# Russell J Boyd

## List of Publications by Year in descending order

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|---|---|---|---|
| 313 papers | 9,252 citations | 47006 47 h-index | 71685 76 g-index |
| 325 all docs | 325 docs citations | 325 times ranked | 6131 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | On the Importance of Prereactive Complexes in Moleculeâ^'Radical Reactions:â€‰ Hydrogen Abstraction from Aldehydes by OH. Journal of the American Chemical Society, 2001, 123, 2018-2024. | 13.7 | 244 |
| 2 | Electron affinities and ionization potentials of nucleotide bases. Chemical Physics Letters, 2000, 322, 129-135. | 2.6 | 226 |
| 3 | Extended Weak Bonding Interactions in DNA:Â Ï€-Stacking (Baseâ^'Base), Baseâ^'Backbone, and Backboneâ^'Backbone Interactionsâ€. Journal of Physical Chemistry B, 2006, 110, 563-578. | 2.6 | 215 |
| 4 | Density Functional Study of the Proline-Catalyzed Direct Aldol Reaction. Journal of Physical Chemistry A, 2002, 106, 5155-5159. | 2.5 | 188 |
| 5 | Sulfur-sulfur bond lengths, or can a bond length be estimated from a single parameter?. Journal of the American Chemical Society, 1988, 110, 7299-7301. | 13.7 | 179 |
| 6 | Polarizable pointâ€charge model for water: Results under normal and extreme conditions. Journal of Chemical Physics, 1996, 105, 4742-4750. | 3.0 | 167 |
| 7 | Characterization of a Closed-Shell Fluorineâ^'Fluorine Bonding Interaction in Aromatic Compounds on the Basis of the Electron Density. Journal of Physical Chemistry A, 2005, 109, 3669-3681. | 2.5 | 165 |
| 8 | Group electronegativities from the bond critical point model. Journal of the American Chemical Society, 1992, 114, 1652-1655. | 13.7 | 145 |
| 9 | The shell structure of atoms and the Laplacian of the charge density. Journal of Chemical Physics, 1988, 88, 4375-4377. | 3.0 | 140 |
| 10 | Hydrogen bonding between nitriles and hydrogen halides and the topological properties of molecular charge distributions. Chemical Physics Letters, 1986, 129, 62-65. | 2.6 | 136 |
| 11 | A Density Functional Study of Methanol Clusters. Journal of Chemical Theory and Computation, 2007, 3, 54-61. | 5.3 | 128 |
| 12 | Atomic and group electronegativities from the electron-density distributions of molecules. Journal of the American Chemical Society, 1988, 110, 4182-4186. | 13.7 | 123 |
| 13 | A bond-length-bond-order relationship for intermolecular interactions based on the topological properties of molecular charge distributions. Chemical Physics Letters, 1985, 120, 80-85. | 2.6 | 122 |
| 14 | An Introduction to the Quantum Theory of Atoms in Molecules. , 0, , 1-34. | | 121 |
| 15 | A theoretical study of 5-halouracils: electron affinities, ionization potentials and dissociation of the related anions. Chemical Physics Letters, 2001, 343, 151-158. | 2.6 | 118 |
| 16 | The 28-Electron Tetraatomic Molecules:â€‰ N4, CN2O, BFN2, C2O2, B2F2, CBFO, C2FN, and BNO2. Challenges for Computational and Experimental Chemistry. The Journal of Physical Chemistry, 1996, 100, 5702-5714. | 2.9 | 113 |
| 17 | An SCFâ€“MOâ€“CNDO study of equilibrium geometries, force constants, and bonding energies: CNDO/BW. Part I. Parameterization. Journal of the Chemical Society Dalton Transactions, 1972, , 73-77. | 1.1 | 110 |
| 18 | Coming to Grips with Nâ^'HÂ·Â·Â·N Bonds. 1. Distance Relationships and Electron Density at the Bond Critical Point. Journal of Physical Chemistry A, 2001, 105, 6552-6566. | 2.5 | 101 |

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| 19 | Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16. | 2.5 | 99 |
| 20 | Selenium stories. Nature Chemistry, 2011, 3, 570-570. | 13.6 | 97 |
| 21 | A quantum mechanical explanation for Hund's multiplicity rule. Nature, 1984, 310, 480-481. | 27.8 | 92 |
| 22 | A theoretical investigation of the structures and properties of peroxyl radicals. Journal of the American Chemical Society, 1990, 112, 5724-5730. | 13.7 | 91 |
| 23 | Coulomb hole in some excited states of helium. Journal of Physics B: Atomic and Molecular Physics, 1973, 6, 782-793. | 1.6 | 88 |
| 24 | Coming to Grips with Nâ^'HÂ·Â·Â·N Bonds. 2. Homocorrelations between Parameters Deriving from the Electron Density at the Bond Critical Point. Journal of Physical Chemistry A, 2003, 107, 272-284. | 2.5 | 86 |
| 25 | Molecular Model with Quantum Mechanical Bonding Information. Journal of Physical Chemistry A, 2011, 115, 12991-12997. | 2.5 | 86 |
| 26 | Radiation Products of Thymine, 1-Methylthymine, and Uracil Investigated by Density Functional Theory. Journal of Physical Chemistry B, 1998, 102, 5369-5377. | 2.6 | 83 |
| 27 | Comparison of Experimental and Calculated Hyperfine Coupling Constants. Which Radicals Are Formed in Irradiated Guanine?. Journal of Physical Chemistry B, 1998, 102, 9332-9343. | 2.6 | 82 |
| 28 | Tautomeric Equilibria of Hydroxypyridines in Different Solvents:Â An ab Initio Study. The Journal of Physical Chemistry, 1996, 100, 16141-16146. | 2.9 | 78 |
| 29 | The Fermi hole in atoms. Journal of Physics B: Atomic and Molecular Physics, 1974, 7, 1805-1816. | 1.6 | 70 |
| 30 | Theoretical Investigation of Adenine Radicals Generated in Irradiated DNA Components. Journal of Physical Chemistry B, 1998, 102, 10602-10614. | 2.6 | 69 |
| 31 | Effects of Ionizing Radiation on Crystalline Cytosine Monohydrate. Journal of Physical Chemistry B, 1998, 102, 7484-7491. | 2.6 | 68 |
| 32 | The relative sizes of atoms. Journal of Physics B: Atomic and Molecular Physics, 1977, 10, 2283-2291. | 1.6 | 67 |
| 33 | An ab initio study of model SN2 reactions with inclusion of electron correlation effects through second-order Moeller-Plesset perturbation calculations. Journal of the American Chemical Society, 1990, 112, 6789-6796. | 13.7 | 67 |
| 34 | Cooperativity between hydrogen bonds and beryllium bonds in (H2O)nBeX2 (n = 1â€“3, X = H, F) complexes. A new perspective. Physical Chemistry Chemical Physics, 2012, 14, 14540. | 2.8 | 67 |
| 35 | Alkoxy radicals in the gaseous phase: Î²-scission reactions and formation by radical addition to carbonyl compounds. Canadian Journal of Chemistry, 2003, 81, 431-442. | 1.1 | 58 |
| 36 | Electronegativities of the elements from a nonempirical electrostatic model. Journal of Chemical Physics, 1981, 75, 5385-5388. | 3.0 | 57 |

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| 37 | Transition-state electronic structures in SN2 reactions. Journal of the American Chemical Society, 1989, 111, 1575-1579. | 13.7 | 56 |
| 38 | Changing Weak Halogen Bonds into Strong Ones through Cooperativity with Beryllium Bonds. Journal of Physical Chemistry A, 2014, 118, 4205-4213. | 2.5 | 54 |
| 39 | Electron density partitioning in atoms. Journal of Chemical Physics, 1977, 66, 356-358. | 3.0 | 53 |
| 40 | Atomic contributions to bond dissociation energies in aliphatic hydrocarbons. Journal of Chemical Physics, 2006, 125, 204103. | 3.0 | 53 |
| 41 | Sulfonyl radicals, sulfinic acid, and related species: an abinitio molecular orbital study. Canadian Journal of Chemistry, 1980, 58, 331-338. | 1.1 | 52 |
| 42 | Ab initio studies of reactions of hydroxyl radicals with fluorinated ethanes. The Journal of Physical Chemistry, 1995, 99, 13402-13411. | 2.9 | 52 |
| 43 | A hybrid quantum mechanical force field molecular dynamics simulation of liquid methanol: Vibrational frequency shifts as a probe of the quantum mechanical/molecular mechanical coupling. Journal of Chemical Physics, 1996, 104, 7261-7269. | 3.0 | 52 |
| 44 | QTAIM Study of an Î±-Helix Hydrogen Bond Network. Journal of Physical Chemistry B, 2009, 113, 10957-10964. | 2.6 | 52 |
| 45 | Density Functional Theory Study of the Reaction Mechanism and Energetics of the Reduction of Hydrogen Peroxide by Ebselen, Ebselen Diselenide, and Ebselen Selenol. Journal of Physical Chemistry A, 2007, 111, 3152-3160. | 2.5 | 51 |
| 46 | Stereoselective Synthesis of a Potent Thrombin Inhibitor by a Novel P2â˜’P3 Lactone Ring Opening. Journal of Organic Chemistry, 2004, 69, 3620-3627. | 3.2 | 50 |
| 47 | Electronic and structural properties of borazine and related molecules. Chemical Physics Letters, 1984, 112, 136-141. | 2.6 | 49 |
| 48 | Effects of electron correlation on the series C2HnF6-n (n = 0-6): geometries, total energies, and C-C and C-H bond dissociation energies. The Journal of Physical Chemistry, 1993, 97, 7208-7215. | 2.9 | 48 |
| 49 | A Comprehensive Study of Sugar Radicals in Irradiated DNA. Journal of Physical Chemistry B, 1998, 102, 7674-7686. | 2.6 | 48 |
| 50 | The effect of electron correlation on the topological and atomic properties of the electron density distributions of molecules. Journal of Computational Chemistry, 1989, 10, 367-375. | 3.3 | 47 |
| 51 | Recent applications of density functional theory calculations to biomolecules. Theoretical Chemistry Accounts, 2002, 108, 1-11. | 1.4 | 47 |
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| 53 | The first example of a cage critical point in a single ring: A novel twisted Î±-helical ring topology. Chemical Physics Letters, 2005, 409, 265-269. | 2.6 | 46 |
| 54 | Electronic structure calculations of hydrocarbon radical cations: a density functional study. Journal of the American Chemical Society, 1993, 115, 6896-6900. | 13.7 | 45 |

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| 55 | Fluorineâ^'Fluorine Spinâ^'Spin Coupling Constants in Aromatic Compounds:â€‰ Correlations with the Delocalization Index and with the Internuclear Separation. Journal of Chemical Information and Modeling, 2005, 45, 354-359. | 5.4 | 45 |
| 56 | The Ionezation Potentials of BF3, BC13 and BBr3. Chemical Physics Letters, 1968, 1, 649-650. | 2.6 | 44 |
| 57 | The shell structure of atoms. Journal of Physics B: Atomic and Molecular Physics, 1976, 9, L69-L72. | 1.6 | 44 |
| 58 | A Density-Functional Theory Investigation of the Radiation Products of l-Î±-Alanine. Journal of Physical Chemistry A, 1999, 103, 4303-4308. | 2.5 | 44 |
| 59 | A Quantum Chemical and TST Study of the OH Hydrogen-Abstraction Reaction from Substituted Aldehydes:Â FCHO and ClCHO. Journal of Physical Chemistry A, 2001, 105, 9034-9039. | 2.5 | 43 |
| 60 | A comparative study of the hyperfine structures of neutral nitrogen oxides: DFT vs CISD results. The Journal of Physical Chemistry, 1994, 98, 792-799. | 2.9 | 42 |
| 61 | The radial density function for the neutral atoms from helium to xenon. Canadian Journal of Physics, 1977, 55, 452-455. | 1.1 | 41 |
| 62 | Effect of Substituents on the GPx-like Activity of Ebselen:â€‰ Steric versus Electronic. Journal of Physical Chemistry A, 2008, 112, 1013-1017. | 2.5 | 41 |
| 63 | Density functional theory investigation of hyperfine coupling constants in peroxyl radicals. Journal of Chemical Physics, 1997, 106, 7738-7748. | 3.0 | 40 |
| 64 | Intracule densities and electron correlation in the hydrogen molecule. Journal of Physics B: Atomic, Molecular and Optical Physics, 1988, 21, 2555-2561. | 1.5 | 39 |
| 65 | Theoretical study of metastable N2CO isomers. New candidates for high energy materials?. Chemical Physics Letters, 1994, 227, 312-320. | 2.6 | 39 |
| 66 | Structure sensitivity and cluster size convergence for formate adsorption on copper surfaces: A DFT cluster model study. Journal of Chemical Physics, 2000, 112, 9562-9568. | 3.0 | 39 |
| 67 | A localized electrons detector for atomic and molecular systems. Theoretical Chemistry Accounts, 2010, 127, 393-400. | 1.4 | 39 |
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| 69 | Diazasilene (SiNN): a comparative study of electron density distributions derived from Hartree-Fock, second-order Moller-Plesset perturbation theory, and density functional methods. The Journal of Physical Chemistry, 1994, 98, 1844-1850. | 2.9 | 37 |
| 70 | A Theoretical Study of the Effects of Protonation and Deprotonation on Bond Dissociation Energies. Journal of the American Chemical Society, 1995, 117, 8816-8822. | 13.7 | 37 |
| 71 | Modeling the Reaction Mechanisms of the Amide Hydrolysis in anN-(o-Carboxybenzoyl)-l-amino Acid. Journal of the American Chemical Society, 2003, 125, 6994-7000. | 13.7 | 37 |
| 72 | An SCFâ€"MOâ€"CNDO study of equilibrium geometries, force constants, and bonding energies: CNDO/BW. Part II. Diatomics. Journal of the Chemical Society Dalton Transactions, 1972, , 78-81. | 1.1 | 36 |

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| 73 | The Laplacian of the charge density as a probe of reaction paths and reactivity: a comparison of SN2 reactions at carbon and silicon. The Journal of Physical Chemistry, 1991, 95, 4698-4701. | 2.9 | 36 |
| 74 | Secondary H/D isotope effects and transition state looseness in nonidentity methyl transfer reactions. Implications for the concept of enzymic catalysis via transition state compression. Journal of the American Chemical Society, 1993, 115, 10147-10152. | 13.7 | 36 |
| 75 | A Density Functional Theory Study of the Radiation Products of Glycine. Journal of Physical Chemistry A, 2000, 104, 5080-5086. | 2.5 | 36 |
| 76 | The Spin Dependence of the Spatial Size of Fe(II) and of the Structure of Fe(II)-Porphyrins. Journal of Physical Chemistry A, 2004, 108, 4653-4657. | 2.5 | 36 |
| 77 | Topological Atomâ€“Atom Partitioning of Molecular Exchange Energy and its Multipolar Convergence. , 0, , 121-140. | | 36 |
| 78 | Charge development at the transition state: a second-order Moeller-Plesset perturbation study of gas-phase SN2 reactions. Journal of the American Chemical Society, 1991, 113, 1072-1076. | 13.7 | 35 |
| 79 | Intrinsic barriers of some model SN2 reactions: second-order Moeller-Plesset perturbation calculations. Journal of the American Chemical Society, 1991, 113, 2434-2439. | 13.7 | 35 |
| 80 | A density functional theory study of the hyperfine structures of the atoms B to O and the species NH2 and NH+3. Chemical Physics Letters, 1994, 217, 24-30. | 2.6 | 35 |
| 81 | Electron Densities of Several Small Molecules As Calculated from Density Functional Theory. The Journal of Physical Chemistry, 1996, 100, 6317-6324. | 2.9 | 35 |
| 82 | Theoretical Studies of the Cross-Linking Mechanisms between Cytosine and Tyrosine. Journal of the American Chemical Society, 2002, 124, 2753-2761. | 13.7 | 35 |
| 83 | Modeling the Reduction of Hydrogen Peroxide by Glutathione Peroxidase Mimics. Journal of Physical Chemistry A, 2006, 110, 8979-8985. | 2.5 | 35 |
| 84 | The localized electrons detector as an ab initio representation of molecular structures. International Journal of Quantum Chemistry, 2010, 110, 2418-2425. | 2.0 | 35 |
| 85 | The Hydrated Electron as a Pseudo-Atom in Cavity-Bound Water Clusters. Journal of Chemical Theory and Computation, 2007, 3, 1054-1063. | 5.3 | 34 |
| 86 | Hydrogen Bond Cooperativity in Water Hexamers: Atomic Energy Perspective of Local Stabilities. Journal of Physical Chemistry A, 2013, 117, 10790-10799. | 2.5 | 34 |
| 87 | Density difference representation of electron correlation. Journal of Chemical Physics, 1978, 68, 1951-1957. | 3.0 | 33 |
| 88 | Angular aspects of electron correlation and the Coulomb hole. Journal of Chemical Physics, 1982, 77, 3578-3582. | 3.0 | 33 |
| 89 | The Radius of the Coulomb Hole. Canadian Journal of Physics, 1975, 53, 592-597. | 1.1 | 32 |
| 90 | Hundâ€™s rule and singletâ€“triplet energy differences for molecular systems. Journal of Chemical Physics, 1987, 87, 5329-5332. | 3.0 | 32 |

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| 91 | Energy component analysis of the Jahnâ€“Teller effect in the methane radical cation. Journal of Chemical Physics, 1991, 94, 8083-8088. | 3.0 | 32 |
| 92 | A density functional theory study of the free radicals NH2, NF2, NCl2, PH2, PF2, and PCl2. Canadian Journal of Chemistry, 1994, 72, 695-704. | 1.1 | 32 |
| 93 | An Evaluation of Various Computational Methods for the Treatment of Organoselenium Compounds. Journal of Physical Chemistry A, 2005, 109, 10373-10379. | 2.5 | 32 |
| 94 | On the local representation of the electronic momentum operator in atomic systems. Journal of Chemical Physics, 2008, 129, 024110. | 3.0 | 32 |
| 95 | The effect of electron correlation on the electron density distributions of molecules: Comparison of perturbation and configuration interaction methods. Journal of Chemical Physics, 1989, 90, 1083-1090. | 3.0 | 31 |
| 96 | Visualizing Internal Stabilization in Weakly Bound Systems Using Atomic Energies: Hydrogen Bonding in Small Water Clusters. Journal of Physical Chemistry A, 2012, 116, 3946-3951. | 2.5 | 31 |
| 97 | The Coulomb hole in the 23S state of the helium isoelectronic sequence. International Journal of Quantum Chemistry, 1974, 8, 255-261. | 2.0 | 30 |
| 98 | An ab initio SCF calculation of the effect of water-anion and water-cation interactions on the vibrational frequencies of water. Spectrochimica Acta Part A: Molecular Spectroscopy, 1986, 42, 175-180. | 0.1 | 30 |
| 99 | Recombination of methyl radicals: ab initio potential and transition-state theory calculations. The Journal of Physical Chemistry, 1989, 93, 4772-4779. | 2.9 | 30 |
| 100 | A Computational Study of the Kinetics of the NO3Hydrogen-Abstraction Reaction from a Series of Aldehydes (XCHO:Â X = F, Cl, H, CH3). Journal of Physical Chemistry A, 2002, 106, 384-394. | 2.5 | 30 |
| 101 | A density functional theory study of the mechanism of the Paalâ€“Knorr pyrrole synthesis. Computational and Theoretical Chemistry, 2007, 811, 97-107. | 1.5 | 30 |
| 102 | Can correlation bring electrons closer together?. Molecular Physics, 2009, 107, 1089-1093. | 1.7 | 30 |
| 103 | Interpretation of Hund's rule for first-row hydrides AH (A = lithium, boron, nitrogen, fluorine). The Journal of Physical Chemistry, 1990, 94, 3480-3484. | 2.9 | 29 |
| 104 | An ab initio study of the series of fluorinated ethanes C2HnF6-n (n = 0-6): geometries, total energies, and carbon-carbon bond dissociation energies. The Journal of Physical Chemistry, 1992, 96, 6287-6290. | 2.9 | 29 |
| 105 | Charge and intracule densities in singly excited heliumlike ions. Journal of Chemical Physics, 1993, 98, 7132-7139. | 3.0 | 29 |
| 106 | Reduction of Hydrogen Peroxide by Glutathione Peroxidase Mimics: Reaction Mechanism and Energetics. Journal of Physical Chemistry A, 2010, 114, 1996-2000. | 2.5 | 29 |
| 107 | Systematic Study of the Performance of Density Functional Theory Methods for Prediction of Energies and Geometries of Organoselenium Compounds. Journal of Physical Chemistry A, 2011, 115, 4827-4831. | 2.5 | 29 |
| 108 | Torquoselectivity in the Nazarov Reactions of Allenyl Vinyl Ketones. Journal of Organic Chemistry, 2015, 80, 1042-1051. | 3.2 | 29 |

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| 109 | Relative sizes of high and low spin states of atoms. Nature, 1974, 250, 566-567. | 27.8 | 28 |
| 110 | A Comparative Study of Electron Densities in Carbon Monoxide Calculated from Conventional ab Initio and Density Functional Methods. The Journal of Physical Chemistry, 1994, 98, 6988-6994. | 2.9 | 28 |
| 111 | Properties of Transition Species in the Reaction of Hydroxyl with Ethane from ab Initio Calculations and Fits to Experimental Data. The Journal of Physical Chemistry, 1995, 99, 8661-8668. | 2.9 | 27 |
| 112 | Molecular Structures and Excited States of CpM(CO)2(Cp = Î·5-C5H5; M = Rh, Ir) and [Cl2Rh(CO)2]-. Theoretical Evidence for a Competitive Charge Transfer Mechanism. Journal of the American Chemical Society, 2002, 124, 2664-2671. | 13.7 | 27 |
| 113 | Evaluation of Effective Core Potentials and Basis Sets for the Prediction of the Geometries of Alkyltin Halides. Journal of Physical Chemistry A, 2006, 110, 5893-5896. | 2.5 | 27 |
| 114 | The effect of electron correlation on one-electron distributions. Chemical Physics Letters, 1976, 44, 363-365. | 2.6 | 26 |
| 115 | A density functional theory study of the dimers of HX (Xâ€‰=â€‰F, Cl, and Br). Journal of Computational Chemistry, 2001, 22, 1590-1597. | 3.3 | 26 |
| 116 | 1,n-Radical ions: an abinitio study of racemization and isomerization of the cyclopropane radical cation. Canadian Journal of Chemistry, 1985, 63, 3283-3289. | 1.1 | 25 |
| 117 | Hundâ€™s rule and singletâ€“triplet energy differences for the lowest nÏ€* states of formaldehyde, H2CO. Journal of Chemical Physics, 1989, 90, 5638-5643. | 3.0 | 25 |
| 118 | The Effect of Multiplicity on the Size of Iron(II) and the Structure of Iron(II) Porphyrins. Journal of Physical Chemistry A, 2010, 114, 10315-10319. | 2.5 | 25 |
| 119 | Assessment of Several DFT Functionals in Calculation of the Reduction Potentials for Niâ€“, Pdâ€“, and Ptâ€“Bis-ethylene-1,2-dithiolene and -Diselenolene Complexes. Journal of Physical Chemistry A, 2015, 119, 911-918. | 2.5 | 25 |
| 120 | Conformations of simple disulfides and L-cystine. Canadian Journal of Chemistry, 1983, 61, 1082-1085. | 1.1 | 24 |
| 121 | Stereoselectivity of nucleophilic addition to substituted cyclohexanones: a structure and charge density study. Journal of the American Chemical Society, 1993, 115, 9614-9619. | 13.7 | 24 |
| 122 | Is the size of an atom determined by its ionization energy?. Chemical Physics Letters, 2009, 480, 127-131. | 2.6 | 24 |
| 123 | Photoelectron spectra of diazabasketene, diazadeltacyclene, and related polycyclic cis-azoalkanes. Journal of the American Chemical Society, 1976, 98, 2398-2406. | 13.7 | 23 |
| 124 | The evaluation of extracule and intracule densities in the first-row hydrides, LiH, BeH, BH, CH, NH, OH and FH, from self-consistent field molecular orbital wavefunctions. Journal of Physics B: Atomic, Molecular and Optical Physics, 1990, 23, 1095-1105. | 1.5 | 23 |
| 125 | An assessment of theoretical methods for the study of transition metal carbonyl complexes: [Cl2Rh(CO)2]â^' and [Cl2Rh(CO)]â^' as case studies. Journal of Chemical Physics, 2000, 113, 9393-9401. | 3.0 | 23 |
| 126 | Addition vs Abstraction Reactions of the Methyl Radical with Nitrones, Alkenes, Aldehydes, and Imines. Journal of Physical Chemistry A, 2001, 105, 7096-7105. | 2.5 | 23 |

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| 127 | Modeling the Action of an Antitumor Drug:Â A Density Functional Theory Study of the Mechanism of Tirapazamine. Journal of the American Chemical Society, 2001, 123, 7320-7325. | 13.7 | 23 |
| 128 | A Computational Study of the Isomerization of Prolyl Amides As Catalyzed by Intramolecular Hydrogen Bonding. Journal of Physical Chemistry A, 2002, 106, 11168-11172. | 2.5 | 23 |
| 129 | Atomic energy analysis of cooperativity, anti-cooperativity, and non-cooperativity in small clusters of methanol, water, and formaldehyde. Computational and Theoretical Chemistry, 2015, 1053, 328-336. | 2.5 | 23 |
| 130 | Computational Study of Engineered Cytochrome P450-Catalyzed Câ€“H Amination: The Origin of the Regio- and Stereoselectivity. Journal of Physical Chemistry B, 2017, 121, 10859-10868. | 2.6 | 23 |
| 131 | Thermal and photochemical reactivity of cyclopropene derivatives: a semi-empirical molecular orbital study. Canadian Journal of Chemistry, 1977, 55, 2482-2491. | 1.1 | 22 |
| 132 | Angular aspects of exchange correlation and the fermi hole. International Journal of Quantum Chemistry, 1985, 27, 439-449. | 2.0 | 22 |
| 133 | The effect of a neon matrix on the hyperfine structure of CH+4. A model study. Chemical Physics Letters, 1993, 211, 88-93. | 2.6 | 22 |
| 134 | Statistical electron correlation coefficients for 29 states of the heliumlike ions. International Journal of Quantum Chemistry, 1993, 48, 33-42. | 2.0 | 22 |
| 135 | Validation of a computational scheme to study 15N and 13C nuclear shielding constants. Chemical Physics Letters, 2005, 401, 7-12. | 2.6 | 22 |
| 136 | Balancing Exchange Mixing in Density-Functional Approximations for Iron Porphyrin. Journal of Chemical Theory and Computation, 2015, 11, 3022-3028. | 5.3 | 22 |
| 137 | cis-Azoxyalkanes. III. Dichotomy in the thermal stability of azo- and azoxyalkanes. Journal of the American Chemical Society, 1972, 94, 3260-3261. | 13.7 | 21 |
| 138 | Photoelectron spectra of 2,3-diazabicyclo[2.2.n]alk-2-enes (n = 1,2,3,4). Journal of the American Chemical Society, 1973, 95, 6478-6480. | 13.7 | 20 |
| 139 | Conformational aspects of L-histidine. Canadian Journal of Chemistry, 1981, 59, 3232-3236. | 1.1 | 20 |
| 140 | Molecular orbital treatment of substituent effects. I. Structures of some carbon acids and their conjugate bases. Canadian Journal of Chemistry, 1983, 61, 45-49. | 1.1 | 20 |
| 141 | Atomic orbital populations and atomic charges from self-consistent field molecular orbital wavefunctions. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 1307. | 1.1 | 20 |
| 142 | The lone electron pair and crystal packing: observations on pyramidal YEL3Îµ species, abinitio calculations, and the crystal structures of Me3SOI, Et3SI, (Me3S)2SnCl6, (Me3SO)2SnCl6, and (Et3S)2SnCl6. Canadian Journal of Chemistry, 1989, 67, 1984-2008. | 1.1 | 20 |
| 143 | Electron Densities of Homonuclear Diatomic Molecules As Calculated from Density Functional Theory. The Journal of Physical Chemistry, 1996, 100, 5274-5280. | 2.9 | 20 |
| 144 | Theoretical Study of the Effects of Protonation and Deprotonation on Bond Dissociation Energies of Second-Row Elements:Â Comparison with First-Row Elements. Journal of the American Chemical Society, 1997, 119, 4214-4219. | 13.7 | 20 |

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| 145 | Theoretical Studies of the Radiation Products of Hydroxyproline. Journal of Physical Chemistry A, 2000, 104, 8583-8592. | 2.5 | 20 |
| 146 | Modeling Competitive Reaction Mechanisms of Peroxynitrite Oxidation of Guanine. Journal of Physical Chemistry A, 2006, 110, 9908-9914. | 2.5 | 20 |
| 147 | AB initio calculations of 2H and 14N quadrupolar coupling constants in hydrogen bonded dimers. Chemical Physics Letters, 1982, 89, 478-482. | 2.6 | 19 |
| 148 | 1,n-Radical ions: the nature of the one-electron two-centre bond in cyclopropane radical cations. An abinitio SCF MO approach. Canadian Journal of Chemistry, 1983, 61, 2310-2315. | 1.1 | 19 |
| 149 | Hyperfine Structures of the Series C2HnF5-n, n = 0-5: A Density Functional Theory Study. The Journal of Physical Chemistry, 1995, 99, 623-629. | 2.9 | 19 |
| 150 | A theoretical study of the change in homolytic bond dissociation energy on conversion of A-B to A-B+H. Journal of the American Chemical Society, 1989, 111, 5152-5155. | 13.7 | 18 |
| 151 | Cleavage of the radical cations of alkenes; 1-butene and 4,4-dimethyl-1-pentene. Ab initio calculations on the interaction between the allyl and alkyl radical and carbocation moieties. Canadian Journal of Chemistry, 1991, 69, 1365-1375. | 1.1 | 18 |
| 152 | Calculation of Quadrupole Moments of Polycyclic Aromatic Hydrocarbons:â€‰ Applications to Chromatography. Journal of Physical Chemistry A, 1997, 101, 5374-5377. | 2.5 | 18 |
| 153 | Efficient synthesis of the optically active dihydropyrimidinone of a potent Î±1A- selective adrenoceptor antagonist. Canadian Journal of Chemistry, 2002, 80, 646-652. | 1.1 | 18 |
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| 155 | Fermi and Coulomb correlations in the 21 S state of the helium isoelectronic sequence. Theoretica Chimica Acta, 1977, 45, 61-67. | 0.8 | 17 |
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