

Roger L. DeKock
Publications

(Student co-authors are listed with an asterisk)

- 1) A Comparison of Carbon Monoxide and Nitrogen as Ligands in Transition Metal Complexes, K. G. Caulton, R. L. DeKock, and R. F. Fenske, *J. Am. Chem. Soc.*, **1970**, *92*, 515-518.
- 2) Electronic Structure and Bonding in Manganese Pentacarbonyl Halides and Hydride, R. F. Fenske and R. L. DeKock, *Inorg. Chem.*, **1970**, *9*, 1053-1060.
- 3) Intramolecular Environmental Effects on the Bonding of Cyanide and Carbonyl, R. L. DeKock, A. C. Sarapu, and R. F. Fenske, *Inorg. Chem.*, **1971**, *10*, 38-43.
- 4) Spectroscopy of Rare Earth Oxide Molecules in Inert Matrices at 4 K, R. L. DeKock and W. Weltner, Jr., *J. Phys. Chem.*, **1971**, *75*, 514-525.
- 5) Preparation and Identification of Intermediate Carbonyls of Nickel and Tantalum by Matrix Isolation, R. L. DeKock, *Inorg. Chem.*, **1971**, *10*, 1205-1211.
- 6) Spectroscopy of Carbon Molecules, IV., K. R. Thompson, R. L. DeKock, and W. Weltner, Jr., *J. Am. Chem. Soc.*, **1971**, *93*, 4688-4695.
- 7) C₂O, CN₂, and C₃O Molecules, R. L. DeKock and W. Weltner, Jr., *J. Am. Chem. Soc.*, **1971**, *93*, 7106-7107.
- 8) Intramolecular Environmental Effects on the Bonding in Transition Metal-Pentacyanonitrosyl Complexes, R. F. Fenske and R. L. DeKock, *Inorg. Chem.*, **1972**, *11*, 437-444.
- 9) Experimental and Theoretical Study of the Electronic Structures of Sulphuryl Fluoride and Perchloryl Fluoride, R. L. DeKock and D. R. Lloyd, *Proc. R. Soc. Lond. A.*, **1972**, *328*, 401-411.
- 10) Photoelectron Spectroscopy and ab initio LCAO MO SCF Calculations on Thiazyl Fluoride, R. L. DeKock, D. R. Lloyd, A. Breeze, G. A. D. Collins, and D. W. J. Cruickshank, *Chem. Phys. Lett.*, **1972**, *14*, 525-527.
- 11) Photoelectron Spectra of Halides V. Experimental and Theoretical Study of the Electronic Structures of ClF, ClF₃, BrF and BrF₃, R. L. DeKock, B. R. Higginson, and D. R. Lloyd, *Mol. Phys.*, **1972**, *24*, 1059-1072.
- 12) Photoelectron Spectra of Halides Part 6. The Spectra of SF₅Cl, BrF₅ and IF₅, R. L. DeKock, B. R. Higginson, and D. R. Lloyd, *Faraday Disc. Chem. Soc.*, **1972**, *54*, 84-92.
- 13) The He^I Photoelectron Spectrum of Sulphur Trioxide, R. L. DeKock and D. R. Lloyd, *J. Chem. Soc.*, **1973**, 526-529.
- 14) HeII Photoelectron Spectra of XeF₂ and KrF₂, R. L. DeKock, *J. Chem. Phys.*, **1973**, *58*, 1267-1268.

- 15) Vacuum Ultraviolet Photoelectron Spectroscopy of Inorganic Molecules, R. L. DeKock and D. R. Lloyd, *Advances in Inorg. Chem. and Radiochem.*, **1974**, *16*, 65-107.
- 16) Some Comments on a "Breakdown" in Koopmans' Theorem, R. L. DeKock, *Chem. Phys. Lett.*, **1974**, *27*, 297-299.
- 17) Correlation of Electronic States of the Positive Ions of Xenon Tetrafluoride, Xenon Oxide Tetrafluoride, and Iodine Pentafluoride, R. L. DeKock, *J. Electron Spectr. and Related Phenomena*, **1974**, *4*, 155-161.
- 18) Proton Affinity and the Frontier Orbital Concept. Predictions and Pitfalls, R. L. DeKock, *J. Am. Chem. Soc.*, **1975**, *97*, 5592-5593.
- 19) Stability of Zerovalent Compounds in the Nickel Triad. Interplay of Ionization Potential and Electron Affinity, R. L. DeKock, *Inorg. Chim. Acta*, **1976**, *19*, L27-L28.
- 20) Ultraviolet Photoelectron Spectra of Thiazyl Chloride, R. L. DeKock, M. A. Shehfeh*, D. R. Lloyd, and P. J. Roberts, *J.C.S. Faraday II*, **1976**, 807-813.
- 21) Gas-Phase Reaction of Ammonia with Thionyl Chloride, R. L. DeKock and M. S. Haddad*, *Inorg. Chem.*, **1977**, *16*, 216-217.
- 22) Ultraviolet Photoelectron Spectroscopy of Inorganic Molecules, R. L. DeKock, *Electron Spectroscopy. Theory, Techniques, and Applications*, Vol. 1, **1977**, pp. 293-353.
- 23) The Symmetry of Atomic States and Atomic Orbitals, R. L. DeKock, A. J. Kromminga and T. S. Zwier*, *J. Chem. Educ.* **1979**, *56*, 510-511.
- 24) Proton Affinity, Ionization Energy, and the Nature of Frontier Orbital Electron Density, R. L. DeKock and M. R. Barbachyn*, *J. Am. Chem. Soc.*, **1979**, *101*, 6516-6519.
- 25) Structure of the Tricyano Ion, R. L. DeKock and D. S. Caswell*, *Inorg. Chim. Acta*, **1979**, *37*, L469-L470.
- 26) Substituent Effects in Cluster Species.3. Structural Consequences of Intercage B Interactions in the Dimer and Trimer of 1,5-C₂B₃H₅, E. L. Andersen, R. L. DeKock, and T. P. Fehlner, *J. Am. Chem. Soc.*, **1980**, *102*, 2644-2650.
- 27) Nature of the Highest Occupied Molecular Orbital in R₂C₂CO₂(CO)₆, R. L. DeKock, T. V. Lubben*, J. Hwang, and T. P. Fehlner, *Inorg. Chem.*, **1981**, *20*, 1627-1628.
- 28) Quantum-Chemical Studies of the Interaction between Hydrogen Fluoride and Cyanide, R. L. DeKock and D. S. Caswell*, *J. Phys. Chem.*, **1981**, *85*, 2639-2642.
- 29) Electronic Structure of Diiron Ferraboranes, E. L. Andersen, R. L. DeKock, and T. P. Fehlner, *Inorg. Chem.*, **1981**, *20*, 3291-3298.
- 30) Electronic Structure and Molecular Topology of Boron and Aluminum Suboxides, R. L. DeKock and M. R. Barbachyn*, *J. Inorg. Nucl. Chem.*, **1981**, *43*, 2645-2647.

- 31) Incorporation of Unsaturated Hydrocarbons into a Borane Cage. A Model for the Irreversible Adsorption of Alkynes, R. L. DeKock, T. P. Fehlner, C. E. Housecroft, T. V. Lubben*, and K. Wade, *Inorg. Chem.*, **1982**, *21*, 25-30.
- 32) Effects of Bridging Hydrogens on Metal-Metal Bonds. 2. UV Photoelectron and UV-Visible Spectra and Quantum-Chemical Calculations for $\text{Fe}_3(\mu_3\text{-CCH}_3)$ and $\text{Co}_3(\text{CO})_9(\mu_3\text{-CCH}_3)$, R. L. DeKock, K. S. Wong, and T. P. Fehlner, *Inorg. Chem.*, **1982**, *21*, 3203-3209.
- 33) On the Validity of the Isolobal Principle: Pentaborane(9) and its Ferraborane Derivatives, R. L. DeKock and T. P. Fehlner, *Polyhedron*, **1982**, *6*, 521-523.
- 34) Calculations on the Orientation of the CH Fragment in $\text{Co}_3(\text{CO})_9(\mu_3\text{-CH})$: Implications for Metal Surfaces, R. L. DeKock and T. P. Fehlner, *Surface Science*, **1982**, *119*, 391-398.
- 35) UV Photoelectron Spectra and Electronic Structure of $(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_2\text{FeB}_2\text{H}_5$. Comparison of the Fe-B Bonding with the Fe-C Bonding in $(\text{CO})_4\text{FeC}_2\text{H}_4$, R. L. DeKock, P. Deshmukh, T. P. Fehlner, C. E. Housecroft, J. S. Plotkin, and S. G. Shore, *J. Am. Chem. Soc.*, **1983**, *105*, 815-822.
- 36) MNDO Study of the Proton Affinity of Fluorinated Formaldehydes and Acetones, R. L. DeKock, C. P. Jasperse* and M. S. Konings*, *J. Mol. Structure*, **1983**, *94*, 343-350.
- 37) Quantum Chemical Calculations on the Structure of $(\text{Cl}_2\text{F})^+$ and Related Molecules, R. L. DeKock, C. P. Jasperse*, D. T. Dao, J. H. Bieda, and J. F. Liebman, *J. Fluorine Chem.*, **1983**, *22*, 575-584.
- 38) On the Structures of $\text{H}^+(\text{CO})_5$ and $\text{H}^+(\text{N}_2)_5$, R. L. DeKock and C. P. Jasperse*, *J. Mol. Structure*, **1983**, *105*, 231-232.
- 39) Fe-Fe B Bonding in $\text{Fe}_2(\text{CO})_6\text{S}_2?$, R. L. DeKock, E. J. Baerends, and A. Oskam, *Inorg. Chem.*, **1983**, *22*, 4158-4159.
- 40) MNDO Studies of Proton Affinity as a Probe of Electronic Structure. 1. General Overview, R. L. DeKock and C. P. Jasperse*, *Inorg. Chem.*, **1983**, *22*, 3839-3843.
- 41) MNDO Studies of Proton Affinity as a Probe of Electronic Structure. 2. Boranes and Carboranes, R. L. DeKock and C. P. Jasperse*, *Inorg. Chem.*, **1983**, *22*, 3843-3848.
- 42) Substituent Effects in Cluster Species. 4. Ultraviolet-Photoelectron Spectroscopic and Molecular Orbital Studies of Carbyne Complexes of Multinuclear Cobalt Carbonyls, R. L. DeKock, P. Deshmukh, T. K. Dutta, T. P. Fehlner, C. E. Housecroft, and J. L-S. Hwang, *Organometallics*, **1983**, *2*, 1108-1116.
- 43) The Nature of the LUMO in $\text{Fe}_2(\text{CO})_6\text{S}_2$ and the Bonding in $\text{Fe}_2(\text{CO})_6\text{S}_2^{2-}$, R. L. DeKock, E. J. Baerends, and R. Hengelmolen*, *Organometallics*, **1984**, *3*, 289-292.

- 44) On the Nature of the First Excited States of the Uranyl Ion, R. L. DeKock, E. J. Baerends, P. M. Boerrigter, and J. G. Snijders, *Chem. Phys. Lett.*, **1984**, *105*, 308-316.
- 45) Electronic Structure and Bonding of $\text{Hg}(\text{CH}_3)_2$, $\text{Hg}(\text{CN})_2$, $\text{Hg}(\text{CH}_3)(\text{CN})$, $\text{Hg}(\text{CCCH}_3)_2$, and $\text{Au}(\text{PMe}_3)(\text{CH}_3)$, R. L. DeKock, E. J. Baerends, P. M. Boerrigter, and R. Hengelmolen*, *J. Am. Chem. Soc.*, **1984**, *106*, 3387-3396.
- 46) Ultraviolet Photoelectron Spectra of Square-Planar Complexes of Nickel Triad Metals. 3. He I and He II Spectra of trans- $[(\text{Pet}_3)_2\text{MXY}]$ (M = Pd, Pt; X = Y = C/C-H, C/C-CH₃, C/N; X = Cl, Y = C/N) and Hartree-Fock-Slater Calculations on Model Compounds, J. N. Louwen, R. Hengelmolen*, D. M. Grove, and A. Oskam, *Organometallics*, **1984**, *3*, 908-918.
- 47) Can F_2H^+ Exist in the Topological Form FHF^+ ?, R. L. DeKock, R. Dutler A. Rauk, and R. D. van Zee*, *Inorg. Chem.*, **1986**, *25*, 3329-3330.
- 48) Structure and Fragmentation of Ag_2H^+ and Ag_2CH_3^+ , R. L. DeKock, R. D. van Zee*, and T. Ziegler, *Inorg. Chem.*, **1987**, *26*, 563-567.
- 49) The Chemical Bond, R. L. DeKock, *J. Chem. Educ.*, **1987**, *64*, 934-941.
- 50) The Three-Center Two-Electron Chemical Bond, R. L. DeKock and W. B. Bosma*, *J. Chem. Educ.*, **1988**, *65*, 194-197.
- 51) The Valence Isoelectronic Molecules CCO , CNN , SiCO , and SiNN in their Triplet Sigma Ground States: Theoretical Predictions of Structures and Infrared Spectra, R. L. DeKock, R. S. Grev, and H. F. Schaefer III, *J. Chem. Phys.*, **1988**, *89*, 3016-3027.
- 52) The Chemistry of μ -dithio-bis-(tricarbonyliron), an Inorganic Mimic of Organic Disulfides 3. Reactions with low Valent Metal Compounds and some Interesting Isolobal Analogies Involving the Products, M. Cowie, R. L. DeKock, T. R. Wagenmaker*, D. Seyferth, R. S. Henderson, and Michael K. Gallagher, *Organometallics*, **1988**, *8*, 119-132.
- 53) The Electronic Structure of the Triplet Sigma States of SiOSi and SiSiO , R. L. DeKock, B. F. Yates, and H. F. Schaefer III, *Inorg. Chem.*, **1989**, *28*, 1680-1684.
- 54) The Lithium Superoxide Radical: Symmetry Breaking Phenomena and Potential Energy Surfaces, W. D. Allen, D. A. Horner, R. L. DeKock, R. B. Remington, and H. F. Schaefer III, *Chem. Phys.*, **1989**, *133*, 11-45.
- 55) Comments upon Correlation of Ionization Energies with a New Electronegativity Scale, R. L. DeKock, *J. Phys. Chem.*, **1990**, *94*, 1713-1714.
- 56) Theoretical Study of the Linear Versus Bent Geometry for Several MX_2 Molecules: MgF_2 , CaH_2 , CaF_2 , CeO_2 , and YbCl_2 , R. L. DeKock, M. A. Peterson*, L. K. Timmer*, E. J. Baerends, and P. Vernooijs, *Polyhedron*, **1990**, *9*, 1919-1934.

- 57) The Electronic Structure and Vibrational Frequencies of CNN and SiNN from Local Density Functional Methods, D. A. Dixon and R. L. DeKock, *J. Chem. Phys.*, **1992**, *97*, 1157-1161.
- 58) Computational Chemistry in the Undergraduate Curriculum, R. L. DeKock, J. D. Madura, F. Rioux, and J. Casanova, *Reviews in Computational Chemistry*, edited by K. B. Lipkowitz and D. B. Boyd, VCH Publishers, New York, **1993**, Vol. 4, 149-228.
- 59) Theoretical Study of the Nature of the Bonding in $[\text{Cp}_2\text{M}(\mu\text{-X})]_2$, Where M = Zr (X = I, PH_2 , and NH) and M = Ti (X = Cl), R. L. DeKock, M. A. Peterson*, L. E. L. Reynolds*, L. H. Chen, E. J. Baerends, and P. Vernooijs, *Organometallics*, **1993**, *12*, 2794-2805.
- 60) Tendency of Reaction, Electrochemistry, and Units, R. L. DeKock, *J. Chem. Educ.*, **1996**, *73*, 955-956.
- 61) Invited book review of Modelling Molecular Structures by Alan Hinchliffe. Review by R. L. DeKock, *J. Molecular Structure (Theochem)*, *369*, 213-214, 1996.
- 62) An invited encyclopedia entry, "Multicenter Bond", R. L. DeKock, in *Macmillan Encyclopedia of Chemistry*, Joseph J. Lagowski, Editor in Chief, Macmillan Reference USA, Simon and Schuster Macmillan, New York, 1997, Volume 3, 989-991.
- 63) A Computational Study of M-M Multiple Bonding in $\text{Ph}_2\text{MMPh}_2^{n-}$, where M = B or Al, and n = 0, 1, or 2, E. L. Hamilton*, J. G. Pruis*, R. L. DeKock, and K. J. Jalkanen, *Main Group Metal Chemistry*, **1998**, *21*, 219-224.
- 64) A Mechanical Analogue for Chemical Potential, Extent of Reaction, and the Gibbs Energy, S. V. Glass* and R. L. DeKock, *J. Chem. Educ.*, **1998**, *75*, 190-193.
- 65) The Crucial Role of Kinetic Energy in Interpreting Ionization Energies, F. Rioux and R. L. DeKock, *J. Chem. Educ.*, **1998**, *75*, 537-539.
- 66) Reaction of NH (X) with Oxygen in a Solid Xenon Matrix: Formation and Infrared Spectrum of Imine Peroxide, HNOO , S. L. Laursen, J. E. Grace, R. L. DeKock, and S. A. Spronk*, *J. Am. Chem. Soc.*, **1998**, *120*, 12583-12594.
- 67) Metal-Metal Cooperativity Effects in Promoting C-H Bond Cleavage of a Methyl Group by an Adjacent Metal Center, J. R. Torkelson, F. H. Antwi-Nsiah, R. MacDonald, M. Cowie, J. G. Pruis*, K. J. Jalkanen, and R. L. DeKock, *J. Am. Chem. Soc.*, **1999**, *121*, 3666-3683.
- 68) The Electronic Structure of Titanacycloalkenes, D. B. Lawson and R. L. DeKock, *J. Phys. Chem. A*, **1999**, *103*, 1627-1633.
- 69) An Instructive Analogy for the Virial Theorem in the H Atom, R. L. DeKock, *J. Chem. Educ.*, **1999**, *76*, 605-606.
- 70) Response to Potential-Energy-Only Models, F. Rioux and R. L. DeKock, *J. Chem. Educ.*, **2002**, *79*, 29-30.

- 71) The Short N–F Bond in N_2F^+ and How Pauli Repulsion Influences Bond Lengths. Theoretical Study of N_2X^+ , NF_3X^+ , and NH_3X^+ (X = F, H), F. M. Bickelhaupt, R. L. DeKock, and E. J. Baerends, *J. Am. Chem. Soc.*, **2002**, *124*, 1500-1505.
- 72) The Electronic Structure and Vibrational Spectrum of *trans*-HNOO, R. L. DeKock, M. J. McGuire, P. Piecuch, W. D. Allen, H. F. Schaefer, III, K. Kowalski, S. A. Kucharski, M. Musial, A. R. Bonner*, S. A. Spronk*, D. B. Lawson, and S. L. Laursen, *J. Phys. Chem. A*, **2004**, *108*, 2893-2903.
- 73) Possible Side Reactions Due to Water in Emulsion Polymerization by Late Transition Metal Complexes II: Deactivation of the Catalyst by a Wacker-Type Reaction, R. L. DeKock, I. H. Hristov, G. D. W. Anderson, I. Göttker-Schnetmann, S. Mecking, and T. Ziegler, *Organometallics*, **2005**, *24*, 2679-2687.
- 74) "Possible Side Reactions Due to Water in Emulsion Polymerization by Late Transition Metal Complexes. 1. Water Complexation and Hydrolysis of the Growing Chain", I. H. Hristov, R. L. DeKock, G. D. W. Anderson, I. Göttker-Schnetmann, S. Mecking, and T. Ziegler, *Inorg. Chem.* **2005**, *44*, 7806-7818.
- 75) "Bond Multiplicity in Transition-Metal Complexes: Applications of Two-Electron Valence Indices", by A. Michalak, R. L. DeKock, and T. Ziegler, *J. of Phys. Chem. A*, **2008**, *112*, 7256-7263
- 76) "Ion Pairs or Neutral Molecule Adducts? Cooperativity in Hydrogen Bonding", by Roger L. DeKock, Laura A. Schipper*, Stephanie C. Dykhouse*, Lee P. Heeringa*, and Benjamin M. Brandsen*, *Journal of Chemical Education*, **2009**, *86*, 1459-1464.