# David F Feller

## List of Publications by Year in Descending Order



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| 183 papers | 16,246 citations | 64 h-index | 124 g-index |
| 189 ext. papers | 17,073 ext. citations | 5.3 avg, IF | 6.87 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 183 | Atomic isotropic hyperfine properties for first row elements (B-F) revisited.. *Journal of Chemical Physics*, **2022**, 156, 034304 | 3.9 | 2 |
| 182 | Elaborated thermochemical treatment of HF, CO, N, and HO: Insight into HEAT and its extensions. *Journal of Chemical Physics*, **2021**, 155, 184109 | 3.9 | 4 |
| 181 | Enthalpy of Formation of CHO (Oxalic Acid) from High-Level Calculations and the Active Thermochemical Tables Approach. *Journal of Physical Chemistry A*, **2019**, 123, 3481-3496 | 2.8 | 5 |
| 180 | Density Functional Theory and the Basis Set Truncation Problem with Correlation Consistent Basis Sets: Elephant in the Room or Mouse in the Closet?. *Journal of Physical Chemistry A*, **2018**, 122, 2598-2603 | 2.8 | 11 |
| 179 | A theoretical study of the adiabatic and vertical ionization potentials of water. *Journal of Chemical Physics*, **2018**, 148, 234308 | 3.9 | 4 |
| 178 | Enthalpy of Formation of NH (Hydrazine) Revisited. *Journal of Physical Chemistry A*, **2017**, 121, 6187-6198 | 2.8 | 21 |
| 177 | Estimating the intrinsic limit of the Feller-Peterson-Dixon composite approach when applied to adiabatic ionization potentials in atoms and small molecules. *Journal of Chemical Physics*, **2017**, 147, 034103 | 3.9 | 9 |
| 176 | The Impact of Larger Basis Sets and Explicitly Correlated Coupled Cluster Theory on the FellerPetersonDixon Composite Method. *Annual Reports in Computational Chemistry*, **2016**, 47-78 | 1.8 | 20 |
| 175 | Application of a convergent, composite coupled cluster approach to bound state, adiabatic electron affinities in atoms and small molecules. *Journal of Chemical Physics*, **2016**, 144, 014105 | 3.9 | 17 |
| 174 | Statistical Electronic Structure Calibration Study of the CCSD(T*)-F12b Method for Atomization Energies. *Journal of Physical Chemistry A*, **2015**, 119, 7375-87 | 2.8 | 11 |
| 173 | Improved accuracy benchmarks of small molecules using correlation consistent basis sets. *Highlights in Theoretical Chemistry*, **2015**, 31-46 | | 1 |
| 172 | A systematic approach to vertically excited states of ethylene using configuration interaction and coupled cluster techniques. *Journal of Chemical Physics*, **2014**, 141, 104302 | 3.9 | 27 |
| 171 | Improved accuracy benchmarks of small molecules using correlation consistent basis sets. *Theoretical Chemistry Accounts*, **2014**, 133, | 1.9 | 59 |
| 170 | Active Thermochemical Tables: dissociation energies of several homonuclear first-row diatomics and related thermochemical values. *Theoretical Chemistry Accounts*, **2014**, 133, 1 | 1.9 | 72 |
| 169 | An expanded calibration study of the explicitly correlated CCSD(T)-F12b method using large basis set standard CCSD(T) atomization energies. *Journal of Chemical Physics*, **2013**, 139, 084110 | 3.9 | 43 |
| 168 | Benchmarks of improved complete basis set extrapolation schemes designed for standard CCSD(T) atomization energies. *Journal of Chemical Physics*, **2013**, 138, 074103 | 3.9 | 66 |
| 167 | Anharmonic zero point vibrational energies: tipping the scales in accurate thermochemistry calculations?. *Journal of Chemical Physics*, **2013**, 138, 044311 | 3.9 | 49 |

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| 166 | Chemical accuracy in ab initio thermochemistry and spectroscopy: current strategies and future challenges. *Theoretical Chemistry Accounts*, **2012**, 131, 1 | 1.9 | 317 |
| 165 | High-level ab initio enthalpies of formation of 2,5-dimethylfuran, 2-methylfuran, and furan. *Journal of Physical Chemistry A*, **2012**, 116, 11768-75 | 2.8 | 32 |
| 164 | Heats of formation of MHxCly (M = Si, P, As, Sb) compounds and main group fluorides from high level electronic structure calculations. *Journal of Physical Chemistry A*, **2012**, 116, 3717-27 | 2.8 | 12 |
| 163 | A Practical Guide to Reliable First Principles Computational Thermochemistry Predictions Across the Periodic Table. *Annual Reports in Computational Chemistry*, **2012**, 1-28 | 1.8 | 74 |
| 162 | Further benchmarks of a composite, convergent, statistically calibrated coupled-cluster-based approach for thermochemical and spectroscopic studies. *Molecular Physics*, **2012**, 110, 2381-2399 | 1.7 | 139 |
| 161 | Chemical accuracy in ab initio thermochemistry and spectroscopy: current strategies and future challenges **2012**, 161-180 | | |
| 160 | Ab initio coupled cluster determination of the heats of formation of C2H2F2, C2F2, and C2F4. *Journal of Physical Chemistry A*, **2011**, 115, 1440-51 | 2.8 | 34 |
| 159 | Ab initio coupled cluster determination of the equilibrium structures of cis- and trans-1,2-difluoroethylene and 1,1-difluoroethylene. *Journal of Physical Chemistry A*, **2011**, 115, 94-8 | 2.8 | 25 |
| 158 | On the effectiveness of CCSD(T) complete basis set extrapolations for atomization energies. *Journal of Chemical Physics*, **2011**, 135, 044102 | 3.9 | 210 |
| 157 | Correction to Ab Initio Coupled Cluster Determination of the Heats of Formation of C2H2F2, C2F2, and C2F4 *Journal of Physical Chemistry A*, **2011**, 115, 3182-3182 | 2.8 | 6 |
| 156 | Thermodynamic properties of arsenic compounds and the heat of formation of the As atom from high level electronic structure calculations. *Journal of Physical Chemistry A*, **2011**, 115, 14667-76 | 2.8 | 14 |
| 155 | Structures and heats of formation of simple alkali metal compounds: hydrides, chlorides, fluorides, hydroxides, and oxides for Li, Na, and K. *Journal of Physical Chemistry A*, **2010**, 114, 4272-81 | 2.8 | 31 |
| 154 | Refined theoretical estimates of the atomization energies and molecular structures of selected small oxygen fluorides. *Journal of Physical Chemistry A*, **2010**, 114, 613-23 | 2.8 | 34 |
| 153 | Infrared spectra of CF(2)=CHD and CF(2)=CD(2): scaled quantum-chemical force fields and an equilibrium structure for 1,1-difluoroethylene. *Journal of Physical Chemistry A*, **2010**, 114, 9309-18 | 2.8 | 17 |
| 152 | Calibration study of the CCSD(T)-F12a/b methods for C2 and small hydrocarbons. *Journal of Chemical Physics*, **2010**, 133, 184102 | 3.9 | 50 |
| 151 | Structures and heats of formation of simple alkaline earth metal compounds: fluorides, chlorides, oxides, and hydroxides for Be, Mg, and Ca. *Journal of Physical Chemistry A*, **2010**, 114, 9349-58 | 2.8 | 37 |
| 150 | High level coupled cluster determination of the structure, frequencies, and heat of formation of water. *Journal of Chemical Physics*, **2009**, 131, 154306 | 3.9 | 34 |
| 149 | High level ab initio energies and structures for the rotamers of 1,3-butadiene. *Journal of Physical Chemistry A*, **2009**, 113, 1601-7 | 2.8 | 36 |

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| 148 | Heats of formation of the H1,2OmSn (m, n = 0-3) molecules from electronic structure calculations. *Journal of Physical Chemistry A*, **2009**, 113, 11343-53 | 2.8 | 50 |
| 147 | A survey of factors contributing to accurate theoretical predictions of atomization energies and molecular structures. *Journal of Chemical Physics*, **2008**, 129, 204105 | 3.9 | 302 |
| 146 | Ab initio structures for 90 degrees -twisted s-trans-1,3-butadiene and cyclooctatetraene: the naked sp2-sp2 bond. *Journal of Physical Chemistry A*, **2008**, 112, 2131-3 | 2.8 | 35 |
| 145 | The CCSD(T) complete basis set limit for Ne revisited. *Journal of Chemical Physics*, **2008**, 129, 194115 | 3.9 | 38 |
| 144 | Vibrational spectroscopy of 1,1-difluorocyclopropane-d0, -d2, and -d4: the equilibrium structure of difluorocyclopropane. *Journal of Physical Chemistry A*, **2007**, 111, 2498-506 | 2.8 | 20 |
| 143 | Basis Sets for Ab Initio Molecular Orbital Calculations and Intermolecular Interactions. *Reviews in Computational Chemistry*, **2007**, 1-43 | | 22 |
| 142 | Probing the limits of accuracy in electronic structure calculations: is theory capable of results uniformly better than "chemical accuracy"?. *Journal of Chemical Physics*, **2007**, 126, 114105 | 3.9 | 82 |
| 141 | Sources of error in electronic structure calculations on small chemical systems. *Journal of Chemical Physics*, **2006**, 124, 054107 | 3.9 | 168 |
| 140 | Comment on Pople versus Dunning basis sets for group IA metal hydrides and some other second row hydrides: The case against a De Facto standard by R.A. Klein and M.A. Zottola [Chem. Phys. Lett. 419 (2006) 254258]. *Chemical Physics Letters*, **2006**, 430, 459-463 | 2.5 | 7 |
| 139 | Enthalpies of formation of gas-phase N3, N3-, N5+, and N5- from Ab initio molecular orbital theory, stability predictions for N5(+)N3(-) and N5(+)N5(-), and experimental evidence for the instability of N5(+)N3(-). *Journal of the American Chemical Society*, **2004**, 126, 834-43 | 16.4 | 182 |
| 138 | The gas and solution phase acidities of HNO, HOONO, HONO, and HONO2. *International Journal of Mass Spectrometry*, **2003**, 227, 421-438 | 1.9 | 37 |
| 137 | Coupled Cluster Theory Determination of the Heats of Formation of Combustion-Related Compounds: CO, HCO, CO2, HCO2, HOCO, HC(O)OH, and HC(O)OOH. *Journal of Physical Chemistry A*, **2003**, 107, 1604-1617 | 2.8 | 94 |
| 136 | Molecular Structure, Vibrational Frequencies, and Energetics of the HCO, HOCO, and HCO2 Anions. *Journal of Physical Chemistry A*, **2003**, 107, 186-190 | 2.8 | 40 |
| 135 | Collision-Induced Dissociation and Theoretical Studies of Ag+(methanol)n, n = 1 4. *Journal of Physical Chemistry A*, **2003**, 107, 2829-2838 | 2.8 | 17 |
| 134 | A Nonparametrized Ab Initio Determination of the Heat of Formation of Hydroxylamine, NH2OH. *Journal of Physical Chemistry A*, **2003**, 107, 10419-10427 | 2.8 | 25 |
| 133 | Coupled Cluster Theory and Multireference Configuration Interaction Study of FO, F2O, FO2, and FOOF. *Journal of Physical Chemistry A*, **2003**, 107, 9641-9651 | 2.8 | 83 |
| 132 | Accurate ab initio study of the energetics of phosphorus nitride: Heat of formation, ionization potential, and electron affinity. *Journal of Chemical Physics*, **2003**, 118, 8290-8295 | 3.9 | 28 |
| 131 | Performance of coupled cluster theory in thermochemical calculations of small halogenated compounds. *Journal of Chemical Physics*, **2003**, 118, 3510-3522 | 3.9 | 184 |

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| 130 | Decomposition Pathways of Peroxynitrous Acid: Gas-Phase and Solution Energetics. *Journal of Physical Chemistry A*, **2002**, 106, 3191-3196 | 2.8 | 77 |
| 129 | On the Enthalpy of Formation of Hydroxyl Radical and Gas-Phase Bond Dissociation Energies of Water and Hydroxyl. *Journal of Physical Chemistry A*, **2002**, 106, 2727-2747 | 2.8 | 422 |
| 128 | Metal Ion Binding: An Electronic Structure Study of M+(Dimethyl Ether)n, M = Cu, Ag, and Au and (n= 1-4), Complexes. *Journal of Physical Chemistry A*, **2002**, 106, 5136-5143 | 2.8 | 17 |
| 127 | Promise and challenge of high-performance computing, with examples from molecular modelling. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2002**, 360, 1079-105 | 3 | 9 |
| 126 | Heats of formation and ionization energies of NHx, x=0-3. *Journal of Chemical Physics*, **2001**, 115, 2576-2581 | 3.9 | 112 |
| 125 | Extended benchmark studies of coupled cluster theory through triple excitations. *Journal of Chemical Physics*, **2001**, 115, 3484-3496 | 3.9 | 236 |
| 124 | Evidence for a Lower Enthalpy of Formation of Hydroxyl Radical and a Lower Gas-Phase Bond Dissociation Energy of Water. *Journal of Physical Chemistry A*, **2001**, 105, 1-4 | 2.8 | 161 |
| 123 | A complete basis set estimate of cation-π bond strengths: Na+(ethylene) and Na+(benzene). *Chemical Physics Letters*, **2000**, 322, 543-548 | 2.5 | 90 |
| 122 | Theoretical study of cation/ether complexes: 15-crown-5 and its alkali metal complexes. *International Journal of Mass Spectrometry*, **2000**, 201, 41-58 | 1.9 | 45 |
| 121 | Barrier for the H2CO-H2+CO reaction: A discrepancy between high-level electronic structure calculations and experiment. *Journal of Chemical Physics*, **2000**, 113, 218-226 | 3.9 | 51 |
| 120 | A CCSDT study of the effects of higher order correlation on spectroscopic constants. I. First row diatomic hydrides. *Journal of Chemical Physics*, **2000**, 112, 5604-5610 | 3.9 | 107 |
| 119 | Performance of CCSDT for diatomic dissociation energies. *Journal of Chemical Physics*, **2000**, 113, 485-493 | 3.9 | 168 |
| 118 | Predicting the Heats of Formation of Model Hydrocarbons up to Benzene. *Journal of Physical Chemistry A*, **2000**, 104, 3048-3056 | 2.8 | 140 |
| 117 | Molecular Dynamics Study of Water-Benzene Interactions at the Liquid/Vapor Interface of Water. *Journal of Physical Chemistry B*, **2000**, 104, 4403-4407 | 3.4 | 42 |
| 116 | Theoretical Conformational Analysis of Thiacrown Macrocycles. *Journal of Physical Chemistry A*, **2000**, 104, 652-660 | 2.8 | 68 |
| 115 | A Theoretical Determination of the Heats of Formation of Furan, Tetrahydrofuran, THF-2-yl, and THF-3-yl. *Journal of Physical Chemistry A*, **2000**, 104, 9017-9025 | 2.8 | 35 |
| 114 | Estimating the Strength of the Water/Single-Layer Graphite Interaction. *Journal of Physical Chemistry A*, **2000**, 104, 9971-9975 | 2.8 | 119 |
| 113 | The Molecular Structure and Ionization Potential of Si2: The Role of the Excited States in the Photoionization of Si2. *Journal of Physical Chemistry A*, **2000**, 104, 2326-2332 | 2.8 | 28 |

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| 112 | Binding Enthalpies for Alkali CationBenzene Complexes Revisited. *Journal of Physical Chemistry A*, **2000**, 104, 11414-11419 | 2.8 | 115 |
| 111 | Novel Binding Modes in Tetramethoxycalix[4]arene:Implications for Ligand Design. *Journal of the American Chemical Society*, **2000**, 122, 10083-10089 | 16.4 | 48 |
| 110 | A comparison of techniques for predicting higher order correlation effects: Diatomic dissociation energies. *Journal of Chemical Physics*, **1999**, 111, 4373-4382 | 3.9 | 75 |
| 109 | Ab initio study of the Wolff rearrangement of C6H4O intermediate in the gas phase. *Russian Chemical Bulletin*, **1999**, 48, 1642-1646 | 1.7 | 3 |
| 108 | Structures and binding enthalpies of M+(H2O)n clusters, M=Cu, Ag, Au. *Journal of Chemical Physics*, **1999**, 110, 1475-1491 | 3.9 | 105 |
| 107 | Strength of the BenzeneWater Hydrogen Bond. *Journal of Physical Chemistry A*, **1999**, 103, 7558-7561 | 2.8 | 136 |
| 106 | Re-examination of atomization energies for the Gaussian-2 set of molecules. *Journal of Chemical Physics*, **1999**, 110, 8384-8396 | 3.9 | 251 |
| 105 | Theoretical Study of the Heats of Formation of Small Silicon-Containing Compounds. *Journal of Physical Chemistry A*, **1999**, 103, 6413-6419 | 2.8 | 118 |
| 104 | Heats of Formation of Simple Perfluorinated Carbon Compounds. *Journal of Physical Chemistry A*, **1999**, 103, 4744-4751 | 2.8 | 129 |
| 103 | Computational Chemistry in the Environmental Molecular Sciences Laboratory **1999**, 215-228 | | 2 |
| 102 | An examination of intrinsic errors in electronic structure methods using the Environmental Molecular Sciences Laboratory computational results database and the Gaussian-2 set. *Journal of Chemical Physics*, **1998**, 108, 154-176 | 3.9 | 235 |
| 101 | Heats of Formation of CF2, FCO, and CF2O. *Journal of Physical Chemistry A*, **1998**, 102, 8209-8216 | 2.8 | 100 |
| 100 | Heats of Formation of Simple Boron Compounds. *Journal of Physical Chemistry A*, **1998**, 102, 7053-7059 | 2.8 | 84 |
| 99 | Theoretical Study of Cation/Ether Complexes:Alkali Metal Cations with 1,2-Dimethoxyethane and 12-Crown-4. *Journal of Physical Chemistry A*, **1998**, 102, 3813-3819 | 2.8 | 87 |
| 98 | Configuration interaction calculations on the state of CP and the - transition bands. Miscellaneous properties. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1998**, 31, 5053-5075 | 1.3 | 12 |
| 97 | Improved estimates of the total correlation energy in the ground state of the water molecule. *Journal of Chemical Physics*, **1997**, 106, 7706-7708 | 3.9 | 32 |
| 96 | A Theoretical Case Study of Substituent Effects and Microsolvation on the Binding Specificity of Crown Ethers. *Journal of Physical Chemistry A*, **1997**, 101, 7292-7298 | 2.8 | 36 |
| 95 | Accurate Calculations of the Electron Affinity and Ionization Potential of the Methyl Radical. *Journal of Physical Chemistry A*, **1997**, 101, 9405-9409 | 2.8 | 60 |

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| 94 | Ab InitioStudy of M+:18-Crown-6 Microsolvation. *Journal of Physical Chemistry A*, **1997**, 101, 2723-2731 | 2.8 | 103 |
| 93 | Theoretical Study of Cation/Ether Complexes: The Alkali Metals and Dimethyl Ether. *Journal of Physical Chemistry A*, **1997**, 101, 6125-6131 | 2.8 | 57 |
| 92 | Hydrogen fluoride: a critical comparison of theoretical and experimental results. *Computational and Theoretical Chemistry*, **1997**, 400, 69-92 | | 35 |
| 91 | Towards a confirmation of theoretical predictions of selected spectroscopic constants for the state of PN. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1996**, 29, 6069-6074 | 1.3 | 6 |
| 90 | An Ab Initio Investigation of the Structure and Alkaline Earth Divalent Cation Selectivity of 18-Crown-6. *Journal of the American Chemical Society*, **1996**, 118, 6052-6059 | 16.4 | 91 |
| 89 | Hydrogen Bond Energy of the Water Dimer. *The Journal of Physical Chemistry*, **1996**, 100, 2993-2997 | | 433 |
| 88 | The structure and binding energy of K+Ether complexes: A comparison of MP2, RI-MP2, and density functional methods. *Journal of Chemical Physics*, **1996**, 105, 1940-1950 | 3.9 | 55 |
| 87 | The role of databases in support of computational chemistry calculations. *Journal of Computational Chemistry*, **1996**, 17, 1571-1586 | 3.5 | 1909 |
| 86 | Configuration-interaction calculations of miscellaneous properties of the CP and molecules: I. CP ground state. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1996**, 29, 5283-5303 | 1.3 | 15 |
| 85 | Electron spin resonance rare gas matrix studies of 12CO2+13CO2+and C17O2: Comparison with ab initio calculations. *Journal of Chemical Physics*, **1996**, 105, 5672-5686 | 3.9 | 16 |
| 84 | CationEther Complexes in the Gas Phase: Bond Dissociation Energies and Equilibrium Structures of Li+(1,2-dimethoxyethane)x, x = 1 and 2, and Li+(12-crown-4). *The Journal of Physical Chemistry*, **1996**, 100, 16116-16125 | | 140 |
| 83 | CationEther Complexes in the Gas Phase: Bond Dissociation Energies and Equilibrium Structures of Li+[O(CH3)2]x, x = 1. *The Journal of Physical Chemistry*, **1996**, 100, 1605-1614 | | 138 |
| 82 | DicationWater Interactions: M2+(H2O)n Clusters for Alkaline Earth Metals M = Mg, Ca, Sr, Ba, and Ra. *The Journal of Physical Chemistry*, **1996**, 100, 4790-4797 | | 140 |
| 81 | The role of databases in support of computational chemistry calculations **1996**, 17, 1571 | | 75 |
| 80 | The dipole moment and magnetic hyperfine properties of the excited A 2(3s)Rydberg state of nitric oxide. *Journal of Chemical Physics*, **1995**, 103, 3517-3525 | 3.9 | 17 |
| 79 | An extended basis set ab initio study of alkali metal cationwater clusters. *Journal of Chemical Physics*, **1995**, 103, 3526-3542 | 3.9 | 214 |
| 78 | Configuration interaction calculations on the P2molecule. III. Spectroscopic properties of the A1Pigstate, the A1Pig- X1Sigmag+transition bands and a comparison with the results for the X1Sigmag+, a3Sigmau+, and b3Pi2,gstates and related transition bands. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1995**, 28, 3135-3146 | 1.3 | 8 |
| 77 | Configuration interaction calculations on the P2molecule. II. Spectroscopic properties of the b32,gstate, the b32,g- a3+transition bands and the a3+state revisited. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1995**, 28, 1393-1410 | 1.3 | 11 |

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| 76 | Cation-Water Interactions: The M+(H2O)n Clusters for Alkali Metals, M = Li, Na, K, Rb, and Cs. *The Journal of Physical Chemistry*, **1995**, 99, 3060-3067 | | 222 |
| 75 | Configuration interaction calculations on the P2molecule. I. Potential energy curves of the X1Sigmag+and a3Sigmau+states of P2; spectroscopic properties. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1994**, 27, 1657-1670 | 1.3 | 15 |
| 74 | An extended basis set ab initio study of Li+(H2O)n, n=1 . *Journal of Chemical Physics*, **1994**, 100, 4981-4997 | 3.9 | 151 |
| 73 | An Ab Initio Investigation of the Structure and Alkali Metal Cation Selectivity of 18-Crown-6. *Journal of the American Chemical Society*, **1994**, 116, 10657-10669 | 16.4 | 335 |
| 72 | The Nature of K+/Crown Ether Interactions: A Hybrid Quantum Mechanical-Molecular Mechanical Study. *The Journal of Physical Chemistry*, **1994**, 98, 10465-10476 | | 154 |
| 71 | Comment on the Hyperfine Structure of the X2.PI. Ground State of Nitric Oxide. *The Journal of Physical Chemistry*, **1994**, 98, 10375-10375 | | 4 |
| 70 | Configuration interaction calculations on the X1Sigma+ground state and low-lying A1Pi and1Delta excited states of the PN molecule. II. Potential energy curves of the A1Pi and1Delta excited states of PN and spectroscopic properties. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1993**, 26, 1915-1934 | 1.3 | 13 |
| 69 | The use of systematic sequences of wave functions for estimating the complete basis set, full configuration interaction limit in water. *Journal of Chemical Physics*, **1993**, 98, 7059-7071 | 3.9 | 526 |
| 68 | A comparison of unrestricted Hartree Fock- and restricted open-shell Hartree Fock-based methods for determining the magnetic hyperfine parameters of NO (X 2 ). *Journal of Chemical Physics*, **1993**, 99, 2829-2840 | 3.9 | 60 |
| 67 | Ab initio study of hydrogen bonding in the phenol water system. *Journal of Computational Chemistry*, **1993**, 14, 1027-1035 | 3.5 | 92 |
| 66 | Valence electron momentum distributions of the hydrogen halides. I. Comparison of EMS measurements and calculations using Hartree Fock limit and configuration interaction wavefunctions for hydrogen fluoride.. *Chemical Physics*, **1993**, 171, 303-317 | 2.3 | 18 |
| 65 | Configuration interaction calculations on the X1Sigma+ground state and low-lying A1Pi and1Delta excited states of the PN molecule. I. Potential energy curve of the X1Sigma+state of PN. Miscellaneous spectroscopic observables. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1992**, 25, 4433-4445 | 1.3 | 18 |
| 64 | Application of systematic sequences of wave functions to the water dimer. *Journal of Chemical Physics*, **1992**, 96, 6104-6114 | 3.9 | 1007 |
| 63 | Theoretical and neon matrix electron spin resonance studies of the methanol cation: CH3OH+, CH3OD+, CH2DOH+, and 13CH3OH+. *Journal of Chemical Physics*, **1992**, 97, 5363-5376 | 3.9 | 40 |
| 62 | Exploiting regularity in systematic sequences of wavefunctions which approach the full CI limit. *Theoretica Chimica Acta*, **1992**, 83, 31-55 | | 39 |
| 61 | Molecular orbital studies of hyperfine coupling constants in the H2CN and H(HO)CN radicals. *The Journal of Physical Chemistry*, **1991**, 95, 4702-4708 | | 46 |
| 60 | Theoretical Approaches to ESR Spectroscopy **1991**, 429-455 | | 7 |
| 59 | Ab initio calculations of the 13C magnetic hyperfine parameters in C+2 using numerical and Gaussian basis set methods. *Chemical Physics Letters*, **1990**, 175, 629-632 | 2.5 | 9 |

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| 58 | Configuration interaction calculations on the propane radical cation, C3H +8. *Theoretica Chimica Acta*, **1990**, 77, 111-122 | | 18 |
| 57 | Hartree-Fock limit and configuration interaction calculations of the ion-molecule overlap amplitude for hydrogen fluoride: Comparison with EMS experiments. *Chemical Physics*, **1990**, 147, 45-50 | 2.3 | 13 |
| 56 | An ab initio study of the magnetic hyperfine properties of F2(2u). *Journal of Chemical Physics*, **1990**, 93, 579-589 | 3.9 | 54 |
| 55 | The electron affinity of oxygen: A systematic configuration interaction approach. *Journal of Chemical Physics*, **1989**, 90, 1024-1030 | 3.9 | 65 |
| 54 | Neon matrix electron spin resonance and theoretical investigations of 10,11BH2, 12,13CH2, and 12,13CH+2. *Journal of Chemical Physics*, **1989**, 91, 4468-4476 | 3.9 | 45 |
| 53 | Electron spin resonance investigations of 11B12C, 11B13C, and 10B12C in neon, argon, and krypton matrices at 4 K: Comparison with theoretical results. *Journal of Chemical Physics*, **1989**, 90, 690-699 | 3.9 | 58 |
| 52 | A multireference CI determination of the isotropic hyperfine constants for first row atoms B. *Journal of Chemical Physics*, **1988**, 88, 7580-7587 | 3.9 | 93 |
| 51 | The generation of 12C31P and 13C31P by reactive laser vaporization for rare gas matrix electron spin resonance studies: Comparison with ab initio theoretical calculations. *Journal of Chemical Physics*, **1988**, 88, 3441-3450 | 3.9 | 21 |
| 50 | CI effects on one-electron properties: the case of the electric quadrupole moment of OCS. *Journal of Physics B: Atomic and Molecular Physics*, **1987**, 20, 5325-5334 | | 4 |
| 49 | ESR and ab initio theoretical studies of the cation radicals 14N+4 and 15N+4: The trapping of ion–neutral reaction products in neon matrices at 4 K. *Journal of Chemical Physics*, **1987**, 87, 885-897 | 3.9 | 82 |
| 48 | One-electron properties of several small molecules using near Hartree–Fock limit basis sets. *Journal of Chemical Physics*, **1987**, 86, 3424-3440 | 3.9 | 221 |
| 47 | Laser sputtering generation of B2 for ESR matrix isolation studies: comparison with ab initio CI theoretical calculations. *Journal of the American Chemical Society*, **1987**, 109, 3521-3525 | 16.4 | 57 |
| 46 | Ab initio studies of [1.1.1]- and [2.2.2]propellane. *Journal of the American Chemical Society*, **1987**, 109, 4133-4139 | 16.4 | 63 |
| 45 | Electron momentum spectroscopy of the valence orbitals of H2O and D2O: Quantitative comparisons using Hartree–Fock limit and correlated wavefunctions. *Chemical Physics*, **1987**, 113, 19-42 | 2.3 | 169 |
| 44 | Basis set selection for molecular calculations. *Chemical Reviews*, **1986**, 86, 681-696 | 68.1 | 680 |
| 43 | Neon matrix ESR and CI theoretical investigation of 10BF+ and 11BF+: Photoionization of BF from reactive laser sputtering and high temperature sources. *Journal of Chemical Physics*, **1986**, 85, 5437-5445 | 3.9 | 29 |
| 42 | Neon matrix ESR and CI theoretical investigation of AlF+; photoionization of AlF from thermal and laser sputtering generation methods. *Journal of the American Chemical Society*, **1986**, 108, 5065-5071 | 16.4 | 39 |
| 41 | Theoretical investigations of the electronic states of porphyrins. III. Low-lying electronic states of porphinatoiron(II). *International Journal of Quantum Chemistry*, **1985**, 28, 773-796 | 2.1 | 36 |

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| 40 | Difficulties inab initio CI calculations of the hyperfine structure of small radicals. *Theoretica Chimica Acta*, **1985**, 68, 57-67 | | 86 |
| 39 | Theoretical investigations of the electronic states of porphyrins. IV. Low-lying electronic states of bisammineporphinatoiron(II). *International Journal of Quantum Chemistry*, **1985**, 28, 797-822 | 2.1 | 4 |
| 38 | Theoretical investigations of Fe porphyrins. V. Low-lying electronic states of bisammineporphinatoiron(III). *International Journal of Quantum Chemistry*, **1985**, 28, 823-842 | 2.1 | 4 |
| 37 | Ab initio multireference CI determinations of the electron affinity of carbon and oxygen. *Journal of Chemical Physics*, **1985**, 82, 4135-4141 | 3.9 | 54 |
| 36 | Some aspects of the triplet di-.pi.-methane rearrangement: comparison of the ring opening of cyclopropyldicarbinyl and cyclopropylcarbinyl. *Journal of the American Chemical Society*, **1985**, 107, 5054-5059 | 16.4 | 12 |
| 35 | Ab initio calculations on the diphosphine radical cation (P2H4+.cntdot.). *Journal of the American Chemical Society*, **1985**, 107, 2596-2597 | 16.4 | 10 |
| 34 | The generation and trapping of the high-temperature oxosilyliumyl cation radicals (28SiO+ and 29SiO+) in neon matrixes at 4 K; an ESR and ab initio CI theoretical investigation. *Journal of the American Chemical Society*, **1985**, 107, 2857-2864 | 16.4 | 56 |
| 33 | Ab initio configuration interaction calculations of the hyperfine structure in small radicals. *Journal of Chemical Physics*, **1984**, 80, 1006-1017 | 3.9 | 158 |
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