# A Bibliography of Publications in *The International Journal of Quantum Chemistry*: 1980–1989


Nelson H. F. Beebe
University of Utah
Department of Mathematics, 110 LCB
155 S 1400 E RM 233
Salt Lake City, UT 84112-0090
USA

Tel: +1 801 581 5254
FAX: +1 801 581 4148

E-mail: `beebe@math.utah.edu`, `beebe@acm.org`, `beebe@computer.org` (Internet)
WWW URL: `https://www.math.utah.edu/~beebe/`



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## Title word cross-reference

Sch81, Sch83a, ZJŻ88, vDTBN80]. $^{+}_{3}$ [NPL89a]. $^{-}$ [AM83a, BN84, CS83c, HL80, LS86, SOS84a, SOS84b, SJ85, SHP+80, vDTBN80, NS82b]. $^{-1}$ [Del87]. $^{0}$ [GLLOB88, Ing80, LC82a]. $^{1}$ [DS80a, LR89, MASF88, NS82b, SG81a, Vog86]. $^{1+}$ [TL82]. $^{1,3}$ [Mül81, DMB86]. $^{13}$ [FGM87]. $^{14}$ [JMS+85]. $^{17}$ [LCCW87]. $^{19}$ [KGEP89, KG89, RDG+86]. $^{1}\Sigma^{+}$ [DG85]. $^{2}$ [AM84, Kun86, Sim81, Var87]. $^{2+}$ [GM86a, GP83a, KD80b, LG84, TL82]. $^{2+}_{2}$ [VBS85]. $^{2}\Delta$ [KG86a, KG86b]. $^{2}p$ [Yar87]. $^{2}\Pi$ [LLS83]. $^{2}S_{1/2}$ [ST84]. $^{2}\Sigma^{+}$ [KG86a, KG86b, LLS83]. $^{3}$ [Bri87, GT86, KS89b, LCLC88, Lee83]. $^{3+}$ [CPS81]. $^{31}$ [Gup80, MG80]. $^{35}$ [KG89]. $^{3}\Sigma$ [NP80]. $^{4}$ [Bha80, Bri87, LC82a, PKP+81, SS80b]. $^{5}$ [VARPU84]. $^{6}$ [PKP+81, Tew87, Tew88a, Tew88b]. $^{N}$ [KG85, KG86c, SMJ83]. $^{N-1}$ [Win83]. $^{Phe}$ [LCP81]. $'$ [Gre82]. $''_{2}$ [Mül81]. $_{1}$ [ES81, FCPL84, KD80b, MASF88, PDMC80]. $_{1-x}$ [CE86, CE87, CE88, GOLC87, LOGC86]. $_{10}$ [KKTE80]. $_{1u}$ [LR89]. $_{2}$ [AYBP83, AJY80, AM82, ADT+89, BBH87, BLR81, BMMS81, BF83a, BDK86, Bow86, CBV85, CMDBVMA89, CEB86, CKM81, CV82a, CHKB83, CL83b, CF81b, CH82, CP85b, Dat82, DPC82, DS81b, Del87, DF89, DLVÖ84, DYD89, Don82, DWQ86, ESKG83, ES81, Enz80, EHK83, ESCC85, FD89b, GVVDB89, GT86, GG82a, GDBRV87, GJMLRGSA85, GLLOB86a, GLLOB86b, GLLOB88, GA82, Gub82, HDFL84, HL80, Ish86, Ish88b, INO88, JTST87, JŻ85, JRK84, JR85, KH85, Kat80, KHCH85, KU80, KBT80, KTS86, KM89b, LPS83b, LJC83, LHC80, LB83, LFL+81, LL89, LC88b, LGL+84, MS87, MTWO83, MSI80, MK80, NT80, Nov83a, NP80, PZ84, PMOW89, PR83, PDC80, PDMC82, PDKC84, PSBB83, RS86, Rér89, RBL84, RS88, RKHK88, RKO+89, SD80, SOS84a, SOS84b, SJ85, SJ88, SBE87, Sch80a]. $_{2}$ [Sch81, Sch83a, SAS86, SBB87, SNNG86, Sie83b, Sok81, SSC83, SRL+83, SR87, SS87, STG86, SS88, TNY86, TST89, TL80, VP84, VŻH82, Wea83, WHT86, Wój86a, Wój86b, YOJ81, YKZ+89, ZW83, ZJŻ88]. $_{2-x}$ [MS88]. $^{+}_{2}$ [CEB86, CS80b, SBE87]. $^{-}_{2}$ [AM83a]. $_{2n}$ [GBO86a]. $_{2n+2}$ [GBO86a]. $_{2V}$ [PSBB83]. $_{3}$ [BLR81, BMMS81, BR80, BFOP83, CBV85, CPS89, CD87a, CV82a, CHKB83, CF81b, DK87, DS81b, DSB84, Del87, ES81, FD89b, Ish86, Ish88b, KHCH85, KBT80, KKTE80, KTS86, LJC83, LS86, LWZ88, LGL+84, Mül81, PXLC86, RKHK88, RKO+89, SJ88, Sch83a, SRL+83, SS87, SR80, SS88, TMO86, Wój86a, Wój86b]. $^{+}_{3}$ [LWZ88]. $_{4}$ [BLR81, BR80, FN84, FD89b, GA82, KBT80, KKTE80, KTS86, LH85, LLAG89, LGL+84, MS88, NC84, PDC81b, SM85, TST89, VŻH82, WHT86]. $^{2-}_{4}$ [LOR84]. $_{5}$ [BLR81, BR80, BDK86, KBT80, LH85, MMB84, Sch80a, SJRP88, SHP+80, TWL82]. $_{6}$ [BR82, Dat82, GP86b, GVB80, HDTR83, KFD85, KKTE80, MOT+83, PZ84, PG89, SHP+80, TWL82]. $^{n-}_{6}$ [MTO+81, MK83]. $_{7}$ [BFOP83, MMB84, Sch81]. $_{8}$ [CH82]. $_{a}$ [Cal84, PO85, XYSJ81]. $_{\alpha}$ [CPGP83, GLP83, GBO86b, IST89, OM81, PXLC86, RSGK88, RLS87]. $_{b}$ [Cal84]. $_{c}$ [LSW89, Sch88, SS88]. $_{e}$ [DYD89]. $_{eff}$ [FN83]. $_{f}$ [YKZ+89]. $_{II}$ [MMB84]. $_{K}$ [Nas83]. $_{m}$ [Che80]. $_{N}$ [Ser84, CBV85, Che80, Del87, INFU84, PFLB83, SOS84a, SOS84b, SJ85, Sin89, TL80, Wor81]. $_{n-1}$ [SMD83, Del87]. $^{2+}_{n}$ [GLLOB86a]. $_{\pi}$ [HDFL84]. $_{rs}$ [BAG83a]. $_{\sigma}$ [HDFL84]. $_{x}$ [CE86, CE87, CE88, GOLC87, KKA80b, LOGC86, MS88]. $A+BC \rightarrow AC+B$ [Var85]. $\alpha$ [Blo83b, BF81, BS80c, CY80, DG86, DC86, EHK83, GN87, HKK+82, Jon84, JBW87, JR85, KT80a, LHC80, LHK81, Mof81, Mof82, MP84a, Nag87, SA80, SRP81, SC89, SPSG85, SNSM82, TMO86, TH81b, Vol88, vDTBN80]. $\alpha_R$ [MMB84]. $B$ [Lee83]. $\beta$ [Cio88b, DS80b, DM83a, EHK83, HKK+82, LCP+88, MSC+83b, PKH+81, SHH+83a, Tho80, VU85]. $\beta(1 \rightarrow 3)$ [YL83]. $\beta(1 \rightarrow 4)$ [Yad83]. $\beta^-$ [IHI80]. $c$ [AWCL89]. $\mathcal{L}^2$ [YKZ+89]. $\cdot$ [CLP83, Del87, LG84, LP80, SHP+80, TTRL88, VŻH82, Wój86a]. $d$ [BSZ81, FFF88, JN88, LÖ85b, Mod81, Mor83, RFST85, SIJ85, Yan85]. $\delta$ [HKK+82]. $\Delta^2$ [Tew88a]. $\delta E/\delta R$ [Eps87]. $\Delta E_{\mathrm{SCF}}$ [PZ84]. $E$ [JBW87]. $E \otimes \epsilon$ [Sin81]. $\eta^5$ [XHR86]. $\exp(-r)$ [Ten88a]. $f$ [FF80, LÖ85b]. $g$ [LHC80]. $G(1,2)$ [SL86]. $\gamma$ [GM86c]. $K$ [MTLL82, Ish83, Kut80]. $k \cdot p$ [DDP81a, DDP81b]. $m$ [AW82]. $\mu$ [NDBE82]. $\mu^+$ [KB80]. $N$ [BFC80, ERB82, GM86b, Gru85, HDO88, Kry82c, Mor89, ST89, WB89, BB82a, BKJ88, GOLC87, Gre81b, MMN87, OG86, Sch83b, SV82, TV83a, TV83b, TV84, TV89, Van85, VT85, Van86]. $n = 0,2,3,4$ [SOS84a]. $n = 1,2$ [SOS84b, SJ85]. $n = 1--4$ [TL80]. $n = 3--7$ [GBO86a]. $n = 4,3$ [MOT+83, MK83]. $n^{i\grave{e}me}$ [SV82]. $nl4f$ [JMS88]. $ns^2$ [SB83a]. $\Omega$ [WS82]. $O \supset T \supset D_2$ [Her84]. $p$ [FC80a, FC81a, LÖ85b]. $\pi$ [BB82a, CGT86b, Cio88b, DMB86, FMF80, GTB80, Gre87, Has82a, Has82b, Has82c, KSSH85, PMT84, TN80, WK83, YZ85, Živ86, Živ87c]. $R$ [EKBE86, Lin89]. $r_{12}^{-1}$ [LKB89]. $\rho_2$ [CL85]. $\rightarrow$ [AM82, ES81, GT86, GT87a, HDFL84, KS89b, LB83, NS82b, SBE87, SS87, YKZ+89]. $\rightleftharpoons$ [TOK80]. $S$ [Ave84c, CJZ+86, LÖ85b, RSST86, STS83]. $S_{N1+N2} \supset S_{N1} \otimes s_{n2}$ [Wen86]. $\sigma$ [Bha82c, Kle83, PMT84]. SO(3) [ACCYCC80]. SU(2) [ZS85]. su($n$) [TV83a, TV83b, TV84, TV89, Van85, VT85, Van86]. $T$ [WS82, Lin81b]. $T_d \supset T \supset D_2$ [Her84]. U($n$) [Bor82]. $U(n = n_1 + n_2){:}\,U(n_1) \times u(n_2)$ [GP86a]. $U(n_1 + n_2) \supset u(n_1) \otimes u(n_2)$ [Wen86]. $V$ [ACCYCC80]. $\varphi = A\exp(-\alpha r^{\nu})$ [Tay81]. $\varphi_4$ [ECM89]. $xy$ [LB86]. $Z$ [BVGV89, Kin89, Mez83d].

***** [BB82a].

**-5** [Gre82]. **-adrenergic** [PKH+81]. **-adrenoceptor** [DS80b]. **-aminobutyric** [GM86c]. **-ary** [OG86]. **-band** [Mor83]. **-bonded** [Kle83]. **-carbolines** [MSC+83b]. **-catalyzed** [SRC84]. **-chymotrypsin** [SNSM82]. **-classes** [FEKC84]. **-coupled** [ERB82]. **-coupling** [ACCYCC80]. **-cyano** [Mof82]. **-cyanocarbonium** [Mof81]. **-cyclodextrin** [MP84a]. **-cyclopentadienyl** [XHR86]. **-D** [ddF86]. **-Decay** [IHI80]. **-deoxy-** [LMG85]. **-deoxyfuranose** [LMG85]. **-deoxyuridines** [SP82a]. **-dimensional** [AW82, GM86b]. **-donor** [Bha82c]. **-doped** [BKJ88]. **-electron** [Cio88b, Sch83b, Živ86, Živ87c]. **-end** [KG80]. **-endorphins**

[OM82c]. **Pseudodegenerate** [EB82b]. **Pseudopotential** [SSF$^+$84, Sza85, TLDK89, BL81c, DF86, Gás83, GG85, KSO84, Mor83, WBK86, GPN80, Bra86b]. **pseudopotential-CI** [WBK86]. **pseudopotentials** [Coh83, GG81, GG82b, GG82a, GG83]. **pseudoresonances** [WOT89]. **pseudorotation** [LMG85]. **Pt** [PR83, BDK86, KKTE80]. **PtCl** [LOR84]. **Publications** [Ano89-29, Cal81a]. **publishers** [Ågr87c]. **Publishing** [Ågr80, Ågr87a, Cal86a, Dun80, Gos80, Mic87, Ågr87b]. **puckering** [Wol88]. **Pullman** [LM81, Mar81a]. **Pulsed** [KKCM85, KKC$^+$86, KKCM87]. **pulses** [BSD82]. **pure** [Gos82b, KS82, Was89]. **Purine** [LGPP$^+$80, KBR83]. **purines** [Cal84, Eis88, SS81b]. **purity** [LW81]. **putative** [CLL86]. **pyramidal** [RK82]. **pyran** [FA86]. **pyrazofurins** [CS81]. **pyrazolones** [KKA$^+$84]. **pyrene** [PZPL86, SG80a, UT80]. **pyridine** [BH89b, IHI80, TW88, YZ85, TS81]. **pyridines** [POK85]. **pyridinone** [Sch82]. **pyrimidines** [BCD$^+$80, Eis88, SS81b]. **pyrolysis** [GMP84b]. **pyrrole** [IHI80, LP80, RDG84b, SRS81]. **pyrrolidine** [Sap80]. **pyruvate** [KK83, MSM81]. **Pyykkö** [Ågr88].

**QCLDB** [OYH$^+$80]. **QSAR** [BNS$^+$87, CNT89, MFM89, RSNT88]. **QSARs** [Lew88]. **quadratic** [CV85, Niu84a]. **Quadratically** [HGPF89, Sla85]. **quadruple** [Cul89]. **quadrupole** [JD85, Mak80, SS81a]. **qualitative** [BW80, SL81, TP87]. **Qualitatively** [Dav81]. **quality** [DPC82, GG82b, GG82a, LT89, Mcd81a, PDMC80, PDC80, PDC81a, PDC81b, PDMC82, RSST86, RST87, STS83, SP85]. **Quantal** [GVVDB89, CMDBVMA89, DBVMB85, YKZ$^+$89]. **quantique** [Cal81a, SV85a, SV85b]. **quantiques** [TV83a, TV83b, TV84, TV89, Van85, VT85, Van86]. **Quantitative** [AABW80, AAW82b, BJR86, GDR85, SL81, Sey81]. **quantities** [BAG83a]. **quantization** [AL81, GSL86, Gir80, HA84, LAGS89, Ols86]. **Quantum** [BNK86, Ber88, BS83b, BCV80, BVGV89, CBV85, Cal89a, CLL86, Con88b, CAML87, Del83, FGMM80, GGDG86, GGDG87, GD82b, GM83, Gol88, GJMLRGSA85, GK80b, GSS85a, HLKK82, H$^+$90, IMTG80, JL84, JRK84, KJMS85, LOBS86, LM89, LHKK82, LP81b, MG83, Mar89, Mar81a, MSC$^+$83a, MSC$^+$83b, MMI$^+$82, OM82a, OM82b, OM83b, OM83a, OM84, OM85, OM86, OMH89, Pul79, PTG80, RBL84, RBH$^+$86, SZ84, Sew86, SBE$^+$83, SPSG85, Tap86, VMMV80, Woo80, Yad83, Ågr87a, ACP82b, Ano84a, AZY84, Ave86, ALH86, AA89, Bar85, Bec89, Bel80a, Ben81, Ber81, BQS87, BERE85, BV86, Cal82c, CDL82, CD83, CSK87, CB85, ČV88, CCD$^+$84, CT84, CT98, CE86, CE87, CE88, De 80, DFP80, DAPS81, Dew88, Dun87, Eri89, FC81b, FC81c, FC81d, FC83, FC82e, GS89]. **quantum** [GPLP85, GOLC87, GJ83, Gos80, Gre80, Hal80, HKLM85, HCCB86, Hay82, HM85a, HM81, HYS89, Hun80, Jac80, Jas80, Jor89, JJ83, Kau81, Kib83, Kim81, Kot84, Kot82, Kou80, KLDD84, KPS87a, KPS87b, KPS88, KEB87, KB87a, Kun83, LOF83, Lan84, LM81, Lar86b, Law87, LFL$^+$81, LOGC86,

**R**

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