Quantum Chemistry*, 60(1):147–156, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60577.

Sambrano:1997:ISO

[SAB+97] J. R. Sambrano, J. Andrés, A. Beltrán, F. R. Sensato, E. R. Leite, F. M. L. G. Stamato, and E. Longo. An ab initio study of oxygen vacancies and doping process of Nb and Cr atoms on TiO_2 (110) surface models. *International Journal of Quantum Chemistry*, 65(5):625–631, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42793; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42793&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Sadlej:1997:CSE

[Sad97] Andrzej J. Sadlej. Constrained solutions of the eigenvalue problem in truncated basis sets. *International Journal of Quantum Chemistry*, 63(1):35–38, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42578; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42578&PLACEBO=IE.pdf.

Serrano-Andres:1997:SEE

[SAFK97] Luis Serrano-Andrés, Markus P. Fülscher, and Gunnar Karlström. Solvent effects on electronic spectra studied by multiconfigurational perturbation theory. *International Journal of Quantum Chemistry*, 65(2):167–181, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42754`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42754&PLACEBO=IE.pdf`.

Sahni:1995:DRA

[Sah95a] V. Sahni. Derivation and reinterpretation of approximations in Schrödinger and Kohn–Sham theory via a hierarchy within the work formalism. *International Journal of Quantum Chemistry*, 53(6):591–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sahni:1995:WFE

[Sah95b] V. Sahni. The work formalism of electronic structure. *International Journal of Quantum Chemistry*, 56(4):265–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sakai:1997:ISZ

[Sak97] Shogo Sakai. Ab initio studies on the Ziegler-Natta polymerization mechanisms of ethylene and propylene. role of cocatalysis and stereoregulation. *International Journal of Quantum Chemistry*, 65(5):739–747, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42807`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42807&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Sakai:1998:TMR

[Sak98] Shogo Sakai. Theoretical model for the reaction mechanisms of singlet carbene analogs into unsaturated hydrocarbon and the origin of the activation barrier. *International Journal of Quantum Chemistry*, 70(2):291–302, ???? 1998. CODEN

IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74997; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74997&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Sosa:1994:ESC

[SAL+94] C. Sosa, J. Andelm, C. Lee, J. F. Blake, and B. L. Chenard. Electronic structure calculations of 1,3-Dipolar cycloadditions using density functional and Hartree–Fock methods. *International Journal of Quantum Chemistry*, 49(4):511–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Samvelyan:1997:RDE

[Sam97] S. Kh. Samvelyan. N-representability of diagonal elements of second-order reduced density matrices. *International Journal of Quantum Chemistry*, 65(2):127–142, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42750; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42750&PLACEBO=IE.pdf.

Santamaria:1997:DEF

[San97] R. Santamaria. Design of an exchange functional with correct asymptotics. *International Journal of Quantum Chemistry*, 61(6):891–898, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42473; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42473&PLACEBO=IE.pdf.

Sarma:1996:GAP

[SAR96] C. R. Sarma, M. A. H. Ahsan, and Sten Rettrup. A graphical approach to permutation group representations for many-electron systems. *International Journal of Quantum Chemistry*, 58(6):637–643, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60517.

Sasaki:1974:MEC

[Sas74] F. Sasaki. Matrix elements in configuration interaction calculations. *International Journal of Quantum Chemistry*, 8(??): 605–617, ?? 1974. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shiga:1999:DHM

[SAS99] Motoyuki Shiga, Fumihiko Aiga, and Kotoku Sasagane. Dynamic hyperpolarizabilities in Møller–Plesset perturbation theory. *International Journal of Quantum Chemistry*, 71 (3):251–271, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10016710; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10016710&PLACEBO=IE.pdf.

Suarez:1994:ASO

[SATP94] C. Suarez, A. Aguado, C. Tablero, and M. Paniagua. Application of second-order density functional methods to the calculation of the LiFH potential energy surface. *International Journal of Quantum Chemistry*, 52(4):935–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saenz:1997:MCS

[SAW97] Alejandro Saenz, Tanja Asthalter, and Wolf Weyrich. Methods for the calculation of spherically averaged Compton profiles with GTOs. *International Journal of Quantum Chemistry*, 65(3):213–223, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42759; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42759&PLACEBO=IE.pdf.

Sekino:1990:RCC

[SB90] H. Sekino and R. J. Bartlett. Relativistic coupled cluster calculations on neutral and highly ionized atoms. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:241–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Szalay:1992:AAC

[SB92] P. G. Szalay and R. J. Bartlett. Alternative Ansatze in coupled-cluster theory. IV. comparison for the two electron problem and the role of exclusion principle violating (EPV) terms. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:85–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Sarkar:1995:ESQ

[SB95] P. Sarkar and S. P. Bhattacharyya. The effects of static quartic anharmonicity on the quantum dynamics of a linear oscillator with time-dependent harmonic frequency: Perturbative analysis and numerical calculations. *International Journal of Quantum Chemistry*, 54(6):337–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Seijo:1996:AGF

[SB96] Luis Seijo and Zoila Barandiarán. Applications of the group-function theory to the field of materials science. *International Journal of Quantum Chemistry*, 60(1):617–636, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60624`.

Sarkar:1997:DLN

[SB97a] Pranab Sarkar and S. P. Bhattacharyya. On the dynamics of a linear and a nonlinear quantum oscillator with randomly changing harmonic frequency. *International Journal of Quantum Chemistry*, 62(3):265–272, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42511`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42511&PLACEBO=IE.pdf`.

Sarkar:1997:TDO

[SB97b] Pranab Sarkar and S. P. Bhattacharyya. Tunneling dynamics of one- and two-dimensional cubic oscillators with randomly fluctuating harmonic force constants: A numerical experiment. *International Journal of Quantum Chemistry*, 64(4):403–409, September 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42698`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42698&PLACEBO=IE.pdf`.

Sarkar:1998:AEE

[SB98] Pranab Sarkar and S. P. Bhattacharyya. Adiabatic evolution of eigenspectra of model 1-D and 2-D Hamiltonians: Quantum adiabatic switching algorithm in a time-independent Fourier grid Hamiltonian framework. *International Journal of Quantum Chemistry*, 67(3):133–141, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29894; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29894&PLACEBO=IE.pdf.

Schwarz:1990:CDE

[SBAD90] K. Schwarz, P. Blaha, and C. Ambrosch-Draxl. Charge distribution and electric field gradients in YBasub 2 cu_3 osub 7 by band structure calculations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:339–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Sola:1992:VBC

[SBD+92] M. Sola, M. Balcells, M. Duran, A. Lledos, and J. Bertran. Valence-bond calculations on ZnO and HgO using integrals computed through the semiempirical am1 method. *International Journal of Quantum Chemistry*, 44(5):887–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sizova:1997:ESS

[SBIP97a] O. V. Sizova, V. I. Baranovski, N. V. Ivanova, and A. I. Panin. Electronic structure and spectra of ruthenium binuclear complexes: Localized versus delocalized model. *International Journal of Quantum Chemistry*, 65(2):183–193, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42755; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42755&PLACEBO=IE.pdf.

Sizova:1997:SCE

[SBIP97b] O. V. Sizova, V. I. Baranovski, N. V. Ivanova, and A. I. Panin. Semiempirical calculations of electronic spectra of Ru(II) and Ru(III) compounds in restricted active space CI approximation. *International Journal of Quantum Chemistry*,

63(4):853–860, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42636; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42636&PLACEBO=IE.pdf.

Scolfaro:1994:EPM

[SBLL94] L. M. R. Scolfaro, D. Beliaev, J. R. Leite, and A. T. Lino. Electronic properties of multiple delta-doped layers in silicon and GaAs. *International Journal of Quantum Chemistry. Symposium*, 28:667–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Sarkar:1997:LSF

[SBM97] Jayanta Sarkar, Manas Banerjee, and Asok K. Mukherjee. Lucas sequences and Fibonacci triads of graphs in PMO calculation on the charge-transfer bands of a series of EDA complexes: Correlation with experimental and AM1 results. *International Journal of Quantum Chemistry*, 63 (4):817–825, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42632; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42632&PLACEBO=IE.pdf.

Sodupe:1997:TSS

[SBOB97] Mariona Sodupe, Vicenç Branchadell, Antonio Oliva, and Juan Bertran. Theoretical study of $ScCO_2^+$. *International Journal of Quantum Chemistry*, 63(2):523–528, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42595; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42595&PLACEBO=IE.pdf.

Schmelcher:1991:MIS

[SC91] P. Schmelcher and L. S. Cederbaum. On molecules and ions in strong magnetic fields. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:371–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Sengupta:1994:RTH

[SC94] D. Sengupta and A. K. Chandra. Role of tunneling of hydrogen in photoenolization of a ketone. *International Journal of*

Quantum Chemistry, 52(6):1317–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Su:1995:SBS

[SC95] Y.-N. Su and S.-Y. Chu. Structure and bonding study of the $P_2 + P_2^+$ system. *International Journal of Quantum Chemistry*, 54(1):43–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schulz:1996:RAMa

[SC96a] L. Schulz and H. Chojnacki. Resemblance analysis of molecular systems on the grounds of DFT-evaluated parameters. platinum complexes and their anticancer activity. *International Journal of Quantum Chemistry*, 60(7):173–??, 1996. CODEN IJQCB2.

Schulz:1996:RAMb

[SC96b] L. Schulz and H. Chojnacki. Resemblance analysis of molecular systems on the grounds of DFT-evaluated parameters. Platinum complexes and their anticancer activity. *International Journal of Quantum Chemistry*, 60(7):1385–1391, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60697`.

Schulz:1996:RAMc

[SC96c] L. Schulz and H. Chojnacki. Resemblance analysis of molecular systems on the grounds of DFT-Evaluated parameters. platinum complexes and their anticancer activity. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):173–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Schmelcher:1997:MSM

[SC97a] P. Schmelcher and L. S. Cederbaum. Molecules in strong magnetic fields: Some perspectives and general aspects. *International Journal of Quantum Chemistry*, 64(5):501–511, September 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42715; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42715&PLACEBO=IE.pdf`. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

SreedharaRao:1997:SBC

[SC97b] V. Sreedhara Rao and A. K. Chandra. A study of bond-cleavage and bond-formation processes in some simple metathesis reactions. *International Journal of Quantum Chemistry*, 63 (6):1099–1106, July 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42653; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42653&PLACEBO=IE.pdf.

Serrano:1998:SDL

[SC98a] Agostinho Serrano and Sylvio Canuto. Structure dependence of the low-lying excited states and the first dipole hyperpolarizability of phenol blue. *International Journal of Quantum Chemistry*, 70(4-5):745–750, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75052; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75052&PLACEBO=IE.pdf.

Su:1998:STS

[SC98b] Ming-Der Su and San-Yan Chu. Singlet-triplet splitting and the activation of C — H bond for (η^5-C_5H_5)M(CO) isoelectronic fragments: A theoretical study. *International Journal of Quantum Chemistry*, 70(4-5):961–971, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75074; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75074&PLACEBO=IE.pdf.

Su:1999:DFT

[SC99] Ming-Der Su and San-Yan Chu. Density functional theory of C — H bond activation by transition-metal complex: A (η^5-C_5H_5)ML (M = Rh, Ir; L = CH_2, CO, SH_2, PH_3)+CH_4 case study. *International Journal of Quantum Chemistry*, 72(4):405–410, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006318; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006318&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Saragoni:1993:TSC

[SCA93] V. G. Saragoni, R. R. Contreras, and A. J. Aizman. Theoretical study of the C- vs. O-acylation of metal enolates frontier molecular orbital analysis including solvent effects. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:713–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Schuch:1990:NLH

[Sch90] D. Schuch. A new Lagrange–Hamilton formalism for dissipative systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:767–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Schlegel:1992:CGO

[Sch92] H. B. Schlegel. A comparison of geometry optimization with internal, cartesian, and mixed coordinates. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:243–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Schuch:1993:ANS

[Sch93] D. Schuch. On the applicability of a nonlinear Schrödinger equation to the determination of rate constants in Kramers' theory of chemical reactions. *International Journal of Quantum Chemistry*, 45(3):235–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schuch:1994:FND

[Sch94] D. Schuch. On a form of nonlinear dissipative wave mechanics valid in position- and momentum-space. *International Journal of Quantum Chemistry. Symposium*, 28:251–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Schmidt:1995:EMEa

[Sch95a] P. P. Schmidt. The evaluation of matrix elements in the analysis of anharmonic molecular vibrations: Functional Taylor series vibrations. *International Journal of Quantum Chemistry*, 53 (6):651–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schmidt:1995:EMEb

[Sch95b] P. P. Schmidt. The evaluation of matrix elements in the analysis of anharmonic molecular vibrations: Optimized expansions and quadratures. *International Journal of Quantum Chemistry*, 53 (6):663–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schmidt:1995:SCM

[Sch95c] P. P. Schmidt. Self-consistent methods for the treatment of low-lying molecular vibrations. *International Journal of Quantum Chemistry*, 53(6):635–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schmelcher:1997:ETP

[Sch97] P. Schmelcher. Exploring the topology of potential energy surfaces of the H_2^+ ion in the presence of a strong magnetic field. *International Journal of Quantum Chemistry*, 64 (5):553–560, September 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42718; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42718&PLACEBO=IE.pdf`. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

Schmelcher:1998:GSA

[Sch98] P. Schmelcher. Ground states of atoms and molecules in strong magnetic fields. *International Journal of Quantum Chemistry*, 70(4-5):789–795, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75057; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75057&PLACEBO=IE.pdf`.

Schmidt:1999:HMR

[Sch99a] P. P. Schmidt. Hall model reaction surface for HCN. *International Journal of Quantum Chemistry*, 72(5):473–482, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006350; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006350&PLACEBO=IE.pdf`.

Schuch:1999:EDD

[Sch99b] Dieter Schuch. Effective description of the dissipative interaction between simple model-systems and their environment. *International Journal of Quantum Chemistry*, 72

(6):537–547, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=50000012; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=50000012&PLACEBO=IE.pdf.

Shillady:1990:MOV

[SCJK90] D. D. Shillady, S. Cutler, L. F. Jones, and L. B. Kier. A molecular orbital valence bond study of 3-Methyl sydnone and 3-Methyl pseudosydnone. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:153–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Saba:1996:AQX

[SCL96] Giuseppe Saba, Mariano Casu, and Adolfo Lai. Application of quadrupolar ^{131}Xe-NMR relaxation to the study of macromolecular systems. *International Journal of Quantum Chemistry*, 59(4):343–348, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60553.

Scharnagl:1993:RPA

[SCMF93] C. Scharnagl, C. Cometta-Morini, and S. F. Fischer. Reversible photochemistry in the alpha-subunit of phycoerythrocyanin: Characterization of chromophore and protein by electrostatic calculations. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 20:199–??, 1993. CODEN IJQBDZ. ISSN 0360-8832.

Scoles:1990:PIF

[Sco90] G. Scoles. On the prediction of intermolecular forces between unlike atoms and molecules. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:475–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Seminario:1991:CMG

[SCP91] Jorge M. Seminario, Monica C. Concha, and Peter Politzer. Calculation of molecular geometries and energies by a local density functional approach. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:249–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Seminario:1993:DFI

[SCP93] J. M. Seminario, M. C. Concha, and P. Politzer. Density-functional and ab initio computational studies of palladium clusters. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:263–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Salazar:1995:ICS

[SCP+95a] M. C. Salazar, A. De Castro, J. L. Paz, G. H. F. Diercksen, and A. J. Hernadez. Ab initio conformational study of the CO ... H_2 Van der Waals dimer. *International Journal of Quantum Chemistry*, 55(3):251–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Seminario:1995:MDS

[SCP95b] J. M. Seminario, M. C. Concha, and P. Politzer. Molecular dynamics simulation of liquid nitromethane shocked to 143 kbar. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:621–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Sirois:1994:DFS

[SCS94] S. Sirois, M. Castro, and D. R. Salahub. A density functional study of the interaction of CO_2 with a Pd atom. *International Journal of Quantum Chemistry. Symposium*, 28:645–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Scuseria:1995:CBB

[Scu95] G. E. Scuseria. On the connections between Brueckner-coupled-cluster, density-dependent Hartree–Fock, and density functional theory. *International Journal of Quantum Chemistry*, 55(2):165–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schmider:1996:NSE

[SD96a] Hartmut Schmider and Jens Peder Dahl. Nodal structure of the electronic Wigner function of many-electron atoms and molecules. *International Journal of Quantum Chemistry*, 60 (1):439–452, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60607`.

Smith:1996:NPD

[SD96b] Lorna J. Smith and Christopher M. Dobson. NMR and protein dynamics. *International Journal of Quantum Chemistry*, 59(4): 315–332, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60551.

Schafer:1997:MHS

[SD97] Olivier Schafer and Claude Daul. Modeling of the hydration sphere of gadolinium(III) ion using density functional theory. *International Journal of Quantum Chemistry*, 61(3): 541–546, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42424; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42424&PLACEBO=IE.pdf.

Schranz:1998:IAI

[SD98] D. W. Schranz and S. G. Davison. Indirect adatom interactions via III-V semiconductor substrates. *International Journal of Quantum Chemistry*, 67(6):377–397, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29918; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29918&PLACEBO=IE.pdf.

Shcheka:1994:QCS

[SDE94] O. L. Shcheka, N. V. Dobrodey, and T. B. Emelina. Quantum chemical study of catalysts based on oxides of transition metals. *International Journal of Quantum Chemistry*, 50(3): 181–??, April 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stuckl:1997:DFC

[SDG97] A. C. Stückl, C. A. Daul, and H. U. Güdel. Density functional calculations of optical excitation energies by a transition-state method. *International Journal of Quantum Chemistry*, 61(3):579–588, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42429; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42429&PLACEBO=IE.pdf.

Sankey:1998:AAD

[SDW+98] Otto F. Sankey, Alexander A. Demkov, Wolfgang Windl, Jürgen H. Fritsch, James P. Lewis, and Miguel Fuentes-Cabrera. The application of approximate density functionals to complex systems. *International Journal of Quantum Chemistry*, 69(3):327–340, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29988; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29988&PLACEBO=IE.pdf`. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Sadlej:1992:CIG

[SE92] J. Sadlej and W. D. Edwards. Correlated ab initio geometry and vibrational spectra of imidazole and its different forms. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:409–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Sadlej:1993:ISG

[SE93a] J. Sadlej and W. D. Edwards. Ab initio study of the ground and excited states of LiNe. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:731–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Sadlej:1993:SWI

[SE93b] J. Sadlej and W. D. Edwards. A study of the weak interactions in SCO/He and SCO/N_2 systems. *International Journal of Quantum Chemistry*, 46(5):623–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sadlej:1995:ISG

[SE95a] J. Sadlej and W. D. Edwards. Ab initio study of the ground and first excited state of LiAr. *International Journal of Quantum Chemistry*, 53(6):607–615, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shroll:1995:ESG

[SE95b] R. M. Shroll and W. D. Edwards. Excited-state gradients via CPHF equations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:395–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Shroll:1997:RCG

[SE97] R. M. Shroll and W. D. Edwards. Restricted CIS gradients via CPHF equations. *International Journal of Quantum Chemistry*, 63(6):1037–??, July 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Seel:1997:CLS

[See97] M. Seel. Core-level shifts and their relation to surface effects and dimensionality of a system. *International Journal of Quantum Chemistry*, 63(3):623–629, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42623; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42623&PLACEBO=IE.pdf.

Shalabi:1998:CSE

[SEKEB98] A. S. Shalabi, Kh. M. Eid, M. A. Kamel, and A. A. El-Barbary. Comparative study of errors in HeH^- interaction energy calculations. *International Journal of Quantum Chemistry*, 68(5):329–350, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29953; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29953&PLACEBO=IE.pdf.

Sellers:1993:CDC

[Sel93] H. Sellers. The C^2-DIIS convergence acceleration algorithm. *International Journal of Quantum Chemistry*, 45(1):31–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Seminario:1994:SSS

[Sem94] J. M. Seminario. A study of small systems containing H and O atoms using nonlocal functionals: Comparisons with ab initio and experiment. *International Journal of Quantum Chemistry. Symposium*, 28:655–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Seminario:1996:CIFa

[Sem96a] J. M. Seminario. Calculation of intramolecular force fields from second-derivative tensors. *International Journal of Quantum Chemistry*, 60(7):59–??, 1996. CODEN IJQCB2.

Seminario:1996:CIFc

[Sem96b] J. M. Seminario. Calculation of intramolecular force fields from second-derivative tensors. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):59–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Seminario:1996:CIFb

[Sem96c] Jorge M. Seminario. Calculation of intramolecular force fields from second-derivative tensors. *International Journal of Quantum Chemistry*, 60(7):1271–1277, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60738.

Senent:1996:SPI

[Sen96] M. L. Senent. Symmetry properties of inversion-bending Hamiltonian of dimethyl-amine. *International Journal of Quantum Chemistry*, 58(4):399–406, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60496.

Sorensen:1993:QFT

[SES93] T. E. Sorensen, W. B. England, and D. M. Silver. Quantum field theoretical methods in chemically bonded systems. V. potential energy curves for N_2 (xsup 1 sigmasub gsup +)arrr 2N(sup 4 S sup *). *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:467–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Schork:1994:CEE

[SF94] T. Schork and P. Fulde. Calculating excitations energies with the help of cumulants. *International Journal of Quantum Chemistry*, 51(3):113–??, July 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Savin:1995:DFY

[SF95a] A. Savin and H. J. Flad. Density functionals for the Yukawa electron-electron interaction. *International Journal of Quantum Chemistry*, 56(4):327–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schlegel:1995:TBC

[SF95b] H. B. Schlegel and M. J. Frisch. Transformation between Cartesian and pure spherical harmonic Gaussians. *International Journal of Quantum Chemistry*, 54(2):83–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Steiner:1996:RCA

[SF96] Erich Steiner and Patrick W. Fowler. Ring currents in aromatic hydrocarbons. *International Journal of Quantum Chemistry*, 60(1):609–617, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60623.

Sjovoll:1998:SOC

[SFG+98] Merethe Sjøvoll, Hilde Fagerli, Odd Gropen, Jan Almlöf, Jeppe Olsen, and Trygve U. Helgaker. Spin-orbit and correlation effects in platinum hydride (PtH). *International Journal of Quantum Chemistry*, 68(1):53–64, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29922; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29922&PLACEBO=IE.pdf.

Swang:1996:CHO

[SFGW96] Ole Swang, Knut Faegri Jr., Odd Gropen, and Ulf Wahlgren. Chemisorption of hydrogen and oxygen atoms on a cobalt surface: A quantum chemical cluster model study. *International Journal of Quantum Chemistry*, 57(1):105–111, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60349.

Soirat:1994:ARD

[SFM94] A. Soirat, M. Flocco, and L. Massa. Approximately N-representable density functional density matrices. *International Journal of Quantum Chemistry*, 49(3):291–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shim:1993:ESN

[SG93] I. Shim and K. A. Gingerich. Electronic states and nature of bonding in the molecule YN by all-electron ab initio CASSCF calculations. *International Journal of Quantum Chemistry*, 46 (1):145–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shrivastava:1994:MEC

[SG94] I. H. Shrivastava and S. R. Gadre. Molecular electrostatic charge models: A topographical approach. *International Journal of Quantum Chemistry*, 49(4):397–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sosa:1996:ESPa

[SG96a] R. M. Sosa and P. Gardiol. Electronic structure and properties of MCO and M_5CO carbonyls (M = Fe, Ni, Cu) by density functional methods. *International Journal of Quantum Chemistry*, 60(7):217–??, 1996. CODEN IJQCB2.

Sosa:1996:ESPc

[SG96b] R. M. Sosa and P. Gardiol. Electronic structure and properties of MCO and M_5CO carbonyls (M = Fe, Ni, Cu) by density functional methods. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):217–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Sosa:1996:ESPb

[SG96c] Ramon M. Sosa and Patricia Gardiol. Electronic structure and properties of MCO and M_5CO carbonyls (M = Fe, Ni, Cu) by density functional methods. *International Journal of Quantum Chemistry*, 60(7):1429–1441, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60702.

Sosa:1997:ESP

[SG97] Ramon M. Sosa and Patricia Gardiol. Electronic structure and properties of the carbonyls TiCO, and Ti_7CO and carbenes $TiCH_2$ and Ti_7CH_2 by density functional methods. *International Journal of Quantum Chemistry*, 65 (1):65–73, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42742; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42742&PLACEBO=IE.pdf.

Sergeev:1998:SSC

[SG98] Alexei V. Sergeev and David Z. Goodson. Semiclassical self-consistent field perturbation theory for the hydrogen atom in a magnetic field. *International Journal of Quantum Chemistry*, 69(2):183–192, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29981; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29981&PLACEBO=IE.pdf.

Sosa:1997:TSE

[SGB97] Ramón M. Sosa, Patricia Gardiol, and Gerardo Beltrame. A theoretical study of the electronic structure of transition-element carbides MnC (M = Fe, Ni, Cu, $n = 1, 5$; and M = Ti, $n = 1, 7$) and their interactions with an O atom by DFT methods. *International Journal of Quantum Chemistry*, 65(5):919–928, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42823; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42823&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Sosa:1998:TST

[SGB98] Ramón M. Sosa, Patricia Gardiol, and Gerardo Beltrame. Theoretical study of transition-element carbonyls MCO and carbenes MCH_2 (M = Ti, Fe, Ni) in the ground and first electronic excited states by DFT methods. *International Journal of Quantum Chemistry*, 69(3):371–386, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29992; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29992&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Schurer:1999:APV

[SGGC99] Gudrun Schürer, Peter Gedeck, Maik Gottschalk, and Timothy Clark. Accurate parametrized variational calculations of the molecular electronic polarizability by NDDO-based methods. *International Journal of Quantum Chemistry*, 75 (1):17–31, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63003146; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63003146&PLACEBO=IE.pdf.

Smeyers:1996:SMO

[SGGMGFS96] Yves G. Smeyers, A. González-Guerra, J. Martín-González, and P. Fernández-Serra. A study of the molecular orbital localization into an extended Hartree–Fock approach: Application to the BeH_2 ground state. *International Journal of Quantum Chemistry*, 60(1):493–504, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60612.

Sen:1995:ALE

[SGK+95] K. D. Sen, T. V. Gayatri, R. Krishnaveni, M. Kakkar, H. Toufar, G. O. A. Janssens, B. G. Baekelandt, R. A. Schoonheydt, and W. J. Mortier. Average local electrostatic potential and the core-valency separation in atoms. *International Journal of Quantum Chemistry*, 56(4):399–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sarma:1999:GAC

[SGK99] C. R. Sarma, Dipan K. Ghosh, and C. Y. Kadolkar. Graphical approach to correlations in high-spin systems. *International Journal of Quantum Chemistry*, 73(5):389–393, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61004337; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61004337&PLACEBO=IE.pdf.

Stanton:1992:AIP

[SGW+92] J. F. Stanton, J. Gauss, J. D. Watts, W. J. Lauderdale, and R. J. Bartlett. The ACES II program system. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:879–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Sahni:1990:QMI

[SH90a] V. Sahni and M. K. Harbola. Quantum-mechanical interpretation of the local many-body potential of density-functional theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:569–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Steinborn:1990:MTQ

[SH90b] E. O. Steinborn and H. H. H. Homeier. Möbius-type quadrature of electron repulsion integrals with B functions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:349–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Sham:1995:SEB

[Sha95] L. J. Sham. Some efforts beyond the local density approximation. *International Journal of Quantum Chemistry*, 56(4): 345–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schramm:1996:ETSc

[SHB+96a] V. L. Schramm, B. A. Horenstein, C. K. Bagdassarian, S. D. Schwartz, P. J. Berti, K. A. Rising, J. Scheuring, P. C. Kline, D. W. Parkin, and D. J. Merkler. Enzymatic transition states and inhibitor design from principles of classical and quantum chemistry. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 23 (??):81–??, ???? 1996. CODEN IJQBDZ. ISSN 0360-8832.

Schramm:1996:ETSb

[SHB+96b] Vern L. Schramm, Benjamin A. Horenstein, Carey K. Bagdassarian, Steven D. Schwartz, Paul J. Berti, Kathleen A. Rising, Johannes Scheuring, Paul C. Kline, David W. Parkin, and David J. Merkler. Enzymatic transition states and inhibitor design from principles of classical and quantum chemistry. *International Journal of Quantum Chemistry*, 60(8):1805–1813, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60752`.

Schramm:1996:ETSa

[SHBS96] V. L. Schramm, B. A. Horenstein, C. K. Bagdassarian, and S. D. Schwartz. Enzymatic transition states and inhibitor design from principles of classical and quantum chemistry. *International Journal of Quantum Chemistry*, 60(8):81–??, 1996. CODEN IJQCB2.

Soscun:1998:ISM

[SHC+98] Humberto Soscún, Javier Hernández, Olga Castellano, Gilberto Díaz, and Alan Hinchliffe. Ab initio SCF-MO study of the topology of the charge distribution of acid sites of zeolites. *International Journal of Quantum Chemistry*, 70(4-5):951–960, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75073; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75073&PLACEBO=IE.pdf.

Scharnagl:1994:PRP

[SHF94] C. Scharnagl, J. Hettenkofer, and S. F. Fischer. Proton release pathway in bacteriorhodopsin: Molecular dynamics and electrostatic calculations. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21:33–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Shuto:1996:QHN

[Shu96] Yoshito Shuto. Quadratic hyperpolarizabilities of nitro-substituted pseudo-linear dye molecules with ethylenic and azo bridges. *International Journal of Quantum Chemistry*, 58(4):407–418, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60487.

Siedentop:1993:FOC

[Sie93] H. Siedentop. First-order corrections to sums of zeroth and first power of absolute values of negative eigenvalues of Schrödinger operators with potentials with Coulomb singularity in the semi-classical limit. *International Journal of Quantum Chemistry*, 46(3):383–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sebasdiyar:1993:EPB

[SIM93a] I. Sebasdiyar, K. Iyakutti, and M. Mahendran. Effect of positive background on the ground-state energy of a Wigner lattice. *International Journal of Quantum Chemistry*, 47(3):177–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Simons:1993:FTS

[Sim93b] J. Simons. Finding transition states when second-order Jahn–Teller instability occurs. *International Journal of Quantum Chemistry*, 48(3):211–??, November 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Simos:1995:PCP

[Sim95] T. E. Simos. Predictor-corrector phase-fitted methods for $Y^{11} = F(X, Y)$ and an application to the Schrödinger equation. *International Journal of Quantum Chemistry*, 53(5):473–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Simos:1997:NNT

[Sim97] T. E. Simos. New Numerov-type methods for computing eigenvalues, resonances, and phase shifts of the radial Schrödinger equation. *International Journal of Quantum Chemistry*, 62 (5):467–475, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42534; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42534&PLACEBO=IE.pdf.

Simos:1998:EOM

[Sim98] T. E. Simos. Eighth-order method for accurate computations for the elastic scattering phase-shift problem. *International Journal of Quantum Chemistry*, 68(3):191–200, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29939; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29939&PLACEBO=IE.pdf.

Simonson:1999:DRP

[Sim99a] Thomas Simonson. Dielectric relaxation in proteins: Microscopic and macroscopic models. *International Journal of Quantum Chemistry*, 73(1):45–57, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL

http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55001580; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55001580&PLACEBO=IE.pdf.

Simonson:1999:EDR

[Sim99b] Thomas Simonson. Erratum: Dielectric relaxation in proteins: Microscopic and macroscopic models. *International Journal of Quantum Chemistry*, 75(3):331, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000674/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000674&PLACEBO=IE.pdf.

Simos:1999:HAO

[Sim99c] T. E. Simos. High algebraic order explicit methods with reduced phase-lag for an efficient solution of the Schrödinger equation. *International Journal of Quantum Chemistry*, 73(6):479–496, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61007365; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61007365&PLACEBO=IE.pdf.

Sinanoglu:1992:NME

[Sin92] O. Sinanoglu. Nonorthogonality and the MO energy level patterns of molecules deduced directly from structural formulas by the new VIF method as compared with machine computations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:137–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Sironi:1999:NPO

[Sir99] M. Sironi. A new procedure to optimize core orbitals in the spin-coupled wave function. *International Journal of Quantum Chemistry*, 74(2):145–151, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003360; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003360&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt.* Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Szalewicz:1991:NCT

[SJ91] Krzysztof Szalewicz and Bogumił Jeziorski. Nonadiabatic calculations for $td\mu$ relevant for muon catalyzed fusion. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:671–686, 1991. CODEN IJQSDI. ISSN 0161-3642.

Soudackov:1997:EHC

[SJ97] Alexander V. Soudackov and Karl Jug. Effective Hamiltonian-crystal field on the INDO level: Calculations of d-d spectra of some iron (II) compounds. *International Journal of Quantum Chemistry*, 62(4):403–418, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42527; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42527&PLACEBO=IE.pdf`.

Szalewicz:1991:PTC

[SJR91] K. Szalewicz, B. Jeziorski, and S. Rybak. Perturbation theory calculations of intermolecular interaction energies. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:23–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Saha:1999:LES

[SK99a] Bidhan C. Saha and Anil Kumar. Low-energy single-electron capture cross sections in C^{6+}/C^{4+}-Na(3s) and N^{7+}/N^{5+}-Na(3s) collisions: Molecular state approach. *International Journal of Quantum Chemistry*, 75(4–5):385–398, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004938/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004938&PLACEBO=IE.pdf`.

Sergeev:1999:CNC

[SK99b] Alexei V. Sergeev and Sabre Kais. Critical nuclear charges for N-electron atoms. *International Journal of Quantum Chemistry*, 75(4–5):533–542, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004948/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004948&PLACEBO=IE.pdf`.

Seybold:1999:ABS

[SKC99] Paul G. Seybold, Lemont B. Kier, and Chao-Kun Cheng. Aurora borealis: Stochastic cellular automata simulations of the excited-state dynamics of oxygen atoms. *International Journal of Quantum Chemistry*, 75(4–5):751–756, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004971/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004971&PLACEBO=IE.pdf.

Sak:1998:QCM

[SKJ98] Katrin Sak, Mati Karelson, and Jaak Järv. Quantum chemical modelling of the effect of proline residues on peptide conformation. *International Journal of Quantum Chemistry*, 66(5):391–396, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29873; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29873&PLACEBO=IE.pdf.

Skolnick:1999:NPQ

[SKM99] Jeffrey Skolnick, Andrzej Kolinski, and Debasisa Mohanty. De novo predictions of the quaternary structure of leucine zippers and other coiled coils. *International Journal of Quantum Chemistry*, 75(3):165–176, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000658/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000658&PLACEBO=IE.pdf.

Santamaria:1995:TDAa

[SKN95a] R. Santamaria, I. G. Kaplan, and O. Novaro. On the test of different atomic exchange functionals. *International Journal of Quantum Chemistry*, 56(4):307–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Santamaria:1995:TDAb

[SKN95b] R. Santamaria, I. G. Kaplan, and O. Novaro. On the test of different atomic exchange functionals. *International Journal of Quantum Chemistry*, 56(4):421–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sokalski:1990:CAM

[SKRK90] W. A. Sokalski, P. B. Keegstra, S. Roszak, and J. J. Kaufman. Cumulative atomic multiple moments for molecular crystals from ab-initio crystal orbital wave functions and for molecules in excited states from ab-initio MRD-CI wave functions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:51–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Surjan:1998:NPM

[SKS98] Péter R. Surján, Mihály Kállay, and Ágnes Szabados. Nonconventional partitioning of the many-body Hamiltonian for studying correlation effects. *International Journal of Quantum Chemistry*, 70(4-5):571–581, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75035; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75035&PLACEBO=IE.pdf`.

Sakuma:1997:IMS

[SKTN97] Toshihiro Sakuma, Hiroshi Kashiwagi, Toshikazu Takada, and Haruki Nakamura. Ab initio MO study of the chlorophyll dimer in the photosynthetic reaction center. I. A theoretical treatment of the electrostatic field created by the surrounding proteins. *International Journal of Quantum Chemistry*, 61(1):137–151, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42379; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42379&PLACEBO=IE.pdf`.

Sheka:1996:CMA

[SKZ96] E. F. Sheka, V. D. Khavryutchenko, and V. A. Zayetz. Computer modeling of assembly of atoms in an electric field. *International Journal of Quantum Chemistry*, 57(4):741–755, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60413`.

Sana:1993:ESL

[SL93] M. Sana and G. Leroy. Early stages of LiX, BeH_2X, and BH_3X pyrolysis (X stands for NH_3 or OH_2): A theoretical study of weak dative complex stability. *International Journal of*

Quantum Chemistry, 48(2):89–??, October 15, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stashans:1997:SCW

[SL97] Arvids Stashans and Sten Lunell. Semiempirical calculations on WO_3 and M_xWO_3 crystals (M = H, Li, Na). *International Journal of Quantum Chemistry*, 63(3):729–735, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42616; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42616&PLACEBO=IE.pdf.

Subramanian:1998:TGE

[SL98] Hamsa Subramanian and Jolanta B. Lagowski. Trends in geometric and electronic properties of thiophene- and cyclopentadiene-based polymers. *International Journal of Quantum Chemistry*, 66(3):229–240, January 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29856; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29856&PLACEBO=IE.pdf.

Slater:1967:CSS

[Sla67a] J. C. Slater. The current state of solid-state and molecular theory. *International Journal of Quantum Chemistry*, 1(??):37–??, ?? 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slater:1967:QPA

[Sla67b] J. C. Slater. Quantum physics in America between the wars. *International Journal of Quantum Chemistry*, 1S(??):1–??, ?? 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slater:1970:NSP

[Sla70a] J. C. Slater. Note on the space part of antisymmetric wavefunctions. *International Journal of Quantum Chemistry*, 6(??):561–??, ?? 1970. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slater:1970:SCF

[Sla70b] J. C. Slater. The self-consistent field for crystals. *International Journal of Quantum Chemistry*, 3S(??):727–?? (or 158–??), ?? 1970. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slater:1971:TEA

[Sla71] J. C. Slater. Treatment of exchange in atomic, molecular, and solid-state theory. *International Journal of Quantum Chemistry*, 5(??):403–??, ?? 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slanina:1997:CCC

[SLA97] Zdeněk Slanina, Shyi-Long Lee, and Ludwik Adamowicz. C_{80}, C_{86}, C_{88}: Semiempirical and ab initio SCF calculations. *International Journal of Quantum Chemistry*, 63(2): 529–535, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42596; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42596&PLACEBO=IE.pdf`.

Stener:1995:ALD

[SLD95] M. Stener, A. Lisini, and P. Decleva. Accurate local density photoionization cross sections by LCAO Stieltjes imaging approach. *International Journal of Quantum Chemistry*, 53(2): 229–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Suarez:1996:ISE

[SLG+96] D. Suárez, R. López, J. González, T. L. Sordo, and J. A. Sordo. Ab initio study of the effect of CH···O hydrogen bonding on the *exo/endo* stereoselectivity of Diels–Alder reactions of 2-substituted-1,3-dienes with sulfur dioxide. *International Journal of Quantum Chemistry*, 57(3):493–499, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60388`.

Sokalski:1991:ISE

[SLL+91] W. A. Sokalski, J. Lai, N. Luo, S. Sun, M. Shibata, R. Ornstein, and R. Rein. Ab initio study of the electrostatic multiple nature of torsional potentials in CHsub 3 SSCHsub 3, CHsub 3 SSH, and HOOH. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:61–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Smith:1970:IAS

[SLM70] D. W. Smith, E. G. Larson, and R. C. Morrison. On the interpretative aspects of second-order reduced density matrices. *International Journal of Quantum Chemistry*, 3S(??):689–??, ?? 1970. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sagues:1994:DGS

[SLTMR94] F. Sagues, L. Lopez-Tomas, J. Mach, and R. Reigada. Disordered grown systems: Generation and fractal analysis electrodeposition. *International Journal of Quantum Chemistry*, 52(2):375–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Solmajer:1992:MSE

[SM92] T. Solmajer and E. L. Mehler. Modeling solvent effects in molecular dynamics simulations of proteins. *International Journal of Quantum Chemistry*, 44(2):291–??, September 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Santhosh:1994:EPE

[SM94] C. Santhosh and P. C. Mishra. Electrostatic potential and electric field mapping of some sweeteners of the suosan series: A search for the structure-activity relationship. *International Journal of Quantum Chemistry*, 51(4 (or 5??)):335–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Styszynski:1995:ECR

[SM95] J. Styszynski and G. L. Malli. Electron correlation and relativistic effects in xenon tetrafluoride. *International Journal of Quantum Chemistry*, 55(3):227–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sakaki:1996:TSC

[SM96a] Shigeyoshi Sakaki and Yasuo Musashi. A theoretical study on CO_2 insertion into an M — H bond (M = Rh and Cu).

International Journal of Quantum Chemistry, 57(3):481–491, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60387`.

Sarkar:1996:FIG

[SM96b] Jayanta Sarkar and Asok K. Mukherjee. Factorization of interaction graphs with n-fold symmetry: Some applications in PPP calculation and molecular vibrational analysis. *International Journal of Quantum Chemistry*, 60(4):825–832, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60655`.

Schirmer:1996:SCA

[SM96c] J. Schirmer and F. Mertins. Size consistency of an algebraic propagator approach. *International Journal of Quantum Chemistry*, 58(4):329–339, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60489`.

Santhosh:1998:UMA

[SM98] C. Santhosh and P. C. Mishra. Use of molecular analogs for the bases in DNA: Stability of molecular pairs in gas phase and aqueous media and possible role of hydrogen bonding. *International Journal of Quantum Chemistry*, 68(5):351–355, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29954`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29954&PLACEBO=IE.pdf`.

Salam:1999:NOR

[SM99] A. Salam and D. A. Micha. Nonlinear optical response of metal surfaces with adsorbed molecules. *International Journal of Quantum Chemistry*, 75(4–5):429–439, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004941/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004941&PLACEBO=IE.pdf`.

Smit:1999:MIP

[Smi99] Michael J. Smit. Multicenter integrals over polarization potential operators. *International Journal of Quantum Chemistry*, 73(5):403–416, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61004331; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61004331&PLACEBO=IE.pdf.

Scolfaro:1990:ITS

[SMM+90] L. M. R. Scolfaro, C. A. C. Mendonca, E. A. Menezes, J. M. V. Martins, and J. R. Leite. Interband transitions of Sidelta-doped layers in p-Type GaAs. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:447–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Sola:1996:UIQ

[SMO+96] Miquel Solà, Jordi Mestres, Josep M. Oliva, Miquel Duran, and Ramon Carbó. The use of ab initio quantum molecular self-similarity measures to analyze electronic charge density distributions. *International Journal of Quantum Chemistry*, 58(4):361–372, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60492.

Simons:1990:SWP

[SN90] J. Simons and J. Nichols. Strategies for walking on potential energy surfaces using local quadratic approximations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:263–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Shershakov:1998:CWF

[SN98] Dmitry A. Shershakov and Vladimir V. Nechaev. Correlated wave-function theory for many-center many-electron problems. *International Journal of Quantum Chemistry*, 69 (5):639–648, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30028; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30028&PLACEBO=IE.pdf.

Saito:1999:CNR

[SN99] Yoshihiro Saito and Masataka Nagaoka. Characteristics of numerical realization via stochastic partial differential equation: An application to density matrix calculation. *International Journal of Quantum Chemistry*, 74(6):653–660, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001782`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001782&PLACEBO=IE.pdf`. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Suzumura:1999:GSP

[SNH99] Toshihisa Suzumura, Takahito Nakajima, and Kimihiko Hirao. Ground-state properties of MH, MCl, and M_2 (M = Cu, Ag, and Au) calculated by a scalar relativistic density functional theory. *International Journal of Quantum Chemistry*, 75(4–5):757–766, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004972/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004972&PLACEBO=IE.pdf`.

Schwarz:1997:IMD

[SNMB97] K. Schwarz, E. Nusterer, P. Margl, and P. E. Blöchl. Ab initio molecular dynamics calculations to study catalysis. *International Journal of Quantum Chemistry*, 61(3):369–380, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42421`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42421&PLACEBO=IE.pdf`.

Shigeta:1999:DFT

[SNNY99] Y. Shigeta, H. Nagao, K. Nishikawa, and K. Yamaguchi. Density functional theory without the Born–Oppenheimer approximation. II. Green function techniques. *International Journal of Quantum Chemistry*, 75(4–5):875–883, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.`

com/cgi-bin/abstract/66004983/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004983&PLACEBO=IE.pdf.

Sauer:1994:CPP

[SO94] S. P. A. Sauer and J. Oddershede. Correlated polarization propagator calculations of static polarizabilities. *International Journal of Quantum Chemistry*, 50(5):317–??, May 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sundholm:1997:RMH

[SO97] Dage Sundholm and Edgar Ottschofski. Relativistic multiconfiguration Hartree–Fock by means of direct perturbation theory. *International Journal of Quantum Chemistry*, 65(2):151–158, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42752; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42752&PLACEBO=IE.pdf.

Shigeta:1998:NMT

[SOK+98] Y. Shigeta, Y. Ozaki, K. Kodama, H. Nagao, H. Kawabe, and K. Nishikawa. Nonadiabatic molecular theory and its application. II. Water molecule. *International Journal of Quantum Chemistry*, 69(5):629–637, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30027; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30027&PLACEBO=IE.pdf.

Sandoval:1990:OCM

[SP90] L. Sandoval and A. Palma. One-center matrix elements for the Morse oscillator. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:481–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Seel:1991:CIS

[SP91] Max Seel and Ravindra Pandey. Comparative ab initio study of electronic and ionic properties of lithium and ionic properties of lithium nitride (li_3 N), lithium phosphide (li_3 P), and lithium arsenide (li_3 as). *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:461–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Seminario:1992:GDF

[SP92] J. M. Seminario and P. Politzer. Gaussian-2 and density functional studies of H_2N — NO_2 dissociation, inversion, and isomerization. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:497–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Strnad:1994:NAM

[SP94] M. Strnad and R. Ponec. Novel approach to molecular similarity: Second-order similarity indices from geminal expansion of pair densities. *International Journal of Quantum Chemistry*, 49 (1):35–??, January 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schmidt:1996:DDW

[SPC96] Marius Schmidt, Fritz Parak, and Giorgina Corongiu. Density distributions in the water shell of myoglobin. *International Journal of Quantum Chemistry*, 59(4):263–269, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60546`.

Sperber:1971:ARDa

[Spe71a] G. Sperber. Analysis of reduced density matrices in the coordinate representation. I. definitions and basic formulas. *International Journal of Quantum Chemistry*, 5(??):177–??, ?? 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sperber:1971:ARDb

[Spe71b] G. Sperber. Analysis of reduced density matrices in the coordinate representation. II. the structure of closed-shell atoms in the restricted Hartree–Fock approximation. *International Journal of Quantum Chemistry*, 5(??):189–??, ?? 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sperber:1972:ARD

[Spe72a] G. Sperber. Analysis of reduced density matrices in the coordinate representation. III. electron density and correlation in the ground states of H_2 and the H_6 ring system within some approximations of the simple LCAO type. *International Journal of Quantum Chemistry*, 6(??):881–??, ?? 1972. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sperber:1972:CDM

[Spe72b] G. R. Sperber. The computation of density matrix values in configuration space. *International Journal of Quantum Chemistry*, 6(??):795–797, ?? 1972. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Seifert:1996:CMC

[SPF96] G. Seifert, D. Porezag, and Th. Frauenheim. Calculations of molecules, clusters, and solids with a simplified LCAO-DFT-LDA scheme. *International Journal of Quantum Chemistry*, 58(2):185–192, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60474`.

Scolfaro:1993:ESI

[SPFL93] L. M. R. Scolfaro, R. Pintanel, A. Fazzio, and J. R. Leite. Electronic states induced by a Ga vacancy in the $GaAs_{1-x}P_x$ alloy. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:213–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Shah:1997:ABC

[SPG97] Rajiv Shah, M. C. Payne, and J. D. Gale. Acid-base catalysis in zeolites from first principles. *International Journal of Quantum Chemistry*, 61(3):393–398, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42433; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42433&PLACEBO=IE.pdf`.

Safouhi:1998:EEI

[SPH98] H. Safouhi, D. Pinchon, and P. E. Hoggan. Efficient evaluation of integrals for density functional theory: Nonlinear D transformations to evaluate three-center nuclear attraction integrals over B functions. *International Journal of Quantum Chemistry*, 70(1):181–188, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74362; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74362&PLACEBO=IE.pdf`. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Surjan:1997:TOM

[SPL97] Péter R. Surján, C. Pérez Del Valle, and Luis Lain. Third-order many-body perturbation theory for intermolecular interactions. I. Hartree–Fock level. *International Journal of Quantum Chemistry*, 64(1):43–51, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42664; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42664&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Seminario:1996:RETb

[SPM+96] Jorge M. Seminario, Peter Politzer, Humberto J. Soscun M., Angélica G. Zacarías, and Miguel Castro. Reaction energetics of tetrahedrane and other hydrocarbons: Ab initio and density functional treatments. *International Journal of Quantum Chemistry*, 60(7):1351–1360, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60693.

Sanchez-Portal:1997:DFM

[SPOAS97] Daniel Sánchez-Portal, Pablo Ordejón, Emilio Artacho, and José M. Soler. Density-functional method for very large systems with LCAO basis sets. *International Journal of Quantum Chemistry*, 65(5):453–461, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42834; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42834&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Springborg:1993:SDF

[Spr93] M. Springborg. Some density-functional LMTO studies of electronic properties of quasi-one-dimensional systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:227–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Sutjianto:1994:SSB

[SPR94] A. Sutjianto, R. Pandey, and J. M. Recio. Structure and stability of BN microclusters: Ab initio calculations for $(BN)_n$, $(n = 2 - 4)$. *International Journal of Quantum Chemistry*, 52 (1):199–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Springborg:1996:TMB

[Spr96] Michael Springborg. Transfer matrices, band structures, and localized orbitals in quasi-one-dimensional systems. *International Journal of Quantum Chemistry*, 58(6):717–731, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60512`.

Scherbinin:1996:UME

[SPS96a] Andrei V. Scherbinin, Vladimir I. Pupyshev, and Nikolai F. Stepanov. On the use of multipole expansion of the Coulomb potential in quantum chemistry. *International Journal of Quantum Chemistry*, 60(4):843–852, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60657`.

Seong:1996:ISN

[SPS96b] Jeonghee Seong, Jong Keun Park, and Hosung Sun. Ab initio study on NH^+: Transition dipole moments, transition probabilities, and radiative lifetimes. *International Journal of Quantum Chemistry*, 57(1):79–87, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60359`.

Seminario:1996:RETc

[SPSMZ96] J. M. Seminario, P. Politzer, H. J. Soscun-M., and A. G. Zacarias. Reaction energetics of tetrahedrane and other hydrocarbons: Ab initio and density functional treatments. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):139–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Seminario:1996:RETa

[SPSZ96] J. M. Seminario, P. Politzer, H. J. M. Soscun, and A. G. Zacarias. Reaction energetics of tetrahedrane and other hydrocarbons: Ab initio and density functional treatments. *International Journal of Quantum Chemistry*, 60(7):139–??, 1996. CODEN IJQCB2.

Seminario:1996:MDF

[SPT96] J. H. Seminario, P. Politzer, and S. B. Trickey. Modern density functional theory — A tool for chemistry, vol 2 in the series "Theoretical and Computational Chemistry". *International Journal of Quantum Chemistry*, 59(3):259–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sierraalta:1996:LED

[SR96] Anibal Sierraalta and Fernando Ruette. The Laplacian of the electronic density at the valence-shell charge concentration (VSCC): A comparative study of effective core potential and full-electron calculations in Mo compounds. II. *International Journal of Quantum Chemistry*, 60(5):1015–1026, December 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60674.

Sinha:1999:WMQ

[SR99] Anjana Sinha and Rajkumar Roychoudhury. WKB and MAF quantization rules for spatially confined quantum mechanical systems. *International Journal of Quantum Chemistry*, 73(6):497–504, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61007366; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61007366&PLACEBO=IE.pdf.

Srivastava:1997:IQH

[Sri97] Vipin Srivastava. Integer quantum Hall effect on Abacus. *International Journal of Quantum Chemistry*, 63(1):99–104, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42556; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42556&PLACEBO=IE.pdf.

Sierraalta:1998:TED

[SRM98] Anibal Sierraalta, Fernando Ruette, and Erick Machado. Topology of electronic densities taken from parametric methods: A predictive tool? *International Journal of Quantum Chemistry*, 70(1):113–123, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74356; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74356&PLACEBO=IE.pdf`. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Sanz:1998:TMA

[SRP+98] Javier Fernández Sanz, Hasssan Rabaâ, Flor M. Poveda, Antonio M. Márquez, and Carmen J. Calzado. Theoretical models for γ-Al_2O_3 (110) surface hydroxylation: An ab initio embedded cluster study. *International Journal of Quantum Chemistry*, 70(2):359–365, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75004; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75004&PLACEBO=IE.pdf`. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Shelver:1992:MCB

[SRS92] W. L. Shelver, H. Rosenberg, and W. H. Shelver. Molecular conformation of bilirubin from semiempirical molecular orbital calculations. *International Journal of Quantum Chemistry*, 44 (2):141–??, September 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schatz:1996:QMC

[SRW96a] G. C. Schatz, M. A. Ratner, and K. B. Whaley. Quantum mechanics in chemistry. *International Journal of Quantum Chemistry*, 57(6):1131–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schwarz:1996:URE

[SRW96b] W. H. E. Schwarz, A. Rutkowski, and S. G. Wang. Understanding relativistic effects of chemical bonding. *International Journal of Quantum Chemistry*, 57(4):641–653, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60401`.

Slamet:1991:ADG

[SS91] Marlina Slamet and Viraht Sahni. Analysis of the density-gradient-expansion approximation for the exchange-correlation energy of density-functional theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:235–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Samuel:1992:SPI

[SS92a] J. Samuel and K. D. Sen. Static polarizabilities for the Ne-Isoelectronic series using Harbola–Sahni potential. *International Journal of Quantum Chemistry*, 44(6):1041–??, December 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shivaglal:1992:EHB

[SS92b] M. C. Shivaglal and S. Singh. Effect of hydrogen bonding and cooperativity on stretching force constants of formamide. *International Journal of Quantum Chemistry*, 44(5):679–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slamet:1992:GEA

[SS92c] M. Slamet and V. Sahni. The gradient expansion approximation for exchange: A physical perspective. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:333–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Solomatin:1995:EPM

[SS95] A. Solomatin and V. Sahni. Exchange potentials at a metal surface. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:31–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Silverman:1996:MTO

[SS96] M. P. Silverman and E. Sjoqvist. More than one mystery: Explorations in quantum interference. *International Journal of Quantum Chemistry*, 58(5):535–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Solem:1997:EQC

[SS97a] Johndale C. Solem and Maurice G. Sheppard. Experimental quantum chemistry at ultrahigh magnetic fields: Some opportunities. *International Journal of Quantum Chemistry*, 64

(5):619–628, September 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42711; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42711&PLACEBO=IE.pdf. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

Solomatin:1997:SCK

[SS97b] Alexander Solomatin and Viraht Sahni. Structure of the correlation-kinetic component of the Kohn–Sham exchange potential in atoms and at metal surfaces. *International Journal of Quantum Chemistry*, 65(5):893–906, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42821; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42821&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Surjan:1998:DCO

[SS98] Péter R. Surján and Ágnes Szabados. Dyson-corrected orbital energies for the perturbative treatment of electron correlation. *International Journal of Quantum Chemistry*, 69 (6):713–719, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74988; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74988&PLACEBO=IE.pdf.

Sahni:1999:ECK

[SS99a] Viraht Sahni and Marlina Slamet. Electron correlations in Kohn–Sham exchange-only theory. *International Journal of Quantum Chemistry*, 71(6):473–480, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=15000345; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=15000345&PLACEBO=IE.pdf.

Seto:1999:AIH

[SS99b] Rikuzo Seto and Ivan V. Stankevich. On an application of the intermediate Hamiltonian method for molecular systems. *International Journal of Quantum Chemistry*, 72 (2):101–107, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002777; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002777&PLACEBO=IE.pdf.

Singh:1996:ACS

[SSD96] Harjinder Singh, N. Sukumar, and B. M. Deb. "atom" as a complex system: One- and two-dimensional cellular automata simulations. *International Journal of Quantum Chemistry*, 60(1):21–28, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60581.

Sadykova:1992:MSS

[SSK+92] A. Yu. Sadykova, A. S. Saykaeva, A. V. Kostochko, A. N. Glebov, and V. G. Moozyukov. Magnetic susceptibility of some derivatives of cellulose and their mixtures: Theory and experiment. *International Journal of Quantum Chemistry*, 44(6): 935–??, December 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Smeyers:1990:DSS

[SSM90] Y. G. Smeyers, M. L. Senent, and D. C. Moule. Dynamic and spectroscopic studies of nonrigid molecules: Application to the thioacetone electronic ground state. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:835–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Sonavane:1999:PIC

[SSM+99] Uddhavesh B. Sonavane, Kailas D. Sonawane, Annie Morin, Henri Grosjean, and Ravindra Tewari. N(7)-protonation induced conformational flipping in hypermodified nucleic acid bases N^6-(N-threonylcarbonyl)adenine and its 2-methylthio- or N(6)-methyl-derivatives. *International Journal of Quantum Chemistry*, 75(3):223–229, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000664/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000664&PLACEBO=IE.pdf.

Shinoda:1993:ACH

[SSMK93] H. Shinoda, M. Sayama, M. A. Mori, and H. Kozuka. AM1 calculation of hydration to aldehyde group in nitro-substituted benzaldehydes. *International Journal of Quantum Chemistry*, 45(1):97–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Silva:1999:PCG

[SSN99] Clarissa O. Da Silva, Edilson C. Da Silva, and M. A. Chaer Nascimento. Pseudospectral calculation of the gas-phase acidities of aliphatic alcohols. *International Journal of Quantum Chemistry*, 74(4):417–422, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62502085; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62502085&PLACEBO=IE.pdf.

Sato:1997:DND

[SSO+97] Fumitoshi Sato, Yasuhiro Shigemitsu, Isao Okazaki, Shuuichi Yahiro, Masahiro Fukue, Shingo Kozuru, and Hiroshi Kashiwagi. Development of a new density functional program for all-electron calculation of proteins. *International Journal of Quantum Chemistry*, 63(1):245–256, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42570; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42570&PLACEBO=IE.pdf.

Schmiedekamp-Schneeweis:1998:IHB

[SSP98] Lumelle A. Schmiedekamp-Schneeweis and Judy Ozment Payne. Intramolecular hydrogen bonding in resonance-stabilized systems. *International Journal of Quantum Chemistry*, 70(4-5):863–875, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75064; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75064&PLACEBO=IE.pdf.

Shinoda:1993:ESD

[SST93] T. Shinoda, N. Shima, and M. Tsukada. Electronic structure of DNA dimer-units, d(AA) $\cdots$ d(TT), d$(TA)_2$, d$(AT)_2$, in A and B conformations by DV-Xα cluster calculations. *International*

Journal of Quantum Chemistry, 47(1):59–84, July 5, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shinoda:1994:ESD

[SST94] T. Shinoda, N. Shima, and M. Tsukada. Electronic structure of DNA dimer units, d(AG)cdot d(CT),d(TG)cdot d(CA), d(AC)cdot d(GT), and d(TC)cdot d(GA), in A and B conformations by DV-Xalpha cluster calculations. *International Journal of Quantum Chemistry*, 49(6):849–??, March 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Siregar:1993:LLE

[ST93] R. E. Siregar and M. O. Tjia. The low-lying excitation energies of polyenes investigated with a chain-length-dependent screened potential. *International Journal of Quantum Chemistry*, 48(4): 267–??, November 10, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Simos:1996:VSA

[ST96a] T. E. Simos and G. Tougelidis. A variable-step algorithm for computing eigenvalues of the radial Schrödinger equation. *International Journal of Quantum Chemistry*, 59(6):477–485, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60566`.

Stepanov:1996:DAP

[ST96b] A. V. Stepanov and V. L. Tavgin. Development of the activation process model: Compensation effect. *International Journal of Quantum Chemistry*, 59(1):7–14, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60523`.

Seminario:1997:SSLb

[ST97] Jorge M. Seminario and James M. Tour. Systematic study of the lowest energy states of Au_n ($n = 1--4$) using DFT. *International Journal of Quantum Chemistry*, 65(5): 749–758, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42808;`

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42808&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Stanton:1993:AMB

[Sta93] J. F. Stanton. Applied many-body methods in spectroscopy and electronic structure. edited by D. Mukherjee. *International Journal of Quantum Chemistry*, 45(4):401–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Starikov:1995:TDC

[Sta95] E. B. Starikov. Three-dimensional crystal orbital calculations on mononucleotide crystallohydrates. II. diprotonated mononucleotides. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22 (??):145–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Starikov:1996:ICO

[Sta96a] E. B. Starikov. Ab initio crystal orbital calculations on three-dimensional crystals of large bioorganic molecules and polymers. *International Journal of Quantum Chemistry*, 57(5):851–860, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60439.

Starikov:1996:TDC

[Sta96b] E. B. Starikov. Three-dimensional crystal orbital calculations on mononucleotide crystallohydrates. I. Sodium mononucleotide crystallohydrates. *International Journal of Quantum Chemistry*, 58(5):497–515, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60504.

Starikov:1997:PCC

[Sta97] E. B. Starikov. Polyiodide chains in crystalline organic iodides: Ab initio Hartree–Fock crystal orbital study. *International Journal of Quantum Chemistry*, 64(4):473–479, September 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.

interscience.wiley.com/cgi-bin/abstract?ID=42705; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42705&PLACEBO=IE.pdf.

Starikov:1998:IHF

[Sta98a] E. B. Starikov. Ab initio Hartree–Fock crystal orbital studies on charge-transfer complexes: Different crystal modifications of the same compounds. *International Journal of Quantum Chemistry*, 66(1):69–89, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29839; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29839&PLACEBO=IE.pdf.

Starikov:1998:CTD

[Sta98b] E. B. Starikov. A comparative three-dimensional Hartree–Fock crystal orbital study of double-stack organic charge-transfer (semi)conductors: TTF-TCNQ, TTF-DCNQI, and TTF-2,5-Me_2-DCNQI. *International Journal of Quantum Chemistry*, 66(1):47–68, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29838; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29838&PLACEBO=IE.pdf.

Starikov:1998:CAE

[Sta98c] E. B. Starikov. Could alkaline-earth-intercalated fullerites actually be semimetals? *International Journal of Quantum Chemistry*, 69(2):201–208, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29983; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29983&PLACEBO=IE.pdf.

Starikov:1998:TDC

[Sta98d] E. B. Starikov. Three-dimensional crystal-orbital calculations on crystallohydrates of mononucleotide salts. III. Valence-split basis sets. *International Journal of Quantum Chemistry*, 69 (2):209–217, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29984; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29984&PLACEBO=IE.pdf.

Starikov:1998:TDH

[Sta98e] E. B. Starikov. Three-dimensional Hartree–Fock crystal-orbital calculations on conducting polymers: *trans*-polyacetylene and polythiophene. *International Journal of Quantum Chemistry*, 68(6):421–429, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29960; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29960&PLACEBO=IE.pdf.

Su:1996:HLA

[STC96] Yu-Nung Su, Ming-Sung Tsai, and San-Yan Chu. H^+, Li^+, and Na^+ affinity study of N_2, P_2, and their isoelectronic species. *International Journal of Quantum Chemistry*, 59(6):487–493, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60567.

Stewart:1996:ALM

[Ste96] James J. P. Stewart. Application of localized molecular orbitals to the solution of semiempirical self-consistent field equations. *International Journal of Quantum Chemistry*, 58(2):133–146, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60469.

Sakuma:1990:IMC

[STKN90] T. Sakuma, T. Takada, H. Kashiwagi, and H. Nakamura. Ab initio MO calculations of the chlorophyll dimer in the photosynthetic reaction center. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17:93–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Soudackov:1996:CFS

[STM96a] A. V. Soudackov, A. L. Tchougreeff, and I. A. Misurkin. Crystal-field splittings and optical spectra of transition-metal mixed-ligand complexes by effective Hamiltonian method. *International Journal of Quantum Chemistry*, 57(4):663–671, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60403.

Soudackov:1996:GSM

[STM96b] A. V. Soudackov, A. L. Tchougréeff, and I. A. Misurkin. Ground-state multiplicities and *d*-*d* excitations of transition-metal complexes by effective Hamiltonian method. *International Journal of Quantum Chemistry*, 58(2):161–173, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60472`.

Sicilia:1997:DFI

[STMR97] Emilia Sicilia, Marirosa Toscano, Tzonka Mineva, and Nino Russo. Density functional investigation of the molecular geometries, harmonic vibrational frequencies, singlet-triplet energy separations, adiabatic ionization potentials, and electron affinities of XY_2 (X = Si, Ge, Sn; Y = F, Cl) systems. *International Journal of Quantum Chemistry*, 61(3): 571–577, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42428; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42428&PLACEBO=IE.pdf`.

Strich:1993:QHC

[Str93] A. Strich. *Quanta: a Handbook of Concepts*, second edition, by P. W. Atkins. *International Journal of Quantum Chemistry*, 47 (3):239–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sherer:1995:IPE

[STS95] E. C. Sherer, G. M. Turner, and G. C. Shields. Investigation of the potential energy surface for the first step in the alkaline hydrolysis of methyl acetate. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):83–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Shigeta:1998:DFT

[STY+98] Y. Shigeta, H. Takahashi, S. Yamanaka, M. Mitani, H. Nagao, and K. Yamaguchi. Density functional theory without the Born–Oppenheimer approximation and its application. *International Journal of Quantum Chemistry*, 70(4-

5):659–669, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75044; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75044&PLACEBO=IE.pdf.

Stavrev:1996:CTMa

[STZ96a] K. K. Stavrev, T. Tamm, and M. C. Zerner. Comparison of theoretical models of solvation. *International Journal of Quantum Chemistry*, 60(7):373–??, 1996. CODEN IJQCB2.

Stavrev:1996:CTMc

[STZ96b] K. K. Stavrev, T. Tamm, and M. C. Zerner. Comparison of theoretical models of solvation. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):373–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Stavrev:1996:CTMb

[STZ96c] Krassimir K. Stavrev, Toomas Tamm, and Michael C. Zerner. Comparison of theoretical models of solvation. *International Journal of Quantum Chemistry*, 60(7):1585–1594, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60719.

Su:1993:PTD

[Su93] M.-D. Su. Perturbation theory to determine the stable isomer of triatomic linear molecules. *International Journal of Quantum Chemistry*, 48(4):249–??, November 10, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Suhai:1993:TOM

[Suh93] S. Suhai. Third-order Møller–Plesset perturbation theory of electron correlation in infinite systems: A comparison of carbon- and silicon-based polymers. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:131–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Suhai:1994:CEC

[Suh94] S. Suhai. Cooperativity and electron correlation effects on hydrogen bonding in infinite systems. *International Journal of Quantum Chemistry*, 52(2):395–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sukumar:1994:DFT

[Suk94] N. Sukumar. Density functional theory for Jahn–Teller systems. *International Journal of Quantum Chemistry*, 52(4):809–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sukumar:1995:DFT

[Suk95] N. Sukumar. Density functional theory of Born couplings: Consequences for electron flow in Jahn–Teller molecules and superconductors. *International Journal of Quantum Chemistry*, 56 (5):423–432, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sullivan:1997:MSV

[Sul97] N. S. Sullivan. Molecular spectroscopy at very high magnetic fields. *International Journal of Quantum Chemistry*, 64 (5):629–633, September 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42712; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42712&PLACEBO=IE.pdf`. Special Issue: *The Properties of Molecules in Strong Magnetic Fields*.

Surjan:1994:ICB

[Sur94] P. R. Surjan. The interaction of chemical bonds. III. perturbed strictly localized geminals in LMO basis. *International Journal of Quantum Chemistry*, 52(2):563–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Surjan:1995:ICB

[Sur95] P. R. Surjan. The interaction of chemical bonds. IV. interbond charge transfer by a coupled-cluster-type formalism. *International Journal of Quantum Chemistry*, 55(2):109–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Surjan:1997:CVS

[Sur97] Péter R. Surján. Charge vs spin density waves in the fullerene polymer. *International Journal of Quantum Chemistry*, 63 (2):425–435, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42586;`

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42586&PLACEBO=IE.pdf.

Sutcliffe:1996:DIC

[Sut96] Brian T. Sutcliffe. The development of the idea of a chemical bond. *International Journal of Quantum Chemistry*, 58(6): 645–655, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60518.

Sutcliffe:1999:BOC

[Sut99a] Brian T. Sutcliffe. The Born–Oppenheimer correction terms for a triatomic system in the Sutcliffe–Tennyson formulation. *International Journal of Quantum Chemistry*, 74(2): 109–121, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003357; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003357&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Sutcliffe:1999:DMS

[Sut99b] Brian T. Sutcliffe. Dipole moment surfaces and spectroscopic calculations. *International Journal of Quantum Chemistry*, 74(6):681–695, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001785; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001785&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Suzuki:1999:SME

[Suz99] Yoshi-Ichi Suzuki. Structure of molecular energy levels of homonuclear diatomic molecules. *International Journal of Quantum Chemistry*, 72(6):597–604, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=50000017; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=50000017&PLACEBO=IE.pdf.

Svendsen:1995:GEE

[Sv95] P. S. Svendsen and U. von Barth. On the gradient expansion of the exchange energy within linear response theory and beyond. *International Journal of Quantum Chemistry*, 56(4):351–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slater:1971:SET

[SW71] J. C. Slater and J. H. Wood. Statistical exchange and the total energy of A crystal. *International Journal of Quantum Chemistry*, 4(??):3–??, ?? 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Suba:1997:SSB

[SW97] S. Sˇuba and M. A. Whitehead. Spontaneous symmetry breaking and electron correlation. *International Journal of Quantum Chemistry*, 65(1):9–17, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42737; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42737&PLACEBO=IE.pdf.

Sein:1999:AFC

[SWD+99] Lawrence T. Sein, Jr., Yen Wei, Thanh Duong, Mark D. Kemmerer, and Susan A. Jansen. Anomalous failure of configuration interaction — Singles (CIS) method in the computation of the electronic states of N,$N\prime$-bis(4$\prime$-aminophenyl)-1, 4-quinonenediimine. *International Journal of Quantum Chemistry*, 75(4–5):623–629, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004958/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004958&PLACEBO=IE.pdf.

Saenz:1993:CIO

[SWF93] A. Saenz, W. Weyrich, and P. Froelich. A configuration-interaction-oriented implementation of the complex coordinate method. *International Journal of Quantum Chemistry*, 46(3):365–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shelley:1990:SSD

[SWK90] J. Shelley, K. Watanabe, and M. L. Klein. Simulation of a sodium dodecylsulfate micelle in aqueous solution. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17:103–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Schwalm:1994:TIE

[SWMB94] O. Schwalm, J. Weber, B. Minder, and A. Baiker. Theoretical investigation of the enantioselective hydrogenation of α-ketoesters over Pt/alumina modified with cinchonidine. *International Journal of Quantum Chemistry*, 52(1):191–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schierbaum:1996:ESI

[SX96] K. D. Schierbaum and Wei-Xing Xu. The electronic structure of intrinsic defects at TiO_2 (110) surfaces: An ab initio molecular orbital study. *International Journal of Quantum Chemistry*, 57(6):1121–1129, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60447`.

Scheiner:1991:EPT

[SY91] S. Scheiner and W. O. Yu. Effect of proton transfer on neighboring hydrogen-bond strength. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:37–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Sagan:1996:WPG

[SYZ96] Bruce E. Sagan, Yeong-Nan Yeh, and Ping Zhang. The Wiener polynomial of a graph. *International Journal of Quantum Chemistry*, 60(5):959–969, December 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60668`.

Stavrev:1995:AIS

[SZ95] K. K. Stavrev and M. C. Zerner. Absorption and ionization spectra of model rubredoxins. *International Journal of*

Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology., 22(??):155–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Schreckenbach:1996:CNS

[SZ96] Georg Schreckenbach and Tom Ziegler. The calculation of NMR shielding tensors based on density functional theory and the frozen-core approximation. *International Journal of Quantum Chemistry*, 60(3):753–766, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60642`.

Schreckenbach:1997:CNS

[SZ97a] Georg Schreckenbach and Tom Ziegler. Calculation of NMR shielding tensors based on density functional theory and a scalar relativistic Pauli-type Hamiltonian. the application to transition metal complexes. *International Journal of Quantum Chemistry*, 61(6):899–918, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42474`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42474&PLACEBO=IE.pdf`.

Stavrev:1997:SAH

[SZ97b] Krassimir K. Stavrev and Michael C. Zerner. Spin-averaged Hartree–Fock procedure for spectroscopic calculations: The absorption spectrum of Mn^{2+} in ZnS crystals. *International Journal of Quantum Chemistry*, 65(5):877–884, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42819`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42819&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Stavrev:1998:SHS

[SZ98] Krassimir K. Stavrev and Michael C. Zerner. Studies on the hydrogenation steps of the nitrogen molecule at the *Azotobacter vinelandii* nitrogenase site. *International Journal of Quantum Chemistry*, 70(6):1159–1168, ???? 1998. CODEN

IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75083; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75083&PLACEBO=IE.pdf.

Szalay:1995:AED

[Sza95] P. G. Szalay. Analytic energy derivatives for coupled-cluster methods describing excited states: General formulas and comparison of computational costs. *International Journal of Quantum Chemistry*, 55(2):151–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Seminario:1997:SSLa

[SZC97] Jorge M. Seminario, Angélica G. Zacarías, and Miguel Castro. Systematic study of the lowest energy states of Pd, Pd_2, and Pd_3. *International Journal of Quantum Chemistry*, 61(3):515–523, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42420; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42420&PLACEBO=IE.pdf.

Slanina:1999:BAF

[SZCO99] Zdeněk Slanina, Xiang Zhao, Long Y. Chiang, and Eiji Ōsawa. Biologically active fullerene derivatives: Computations of structures, energetics, and vibrations of C_{60} $(OH)_x$ and $C_{60}(NO_2)_y$. *International Journal of Quantum Chemistry*, 74(3):343–349, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62004764; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62004764&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly*.

Schreckenbach:1995:IAE

[SZL95] G. Schreckenbach, T. Ziegler, and J. Li. The implementation of analytical energy gradients based on a quasi-relativistic density functional method: The application to metal carbonyls. *International Journal of Quantum Chemistry*, 56(5):477–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tachibana:1994:WAC

[Tac94] A. Tachibana. Wannier analysis of the Cooper pairing force. *International Journal of Quantum Chemistry*, 49(5):625–??, February 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tachibana:1996:NFA

[Tac96] Akitomo Tachibana. New formulation of the analytical electronic energy and the regional density functional theory. *International Journal of Quantum Chemistry*, 57(3):423–428, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60379`.

Talman:1993:MSC

[Tal93] J. D. Talman. Molecular SCF calculations using a basis of numerical orbitals. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:321–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Taseli:1993:ACE

[Tas93] H. Taseli. Accurate computation of the energy spectrum for potentials with multiminima. *International Journal of Quantum Chemistry*, 46(2):319–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Taseli:1996:ALU

[Taş96a] H. Taşeli. Accurate lower and upper bounds of the energy spectrum for the asymmetrical two-well potentials. *International Journal of Quantum Chemistry*, 60(2):641–648, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60631`.

Taseli:1996:ESS

[Taş96b] H. Taşeli. On the exact solution of the Schrödinger equation with a quartic anharmonicity. *International Journal of Quantum Chemistry*, 57(1):63–71, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60357`.

Taseli:1997:MLB

[Taş97] H. Taşeli. Modified Laguerre basis for hydrogen-like systems. *International Journal of Quantum Chemistry*, 63 (5):949–959, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42645; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42645&PLACEBO=IE.pdf`.

Tanaka:1997:BAC

[TAY+97] Kazuyoshi Tanaka, Hiroki Ago, Tokio Yamabe, Kenji Okahara, and Mayumi Okada. Bond alternation in carbon nanotubes including σ-electrons. *International Journal of Quantum Chemistry*, 63(3):637–644?, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42625; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42625&PLACEBO=IE.pdf`.

Tobisch:1995:TSO

[TB95] S. Tobisch and H. Boegel. Theoretical studies of organonickel compounds. I. A density functional and ab initio HF study. *International Journal of Quantum Chemistry*, 56(5):575–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tasso:1997:PPV

[TBBE97] Silvina Tasso, Luis Bruno-Blanch, and Guillermina L. Estiú. Pharmacophoric pattern in valpromide derivatives. *International Journal of Quantum Chemistry*, 65(6):1107–1114, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42847; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42847&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on the Application of Fundamental Theory to Problems of Biology and Pharmocolgy.* Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Tasso:1998:OLA

[TBBE98] S. M. Tasso, L. Bruno-Blanch, and G. L. Estiú. On the origin of the lack of anticonvulsant activity of some valpromide derivatives. *International Journal of Quantum Chemistry*, 70(6):1127–1136, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75080; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75080&PLACEBO=IE.pdf.

Takahashi:1995:PEG

[TBČP95] M. Takahashi, P. Bracken, J. Čížek, and J. Paldus. Perturbation expansion of the ground-state energy for the one-dimensional cyclic Hubbard system in the Hückel limit. *International Journal of Quantum Chemistry*, 53(5):457–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Trindle:1999:MVS

[TBP99] Carl Trindle, Mark Braiman, and Amy Beth Prager. Modeling vibrational spectra of amino acid side chains in proteins: Effects of chloride and bromide counterions on ethylguanidino vibrational frequencies. *International Journal of Quantum Chemistry*, 74(3):291–297, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62004759; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62004759&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly*.

Tran:1990:DSW

[TBW90] P. X. Tran, D. W. Brenner, and C. T. White. Dynamics of solitary waves induced by shock impulses in a linear atomic chain. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:549–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Telnov:1998:GFT

[TC98a] Dmitry A. Telnov and Shih-I Chu. Generalized Floquet theoretical formulation of time-dependent density functional theory for many-electron systems in multicolor laser fields. *International Journal of Quantum Chemistry*, 69 (3):305–315, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30004;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30004&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Thorsteinsson:1998:MVB

[TC98b] Thorstein Thorsteinsson and David L. Cooper. Modern valence bond descriptions of molecular excited states: An application of CASVB. *International Journal of Quantum Chemistry*, 70(4-5):637–650, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75042; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75042&PLACEBO=IE.pdf.

Tong:1998:TDD

[TC98c] Xiao-Min Tong and Shih-I Chu. Time-dependent density-functional theory with optimized effective potential and self-interaction correction: Application to the study of coherent control of multiple high-order harmonic generation of He atoms in mixed laser fields. *International Journal of Quantum Chemistry*, 69(3):293–303, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30003; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30003&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Terstegen:1999:IPP

[TCB99] Frank Terstegen, Emily A. Carter, and Volker Buss. Interconversion pathways of the protonatedβ-ionone Schiff base: An ab initio molecular dynamics study. *International Journal of Quantum Chemistry*, 75(3):141–145, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000656/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000656&PLACEBO=IE.pdf.

Tchougreeff:1996:QMMb

[Tch96a] A. L. Tchougréeff. Quantum mechanical models for organometallic reactivity. *International Journal of Quantum Chemistry*,

58(1):67–84, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60465.

Tchougreeff:1996:QMMa

[Tch96b] A. L. Tchougréeff. Quantum mechanical models in catalysis. *International Journal of Quantum Chemistry*, 57(3):413–422, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60378.

Tretiak:1998:EES

[TCM98] Sergei Tretiak, Vladimir Chernyak, and Shaul Mukamel. Excited electronic states of carotenoids: Time-dependent density-matrix-response algorithm. *International Journal of Quantum Chemistry*, 70(4-5):711–727, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75049; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75049&PLACEBO=IE.pdf.

Tomasi:1999:MEP

[TCM99] Jacopo Tomasi, Roberto Cammi, and Benedetta Mennucci. Medium effects on the properties of chemical systems: An overview of recent formulations in the polarizable continuum model (PCM). *International Journal of Quantum Chemistry*, 75(4–5):783–803, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004974/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004974&PLACEBO=IE.pdf.

Thomson:1991:TSS

[TCZ91] C. Thomson, M. Cory, and M. Zerner. Theoretical studies of some new anti-malarial drugs. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:231–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Tchougreeff:1996:LRO

[TD96a] A. L. Tchougréeff and M. B. Darkhovskii. Lattice relaxation and order in the low-spin to high-spin transitions in molecular crystals. *International Journal of Quantum Chemistry*, 57(5):903–912, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60428`.

Trindle:1996:MOS

[TD96b] Carl Trindle and Sambhu Nath Datta. Molecular orbital studies on the spin states of nitroxide species: Bis- and trisnitroxymetaphenylene, 1,1-bisnitroxyphenylethylene, and 4,6-Dimethoxy-1,3-dialkylnitroxybenzenes. *International Journal of Quantum Chemistry*, 57(4):781–799, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60417`.

Tang:1999:HES

[TD99] Karen E. S. Tang and Ken A. Dill. How experiments see fluctuations of native proteins: Perspective from an exact model. *International Journal of Quantum Chemistry*, 75(3):147–164, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/65000657/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000657&PLACEBO=IE.pdf`.

Tyutyulkov:1994:BGA

[TDK+94] N. Tyutyulkov, F. Dietz, D. J. Klein, W. A. Seitz, and T. G. Schmalz. The band gap of alternant 1D π-electron systems. *International Journal of Quantum Chemistry*, 51(3):173–??, July 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tyutyulkov:1997:AMI

[TDO97] N. Tyutyulkov, F. Dietz, and G. Olbrich. On alternant molecules with identical energy spectra: Isospectral molecules. *International Journal of Quantum Chemistry*, 62(2):167–169, March 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42499`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42499&PLACEBO=IE.pdf`.

Taseli:1996:ETD

[TE96] H. Taşeli and R. Eid. Eigenvalues of the two-dimensional Schrödinger equation with nonseparable potentials. *International Journal of Quantum Chemistry*, 59(3):183–201, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60538.

Termath:1997:DFI

[Ter97] Volker Termath. Diagonalization free implementation of Kohn–Sham equations with localized basis sets. *International Journal of Quantum Chemistry*, 61(2):349–353, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42399; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42399&PLACEBO=IE.pdf.

Teter:1993:DFT

[Tet93] M. P. Teter. Density-functional theory in glass chemistry. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:155–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Tewari:1994:PIC

[Tew94] R. Tewari. Protonation-induced conformational flipping in hypermodified nucleic acid base N^6-(*N*-glycylcarbonyl) adenine. *International Journal of Quantum Chemistry*, 51(2):105–??, July 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tewari:1997:IPO

[Tew97] Ravindra Tewari. Influence of N(1) protonation on the orientation of the N(6) substituent in hypermodified nucleic acid base N^6-(*N*-glycylcarbonyl) adenine. *International Journal of Quantum Chemistry*, 62(5):551–556, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42532; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42532&PLACEBO=IE.pdf.

Thorsteinsson:1999:SCI

[TFR99] T. Thorsteinsson, A. Famulari, and M. Raimondi. A spin-coupled investigation of the electrophilic addition of hydrochloric acid to ethylene. *International Journal of Quantum Chemistry*, 74(2):231–239, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003367; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003367&PLACEBO=IE.pdf`. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Teng:1995:TPS

[TFSZ95] Q. Teng, J. Feng, C. Sun, and M. C. Zerner. Theoretical predictions of the structures and electronic spectra of $C_{60}NH_2^+$ with comparisons with the isoelectronic molecules $C_{60}O$ and $C_{60}CH_2$. *International Journal of Quantum Chemistry*, 55(1): 35–??, July 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Theophilou:1995:DFT

[TG95] A. K. Theophilou and N. I. Gidopoulos. Density functional theory for excited states. *International Journal of Quantum Chemistry*, 56(4):333–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tolpygo:1996:ESH

[TG96] Kiril B. Tolpygo and Helen A. Grebneva. Effect of the state of $h-b-1$ hydrogen bond on the character of some atom vibrations in guanine-cytosine pair of the DNA molecule. *International Journal of Quantum Chemistry*, 57(2):219–227, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60370`.

Torrent:1997:MVD

[TGDS97] M. Torrent, P. Gili, M. Duran, and M. Solà. Molybdenum (VI) dioxodihalides: Agreement with experiment and prediction of unknown properties through density functional theory. *International Journal of Quantum Chemistry*, 61(3): 405–414, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42435; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42435&PLACEBO=IE.pdf`.

Tanaka:1999:CBM

[TGS99] Kiyoshi Tanaka, Tapas K. Ghosh, and Takeo Sakai. CSF-based multireference coupled-pair approximation. IV. Revision of coupling term and application to Rydberg-valence avoided crossing in lowest two $^1\Sigma^+$ excited states of FH molecule and lowest two $^3\Pi_g$ states of F_2 molecule. *International Journal of Quantum Chemistry*, 74(6):661–668, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001783; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001783&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Tal:1990:MSG

[TH90] Y. Tal and J. Herzfeld. Multicenter spherical Gaussian expansion of molecular orbital wavefunctions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24: 701–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Tang:1997:ESI

[TH97] Au Chin Tang and Fu Qiang Huang. Electronic structure of icosahedral fullerenes. *International Journal of Quantum Chemistry*, 63(2):367–371, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42608; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42608&PLACEBO=IE.pdf.

Theilhaber:1994:DMM

[The94] J. Theilhaber. Dynamics of metallic and molecular hydrogen through density-functional simulations. *International Journal of Quantum Chemistry. Symposium*, 28:611–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Theophilou:1997:DFT

[The97] Andreas K. Theophilou. Density functional theory for excited states and special symmetries. *International Journal of Quantum Chemistry*, 61(2):333–340, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL

http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42397; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42397&PLACEBO=IE.pdf.

Theophilou:1998:RFK

[The98] Andreas K. Theophilou. Rigorous formulation of a Kohn and Sham theory for states with special symmetries. *International Journal of Quantum Chemistry*, 69(4):461–467, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30019; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30019&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Thompson:1996:MDS

[Tho96] Mark A. Thompson. Molecular dynamics study of a new rigidified 18-crown-6 derivative using a QM/MM method. *International Journal of Quantum Chemistry*, 60(6):1133–1141, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60679.

Thulstrup:1969:ALE

[Thu69] E. W. Thulstrup. Assignment of the lowest electronic transitions in benzene, C_6H_6. *International Journal of Quantum Chemistry*, 3S(??):641–??, ?? 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Thulstrup:1975:SIF

[Thu75] P. W. Thulstrup. Smooth interpolation, Fourier transformation, and two-center overlap integrals for numerical atomic orbitals. *International Journal of Quantum Chemistry*, 9(??):789–795, ?? 1975. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tokiwa:1994:OSH

[TI94] H. Tokiwa and H. Ichikawa. Origin of steric hindrance in ethane. *International Journal of Quantum Chemistry*, 50(2):109–??, April 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Thiagarajan:1996:ESA

[TIPM96] M. Thiagarajan, K. Iyakutti, E. Palaniyandi, and M. Mahendran. Electronic structure of Al, P, S, and Cl impurities in silicon. *International Journal of Quantum Chemistry*, 58(4):383–388, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60494.

Titov:1993:VPT

[Tit93] A. V. Titov. Variational principle for transition matrix. *International Journal of Quantum Chemistry*, 45(1):71–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Titov:1996:TSM

[Tit96] A. V. Titov. A two-step method of calculation of the electronic structure of molecules with heavy atoms: Theoretical aspect. *International Journal of Quantum Chemistry*, 57(3):453–463, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60383.

Teunissen:1995:LBS

[TJ95] E. H. Teunissen and A. J. Jansen. Large basis sets and geometry optimizations in embedded cluster calculations. *International Journal of Quantum Chemistry*, 54(1):73–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tanaka:1997:ESC

[TJ97] Kiyoshi Tanaka and Helge Johansen. On the electronic structure of $Cu(H_2O)_6{}^{2+}$. *International Journal of Quantum Chemistry*, 64(4):453–458, September 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42703; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42703&PLACEBO=IE.pdf.

Thakkar:1992:AAM

[TK92] A. J. Thakkar and T. Koga. Analytic approximations to the momentum moments of neutral atoms. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:291–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Tolic:1990:PSB

[TKK+90] Lj. P. Tolic, B. Kovac, L. Klasinc, S. M. Shevchenko, and S. P. McGlynn. Photoelectron spectroscopy of biologically active molecules 20. para-quinones, semiquinones, and aromatic ketones. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:799–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Thakkar:1992:CSC

[TKMA92] A. J. Thakkar, T. Koga, H. Matsuyama, and E. F. Archibong. Constrained self-consistent-field wave functions with improved long-range behavior. *International Journal of Quantum Chemistry*, 44(6):985–??, December 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tachibana:1996:DFT

[TKNI96] Akitomo Tachibana, Susumu Kawauchi, Koichi Nakamura, and Hideyuki Inaba. Density functional theory of chemical reactivity indices in some ion-molecule reaction systems. *International Journal of Quantum Chemistry*, 57(4):673–682, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60404`.

Thakkar:1993:DQZ

[TKSH93] A. J. Thakkar, T. Koga, M. Saito, and R. E. Hoffmeyer. Double and quadruple zeta contracted Gaussian basis sets for hydrogen through neon. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:343–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Thulstrup:1979:BCI

[TL79] P. W. Thulstrup and J. Linderberg. Bounds to Coulomb interaction integrals. *International Journal of Quantum Chemistry*, S13(??):39–50, ?? 1979. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tang:1998:VNS

[TL98] Au Chin Tang and An Yong Li. Vibration and NMR spectra of dihedral fullerenes. *International Journal of Quantum Chemistry*, 68(3):211–217, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29941;`

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29941&PLACEBO=IE.pdf.

Tang:1998:VSI

[TLC98] Au Chin Tang, Qian Shu Li, and Wei Cheng. Vibrational spectra of icosahedral (I_h and I) fullerenes. *International Journal of Quantum Chemistry*, 66(2):113–117, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29844; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29844&PLACEBO=IE.pdf.

Theophilou:1993:OCD

[TM93] A. K. Theophilou and N. H. March. Optimally convergent determinantal expansion of many-electron wave functions. *International Journal of Quantum Chemistry*, 46(6):735–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Titov:1999:GRE

[TM99] A. V. Titov and N. S. Mosyagin. Generalized relativistic effective core potential: Theoretical grounds. *International Journal of Quantum Chemistry*, 71(5):359–401, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10050249; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10050249&PLACEBO=IE.pdf.

Tapia:1997:QET

[TMA97] O. Tapia, V. Moliner, and J. Andrés. A quantum electronic theory of chemical processes — The inverted energy profile case: $CH_3^+ + H_2$ reaction. *International Journal of Quantum Chemistry*, 63(2):373–391, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42609; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42609&PLACEBO=IE.pdf.

Tong:1996:ACBa

[TMD96a] W. Tong, R. C. Morrison, and O. W. Day. Analysis of chemical bonding in C_2 using Dyson orbitals. *International Journal of Quantum Chemistry*, 60(7):411–??, 1996. CODEN IJQCB2.

Tong:1996:ACBc

[TMD96b] W. Tong, R. C. Morrison, and O. W. Day, Jr. Analysis of chemical bonding in C_2 using Dyson orbitals. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30 (??):411–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Tong:1996:ACBb

[TMD96c] Wei Tong, Robert C. Morrison, and Orville W. Day Jr. Analysis of chemical bonding in C_2 using Dyson orbitals. *International Journal of Quantum Chemistry*, 60(7):1623–1631, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60723`.

Tyutyulkov:1998:OPI

[TMDB98] N. Tyutyulkov, G. Madjarova, F. Dietz, and M. Baumgarten. Organic polymers with indirect magnetic interaction caused by the symmetry of the elementary units. *International Journal of Quantum Chemistry*, 66(6):425–434, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29878`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29878&PLACEBO=IE.pdf`.

Trinajstic:1994:NNS

[TMH94] N. Trinajstić, Z. Mihalić, and F. E. Harris. A note on the number of spanning trees in buckminsterfullerene. *International Journal of Quantum Chemistry. Symposium*, 28:525–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Tenan:1997:TRF

[TMM97] Mário A. Tenan, Marcus V. Mesquita, and Ricardo A. Mosna. The transient regime in Frohlich's condensation phenomenon in biosystems. *International Journal of Quantum Chemistry*, 62(4):363–372, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42523`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42523&PLACEBO=IE.pdf`.

Tawa:1997:RFS

[TMP97] Gregory J. Tawa, Richard L. Martin, and Lawrence R. Pratt. Reaction field spectral shifts with semiempirical molecular orbital theory. *International Journal of Quantum Chemistry*, 64(2):143–155, August 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42670; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42670&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Thorndyke:1999:AES

[TMR99] B. Thorndyke, D. A. Micha, and K. Runge. Acceleration effects in slow ion-atom collisions from a first-principles dynamics. *International Journal of Quantum Chemistry*, 75(4–5):361–366, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004996/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004996&PLACEBO=IE.pdf.

Tachikawa:1998:FVM

[TMSI98] Masanori Tachikawa, Kazuhide Mori, Kazunari Suzuki, and Kaoru Iguchi. Full variational molecular orbital method: Application to the positron-molecule complexes. *International Journal of Quantum Chemistry*, 70(3):491–501, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75016; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75016&PLACEBO=IE.pdf.

Tavard:1996:IAR

[TN96] C. Tavard and B. Najjari. Importance of angular and radial electron correlations in first Born (e,2e) spectroscopies of heliumlike targets. *International Journal of Quantum Chemistry*, 60(2):657–665, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60633.

Ten-No:1996:AERa

[TNI96a] S. Ten-No and S. Iwata. On approximating electron repulsion integrals with linear combination of atomic-electron distributions. *International Journal of Quantum Chemistry*, 60(7):107–??, 1996. CODEN IJQCB2.

Ten-No:1996:AERc

[TNI96b] S. Ten-No and S. Iwata. On approximating electron repulsion integrals with linear combination of atomic-electron distributions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):107–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Ten-No:1996:AERb

[TNI96c] Seiichiro Ten-No and Suehiro Iwata. On approximating electron repulsion integrals with linear combination of atomic-electron distributions. *International Journal of Quantum Chemistry*, 60(7):1319–1324, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60689`.

Trinajstic:1997:CMD

[TNM97] N. Trinajstić, S. Nikolić, and Z. Mihalić. On computing the molecular detour matrix. *International Journal of Quantum Chemistry*, 65(5):415–419, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42828`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42828&PLACEBO=IE.pdf`. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Takahashi:1998:QMT

[TNM98] Junko Takahashi, Masataka Nagaoka, and Koichi Masuda. Quantum mechanical treatment for the diffusion process of a hydrogen atom on the amorphous water ice surface. *International Journal of Quantum Chemistry*, 70(2): 379–385, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75007`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75007&PLACEBO=IE.pdf`. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Truong:1996:GCLa

[TNS96a] T. N. Truong, U. N. Nguyen, and E. V. Stefanovich. Generalized conductor-like screening model (GCOSMO) for solvation: An assessment of its accuracy and applicability. *International Journal of Quantum Chemistry*, 60(7):403–??, 1996. CODEN IJQCB2.

Truong:1996:GCLc

[TNS96b] T. N. Truong, U. N. Nguyen, and E. V. Stefanovich. Generalized conductor-like screening model (GCOSMO) for solvation: An assessment of its accuracy and applicability. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):403–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Truong:1996:GCLb

[TNS96c] Thanh N. Truong, Uyen N. Nguyen, and Eugene V. Stefanovich. Generalized conductor-like screening model (GCOSMO) for solvation: An assessment of its accuracy and applicability. *International Journal of Quantum Chemistry*, 60(7):1615–1622, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60722.

Takeuchi:1994:XRS

[TNSE94] H. Takeuchi, M. Nakagawa, T. Saito, and T. Egawa. X-ray scattering by water molecules studied by using synchrotron radiation. *International Journal of Quantum Chemistry*, 52(6):1339–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tachibana:1999:ARD

[TNSM99] Akitomo Tachibana, Koichi Nakamura, Ken Sakata, and Takatoshi Morisaki. Application of the regional density functional theory: The chemical potential inequality in the HeH^+ System. *International Journal of Quantum Chemistry*, 74(6):669–679, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63001784; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63001784&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor* *of George G. Hall (Part II of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Tobias:1999:QTT

[Tob99] Irwin Tobias. Quantum theory of thermal fluctuations in DNA miniplasmids. *International Journal of Quantum Chemistry*, 72(4):357–360, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006312; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006312&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Tomasi:1991:DIM

[Tom91] J. Tomasi. Description and interpretation of molecular phenomena in solution, using effective Hamiltonian operators related to continuous solvent distributions. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:73–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Tossell:1995:UNS

[Tos95] J. A. Tossell. Using NMR shielding calculations to help determine local and midrange order in amorphous materials. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:443–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Thakkar:1990:LDF

[TP90] A. J. Thakkar and W. A. Pedersen. Local density functional approximations and conjectured bounds for momentum moments. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:327–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Taneri:1994:EGT

[TP94] U. Taneri and J. Paldus. Evaluation of group theoretical characteristics using the symbolic manipulation language MAPLE. *International Journal of Quantum Chemistry. Symposium*, 28:139–154, 1994. CODEN IJQSAF. ISSN 0538-821X.

Thompson:1970:MSS

[TPM70] J. Thompson, M. Povich, and B. Musulin. Molecular screening and spectroscopic constants. *International Journal of Quantum Chemistry*, 3S(??):513–??, ?? 1970. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tarroni:1996:LES

[TPR96] Riccardo Tarroni, Paolo Palmieri, and Pavel Rosmus. On the lowest electronic states of the C_2F radical. *International Journal of Quantum Chemistry*, 60(1):467–473, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60609`.

Telezhkin:1994:ITB

[TR94] V. A. Telezhkin and A. A. Rafalovich. Improved tight-binding method. *International Journal of Quantum Chemistry*, 52(5): 1199–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Trickey:1995:MJC

[Tri95] S. B. Trickey. In memoriam: Joseph Callaway, 1931–1994. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:29–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Trickey:1997:BCG

[Tri97] S. B. Trickey. Benchmark comparison of gradient-dependent and local density calculations for bulk silicon and aluminum. *International Journal of Quantum Chemistry*, 61 (4):641–646, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42450; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42450&PLACEBO=IE.pdf`.

Trickey:1998:I

[Tri98a] Sam Trickey. Introduction. *International Journal of Quantum Chemistry*, 69(3):227, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29986;`

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29986&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Trickey:1998:LP

[Tri98b] Sam Trickey. List of Participants. *International Journal of Quantum Chemistry*, 69(3):229–240, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29997; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29997&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part I of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Trindle:1998:PRC

[Tri98c] Carl Trindle. Planarization of 8π rings. I. Confirmation of a speculation by Ermer on the ground state of a strained cyclooctatetraene and studies on analogous oxepins. *International Journal of Quantum Chemistry*, 67(6):367–376, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29917; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29917&PLACEBO=IE.pdf.

Trickey:1999:BR

[Tri99] S. B. Trickey. Book review. *International Journal of Quantum Chemistry*, 72(2):155–156, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002782; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002782&PLACEBO=IE.pdf.

Tkacz-Smiech:1997:MPD

[TSP97] Katarzyna Tkacz-Śmiech and W. S. Ptak. Maximum principles in DFT from reciprocal variational problem. *International Journal of Quantum Chemistry*, 65(5):499–501, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42778;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42778&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Tkacz-Smiech:1996:MPS

[TSPK96] Katarzyna Tkacz-Smiech, Wieslaw S. Ptak, and Andrzej Kolezynski. Model potentials in studies of atomic electron density distribution. *International Journal of Quantum Chemistry*, 57(6):1097–1106, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60453.

Tkacz-Smiech:1997:EDM

[TSPK97] Katarzyna Tkacz-Smiech, Wiesław S. Ptak, and Andrzej Kolezynski. Electron density in metallic crystal as an extremal with moving boundaries. *International Journal of Quantum Chemistry*, 62(5):543–549, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42531; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42531&PLACEBO=IE.pdf.

Tkacz-Smiech:1994:FDP

[TSPKM94] K. Tkacz-Smiech, W. S. Ptak, A. Kolezynski, and J. Mrugalski. Functional derivative E/p in calculation of chemical potential for the Kohn–Sham electronic system. *International Journal of Quantum Chemistry*, 51(6):569–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Theologitis:1999:PSH

[TSRP99] M. Theologitis, G. C. Screttas, S. G. Raptis, and M. G. Papadopoulos. The polarizability and the second hyperpolarizability of tetrakis(phenylethynyl)ethene and several of its lithiated derivatives. *International Journal of Quantum Chemistry*, 72(3):177–187, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40003030; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40003030&PLACEBO=IE.pdf.

Turner:1995:CEP

[TSS95] G. M. Turner, E. C. Sherer, and G. C. Shields. A computationally efficient procedure for modeling the first step in the alkaline hydrolysis of esters. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):103–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

Tulub:1997:QFL

[TSS97] Alexander A. Tulub, Evgenii K. Skaletskii, and Vassilii E. Stefanov. Quantum field lability indexes of ligands for predicting some properties of platinum complexes. *International Journal of Quantum Chemistry*, 65(1):49–57, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42740; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42740&PLACEBO=IE.pdf`.

Tang:1999:TSS

[TST+99] Auchin Tang, Zhenfeng Shang, Qiwen Teng, Yinming Pan, Zunsheng Cai, Xuezhuang Zhao, and Jikang Feng. Theoretical study on the structures and electron spectra of C_{60} M_{12} (M = Li, Na, Be). *International Journal of Quantum Chemistry*, 73(6):505–509, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61007367; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61007367&PLACEBO=IE.pdf`.

Takahashi:1999:SSM

[TSY99] Osamu Takahashi, Ko Saito, and Satoshi Yabushita. Simple SCF method with spin-orbit interaction: SOSCF method. *International Journal of Quantum Chemistry*, 74(5):515–530, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62503003; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62503003&PLACEBO=IE.pdf`. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Torii:1998:IHB

[TT98] Hajime Torii and Mitsuo Tasumi. Intermolecular hydrogen bonding and low-wave-number vibrational spectra of formamide, N-methylformamide, and N-methylacetamide in the liquid state. *International Journal of Quantum Chemistry*, 70(2):241–252, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74993; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74993&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Tamm:1999:QMS

[TTK99] Tarmo Tamm, Jüri Tamm, and Mati Karelson. A quantum-mechanical study of oxidized oligopyrroles. *International Journal of Quantum Chemistry*, 71(1):101–109, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000007; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000007&PLACEBO=IE.pdf.

Tachikawa:1999:SOG

[TTM99] Masanori Tachikawa, Kento Taneda, and Kazuhide Mori. Simultaneous optimization of GTF exponents and their centers with fully variational treatment of Hartree–Fock molecular orbital calculation. *International Journal of Quantum Chemistry*, 75(4–5):497–510, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004945/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004945&PLACEBO=IE.pdf.

Tanaka:1993:EPH

[TTOY93] K. Tanaka, A. Takata, M. Okada, and T. Yamabe. Electronic-phase of the Hartree–Fock solution of the infinite one-dimensional system: Structural change in an arbitrarily doped polyacetylene chain. *International Journal of Quantum Chemistry*, 47(5):325–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tully:1991:NMD

[Tul91] John C. Tully. Nonadiabatic molecular dynamics. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:299–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Thiel:1992:EMO

[TV92] W. Thiel and A. A. Voityuk. Extension of MNDO to d orbitals: Parameters and results for the halogens. *International Journal of Quantum Chemistry*, 44(5):807–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tai:1993:RUL

[TVP93] C. C. Tai, S. R. Vatsya, and H. O. Pritchard. Related upper and lower bounds to atomic binding energies. *International Journal of Quantum Chemistry*, 46(6):675–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Teleman:1990:ESR

[TW90] O. Teleman and A. Wallqvist. Ewald summation retards translational motion in molecular dynamics simulation of water. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:245–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Timms:1992:ITL

[TWK+92] D. Timms, A. J. Wilkinson, D. R. Kelly, K. J. Broadley, and R. H. Davies. Interactions of tyrsup 377 in a ligand-activation model of signal transmission through betasub 1-adrenoceptor alpha-helices. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:197–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Takahashi:1998:SSW

[TWK98] Ohgi Takahashi, Masayuki Watanabe, and Osamu Kikuchi. Structure of the T_1-state wave function of linear polyenes. *International Journal of Quantum Chemistry*, 67(2):101–106, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29890`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29890&PLACEBO=IE.pdf`.

Taseli:1997:BBA

[TZ97a] H. Taşeli and A. Zafer. Bessel basis with applications: N-dimensional isotropic polynomial oscillators. *International Journal of Quantum Chemistry*, 63(5):935–947, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42644`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42644&PLACEBO=IE.pdf`.

Taseli:1997:FBE

[TZ97b] H. Taşeli and A. Zafer. A Fourier–Bessel expansion for solving radial Schrödinger equation in two dimensions. *International Journal of Quantum Chemistry*, 61(5):759–768, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42461`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42461&PLACEBO=IE.pdf`.

Teng:1997:TSS

[TZCT97] Qiwen Teng, Xuezhuang Zhao, Zun-Sheng Cai, and Au Chin Tang. Theoretical studies on the structures and electronic spectra of $C_{70}CH_2$. *International Journal of Quantum Chemistry*, 61(5):815–822, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42465`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42465&PLACEBO=IE.pdf`.

Urban:1992:BSQ

[UBA92] M. Urban, R. J. Bartlett, and S. A. Alexander. Basis set quantum chemistry and quantum Monte Carlo: Selected atomic and molecular results. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:271–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Ukrainskii:1994:ECP

[Ukr94] I. I. Ukrainskii. Electron correlations and pairing in low-dimensional systems. *International Journal of Quantum Chemistry*, 52(2):413–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Urry:1994:PPH

[Urr94] D. W. Urry. Postulates for protein (hydrophobic) folding and function. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21: 3–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Ungier:1996:SMT

[US96] W. Ungier and M. Suffczýnski. A simple method of treating integrals containing Hylleraas–Ore molecular functions. *International Journal of Quantum Chemistry*, 60(5):1001–1005, December 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60672.

Ugalde:1997:ESN

[US97] J. M. Ugalde and C. Sarasola. Evaluation of screened nuclear attraction and electron repulsion molecular integrals over Gaussian basis functions. *International Journal of Quantum Chemistry*, 62(3):273–278, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42512; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42512&PLACEBO=IE.pdf.

Urban:1994:AMP

[UWB94] M. Urban, J. D. Watts, and R. J. Bartlett. On the accuracy of molecular properties by coupled-cluster methods for some difficult examples: Oxygen atom, iron atom, and cyano radical. *International Journal of Quantum Chemistry*, 52(1):211–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vergenz:1990:IED

[VA90] R. A. Vergenz and W. H. Adams. Interaction energies of diatomic molecules using partial antisymmetry and Hartree–Fock atomic wave functions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:753–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Valiente:1994:IOE

[VABM94] R. Valiente, J. A. Aramburu, M. T. Barriuso, and M. Moreno. An insight into optical and EPR properties of $AgCl^-$ and AgF^-

complexes through MS-Xα and SCCEH calculations. *International Journal of Quantum Chemistry*, 52(4):1051–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valone:1994:DSG

[Val94] S. M. Valone. A dimensionally scaled generalization of constrained search energy density functionals. *International Journal of Quantum Chemistry*, 49(5):591–??, February 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valdemoro:1996:CCT

[Val96] C. Valdemoro. Contracting and calculating traces over the N-electron space: Two powerful tools for obtaining averages. *International Journal of Quantum Chemistry*, 60(1):131–139, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60575`.

vanWullen:1996:UCE

[Van96] Christoph Van Wüllen. On the use of common effective core potentials in density functional calculations. I. Test calculations on transition-metal carbonyls. *International Journal of Quantum Chemistry*, 58(2):147–152, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60470`.

Visscher:1991:KBC

[VAVN91] L. Visscher, P. J. C. Aerts, O. Visser, and W. C. Nieuwpoort. Kinetic balance in contracted basis sets for relativistic calculations. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:131–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

VanLeeuwen:1994:AND

[VB94] R. Van Leeuwen and E. J. Baerends. An analysis of nonlocal density functionals in chemical bonding. *International Journal of Quantum Chemistry*, 52(4):711–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vigneron:1998:AMG

[VBD+98] Jean-Pol Vigneron, Abboud Benaissa, Isabelle Derycke, Alain Wiame, and R. Sporken. Atomic motion at germanium surfaces: Scanning tunneling microscopy and Monte Carlo simulations. *International Journal of Quantum Chemistry*, 70 (4-5):1093–1097, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75032; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75032&PLACEBO=IE.pdf.

Vieira:1995:DCS

[VBF95] A. Vieira, M. Brajczewska, and C. Fiolhais. Decay of charged stabilized jellium clusters. *International Journal of Quantum Chemistry*, 56(4):239–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

vanOosten:1995:HEL

[vBN95] A. B. van Oosten, R. Broer, and W. C. Nieuwpoort. Heisenberg exchange in La_2CuO_4. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:241–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Vivier-Bunge:1999:TDT

[VBUS99] A. Vivier-Bunge, V. H. Uc, and Y. G. Smeyers. Two-dimensional treatment of the aldehydic carbonyl torsion and hydrogen wagging in gas-phase propanal. *International Journal of Quantum Chemistry*, 72(4):411–420, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006319; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006319&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Vasilyev:1992:CQC

[VBV92] V. V. Vasilyev, A. A. Bliznyuk, and A. A. Voityuk. A combined quantum chemical/molecular mechanical study of hydrogen-bonded systems. *International Journal of Quantum Chemistry*, 44(5):897–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ventura:1992:SSR

[VC92] O. N. Ventura and M. L. Cubas. A semiempirical study of the reaction of the hemimercaptal of methylglyoxal and glutathione at the active center of glyoxalase I. *International Journal of Quantum Chemistry*, 44(5):699–??, November 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vianna:1992:RHF

[VCCM92] R. O. Vianna, R. Custodio, H. Chacham, and J. R. Mohallem. Reliable Hellmann–Feynman forces for nuclei-centered GTO basis of standard size. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:311–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Villaveces:1990:TAC

[VD90] J. L. Villaveces and E. E. C. Daza. On the topological approach to the concept of chemical structure. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:97–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

vanDuijnen:1995:UD

[vd95] P. Th. van Duijnen and A. H. de Vries. Utopia dielectrica. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:523–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Vancampenhout:1996:ECS

[VDD96] N. Vancampenhout, G. Dive, and D. Dehareng. Energetic and conformational study of four benzylimidazole compounds with $\alpha 2$ agonist profile: The mivazerol and three methylated derivatives. *International Journal of Quantum Chemistry*, 60(4):911–930, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60650`.

Visscher:1995:KRC

[VDL95] L. Visscher, K. G. Dyall, and T. J. Lee. Kramers-restricted closed-shell CCSD theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:411–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

VanDuijnen:1996:DRF

[VdV96] Piet Th. Van Duijnen and Alex H. de Vries. Direct reaction field force field: A consistent way to connect and combine quantum-chemical and classical descriptions of molecules. *International Journal of Quantum Chemistry*, 60(6):1111–1132, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60678`.

Dam:1999:ESC

[vDvLR99] Huub J. J. van Dam, Joop H. van Lenthe, and Paul J. A. Ruttink. Exact size consistency of multireference Møller–Plesset perturbation theory. *International Journal of Quantum Chemistry*, 72(6):549–558, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=50000013`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=50000013&PLACEBO=IE.pdf`.

Vaz:1999:UED

[VES+99] Roy J. Vaz, Michael Edwards, Jian Shen, Robert Pearlstein, and Dorothea Kominos. Use of electron densities in comparative molecular field analysis (CoMFA): O — H bond dissociation energies in phenols. *International Journal of Quantum Chemistry*, 75(3):187–195, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/65000660/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000660&PLACEBO=IE.pdf`.

Vieira:1996:SECa

[VFBP96a] A. Vieira, C. Fiolhais, M. Brajczewska, and J. P. Perdew. Self-expansion and compression of charged clusters of stabilized jellium. *International Journal of Quantum Chemistry*, 60(7):325–??, 1996. CODEN IJQCB2.

Vieira:1996:SECc

[VFBP96b] A. Vieira, C. Fiolhais, M. Brajczewska, and J. P. Perdew. Self-expansion and compression of charged clusters of stabilized jellium. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):325–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Vieira:1996:SECb

[VFBP96c] Armando Vieira, Carlos Fiolhais, Marta Brajczewska, and John P. Perdew. Self-expansion and compression of charged clusters of stabilized jellium. *International Journal of Quantum Chemistry*, 60(7):1537–1548, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60713`.

Vogel:1993:TOM

[VFHL93] S. Vogel, T. H. Fischer, J. Hutter, and H. P. Luthi. Third-order methods for molecular geometry optimizations. *International Journal of Quantum Chemistry*, 45(6):679–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Satkovskiene:1996:ADM

[vG96] D. Šatkovskienė and V. Gineitytė. The application of the density matrix method for the investigation of the *trans*-effect of heteroatom in σ-electron systems. *International Journal of Quantum Chemistry*, 58(5):453–459, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60500`.

Vacek:1996:TCB

[VH96a] Jaroslav Vacek and Pavel Hobza. On the thermodynamic characteristics of the benzene $\cdots$ ar$_2$ complex: An application of the ab initio intermolecular potential. *International Journal of Quantum Chemistry*, 57(4):551–557, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60419`.

Sponer:1996:DBA

[vH96b] Jiří Šponer and Pavel Hobza. DNA base amino groups and their role in molecular interactions: Ab initio and preliminary density functional theory calculations. *International Journal of Quantum Chemistry*, 57(5):959–970, March 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60434`.

Vogel:1993:DSS

[VHFL93] S. Vogel, J. Hutter, T. H. Fischer, and H. P. Luthi. Direct SCF structure optimization of large molecules on networks of workstations. *International Journal of Quantum Chemistry*, 45 (6):665–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vilkas:1998:SOM

[VIK98] Marius Jonas Vilkas, Yasuyuki Ishikawa, and Konrad Koc. Second-order multiconfigurational Dirac–Fock calculations on boronlike ions. *International Journal of Quantum Chemistry*, 70(4-5):813–823, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75060; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75060&PLACEBO=IE.pdf`.

Vinette:1992:QSD

[Vin92] F. Vinette. Quasispin symmetry for the derivation of coupled cluster equations for the Hubbard model of benzene. *International Journal of Quantum Chemistry*, 42(6):1737–1746, June 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vilanove:1995:DVR

[VJ95] H. Vilanove and M. Jacon. Discrete variable representation method applied to the determination of $J = 0$ vibrational bound states of NO_2. *International Journal of Quantum Chemistry*, 55(5):419–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vilanove:1997:DVR

[VJ97] H. Vilanove and M. Jacon. Discrete variable representation method applied to the determination of rotation-vibration bound states of NO_2. *International Journal of Quantum Chemistry*, 62(2):199–211, March 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42503; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42503&PLACEBO=IE.pdf`.

Villar:1991:PST

[VL91] H. O. Villar and G. H. Loew. Properties of selective type I benzodiazepine receptor ligands. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:131–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Valdemoro:1997:RSWa

[VLCBPR97a] C. Valdemoro, M. P. De Lara-Castells, R. Bochicchio, and E. Perez-Romero. Relevant space within the spin-adapted reduced Hamiltonian theory. I. study of the BH molecule. *International Journal of Quantum Chemistry*, 65 (2):97–105, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42746; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42746&PLACEBO=IE.pdf.

Valdemoro:1997:RSWb

[VLCBPR97b] C. Valdemoro, M. P. De Lara-Castells, R. Bochicchio, and E. Pérez-Romero. Relevant space within the spin-adapted reduced Hamiltonian theory. II. Study of the π cloud in benzene and naphthalene. *International Journal of Quantum Chemistry*, 65(2):107–119, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42748; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42748&PLACEBO=IE.pdf.

Valdes:1997:TCC

[VMCK97] Esther Agacino Valdes, Pablo De La Mora, Miguel Castro, and Jaime Keller. Theoretical calculation of carbon clusters. *International Journal of Quantum Chemistry*, 65(5): 867–875, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42818; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42818&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Mourik:1997:RDN

[vMVvLvD97] Tanja van Mourik, Robert Jan Vos, Joop H. van Lenthe, and Frans B. van Duijneveldt. Removal of dependencies from nearly complete basis sets. Calculations on the helium dimer. *International Journal of Quantum Chemistry*, 63 (4):805–815, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42631; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42631&PLACEBO=IE.pdf`.

Vojtik:1996:SCI

[Voj96] Jan Vojtík. Static characteristics of the ionization event in the He(23S)-HD collision system. *International Journal of Quantum Chemistry*, 57(4):543–550, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60410`.

Vail:1995:ESC

[VR95] J. M. Vail and B. K. Rao. Electronic structure of crystals: Embedded quantum cluster with overlap. *International Journal of Quantum Chemistry*, 53(1):67–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

vonSzentpaly:1995:MIP

[vS95] L. von Szentpaly and I. L. Shamovsky. Modeling intercalated PAH metabolites: Explanation for the bay region methyl effect. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 22(??):191–??, ???? 1995. CODEN IJQBDZ. ISSN 0360-8832.

VanCamp:1995:TEC

[VV95] P. E. Van Camp and V. E. Van Doren. Total energy calculations in the DFT on binary compounds. *International Journal of Quantum Chemistry*, 55(4):339–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

vanLenthe:1996:RRT

[vvBS96] E. van Lenthe, R. van Leeuwen, E. J. Baerends, and J. G. Snijders. Relativistic regular two-component Hamiltonians. *International Journal of Quantum Chemistry*, 57(3):281–293, ????

1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60384`.

Viruela:1998:DDF

[VVO98] Pedro M. Viruela, Rafael Viruela, and Enrique Orti. Difficulties of density functional theory in predicting the torsional potential of 2,2′-bithiophene. *International Journal of Quantum Chemistry*, 70(2):303–312, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74998`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74998&PLACEBO=IE.pdf`. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

VanDoren:1994:SCS

[VVS94] V. E. Van Doren, P. E. Van Camp, and G. Straub. Self-consistent second-order screening in many-body theory. *International Journal of Quantum Chemistry*, 51(6):389–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Varandas:1999:VSL

[VX99] A. J. C. Varandas and Z. R. Xu. Vibrational spectrum of Li_3 first-excited electronic doublet state: Geometric-phase effects and statistical analysis. *International Journal of Quantum Chemistry*, 75(2):89–109, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=64000654`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=64000654&PLACEBO=IE.pdf`.

Vracko:1993:SES

[VZ93] M. G. Vracko and M. Zaider. A study of excited states in trans-polyacetylene in the Hartree–Fock, Tamm–Dancoff, and random-phase approximation. *International Journal of Quantum Chemistry*, 47(2):119–??, July 15, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Watt:1994:CPT

[WA94] D. E. Watt and A. S. Alkharam. Charged particle track structure parameters for application in radiation biology and radiation chemistry. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21:195–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Wallace:1994:SMT

[Wal94] D. C. Wallace. Statistical mechanical theory of liquid entropy. *International Journal of Quantum Chemistry*, 52(2):425–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:1994:OBE

[Wan94] X.-Y. Wang. Orbital binding effect in molecular orbital theory. *International Journal of Quantum Chemistry*, 50(3):197–??, April 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wasilewski:1996:COS

[Was96] Jan Wasilewski. A classification of open-shell states of molecules. *International Journal of Quantum Chemistry*, 57(4): 625–640, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60400.

Watts:1993:TEC

[WB93] J. D. Watts and R. J. Bartlett. Triple excitations in coupled-cluster theory: Energies and analytical derivatives. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:51–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Watts:1994:CCS

[WB94] J. D. Watts and R. J. Bartlett. Coupled-cluster singles, doubles, and triples calculations with Hartree–Fock and Brueckner orbital reference determinants: A comparative study. *International Journal of Quantum Chemistry. Symposium*, 28:195–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Wang:1997:EDS

[WBD97] Yi-Xuan Wang, Yu-Xiang Bu, and Cong-Hao Deng. Effect of different subsets on convergence patterns of hyperspherical harmonic expansion for the S states of the helium atom. *International Journal of Quantum Chemistry*, 64(6): 661–668, September 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42727; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42727&PLACEBO=IE.pdf.

Wahl:1970:BNI

[WBKL70] A. C. Wahl, P. Bertoncini, K. Kaiser, and R. Land. BISON: A new instrument for the experimentalist. *International Journal of Quantum Chemistry*, 3S(??):499–??, ?? 1970. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wojcik:1999:STS

[WBS99] Marek J. Wójcik, Marek Boczar, and Marzena Stoma. Spectroscopic and theoretical study of vibrational spectra of hydrogen-bonded tropolone. *International Journal of Quantum Chemistry*, 73(3):275–282, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003695; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003695&PLACEBO=IE.pdf.

Wilkinson:1991:VMA

[WD91] A. J. Wilkinson and R. H. Davies. Vibrational modes in the agonist and antagonist action of ligands on the betasub 1-Adrenoceptor and some receptor site geometry. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:151–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Wang:1995:PCH

[WD95] Y. Wang and C. Deng. PHGLF calculations of heliumlike three-body systems. *International Journal of Quantum Chemistry*, 55(1):47–??, July 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:1997:CCE

[WD97] Yixuan Wang and Conghao Deng. CFPHGLF calculation of 3S excited states for heliumlike three-body systems. *International Journal of Quantum Chemistry*, 61(1):

101–105, January 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42375; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42375&PLACEBO=IE.pdf.

Wouters:1997:EPF

[WDCA97] Johan Wouters, François Durant, Benoît Champagne, and Jean-Marie André. Electronic properties of flavins: Implications on the reactivity and absorption properties of flavoproteins. *International Journal of Quantum Chemistry*, 64 (6):721–733, September 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42733; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42733&PLACEBO=IE.pdf.

Windt:1993:VIM

[WDD93] L. De Windt, M. Defranceschi, and J. Delhalle. Variation-iteration method in momentum space: Determination of Hartree–Fock atomic orbitals. *International Journal of Quantum Chemistry*, 45(6):609–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weatherford:1997:LEE

[WDS97] Charles A. Weatherford, Mei Dong, and Bidhan C. Saha. Low-energy electron scattering from a model H_2 potential using finite elements in two dimensions. *International Journal of Quantum Chemistry*, 65(5):591–600, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42789; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42789&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Wen:1993:NCS

[Wen93] Z. Wen. A note on the calculation of some transformation coefficients. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:303–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Weniger:1996:NSTb

[Wen96a] E. J. Weniger. Nonlinear sequence transformations: A computational tool for quantum mechanical and quantum chemical calculations. *International Journal of Quantum Chemistry*, 58(3):319–??, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weniger:1996:NSTa

[Wen96b] Ernst Joachim Weniger. Nonlinear sequence transformations: A computational tool for quantum mechanical and quantum chemical calculations. *International Journal of Quantum Chemistry*, 57(3):265–280, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60373`.

Wenzel:1998:EEB

[Wen98] W. Wenzel. Excitation energies in Brillouin–Wigner-based multireference perturbation theory. *International Journal of Quantum Chemistry*, 70(4-5):613–622, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75039; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75039&PLACEBO=IE.pdf`.

Wybourne:1997:CTR

[WFK97] Brian G. Wybourne, Norbert Flocke, and Jacek Karwowski. Characters of two-row representations of the symmetric group. *International Journal of Quantum Chemistry*, 62(3):261–264, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42510; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42510&PLACEBO=IE.pdf`.

Warren:1994:MHP

[WG94] D. S. Warren and B. M. Gimarc. Maximum hardness in P_6 isomers. *International Journal of Quantum Chemistry*, 49(3):207–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:1995:DFS

[WG95] J. Z. Wu and B. Goodman. Distortion of the Fermi surface of an anisotropic two-dimensional Fermi gas. *International Journal* *of Quantum Chemistry*, 53(1):77–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:1999:CSS

[WG99] Youliang Wang and John R. Gunn. Computational study of structures and proton transfer in hydrogen-bonded ammonia complexes using semiempirical valence-bond approach. *International Journal of Quantum Chemistry*, 73(4):357–367, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61000532; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61000532&PLACEBO=IE.pdf.

Woolf:1999:IIC

[WGP99] Thomas B. Woolf, Alan Grossfield, and John G. Pearson. Indoles at interfaces: Calculations of electrostatic effects with density functional and molecular dynamics methods. *International Journal of Quantum Chemistry*, 75(3):197–206, November 5, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/65000661/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=65000661&PLACEBO=IE.pdf.

Winkler:1994:MDS

[WGRM94] R. G. Winkler, A. Gerstmair, P. Reineker, and T. Matsuda. Molecular dynamics simulations of n-alkane melts confined between solid surfaces. *International Journal of Quantum Chemistry*, 52(2):437–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wall:1992:PCA

[WHF92] C. G. Wall, E. F. Healy, and M. A. Fox. Peptide conformational analysis using the TRIPOS force field. *International Journal of Quantum Chemistry*, 44(4):543–??, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Whitkop:1999:IEC

[Whi99] Peter G. Whitkop. Integral evaluation in the case of a helium atom positioned off-center in a spherical box. *International Journal of Quantum Chemistry*, 73(6):459–467, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61007370; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61007370&PLACEBO=IE.pdf.

Windt:1995:ECH

[WHPC95] L. De Windt, D. W. M. Hoffmann, L. Pisani, and E. Clementi. Extension of the Coulomb-hole-Hartree–Fock theory to molecules. *International Journal of Quantum Chemistry*, 53(2):131–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Watanabe:1996:DPTa

[WI96a] H. Watanabe and S. Iwata. Does the proton-transfer reaction take place in the ground state of phenol-$(H_2O)_4$ clusters? *International Journal of Quantum Chemistry*, 60(7):395–??, 1996. CODEN IJQCB2.

Watanabe:1996:DPTc

[WI96b] H. Watanabe and S. Iwata. Does the proton-transfer reaction take place in the ground state of Phenol-$(H_2O)_4$ clusters? *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):395–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Watanabe:1996:DPTb

[WI96c] Hidekazu Watanabe and Suehiro Iwata. Does the proton-transfer reaction take place in the ground state of phenol — $(H_2\ O)_4$ clusters? *International Journal of Quantum Chemistry*, 60(7):1607–1613, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60721.

Wilson:1998:NWL

[WI98] Leslie C. Wilson and Stanislav Ivanov. A new Wigner-like correlation-energy functional from coordinate scaling requirements. *International Journal of Quantum Chemistry*, 69 (4):523–532, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30025; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30025&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Wilson:1967:LBE

[Wil67] T. M. Wilson. Lower bounds to eigenvalues of the Schrödinger equation by the partitioning technique. *International Journal of Quantum Chemistry*, 1S(??):511–??, ?? 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wilson:1969:SES

[Wil69] T. M. Wilson. A study of the electronic structure of the first-row transition-metal compounds. *International Journal of Quantum Chemistry*, 3S(??):757–??, ?? 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wilson:1990:ESI

[Wil90] T. M. Wilson. Electronic structure of the V^{2+} impurity states in ZnSe. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:187–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Wilson:1996:DBS

[Wil96] S. Wilson. Distributed basis sets of *s*-type Gaussian functions for molecular electronic structure calculations: Applications of the Gaussian cell model to one-electron polycentric linear molecular systems. *International Journal of Quantum Chemistry*, 60(1):47–57, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60614`.

Wilson:1999:DGB

[Wil99a] S. Wilson. Distributed Gaussian basis sets: A stochastic variational approach for diatomic molecules. *International Journal of Quantum Chemistry*, 74(5):547–552, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62503005`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62503005&PLACEBO=IE.pdf`. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

Wilson:1999:AHO

[Wil99b] S. Wilson. On the application of hierarchical orthogonality restrictions to spin-coupled wave functions. *International Journal of Quantum Chemistry*, 74(2):135–144, ???? 1999. CODEN

IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003359; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003359&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Wang:1998:PRP

[WJC+98] Qinmi Wang, Hualiang Jiang, Jianzhong Chen, Kaixian Chen, and Ruyun Ji. On the possible reaction pathway for the acylation of AChE-catalyzed hydrolysis of ACh: Semiempirical quantum chemical study. *International Journal of Quantum Chemistry*, 70(3):515–525, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75018; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75018&PLACEBO=IE.pdf.

Wang:1999:TSP

[WJC+99] Qin Mi Wang, Hua Liang Jiang, Kai Xian Chen, Ru Yun Ji, and Yuan-Jie Ye. Theoretical studies on the possible reaction pathway for the deacylation of the AChE-catalyzed reaction. *International Journal of Quantum Chemistry*, 74(3):315–325, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62004761; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62004761&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly*.

Wahl:1967:EMI

[WL67] A. C. Wahl and R. 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*, 1S(??):375–??, ?? 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wilson:1992:IFL

[WL92] T. M. Wilson and E. E. Lafon. Ab initio factorized LCAO calculation of the electronic structure of alpha-SiOsub 2. *International Journal of Quantum Chemistry. Quantum Chemistry*

Symposium, 26:703–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Wechsler:1999:CTH

[WL99] D. Wechsler and J. Ladik. Contribution to the theory of high-temperature superconductivity in $YBa_2Cu_3O_7$. *International Journal of Quantum Chemistry*, 71(3):285–294, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10016712; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10016712&PLACEBO=IE.pdf.

Wang:1994:IMD

[WLBL94] J. Wang, A. Laaksonen, R. J. Boyd, and R. Li. Ab initio and molecular dynamics study of dibenzotricyclic calcium antagonists: A rigid model approach. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21:17–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Wlodarz:1994:SDP

[Wlo94] J. J. Wlodarz. Self-dual phase-space representation of quantum mechanics and the variational principle. *International Journal of Quantum Chemistry*, 51(3):123–??, July 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wlodarz:1995:DFT

[Wlo95] J. J. Wlodarz. Density functional theory and self-dual phase-space representations of quantum mechanics. *International Journal of Quantum Chemistry*, 56(4):233–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wojcik:1995:TSL

[WMD95] M. J. Wojcik, G. J. Mains, and J. P. Devlin. Theoretical study of $[Li(H_2O)_n]^+$ and $[K(H_2O)_n]^+$ ($n = 1 \ldots 4$). *International Journal of Quantum Chemistry*, 53(1):49–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

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(??):711–??, ?? 1969.

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

Wu:1992:SSM

[WMW92] C. S. Wu, L. J. Myers, and S. D. Worley. A semiempirical SCF MO study of the interaction of odorant molecules with a biological substrate. *International Journal of Quantum Chemistry*, 44(4):549–563, October 15, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:1998:TIL

[WMZ98] Z. J. Wu, Q. B. Meng, and S. Y. Zhang. Theoretical investigation of $LaC_3{}^{n+}$ ($n = 0, 1, 2$) clusters by density functional theory. *International Journal of Quantum Chemistry*, 66(4):301–307, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29866; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29866&PLACEBO=IE.pdf.

Woolf:1998:BHL

[Woo98] Thomas B. Woolf. Bacteriorhodopsin α-helices in lipid settings: Insights for structure prediction. *International Journal of Quantum Chemistry*, 69(1):105–116, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29965; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29965&PLACEBO=IE.pdf.

Woolley:1999:CPG

[Woo99] R. G. Woolley. Charged particles, gauge invariance, and molecular electrodynamics. *International Journal of Quantum Chemistry*, 74(5):531–545, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62503004; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62503004&PLACEBO=IE.pdf. Special Issue: *The Role of Mathematics in Quantum Chemistry: Special Issue in Honor of George G. Hall (Part I of II)*. Issue Edited by Don Rees, Hiroshi Fujimotoi.

White:1990:MMC

[WP90] T. G. White and G. R. Pack. Molecular mechanics calculations of the noncovalent interaction of aflatoxin bsub 1 and its ultimate carcinogen with various DNA sequences. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 17:133–??, 1990. CODEN IJQBDZ. ISSN 0360-8832.

Wang:1991:PFL

[WP91] J. Wang and A. Pullman. A program for flexible lattice enegy minimization (FLATER) and its application to the study of the protein-lipid copacking. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 18:317–??, 1991. CODEN IJQBDZ. ISSN 0360-8832.

Wong:1992:MOS

[WP92] L. Wong and G. R. Pack. Molecular orbital studies of the hydrolysis reactions of benzo[a]pyrene diol epoxides. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:1–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Wang:1993:BRP

[WP93] X. Wang and Z. Peng. Binding regions in polyatomic molecules. *International Journal of Quantum Chemistry*, 47(5):393–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Windus:1995:PAT

[WP95] T. L. Windus and J. A. Pople. Pinnacle: An approach toward object oriented quantum chemistry. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:485–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Wallace:1998:TCT

[WPB98] R. Wallace, H. Price, and F. Breitbeil. Toward a charge-transfer model of neuromolecular computing. *International Journal of Quantum Chemistry*, 69(1):3–10, ???? 1998. CODEN

IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29967; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29967&PLACEBO=IE.pdf.

Wright:1996:ERI

[WR96] Jonathan D. Wright and Christopher A. Reynolds. Energetics of reactions involving radical species in solution: Calculation of relative electrode potentials for nitroimidazoles using density functional and continuum methods. *International Journal of Quantum Chemistry*, 59(2):135–145, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60533.

Wilson:1999:JG

[WRC99] S. Wilson, M. Raimondi, and D. L. Cooper. J. Gerratt, 1938–1997. *International Journal of Quantum Chemistry*, 74(2):71–76, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62003351; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62003351&PLACEBO=IE.pdf. Special Issue: *Quantum Theory of Chemical Bonding: Special Issue in Memory of Joseph Gerratt*. Issue Edited by S. Wilson, M. Raimondi, D. L. Cooper.

Wang:1994:ECS

[WS94a] J. Wang and V. H. Smith. Evaluation of cross sections for X-ray and high-energy electron scattering from molecular systems. *International Journal of Quantum Chemistry*, 52(5):1145–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:1994:EPD

[WS94b] J. Wang and V. H. Smith, Jr. Electron-pair distributions and chemical bonding. *International Journal of Quantum Chemistry*, 49(3):147–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:1995:FCH

[WS95] J. Wang and V. H. Smith Jr. Fermi and Coulomb holes of molecules in excited states. *International Journal of Quantum*

Chemistry, 56(5):509–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wetzel:1994:ISI

[WSB94] T. L. Wetzel, R. Shorrosh, and R. F. Borkman. Ab initio study of the inversion barrier in NF_3^+. *International Journal of Quantum Chemistry*, 50(2):151–??, April 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

White:1994:CPT

[WSMB94] C. T. White, S. B. Sinnott, J. W. Mintmire, and D. W. Brenner. Chemistry and phase transitions from hypervelocity impacts. *International Journal of Quantum Chemistry. Symposium*, 28: 129–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Wu:1990:MDA

[WSTB90] J. Z. Wu, J. R. Sabin, S. B. Trickey, and J. C. Boettger. Mono- and dilayer analogues of crystalline atomic hydrogen. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 24:873–??, 1990. CODEN IJQSDI. ISSN 0161-3642.

Wenzel:1996:MBSa

[WSW96a] W. Wenzel, M. M. Steiner, and K. G. Wilson. Multireference basis-set reduction. *International Journal of Quantum Chemistry*, 60(7):113–??, 1996. CODEN IJQCB2.

Wenzel:1996:MBSc

[WSW96b] W. Wenzel, M. M. Steiner, and K. G. Wilson. Multireference basis-set reduction. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):113–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Wenzel:1996:MBSb

[WSW96c] Wolfgang Wenzel, Matthew M. Steiner, and Kenneth G. Wilson. Multireference basis-set reduction. *International Journal of Quantum Chemistry*, 60(7):1325–1330, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60690`.

Wenzel:1998:SBD

[WSW98] W. Wenzel, M. M. Steiner, and K. G. Wilson. Scaling behavior of dynamic correlation effects. *International Journal* *of Quantum Chemistry*, 70(1):147–157, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74359; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74359&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Weiner:1998:FSC

[WT98] B. Weiner and S. B. Trickey. Fukutome symmetry classification of the Kohn–Sham auxiliary one-matrix and its associated state or ensemble. *International Journal of Quantum Chemistry*, 69(4):451–460, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30017; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30017&PLACEBO=IE.pdf. Special Issue: *Symposium on Density Functional Theory and Applications (Part II of II)*. Issue Edited by Sam Trickey, Weitao Yang, Mel Levy.

Wilkinson:1994:DEA

[WTDB94] A. J. Wilkinson, D. Timms, R. H. Davies, and K. J. Broadley. Distortion and energetics in the agonist conformation of bound phenoxypropanolamine agents in the 1-Adrenoceptor. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 21:133–??, 1994. CODEN IJQBDZ. ISSN 0360-8832.

Wu:1993:ESP

[WTS93] J. Z. Wu, S. B. Trickey, and J. R. Sabin. Electronic stopping power for protons in an LiF monolayer. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27: 219–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Weinberger:1997:TLM

[WTS97] P. Weinberger, I. Turek, and L. Szunyogh. The TB-LMTO method and its relation to the screened KKR method. *International Journal of Quantum Chemistry*, 63 (1):165–188, May 15, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42562;

http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42562&PLACEBO=IE.pdf.

Wu:1994:EDP

[WTSN94] J. Z. Wu, S. B. Trickey, J. R. Sabin, and J. Nobel. Energy depositions of protons in allotropic carbon ultrathin films. *International Journal of Quantum Chemistry. Symposium*, 28:299–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Wulfman:1994:SEM

[Wul94] C. Wulfman. On the space of eigenvectors of molecular quantum mechanics. *International Journal of Quantum Chemistry*, 49 (3):185–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wesolowski:1997:KSE

[WW97] Tomasz Adam Wesolowski and Jacques Weber. Kohn–Sham equations with constrained electron density: The effect of various kinetic energy functional parametrizations on the ground-state molecular properties. *International Journal of Quantum Chemistry*, 61(2):303–311, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42394; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42394&PLACEBO=IE.pdf.

Wu:1999:SPD

[WWFR99] Jian Hui Wu, Peter J. Winn, György G. Ferenczy, and Christopher A. Reynolds. Solute polarization and the design of cobalt complexes as redox-active therapeutic agents. *International Journal of Quantum Chemistry*, 73(2):229–236, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=55003520; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=55003520&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly. Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology, La Biodola, Elba (Italy), September 8-11, 1998.* Issue Edited by Roman Osman, Guiliano Alagona, Caterina Ghio.

Wu:1998:EAS

[WWM+98] Wei Wu, Anan Wu, Yirong Mo, Menghai Lin, and Qianer Zhang. Efficient algorithm for the spin-free valence bond theory.

I new strategy and primary expressions. *International Journal of Quantum Chemistry*, 67(5):287–297, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29907; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29907&PLACEBO=IE.pdf`.

Whitten:1995:TSS

[WY95] J. L. Whitten and H. Yang. Theoretical studies of surface reactions on metals. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:41–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Wang:1999:TSI

[WY99] Chaojie Wang and Song Ye. Theoretical study on the insertion reactions of Ti^+ (^2F) with HF, HCl, H_2O, H_2S, NH_3, PH_3, CH_4, and SiH_4. *International Journal of Quantum Chemistry*, 75(1):47–54, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63003148; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63003148&PLACEBO=IE.pdf`.

Wang:1996:SSC

[WYW96] Bo-Cheng Wang, Liang-Jye Yu, and Wen-Jwu Wang. A semiempirical study of $C_{24}N_4$ and its boron-nitrogen analogs. *International Journal of Quantum Chemistry*, 57(3):465–470, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60385`.

Wang:1992:SHP

[WYZ+92] Z. Wang, Y. Yan, H. Zhan, J. C. Morrison, and P. Winkler. On the stability of H^- in plasmas. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:869–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Wu:1994:ONR

[WZ94] W. Wu and Q. Zhang. The orthogonal and the natural representation for symmetric groups. *International Journal of Quantum Chemistry*, 50(1):55–??, March 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:1999:CCB

[WZ99] Z. J. Wu and S. Y. Zhang. Calculation of chemical bond parameters in $La_{1-x}Ca_xCrO_3$ ($0.0 \leq x \leq 0.3$). *International Journal of Quantum Chemistry*, 73(5):433–437, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61004334; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61004334&PLACEBO=IE.pdf.

Wasilewski:1996:MVO

[WZW96] J. Wasilewski, S. Zelek, and Małgorzata Wierzbowska. Modifications of virtual orbitals in the limited CI calculations for electron-rich molecules. *International Journal of Quantum Chemistry*, 60(5):1027–1036, December 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60675.

Xincai:1991:SAA

[XAM91] Luo Xincai, Gustavo A. Arteca, and Paul G. Mezey. Shape analysis along reaction paths of ring opening reactions. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:335–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Xu:1998:ISR

[XFF98] Zhen-Feng Xu, De-Cai Fang, and Xiao-Yuan Fu. Ab initio study on the reaction $2NH_2 \rightarrow NH+NH_3$. *International Journal of Quantum Chemistry*, 70(2):321–329, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75000; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75000&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Xiao:1999:REG

[XKB+99] Chuanyun Xiao, Sven Krüger, Thomas Belling, Markus Mayer, and Notker Rösch. Relativistic effects on geometry and electronic structure of small Pd_n species ($n = 1, 2, 4$). *International Journal of Quantum Chemistry*, 74

(4):405–416, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62502084; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62502084&PLACEBO=IE.pdf.

Xu:1999:CSB

[XLW+99] Xin Xu, Xin Lü, Nanqin Wang, Qianer Zhang, Masahiro Ehara, and Hiroshi Nakatsuji. CASSCF study of bonding in NiCO and FeCO. *International Journal of Quantum Chemistry*, 72(3):221–231, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40003034; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40003034&PLACEBO=IE.pdf.

Xantheas:1994:PES

[XR94] S. S. Xantheas and K. Reudenberg. Potential energy surfaces of carbon dioxide. *International Journal of Quantum Chemistry*, 49(4):409–??, February 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:1997:ISE

[XSG97] Wei-Xing Xu, K. D. Schierbaum, and W. Goepel. Ab initio study of electronic structures of Ptn clusters ($n = 2$–12). *International Journal of Quantum Chemistry*, 62(4):427–436, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42519; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42519&PLACEBO=IE.pdf.

Xu:1996:PEC

[Xu96] Wei-Xing Xu. Parallel electron correlation effect and Fermi hole structure. *International Journal of Quantum Chemistry*, 60(4):853–857, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60658.

Xu:1999:AEC

[Xu99] Wei-Xing Xu. The antiparallel electron correlation coefficient and Coulomb hole structure. *International Journal of Quantum Chemistry*, 74(1):1–6, ???? 1999. CODEN IJQCB2. ISSN

0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62000140; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62000140&PLACEBO=IE.pdf.

Xu:1995:TAC

[XY95] Z. Xu and J. Yan. A theoretical approach to the complexation and decomplexation processes in the reaction C_{60} + He $\rightleftharpoons$ (He@C_{60}). *International Journal of Quantum Chemistry*, 53(3): 287–??, February 5, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xie:1998:TPD

[XY98] Daiqian Xie and Guosen Yan. A theoretical procedure for determining rovibrational eigenstates of van der Waals complexes. *International Journal of Quantum Chemistry*, 66 (2):119–122, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29845; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29845&PLACEBO=IE.pdf.

Xiao:1998:ESC

[XYC98] Shen-Xiu Xiao, Sheng-Yong Yang, and Tian-Lang Chen. Electronic structure and catalytic properties of Waugh-type anion $(NiMo_9O_{32})^{6-}$. *International Journal of Quantum Chemistry*, 70(2):375–378, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75006; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75006&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part II of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Yanez:1995:IEM

[YAD95] R. J. Yáñez, J. C. Angulo, and J. S. Dehesa. Information entropies of many-electron systems. *International Journal of Quantum Chemistry*, 56(5):489–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaguchi:1997:IST

[Yam97] Yoichi Yamaguchi. Ab initio study of n-tetrasilane cation and anion radicals as models of doped linear polysilanes. *International Journal of Quantum Chemistry*, 62(4):393–401, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42526; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42526&PLACEBO=IE.pdf.

Yabana:1999:TDL

[YB99] K. Yabana and G. F. Bertsch. Time-dependent local-density approximation in real time: Application to conjugated molecules. *International Journal of Quantum Chemistry*, 75(1):55–66, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=63003149; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=63003149&PLACEBO=IE.pdf.

Yi:1997:TEC

[YBM97] Z.-G. Yi, D. Bekšić, and D. A. Micha. Time evolution of CO vibrational populations during photodesorption by light pulses. *International Journal of Quantum Chemistry*, 64(1):71–83, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42667; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42667&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Yu:1992:COS

[YBZ92] J. Yu, J. D. Baker, and M. C. Zerner. On the calculation of oscillator strength for electronic transitions using "effective core" methods. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 26:475–??, 1992. CODEN IJQSDI. ISSN 0161-3642.

Ye:1996:ISR

[YD96] Song Ye and Shushan Dai. Ab initio study on the reaction of $Y^+ + NH_3 \to Y^+ NH + H_2$. *International Journal of Quantum*

Chemistry, 59(5):421–426, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60560.

Yang:1997:ECA

[YD97] Zhong-Zhi Yang and Ernest R. Davidson. Evaluation of a characteristic atomic radius by an ab initio method. *International Journal of Quantum Chemistry*, 62(1):47–53, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42488; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42488&PLACEBO=IE.pdf.

York:1992:ICI

[YDDP92] D. M. York, T. Darden, D. Deerfield, and L. G. Pedersen. The interaction of na(I), Ca(II), and Mg(II) metal ions with duplex DNA: A theoretical modeling study. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:145–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Yu:1998:CFC

[YDFS98] M. Yu, M. Dolg, P. Fulde, and H. Stoll. Charge fluctuations and correlation strength in chemical bonds: First-row homonuclear diatomic molecules. *International Journal of Quantum Chemistry*, 67(3):157–173, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29896; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29896&PLACEBO=IE.pdf.

Yoshizawa:1993:UHF

[YITY93] K. Yoshizawa, A. Ito, K. Tanaka, and T. Yamabe. Unrestricted Hartee–Fock method for infinite systems with antiferromagnetic array: Analysis of antiferromagnetic state of trans-polyacetylene. *International Journal of Quantum Chemistry*, 45(4):391–??, 1993. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yu:1992:CIE

[YJL92] M. Yu, Q. Jiang, and P. R. LeBreton. Configuration interaction effects on he(I) photoelectron spectra of nucleotide bases: Evidence for valence electron hole-mixing in 1,9-Dimethylguanine. *International Journal of Quantum Chemistry. Quantum Biology Symposium: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.*, 19:27–??, 1992. CODEN IJQBDZ. ISSN 0360-8832.

Younk:1997:IIE

[YK97] Edward H. Younk and A. Barry Kunz. An ab initio investigation of the electronic structure of lithium azide (LiN_3), sodium azide (NaN_3), and lead azide (pb $(N_3)_2$). *International Journal of Quantum Chemistry*, 63(3):615–621, June 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42622; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42622&PLACEBO=IE.pdf.

Yamaki:1999:VTB

[YKN+99] D. Yamaki, Y. Kitagawa, H. Nagao, M. Nakano, Y. Yoshioka, and K. Yamaguchi. Visualization of two-body electron densities and wave functions of magnetic molecules. *International Journal of Quantum Chemistry*, 75(4–5):645–654, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004961/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004961&PLACEBO=IE.pdf.

Ye:1994:THC

[YL94] Y.-Y. Ye and J. Ladik. Theory of hopping conductivity of proteins. *International Journal of Quantum Chemistry*, 52(2):491–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:1997:SCR

[YLD97] Benhui Yang, Shenglu Lin, and Shiliang Ding. Semiclassical calculation of rotational excitation of atom-symmetric top scattering. *International Journal of Quantum Chemistry*, 65(1):89–96, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42736; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42736&PLACEBO=IE.pdf.

Yiannopoulou:1996:TCR

[YLLJ96] A. Yiannopoulou, T. Leininger, A. M. Lyyra, and G-H Jeung. Theoretically calculated rovibronic transition spectra of KRb. *International Journal of Quantum Chemistry*, 57(4):575–585, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60422.

Yao:1999:ONP

[YM99] Xuan Yao and Sean P. McGlynn. Optogalvanism in a neon plasma. *International Journal of Quantum Chemistry*, 72(4):369–377, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006315; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006315&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Yamaguchi:1998:SOA

[YNMT98] Yoichi Yamaguchi, Yosuke Nagasawa, Akinori Murakami, and Kenji Tabata. Stability of oxygen anions and hydrogen abstraction from methane on reduced SnO_2 (110) surface. *International Journal of Quantum Chemistry*, 69(5):669–678, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30031; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30031&PLACEBO=IE.pdf.

Yudanov:1997:DFC

[YNNR97] Ilya V. Yudanov, Vladimir A. Nasluzov, Konstantin M. Neyman, and Notker Rösch. Density functional cluster description of ionic materials: Improved boundary conditions for MgO clusters with the help of cation model potentials. *International Journal of Quantum Chemistry*, 65(5):975–986, December 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42829; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42829&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue

Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Yamada:1999:ECS

[YNNY99] S. Yamada, M. Nakano, H. Nagao, and K. Yamaguchi. Electron correlation and structure dependencies of the second hyperpolarizability of ethylene. *International Journal of Quantum Chemistry*, 71(2):177–183, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000025; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000025&PLACEBO=IE.pdf`.

Yamamoto:1994:ICC

[YNO94] Y. Yamamoto, T. Noro, and K. Ohno. Ab initio CI calculation on benzene with an extended basis set. *International Journal of Quantum Chemistry*, 51(1):27–??, June 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaguchi:1999:RMM

[YNST99] Yoichi Yamaguchi, Yosuke Nagasawa, Satoshi Shimomura, and Kenji Tabata. Reaction model for methane oxidation on reduced SnO_2 (110) surface. *International Journal of Quantum Chemistry*, 74(4):423–433, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62502086; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62502086&PLACEBO=IE.pdf`.

Yamada:1999:CSD

[YNY99] S. Yamada, M. Nakano, and K. Yamaguchi. CAS-SCF and density functional calculations of second hyperpolarizabilities for a nitronyl nitroxide radical. *International Journal of Quantum Chemistry*, 71(4):329–336, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=10049347; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=10049347&PLACEBO=IE.pdf`.

Yamamoto:1992:BSS

[YO92] S. Yamamoto and M.-A. Ozaki. Broken symmetry solutions of the two-dimensional extended Hubbard model and their instability conditions. *International Journal of Quantum Chemistry*, 44(6):949–??, December 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

York:1995:GFE

[Yor95] D. M. York. A generalized formulation of electronegativity equalization from density-functional theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 29:385–??, 1995. CODEN IJQSDI. ISSN 0161-3642.

Yamaguchi:1993:ICB

[YOTY93] K. Yamaguchi, M. Okumura, K. Takada, and S. Yamanaka. Instability in chemical bonds. II. theoretical studies of exchange-coupled open-shell systems. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:501–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Yu:1997:DUG

[YPC97] Yaxiong Yu, Pancracio Palting, and Ying-Nan Chiu. On the decomposition of the unitary group and the multiple coupling of angular momenta. *International Journal of Quantum Chemistry*, 62(4):331–341, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42518; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42518&PLACEBO=IE.pdf.

Ye:1997:ISR

[YSHD97] Song Ye, Nanhua Shi, Jianhua Huang, and Shushan Dai. Ab initio study on the reaction of Sc^+ + CH_4 $\to Sc^+$ — CH_2 + H_2. *International Journal of Quantum Chemistry*, 62 (1):23–27, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42486; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42486&PLACEBO=IE.pdf.

Yoshioka:1997:CMC

[YTYS97] Yasunori Yoshioka, Tsunaki Tsunesada, Kizashi Yamaguchi, and Isao Saito. CASSCF, MP2, and CASMP2 studies on addition reaction of singlet molecular oxygen to ethylene molecule. *International Journal of Quantum Chemistry*, 65 (5):787–801, December 5, 1997. CODEN IJQCB2. ISSN

0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42811; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42811&PLACEBO=IE.pdf. Special Issue: *Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods*. Issue Edited by Per-Olov Löwdin, Yngve Öhrn, John R. Sabin, Michael C. Zerner.

Yu:1995:AIE

[Yu95] Z.-H. Yu. An atomic interaction energy approach to the reactivity of aromatic ring toward electrophilic attack. *International Journal of Quantum Chemistry*, 55(6):485–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yurtsever:1999:QMA

[YUSM99] Mine Yurtsever, Belkis Ustamehmetoglu, A. Sezai Sarac, and A. Mannschreck. A quantum mechanical approach to electrochemical behavior of spirochromics. *International Journal of Quantum Chemistry*, 75(2):111–117, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=64000655; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=64000655&PLACEBO=IE.pdf.

Yuanqi:1992:IST

[YW92] Tao Yuanqi and Duan Wengui. An ab initio study of tautomerism between formhydroxamic acid and formhydroximic acid. *International Journal of Quantum Chemistry*, 44(3):319–??, September 30, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yan:1999:TSF

[YXX99] Guosen Yan, Ying Xue, and Daiqian Xie. Theoretical studies of force fields and IR spectra of isocytosine. *International Journal of Quantum Chemistry*, 72(1):53–60, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002302; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002302&PLACEBO=IE.pdf.

Yamaguchi:1996:ITP

[YY96] Yoichi Yamaguchi and Tokio Yamabe. Ab initio torsional potentials in silole dimers. *International Journal of Quantum Chemistry*, 57(1):73–78, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60358`.

Yan:1996:IIRa

[YZX96a] J.-M. Yan, C.-B. Zhu, and Z.-J. Xu. Investigation on the interaction and the rotation of C_{60} in alkali-doped complexes $A_xA'_{3-x}C_{60}$ ($x = 1, 2, 3$; $a, a' =$ alkali). *International Journal of Quantum Chemistry*, 60(7):365–371, 1996. CODEN IJQCB2.

Yan:1996:IIRc

[YZX96b] J.-M. Yan, C.-B. Zhu, and Z.-J. Xu. Investigation on the interaction and the rotation of C_{60} in alkali-doped complexes AxA'3 — xC_{60} ($X = 1, 2, 3$; A, A' = Alkali). *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??): 365–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Yan:1996:IIRb

[YZX96c] Ji-Min Yan, Chuan-Bao Zhu, and Zhi-Jin Xu. Investigation on the interaction on and the rotation of C_{60} in alkali-doped complexes A_X $A\prime_{3-X}C_{60}$ (X = 1, 2, 3; A, A$\prime$ = alkali). *International Journal of Quantum Chemistry*, 60(7):1577–1583, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60717`.

Zhang:1995:PDE

[ZA95] Z. Zhang and L. Adamowicz. Properties, dynamics, and electronic structure of atoms and molecules. *International Journal of Quantum Chemistry*, 54(5):281–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zapol:1995:IGC

[Zap95] B. P. Zapol. Integral-geometrical consideration of density matrices. *International Journal of Quantum Chemistry*, 56(5):535–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zuniga:1996:MEM

[ZARB96] José Zúñiga, Mercedes Alacid, Alberto Requena, and Adolfo Bastida. Matrix elements for the modified Poschl–Teller potential. *International Journal of Quantum Chemistry*, 57(1):43–51, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60355.

Zhang:1999:TSI

[ZBL99] Dongju Zhang, Yuxiang Bu, and Chengbu Liu. Theoretical study of the inner-sphere energy barrier of the transition-metal complex $M(H_2O)_6{}^{2+/3+}$ in electron-transfer process. *International Journal of Quantum Chemistry*, 75 (2):119–126, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=64000656; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=64000656&PLACEBO=IE.pdf.

Zhi:1991:ACC

[ZC91] He Zhi and Dieter Cremer. Analysis of coupled cluster and quadratic configuration interaction theory in terms of sixth-order perturbation theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 25:43–??, 1991. CODEN IJQSDI. ISSN 0161-3642.

Zupan:1995:DFL

[ZC95] A. Zupan and M. Causa. Density functional LCAO calculations for solids: Comparison among Hartree–Fock, DFT local density approximation, and DFT generalized gradient approximation structural properties. *International Journal of Quantum Chemistry*, 56(4):337–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zacarias:1996:DFSa

[ZC96a] A. Zacarias and M. Castro. Density functional study of Fe_2-N_2. *International Journal of Quantum Chemistry*, 60(7):207–??, 1996. CODEN IJQCB2.

Zacarias:1996:DFSc

[ZC96b] A. Zacarias and M. Castro. Density functional study of Fe_2-N_2. *International Journal of Quantum Chemistry. Quantum Chem-*

istry Symposium, 30(??):207–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Zacarias:1996:DFSb

[ZC96c] Angelica Zacarias and Miguel Castro. Density functional study of Fe_2-N_2. *International Journal of Quantum Chemistry*, 60 (7):1419–1428, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60701.

Zaitsevskii:1999:DFS

[ZC99] Andréi Zaitsevskii and Renzo Cimiraglia. Diagrammatic formulation of the second-order many-body multipartitioning perturbation theory. *International Journal of Quantum Chemistry*, 73(5):395–401, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=61004330; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=61004330&PLACEBO=IE.pdf.

Zheng:1998:RDT

[ZCT98] Weifan Zheng, Sung Jin Cho, and Alexander Tropsha. Rational design of a targeted combinatorial chemical library with opiatelike activity. *International Journal of Quantum Chemistry*, 69(1):65–75, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29974; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29974&PLACEBO=IE.pdf.

Zakrzewski:1996:DARb

[ZDO96a] V. G. Zakrzewski, O. Dolgounitcheva, and J. V. Ortiz. Direct algorithm for the random-phase approximation. *International Journal of Quantum Chemistry*, 60(7):1241–1247, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60718.

Zakrzewski:1996:DARa

[ZDO96b] V. J. Zakrzewski, O. Dolgounitcheva, and J. V. Ortiz. Direct algorithm for the random-phase approximation. *International Journal of Quantum Chemistry*, 60(7):29–??, 1996. CODEN IJQCB2.

Zakrzewski:1996:DARc

[ZDO96c] V. J. Zakrzewski, O. Dolgounitcheva, and J. V. Ortiz. Direct algorithm for the random-phase approximation. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):29–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Zakrzewski:1999:IAR

[ZDO99] V. G. Zakrzewski, O. Dolgounitcheva, and J. V. Ortiz. Improved algorithms for renormalized electron propagator calculations. *International Journal of Quantum Chemistry*, 75(4–5):607–614, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract/66004956/START; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004956&PLACEBO=IE.pdf.

Zerner:1998:BR

[Zer98a] Michael C. Zerner. Books received. *International Journal of Quantum Chemistry*, 69(5):691, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30034; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30034&PLACEBO=IE.pdf.

Zerner:1998:LP

[Zer98b] Michael C. Zerner. List of participants. *International Journal of Quantum Chemistry*, 70(1):3–40, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=74368; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=74368&PLACEBO=IE.pdf. Special Issue: *The Ninth International Congress of Quantum Chemistry (Part I of II)*. Issue Edited by Keiji Morokuma, Ernest R. Davidson, Henry F. Schaefer III.

Zerner:1999:BR

[Zer99a] Michael C. Zerner. Book review. *International Journal of Quantum Chemistry*, 71(2):215, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000020; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000020&PLACEBO=IE.pdf.

Zerner:1999:BRS

[Zer99b] Michael C. Zerner. Book review: *The Symmetric Group in Quantum Chemistry*, by Ruben Pauncz. *International Journal of Quantum Chemistry*, 72(5):533, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006355; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006355&PLACEBO=IE.pdf.

Zhao:1997:ISS

[ZGPS97] Yongfang Zhao, Tingkun Gu, Soufu Pan, and Jing Sun. An ab initio study of the structure, dissociation energy, and heat of formation of Na_2S. *International Journal of Quantum Chemistry*, 61(6):953–957, February 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42479; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42479&PLACEBO=IE.pdf.

Zhang:1999:TMA

[ZH99a] Shao-Wen Zhang and Fu-Chu He. Thermolysis mechanism of *N*-acetylpropanamide. *International Journal of Quantum Chemistry*, 74(3):337–342, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=62004763; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=62004763&PLACEBO=IE.pdf. Special Issue: *Biophysics Quarterly*.

Zilberg:1999:EPO

[ZH99b] Shmuel Zilberg and Yehuda Haas. The electron-pair origin of antiaromaticity: Spectroscopic manifestations. *International Journal of Quantum Chemistry*, 71(2):133–145, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=20000021; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=20000021&PLACEBO=IE.pdf.

Zhan:1992:MOS

[Zha92] C.-G. Zhan. Maximum overlap symmetry molecular orbital model. *International Journal of Quantum Chemistry*, 44(2):123–??, September 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:1996:ISS

[Zha96] Ruiqin Zhang. Improved scheme to solve the atomic Schrödinger equation in hyperspherical coordinates. *International Journal of Quantum Chemistry*, 59(3):203–207, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60539`.

Zhou:1993:KEC

[Zho93] Z. Zhou. Kinetic energy component in the divide-and-conquer method. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:355–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Ziesche:1995:CSI

[Zie95] P. Ziesche. Correlation strength and information entropy. *International Journal of Quantum Chemistry*, 56(4):363–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ziesche:1996:ATPa

[Zie96a] P. Ziesche. Attempts toward a pair density functional theory. *International Journal of Quantum Chemistry*, 60(7):149–??, 1996. CODEN IJQCB2.

Ziesche:1996:ATPc

[Zie96b] P. Ziesche. Attempts toward a pair density functional theory. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):149–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Ziesche:1996:ATPb

[Zie96c] Paul Ziesche. Attempts toward a pair density functional theory. *International Journal of Quantum Chemistry*, 60(7):1361–1374, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60694`.

Zitnan:1994:LUB

[Zit94] P. Zitnan. Lower and upper bounds of the energy spectrum for potentials with multiminima. *International Journal of Quantum Chemistry*, 52(6):1267–??, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zeroka:1999:ISS

[ZJS99] Daniel Zeroka, James O. Jensen, and Alan C. Samuels. Infrared spectra of some isotopomers of isopropylamine: A theoretical study. *International Journal of Quantum Chemistry*, 72(2):109–126, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=30002778; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=30002778&PLACEBO=IE.pdf.

Zerner:1994:IPS

[ZL94] M. C. Zerner and P.-O. Löwdin. Introduction to a paper symposium on "The Role of Quantum Chemistry as a Foundation for the Principles of Chemistry". *International Journal of Quantum Chemistry*, 49(3):129–??, January 20, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhanpeisov:1998:ISS

[ZL98] N. U. Zhanpeisov and J. Leszczynski. Ab initio study of the structure of isocytosine-cytosine standard Watson–Crick base pairs in the gas phase and in water. *International Journal of Quantum Chemistry*, 69(1):37–47, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29971; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29971&PLACEBO=IE.pdf.

Zhao:1994:AMO

[ZLHZ94] H. Zhao, J. Li, S. Hu, and J. Zhang. Applications of the molecular orbital graph theory: A topological method to calculate α_N-K based on α_N. *International Journal of Quantum Chemistry*, 49(2):81–??, January 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zou:1999:EDC

[ZLWES99] B. S. Zou, R. B. Little, J. P. Wang, and M. A. El-Sayed. Effect of different capping environments on the optical properties of CdS nanoparticles in reverse micelles. *International Journal of Quantum Chemistry*, 72(4):439–450, ???? 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=40006321; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=40006321&PLACEBO=IE.pdf. Special Issue: *In Honor of Lionel Goodman*. Issue Edited by Michael Kasha.

Zaitsevskii:1995:SOI

[ZM95] A. Zaitsevskii and J.-P. Malrieu. Second-order intermediate Hamiltonian method: Pilot applications to vertical excitations in p-electron systems. *International Journal of Quantum Chemistry*, 55(2):117–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zimpel:1996:TAM

[ZM96] Zbigniew Zimpel and Paul G. Mezey. A topological analysis of molecular shape and structure. *International Journal of Quantum Chemistry*, 59(5):379–390, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60556.

Zimpel:1997:MGS

[ZM97] Zbigniew Zimpel and Paul G. Mezey. Molecular geometry and symmetry from a differential geometry viewpoint. *International Journal of Quantum Chemistry*, 64(6):669–678, September 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42728; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42728&PLACEBO=IE.pdf.

Zakrzewski:1994:SAE

[ZO94] V. G. Zakrzewski and J. V. Ortiz. Semidirect algorithms in electron propagator calculations. *International Journal of Quantum Chemistry. Symposium*, 28:23–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Zakrzewski:1995:SAT

[ZO95] V. G. Zakrzewski and J. V. Ortiz. Semidirect algorithms for third-order electron propagator calculations. *International Journal of Quantum Chemistry*, 53(6):583–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zakrzewski:1996:CPM

[ZON+96] V. G. Zakrzewski, J. V. Ortiz, Jeffrey A. Nichols, Dodi Heryadi, Danny L. Yeager, and Joseph T. Golab. Comparison of perturbative and multiconfigurational electron propagator methods.

International Journal of Quantum Chemistry, 60(1):29–36, October 5, 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60592.

Zou:1992:REM

[Zou92] P. F. Zou. A regional embedding method. *International Journal of Quantum Chemistry*, 44(6):997–??, December 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zupan:1997:DGA

[ZPBC97] Aleš Zupan, John P. Perdew, Kieron Burke, and Mauro Causà. Density-gradient analysis for density functional theory: Application to atoms. *International Journal of Quantum Chemistry*, 61(5):835–845, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42467; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42467&PLACEBO=IE.pdf.

Zulicke:1997:IVW

[ZRNZ97] L. Zülicke, F. Ragnetti, R. Neumann, and Ch. Zuhrt. Ionized van der Waals systems: Structure and interactions. *International Journal of Quantum Chemistry*, 64(2):211–222, August 5, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42683; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42683&PLACEBO=IE.pdf. Special Issue: *Second Triennial Congress of the International Society for Theoretical Chemical Physics*. Issue Edited by Seán P. McGlynn, Kresimir Rupnik, Janos Ladik.

Zhu:1997:ABN

[ZSK97] H.-Y. Zhu, T. G. Schmalz, and D. J. Klein. Alternant boron nitride cages: A theoretical study. *International Journal of Quantum Chemistry*, 63(2):393–401, May 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42583; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42583&PLACEBO=IE.pdf.

Zacarias:1997:DFS

[ZTC97] Angélica Zacarías, Hugo Torrens, and Miguel Castro. A density functional study of $Fe - N_2$, $Fe - N_2^+$, and $Fe - N_2^-$. *International Journal of Quantum Chemistry*, 61(3):467–473, January 20, 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42414; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42414&PLACEBO=IE.pdf`.

Zhang:1996:NHHa

[ZW96a] L. Zhang and P. Winkler. Negative hydrogen and helium in a variety of Debye plasmas. *International Journal of Quantum Chemistry*, 60(7):431–??, 1996. CODEN IJQCB2.

Zhang:1996:NHHc

[ZW96b] L. Zhang and P. Winkler. Negative hydrogen and helium in a variety of Debye plasmas. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 30(??):431–??, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Zhang:1996:NHHb

[ZW96c] Li Zhang and Peter Winkler. Negative hydrogen and helium in a variety of Debye plasmas. *International Journal of Quantum Chemistry*, 60(7):1643–1650, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60725`.

Zhao:1996:CCC

[ZW96d] Honggang Zhao and Yin Wang. Calculation of the coefficients of the characteristic polynomial from its subgraphs. *International Journal of Quantum Chemistry*, 59(2):97–102, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60529`.

Zicovich-Wilson:1998:USAa

[ZWD98a] C. M. Zicovich-Wilson and R. Dovesi. On the use of symmetry-adapted crystalline orbitals in SCF-LCAO periodic calculations. I. The construction of the symmetrized orbitals. *International Journal of Quantum Chemistry*, 67

(5):299–309, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29908; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29908&PLACEBO=IE.pdf.

Zicovich-Wilson:1998:USAb

[ZWD98b] C. M. Zicovich-Wilson and R. Dovesi. On the use of symmetry-adapted crystalline orbitals in SCF-LCAO periodic calculations. II. Implementation of the self-consistent-field scheme and examples. *International Journal of Quantum Chemistry*, 67(5):311–320, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29909; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29909&PLACEBO=IE.pdf.

Zicovich-Wilson:1995:AMC

[ZWJP95] C. Zicovich-Wilson, W. Jaskólski, and J. Planelles. Atoms and molecules in cavities: A method for study of spatial confinement effects. *International Journal of Quantum Chemistry*, 54(1):61–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zicovich-Wilson:1994:SCS

[ZWPJ94] C. Zicovich-Wilson, J. H. Planelles, and W. Jaskólski. Spatially confined simple quantum mechanical systems. *International Journal of Quantum Chemistry*, 50(6):429–??, June 5, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhong:1996:RIT

[ZWZ96a] Shi-Jun Zhong, Yin-Gui Wang, and Qian-Er Zhang. Real irreducible tensorial sets. *International Journal of Quantum Chemistry*, 59(3):173–182, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60537.

Zhong:1996:SRM

[ZWZ96b] Shi-Jun Zhong, Yin-Gui Wang, and Qian-Er Zhang. Symmetry reduction of the matrix elements of a two-particle operator. *International Journal of Quantum Chemistry*, 60(4):833–841,

???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60656.

Zhu:1994:SAD

[ZY94] T. Zhu and W. Yang. Structure of the ammonia dimer studied density functional theory. *International Journal of Quantum Chemistry*, 49(5):613–??, February 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:1995:SSU

[ZYY95] J. Zhu, J-M Yan, and D.-Y. Yan. Studies on the structural unit and suspending terminal groups in the quasi-one-dimensional periodic system. *International Journal of Quantum Chemistry*, 56(2):81–??, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zheng:1993:EMM

[ZZ93] X. Zheng and M. C. Zerner. Electric multipole moment integrals evaluated over Slater-type orbitals. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, 27:431–??, 1993. CODEN IJQSDI. ISSN 0161-3642.

Zuelicke:1994:IDS

[ZZCSE94] L. Zuelicke, C. Zuhrt, X. Chapuisat, and C. Saint-Espes. Internal dynamics of simple floppy molecules. *International Journal of Quantum Chemistry*, 52(1):227–??, September 15, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhan:1994:CFR

[ZZW94] H. Zhan, Y. Zhang, and P. Winkler. The calculation of Feshbach resonances using coupled propagator equations. *International Journal of Quantum Chemistry. Symposium*, 28:103–??, 1994. CODEN IJQSAF. ISSN 0538-821X.

Zhidomirov:1996:SWM

[ZZZY96] G. M. Zhidomirov, N. U. Zhanpeisov, I. L. Zilberberg, and I. V. Yudanov. On some ways of modifying semiempirical quantum chemical methods. *International Journal of Quantum Chemistry*, 58(2):175–184, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60473.