Russell J Boyd

List of Publications by Year
in descending order

313 papers	9,252 citations	46918 47 h-index	71532 76 g-index
325 all docs	325 docs citations	325 times ranked	6131 citing authors

#	Article	IF	Citations
1	Lewis Acid-Mediated Cyclization of Allenyl Aryl Ketones. Journal of Organic Chemistry, 2019, 84, 13665-13675.	1.7	3
2	An Electron Density Sourceâ€Function Study of DNA Base Pairs in Their Neutral and Ionized Ground States^{â€}. Journal of Computational Chemistry, 2018, 39, 1112-1128.	1.5	15
3	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.	1.2	23
4	A computational investigation into the redox chemistry of Mo- and W-tris(diselenolene) complexes. Structural Chemistry, 2017, 28, 1173-1180.	1.0	7
5	The acidity of Î²-phosphoglucomutase monofluoromethylenephosphonate ligands probed by NMR spectroscopy and quantum mechanical methods. Canadian Journal of Chemistry, 2016, 94, 902-908.	0.6	2
6	Theoretical study on the mechanism of iridium-catalyzed Î³-functionalization of primary alkyl Câ€“H bonds. Canadian Journal of Chemistry, 2016, 94, 1028-1037.	0.6	9
7	Identifying similarities and differences between analogous bisdithiolene and bisdiselenolene complexes: A computational study. International Journal of Quantum Chemistry, 2016, 116, 369-376.	1.0	9
8	Molecular docking study of macrocycles as Fk506-binding protein inhibitors. Journal of Molecular Graphics and Modelling, 2015, 59, 117-122.	1.3	9
9	Computational Examination of (4 + 3) versus (3 + 2) Cycloaddition in the Interception of Nazarov Reactions of Allenyl Vinyl Ketones by Dienes. Journal of Organic Chemistry, 2015, 80, 12535-12544.	1.7	9
10	Role of Fluoride in Accelerating the Reactions of Dialkylstannylene Acetals. Journal of Organic Chemistry, 2015, 80, 2989-3002.	1.7	6
11	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.	1.1	25
12	Torquoselectivity in the Nazarov Reactions of Allenyl Vinyl Ketones. Journal of Organic Chemistry, 2015, 80, 1042-1051.	1.7	29
13	Competing nitrile hydratase catalytic mechanisms: Is cysteine-sulfenic acid acting as a nucleophile?. Computational and Theoretical Chemistry, 2015, 1070, 48-54.	1.1	4
14	Richard (Rick) Francis Langler Memorial Issue. Australian Journal of Chemistry, 2015, 68, 349.	0.5	0
15	Balancing Exchange Mixing in Density-Functional Approximations for Iron Porphyrin. Journal of Chemical Theory and Computation, 2015, 11, 3022-3028.	2.3	22
16	Density Functional Theory Study of BF₃-Mediated Additions of Enols and [(Trimethylsilyl)oxy]alkenes to an Oxyallyl Cation: Homologous Mukaiyama Reactions. Journal of Physical Chemistry A, 2015, 119, 6714-6722.	1.1	6
17	The Importance of the MM Environment and the Selection of the QM Method in QM/MM Calculations. Advances in Protein Chemistry and Structural Biology, 2015, 100, 153-185.	1.0	2
18	Computational insights into the suicide inhibition of Plasmodium falciparum Fk506-binding protein 35. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 3221-3225.	1.0	9

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19	Interception of Nazarov Reactions of Allenyl Vinyl Ketones with Dienes: (3+2)â€•versus (4+3)â€Cycloaddition and Subsequent Rearrangement. European Journal of Organic Chemistry, 2015, 2015, 2952-2959.	1.2	9
20	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.	1.1	23
21	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	1.1	99
22	The one-electron oxidation of a dithiolate molecule: The importance of chemical intuition. Journal of Chemical Physics, 2014, 140, 18A519.	1.2	8
23	Changing Weak Halogen Bonds into Strong Ones through Cooperativity with Beryllium Bonds. Journal of Physical Chemistry A, 2014, 118, 4205-4213.	1.1	54
24	The catalytic formation of leukotriene C₄: a critical step in inflammatory processes. Physical Chemistry Chemical Physics, 2014, 16, 16284.	1.3	3
25	Organotin bond dissociation energies: An interesting challenge for contemporary computational methods. Computational and Theoretical Chemistry, 2014, 1050, 7-14.	1.1	10
26	The one-electron reduction of dithiolate and diselenolate ligands. Physical Chemistry Chemical Physics, 2014, 16, 10897.	1.3	11
27	Effect of Amino Acid Ligands on the Structure of Iron Porphyrins and Their Ability to Bind Oxygen. Journal of Physical Chemistry A, 2014, 118, 4565-4574.	1.1	11
28	Hydrogen Bond Cooperativity in Water Hexamers: Atomic Energy Perspective of Local Stabilities. Journal of Physical Chemistry A, 2013, 117, 10790-10799.	1.1	34
29	The Calculation of the Hyperfine Coupling Tensors of Biological Radicals. Progress in Theoretical Chemistry and Physics, 2013, , 285-322.	0.2	2
30	Revealing Unexpected Mechanisms for Nucleophilic Attack on Sï£¿S and Seï£¿Se Bridges. Chemistry - A European Journal, 2013, 19, 3629-3638.	1.7	14
31	How Do Nucleophiles Accelerate the Reactions of Dialkylstannylene Acetals? The Effects of Adding Fluoride to Dialkoxydi-n-butylstannanes. Journal of Physical Chemistry A, 2013, 117, 12648-12657.	1.1	4
32	Dramatic substituent effects on the mechanisms of nucleophilic attack on Se-S bridges. Journal of Computational Chemistry, 2013, 34, 2537-2547.	1.5	6
33	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.	1.3	67
34	Self-Assembling ADADA Helices Formed by Hydrogen Bonding. Journal of Physical Chemistry A, 2012, 116, 7965-7975.	1.1	3
35	Mechanism of the Reduction of an Oxidized Glutathione Peroxidase Mimic with Thiols. Journal of Chemical Theory and Computation, 2012, 8, 5052-5057.	2.3	14
36	Reaction of group 16 analogues of ethoxyquin with hydrogen peroxide: A computational study. Computational and Theoretical Chemistry, 2012, 981, 68-72.	1.1	5

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37	Stabilizing effect of solvent and guest residue amino acids on a model alpha-helix peptide. Computational and Theoretical Chemistry, 2012, 998, 80-86.	1.1	1
38	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.	1.1	31
39	Theoretical Study of Polaron Formation in Poly(G)â^'Poly(C) Cations. Journal of Physical Chemistry B, 2011, 115, 3136-3145.	1.2	10
40	Reply to the â€œComment on 'Theoretical Study of Polaron Formation in Poly(G)â€“Poly(C) Cations'â€• Journal of Physical Chemistry B, 2011, 115, 8949-8950.	1.2	1
41	Effect of Counterions on the Protonation State in a Poly(G)â€“Poly(C) Radical Cation. Journal of Physical Chemistry B, 2011, 115, 14885-14890.	1.2	4
42	Molecular Model with Quantum Mechanical Bonding Information. Journal of Physical Chemistry A, 2011, 115, 12991-12997.	1.1	86
43	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.	1.1	29
44	Selenium stories. Nature Chemistry, 2011, 3, 570-570.	6.6	97
45	Effect of Sr²⁺association on the tautomerization processes of uracil and its dithio- and diseleno-derivatives. Organic and Biomolecular Chemistry, 2011, 9, 423-431.	1.5	9
46	A theoretical study of the structure and conductivity of polycytosineacetylene. Chemical Physics Letters, 2011, 506, 243-247.	1.2	2
47	A localized electrons detector for atomic and molecular systems. Theoretical Chemistry Accounts, 2010, 127, 393-400.	0.5	39
48	A simple representation of energy matrix elements in terms of symmetry-invariant bases. Journal of Computational Chemistry, 2010, 31, 492-496.	1.5	0
49	The localized electrons detector as an ab initio representation of molecular structures. International Journal of Quantum Chemistry, 2010, 110, 2418-2425.	1.0	35
50	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.	1.1	25
51	Theoretical Investigations on the Reaction of Monosubstituted Tertiary-Benzylamine Selenols with Hydrogen Peroxide. Journal of Physical Chemistry A, 2010, 114, 10706-10711.	1.1	16
52	Kinetics and Thermodynamics of the Monomerâ^'Dimer Equilibria of Dialkoxydibutylstannanes. Organometallics, 2010, 29, 6384-6392.	1.1	16
53	Electronic Energy Changes Associated with Guanine Quadruplex Formation: An Investigation at the Atomic Level. Journal of Physical Chemistry B, 2010, 114, 9833-9839.	1.2	18
54	Reduction of Hydrogen Peroxide by Glutathione Peroxidase Mimics: Reaction Mechanism and Energetics. Journal of Physical Chemistry A, 2010, 114, 1996-2000.	1.1	29

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55	Can correlation bring electrons closer together?. Molecular Physics, 2009, 107, 1089-1093.	0.8	30
56	Is the size of an atom determined by its ionization energy?. Chemical Physics Letters, 2009, 480, 127-131.	1.2	24
57	QTAIM Study of an Î±-Helix Hydrogen Bond Network. Journal of Physical Chemistry B, 2009, 113, 10957-10964.	1.2	52
58	Bond length and the electron density at the bond critical point: Xï£¿X, Zï£¿Z, and Cï£¿Z bonds (X = Liâ€¦, Z =) Tj ETQq0 0 0 rgBT /Overlo	1.5	17
59	Factors controlling extremely strong AAA-DDD triply hydrogen-bonded complexes. Chemical Physics Letters, 2008, 450, 210-213.	1.2	10
60	On the local representation of the electronic momentum operator in atomic systems. Journal of Chemical Physics, 2008, 129, 024110.	1.2	32
61	Gas-Phase Interaction of Calcium (Ca²⁺) with Seleno Derivatives of Uracil. Journal of Chemical Theory and Computation, 2008, 4, 1002-1011.	2.3	14
62	Characterization of the bond between hydrogen and the non-nuclear attractor in anionic water clusters. Physical Chemistry Chemical Physics, 2008, 10, 6814.	1.3	8
63	Effect of Substituents on the GPx-like Activity of Ebselen:â€‰ Steric versus Electronic. Journal of Physical Chemistry A, 2008, 112, 1013-1017.	1.1	41
64	The Development of Computational Chemistry in Canada. Reviews in Computational Chemistry, 2007, , 213-299.	1.5	4
65	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.	1.1	51
66	The Hydrated Electron as a Pseudo-Atom in Cavity-Bound Water Clusters. Journal of Chemical Theory and Computation, 2007, 3, 1054-1063.	2.3	34
67	A Density Functional Study of Methanol Clusters. Journal of Chemical Theory and Computation, 2007, 3, 54-61.	2.3	128
68	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
69	Modeling the reaction mechanisms for redox regulation of protein tyrosine phosphatase 1B activity. Theoretical Chemistry Accounts, 2007, 118, 573-578.	0.5	2
70	A Non-Bornâ€“Oppenheimer Self-consistent Field Method. Journal of Mathematical Chemistry, 2007, 42, 353-365.	0.7	3
71	Modeling the Reduction of Hydrogen Peroxide by Glutathione Peroxidase Mimics. Journal of Physical Chemistry A, 2006, 110, 8979-8985.	1.1	35
72	Theoretical Study of the Thermolysis of Î²-Hydroxyl Aldehydes. Journal of Physical Chemistry A, 2006, 110, 8710-8718.	1.1	3

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73	Modeling Competitive Reaction Mechanisms of Peroxynitrite Oxidation of Guanine. Journal of Physical Chemistry A, 2006, 110, 9908-9914.	1.1	20
74	An Atoms in Molecules Study of the Halogen Resonance Effect. Journal of Chemical Theory and Computation, 2006, 2, 271-280.	2.3	8
75	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.	1.1	27
76	Calibration of a computational scheme for solvation studies: halide ions bound to water X(H2O)â^'(Xâ€‰=â€‰F, Cl, Br). Molecular Physics, 2006, 104, 389-394.	0.8	1
77	Preparation and evaluation of novel stationary phases for improved chromatographic purification of pneumocandin B0. Journal of Chromatography A, 2006, 1101, 204-213.	1.8	2
78	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.	1.2	215
79	Atomic contributions to bond dissociation energies in aliphatic hydrocarbons. Journal of Chemical Physics, 2006, 125, 204103.	1.2	53
80	Validation of a computational scheme to study 15N and 13C nuclear shielding constants. Chemical Physics Letters, 2005, 401, 7-12.	1.2	22
81	A theoretical study of the fluorine valence shell in methyl fluoride. Chemical Physics Letters, 2005, 403, 47-54.	1.2	9
82	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.	1.2	46
83	The hostâ€“guest inclusion complex of p-chlorophenol inside Î±-cyclodextrin: An atoms in molecules study. Chemical Physics Letters, 2005, 416, 70-74.	1.2	3
84	Fluorineâ€”Fluorine Spinâ€”Spin Coupling Constants in Aromatic Compounds: Correlations with the Delocalization Index and with the Internuclear Separation.. ChemInform, 2005, 36, no.	0.1	0
85	Calibration of a computational scheme for solvation: Group I and II metal ions bound to water, formaldehyde and ammonia. Molecular Physics, 2005, 103, 337-344.	0.8	9
86	The effect of electron-withdrawing groups on15N and13C chemical shifts: a density functional study on a series of pyrroles. Molecular Physics, 2005, 103, 1113-1129.	0.8	12
87	An Evaluation of Various Computational Methods for the Treatment of Organoselenium Compounds. Journal of Physical Chemistry A, 2005, 109, 10373-10379.	1.1	32
88	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.	1.1	165
89	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.	2.5	45
90	Computation of Hyperfine Coupling Tensors to Complement EPR Experiments. , 2004, , 565-580.		1

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91	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.	1.1	36
92	Stereoselective Synthesis of a Potent Thrombin Inhibitor by a Novel P2â˜'P3 Lactone Ring Opening. Journal of Organic Chemistry, 2004, 69, 3620-3627.	1.7	50
93	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.	6.6	37
94	Modeling the Reaction Mechanisms of the Imide Formation in anN-(o-Carboxybenzoyl)-l-amino Acid. Journal of the American Chemical Society, 2003, 125, 3642-3648.	6.6	17
95	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.	0.6	58
96	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.	1.1	86
97	The Calculation of the Hyperfine Coupling Tensors of Biological Radicals. Progress in Theoretical Chemistry and Physics, 2003, , 239-265.	0.2	1
98	ELECTRON CORRELATION STUDIES BY MEANS OF ELECTRON-PAIR DENSITY FUNCTIONS. , 2002, , 577-611.		2
99	HYDROXYL RADICAL REACTIONS IN BIOLOGICAL MEDIA. Recent Advances in Computational, 2002, , 387-415.	0.8	5
100	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.	6.6	27
101	Theoretical Studies of the Cross-Linking Mechanisms between Cytosine and Tyrosine. Journal of the American Chemical Society, 2002, 124, 2753-2761.	6.6	35
102	Density Functional Study of the Proline-Catalyzed Direct Aldol Reaction. Journal of Physical Chemistry A, 2002, 106, 5155-5159.	1.1	188
103	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.	1.1	30
104	A Computational Study of the Isomerization of Prolyl Amides As Catalyzed by Intramolecular Hydrogen Bonding. Journal of Physical Chemistry A, 2002, 106, 11168-11172.	1.1	23
105	Crystal chemistry of tetraradial species. Part 10. Tilting at windmills: conformations of the tetraphenyl species ZPh40, Â±1 (Z = B, C, N). Canadian Journal of Chemistry, 2002, 80, 1351-1366.	0.6	16
106	Efficient synthesis of the optically active dihydropyrimidinone of a potent Î±1A- selective adrenoceptor antagonist. Canadian Journal of Chemistry, 2002, 80, 646-652.	0.6	18
107	Recent applications of density functional theory calculations to biomolecules. Theoretical Chemistry Accounts, 2002, 108, 1-11.	0.5	47
108	THEORETICAL STUDY ON THE REACTION MECHANISMS OF THE IMIDE FORMATION IN AN N-(O-CARBOXYBENZOYL)-L-AMINO ACID. , 2002, , .		0

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109	Addition vs Abstraction Reactions of the Methyl Radical with Nitrones, Alkenes, Aldehydes, and Imines. Journal of Physical Chemistry A, 2001, 105, 7096-7105.	1.1	23
110	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.	6.6	23
111	Hydrogen-Bond Mediated Catalysis:â€‰ The Aminolysis of 6-Chloropyrimidine as Catalyzed by Derivatives of Uracil. Journal of the American Chemical Society, 2001, 123, 2047-2052.	6.6	8
112	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.	1.1	43
113	A multi-component model for radiation damage to DNA from its constituents. Theoretical and Computational Chemistry, 2001, 9, 409-466.	0.2	5
114	A density functional theory study of the dimers of HX (Xâ€‰=â€‰F, Cl, and Br). Journal of Computational Chemistry, 2001, 22, 1590-1597.	1.5	26
115	A theoretical study of 5-halouracils: electron affinities, ionization potentials and dissociation of the related anions. Chemical Physics Letters, 2001, 343, 151-158.	1.2	118
116	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.	6.6	244
117	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.	1.1	101
118	Electron affinities and ionization potentials of nucleotide bases. Chemical Physics Letters, 2000, 322, 129-135.	1.2	226
119	Cusp conditions for non-Coulombic interactions. Computational and Theoretical Chemistry, 2000, 527, 27-33.	1.5	10
120	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.	1.2	23
121	Effects of Alkyl Substituents on the Excited States of Naphthalene:â€‰ Semiempirical Study. Journal of Physical Chemistry A, 2000, 104, 1020-1029.	1.1	10
122	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.	1.2	39
123	Radial moments of the electron density: Gas phase results and the effects of solvation. Journal of Chemical Physics, 2000, 112, 1113-1121.	1.2	4
124	Catalysis Mediated by Hydrogen Bonding:Â A Computational Study of the Aminolysis of 6-Chloropyrimidine. Journal of the American Chemical Society, 2000, 122, 5384-5386.	6.6	8
125	Theoretical Studies of the Radiation Products of Hydroxyproline. Journal of Physical Chemistry A, 2000, 104, 8583-8592.	1.1	20
126	A Density Functional Theory Study of the Radiation Products of Glycine. Journal of Physical Chemistry A, 2000, 104, 5080-5086.	1.1	36

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127	Intracule and Extracule Densities: Historical Perspectives and Future Prospects. Mathematical and Computational Chemistry, 2000, , 231-248.	0.3	15
128	Electronic structures of the bound excited quartet states of the helium anion. Physical Review A, 1999, 60, 4375-4378.	1.0	7
129	The topological features of the intracule density of the uniform electron gas. Chemical Physics Letters, 1999, 304, 393-398.	1.2	15
130	A combined quantum mechanics and molecular dynamics study of small Jahnâ€“Teller distorted hydrocarbons: Another difficult test for density-functional theory. Journal of Chemical Physics, 1999, 110, 12059-12069.	1.2	16
131	Protonation and Deprotonation Effects on the Chemistry of the Third-Row Elements:â€‰ Homolytic versus Heterolytic Cleavage. Journal of Physical Chemistry A, 1999, 103, 7087-7093.	1.1	11
132	Reply to â€œComment on Effects of Ionizing Radiation on Crystalline Cytosine Monohydrateâ€• Journal of Physical Chemistry B, 1999, 103, 3051-3052.	1.2	9
133	A Density-Functional Theory Investigation of the Radiation Products of l-Î±-Alanine. Journal of Physical Chemistry A, 1999, 103, 4303-4308.	1.1	44
134	Theoretical Investigation of Adenine Radicals Generated in Irradiated DNA Components. Journal of Physical Chemistry B, 1998, 102, 10602-10614.	1.2	69
135	Effects of Ionizing Radiation on Crystalline Cytosine Monohydrate. Journal of Physical Chemistry B, 1998, 102, 7484-7491.	1.2	68
136	Ab InitioStudies of the Contrasting Butadiene Cheletropic and Dielsâ˜'Alder Cycloaddition Reactivities Observed for â€œCarbenicâ€•Phosphorus (Phosphenium) and Arsenic (Arsenium) Cationsâ€. Organometallics, 1998, 17, 4014-4029.	1.1	10
137	A Comprehensive Study of Sugar Radicals in Irradiated DNA. Journal of Physical Chemistry B, 1998, 102, 7674-7686.	1.2	48
138	van der Waals Complexes of Water with Oxygen and Nitrogen:â€‰ Infrared Spectra and Atmospheric Implications. Journal of Physical Chemistry A, 1998, 102, 7294-7296.	1.1	46
139	Comparison of Experimental and Calculated Hyperfine Coupling Constants. Which Radicals Are Formed in Irradiated Guanine?. Journal of Physical Chemistry B, 1998, 102, 9332-9343.	1.2	82
140	Radiation Products of Thymine, 1-Methylthymine, and Uracil Investigated by Density Functional Theory. Journal of Physical Chemistry B, 1998, 102, 5369-5377.	1.2	83
141	A spin-density polarization index. Journal of Chemical Physics, 1998, 108, 2824-2830.	1.2	4
142	The calculation of accurate 17O hyperfine coupling constants in the hydroxyl radical:â€‚A difficult problem for current quantum chemical methods. Journal of Chemical Physics, 1998, 109, 9451-9462.	1.2	10
143	The convergence of basis set contractions: A case study of the molecular hyperfine structure of NH214. Journal of Chemical Physics, 1997, 107, 6270-6274.	1.2	6
144	Density functional theory investigation of hyperfine coupling constants in peroxyl radicals. Journal of Chemical Physics, 1997, 106, 7738-7748.	1.2	40

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145	Calculation of Quadrupole Moments of Polycyclic Aromatic Hydrocarbons:â€‰ Applications to Chromatography. Journal of Physical Chemistry A, 1997, 101, 5374-5377.	1.1	18
146	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.	6.6	20
147	An orbital-based density difference index for the comparison of electron density distributions. Journal of Chemical Physics, 1997, 107, 6693-6698.	1.2	3
148	Density functional theory studies of the quadrupole moments of benzene and naphthalene. Chemical Physics Letters, 1997, 277, 252-256.	1.2	15
149	Electron Densities of Homonuclear Diatomic Molecules As Calculated from Density Functional Theory. The Journal of Physical Chemistry, 1996, 100, 5274-5280.	2.9	20
150	Tautomeric Equilibria of Hydroxypyridines in Different Solvents:Â An ab Initio Study. The Journal of Physical Chemistry, 1996, 100, 16141-16146.	2.9	78
151	Topological properties of the electronic structures of the reactants, transition states, and products of the reactions of the hydroxyl radical with the series C2HnF6â^'n, nâ€‚=â€‚1â€“6. Canadian Journal of Chemistry, 1996, 74, 786-800.	0.6	4
152	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.	1.2	52
153	Mechanism of C2H4 dehydrogenation to C2H2 on the Ni(111) surface. Chemical Physics Letters, 1996, 253, 129-134.	1.2	3
154	A theoretical study of proton transfers in aqueous para-, ortho-hydroxypyridine and para-, ortho-hydroxyquinoline. Chemical Physics Letters, 1996, 259, 647-653.	1.2	16
155	Electron Densities of Several Small Molecules As Calculated from Density Functional Theory. The Journal of Physical Chemistry, 1996, 100, 6317-6324.	2.9	35
156	The 2Î£+ states of HBeO, HMgO, and HCaO. Journal of Chemical Physics, 1996, 104, 4055-4060.	1.2	15
157	Polarizable pointâ€charge model for water: Results under normal and extreme conditions. Journal of Chemical Physics, 1996, 105, 4742-4750.	1.2	167
158	Electronegativity and Hardness of Disjoint and Transferable Molecular Fragments. The Journal of Physical Chemistry, 1996, 100, 3448-3453.	2.9	17
159	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
160	The interactions between alkali metals and C2H2. Density functional theory as an analytic tool. Chemical Physics Letters, 1995, 235, 422-429.	1.2	16
161	Internal motion of benzene. A molecular dynamics simulation study. Chemical Physics Letters, 1995, 241, 380-386.	1.2	10
162	CaOH has a second linear structure HCaO. Journal of Chemical Physics, 1995, 103, 10070-10073.	1.2	10

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