Russell J Boyd

List of Publications by Year in Descending Order

313 papers	8,294 citations	46 h-index	72 g-index
325 ext. papers	8,647 ext. citations	4.5 avg, IF	5.96 L-index

#	Paper	IF	Citations
313	Lewis Acid-Mediated Cyclization of Allenyl Aryl Ketones. *Journal of Organic Chemistry*, **2019**, 84, 13665-13675	4.2	1
312	An Electron Density Source-Function Study of DNA Base Pairs in Their Neutral and Ionized Ground States. *Journal of Computational Chemistry*, **2018**, 39, 1112-1128	3.5	10
311	Computational Study of Engineered Cytochrome P450-Catalyzed C-H Amination: The Origin of the Regio- and Stereoselectivity. *Journal of Physical Chemistry B*, **2017**, 121, 10859-10868	3.4	19
310	A computational investigation into the redox chemistry of Mo- and W-tris(diselenolene) complexes. *Structural Chemistry*, **2017**, 28, 1173-1180	1.8	6
309	Identifying similarities and differences between analogous bisdithiolene and bisdiselenolene complexes: A computational study. *International Journal of Quantum Chemistry*, **2016**, 116, 369-376	2.1	9
308	The acidity of □phosphoglucomutase monofluoromethylenephosphonate ligands probed by NMR spectroscopy and quantum mechanical methods. *Canadian Journal of Chemistry*, **2016**, 94, 902-908	0.9	2
307	Theoretical study on the mechanism of iridium-catalyzed □functionalization of primary alkyl C□H bonds. *Canadian Journal of Chemistry*, **2016**, 94, 1028-1037	0.9	7
306	Torquoselectivity in the Nazarov reactions of allenyl vinyl ketones. *Journal of Organic Chemistry*, **2015**, 80, 1042-51	4.2	23
305	Competing nitrile hydratase catalytic mechanisms: Is cysteine-sulfenic acid acting as a nucleophile?. *Computational and Theoretical Chemistry*, **2015**, 1070, 48-54	2	4
304	Richard (Rick) Francis Langler Memorial Issue. *Australian Journal of Chemistry*, **2015**, 68, 349	1.2	
303	Balancing Exchange Mixing in Density-Functional Approximations for Iron Porphyrin. *Journal of Chemical Theory and Computation*, **2015**, 11, 3022-8	6.4	21
302	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, 6714-22	2.8	5
301	The Importance of the MM Environment and the Selection of the QM Method in QM/MM Calculations: Applications to Enzymatic Reactions. *Advances in Protein Chemistry and Structural Biology*, **2015**, 100, 153-85	5.3	2
300	Computational insights into the suicide inhibition of Plasmodium falciparum Fk506-binding protein 35. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 3221-5	2.9	4
299	Interception of Nazarov Reactions of Allenyl Vinyl Ketones with Dienes: (3+2)- versus (4+3)-Cycloaddition and Subsequent Rearrangement. *European Journal of Organic Chemistry*, **2015**, 2015, 2952-2959	3.2	6
298	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	16
297	Six questions on topology in theoretical chemistry. *Computational and Theoretical Chemistry*, **2015**, 1053, 2-16	2	81

296	Molecular docking study of macrocycles as Fk506-binding protein inhibitors. *Journal of Molecular Graphics and Modelling*, **2015**, 59, 117-22	2.8	6
295	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, 12535-44	4.2	8
294	Role of fluoride in accelerating the reactions of dialkylstannylene acetals. *Journal of Organic Chemistry*, **2015**, 80, 2989-3002	4.2	6
293	Assessment of several DFT functionals in calculation of the reduction potentials for Ni-, Pd-, and Pt-bis-ethylene-1,2-dithiolene and -diselenolene complexes. *Journal of Physical Chemistry A*, **2015**, 119, 911-8	2.8	23
292	Changing weak halogen bonds into strong ones through cooperativity with beryllium bonds. *Journal of Physical Chemistry A*, **2014**, 118, 4205-13	2.8	51
291	The catalytic formation of leukotriene C4: a critical step in inflammatory processes. *Physical Chemistry Chemical Physics*, **2014**, 16, 16284-9	3.6	2
290	Organotin bond dissociation energies: An interesting challenge for contemporary computational methods. *Computational and Theoretical Chemistry*, **2014**, 1050, 7-14	2	10
289	The one-electron reduction of dithiolate and diselenolate ligands. *Physical Chemistry Chemical Physics*, **2014**, 16, 10897-902	3.6	11
288	Effect of amino acid ligands on the structure of iron porphyrins and their ability to bind oxygen. *Journal of Physical Chemistry A*, **2014**, 118, 4565-74	2.8	9
287	The one-electron oxidation of a dithiolate molecule: the importance of chemical intuition. *Journal of Chemical Physics*, **2014**, 140, 18A519	3.9	8
286	Hydrogen bond cooperativity in water hexamers: atomic energy perspective of local stabilities. *Journal of Physical Chemistry A*, **2013**, 117, 10790-9	2.8	33
285	The Calculation of the Hyperfine Coupling Tensors of Biological Radicals. *Progress in Theoretical Chemistry and Physics*, **2013**, 285-322	0.6	1
284	Revealing unexpected mechanisms for nucleophilic attack on S-S and Se-Se bridges. *Chemistry - A European Journal*, **2013**, 19, 3629-38	4.8	13
283	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, 12648-57	2.8	4
282	Dramatic substituent effects on the mechanisms of nucleophilic attack on Se-S bridges. *Journal of Computational Chemistry*, **2013**, 34, 2537-47	3.5	4
281	Cooperativity between hydrogen bonds and beryllium bonds in (H2O)(n)BeX2 (n = 1-3, X = H, F) complexes. A new perspective. *Physical Chemistry Chemical Physics*, **2012**, 14, 14540-7	3.6	62
280	Self-assembling ADADA helices formed by hydrogen bonding. *Journal of Physical Chemistry A*, **2012**, 116, 7965-75	2.8	3
279	Mechanism of the Reduction of an Oxidized Glutathione Peroxidase Mimic with Thiols. *Journal of Chemical Theory and Computation*, **2012**, 8, 5052-7	6.4	13

278	Reaction of group 16 analogues of ethoxyquin with hydrogen peroxide: A computational study. *Computational and Theoretical Chemistry*, **2012**, 981, 68-72	2	5
277	Stabilizing effect of solvent and guest residue amino acids on a model alpha-helix peptide. *Computational and Theoretical Chemistry*, **2012**, 998, 80-86	2	1
276	Visualizing internal stabilization in weakly bound systems using atomic energies: hydrogen bonding in small water clusters. *Journal of Physical Chemistry A*, **2012**, 116, 3946-51	2.8	31
275	Molecular model with quantum mechanical bonding information. *Journal of Physical Chemistry A*, **2011**, 115, 12991-7	2.8	63
274	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, 4827-31	2.8	22
273	Selenium stories. *Nature Chemistry*, **2011**, 3, 570	17.6	72
272	Effect of Sr2+ association on the tautomerization processes of uracil and its dithio- and diseleno-derivatives. *Organic and Biomolecular Chemistry*, **2011**, 9, 423-31	3.9	9
271	A theoretical study of the structure and conductivity of polycytosineacetylene. *Chemical Physics Letters*, **2011**, 506, 243-247	2.5	2
270	Theoretical study of polaron formation in poly(G)-poly(C) cations. *Journal of Physical Chemistry B*, **2011**, 115, 3136-45	3.4	9
269	Reply to the Comment on 'Theoretical Study of Polaron Formation in Poly(G)Poly(C) Cations' *Journal of Physical Chemistry B*, **2011**, 115, 8949-8950	3.4	1
268	Effect of counterions on the protonation state in a poly(G)-poly(C) radical cation. *Journal of Physical Chemistry B*, **2011**, 115, 14885-90	3.4	4
267	Methods in Biocomputational Chemistry: A Lesson from the Amino Acids **2010**, 403-421		3
266	The effect of multiplicity on the size of iron(II) and the structure of iron(II) porphyrins. *Journal of Physical Chemistry A*, **2010**, 114, 10315-9	2.8	25
265	Theoretical investigations on the reaction of monosubstituted tertiary-benzylamine selenols with hydrogen peroxide. *Journal of Physical Chemistry A*, **2010**, 114, 10706-11	2.8	14
264	Kinetics and Thermodynamics of the MonomerDimer Equilibria of Dialkoxydibutylstannanes. *Organometallics*, **2010**, 29, 6384-6392	3.8	16
263	Electronic energy changes associated with Guanine quadruplex formation: an investigation at the atomic level. *Journal of Physical Chemistry B*, **2010**, 114, 9833-9	3.4	18
262	Reduction of hydrogen peroxide by glutathione peroxidase mimics: reaction mechanism and energetics. *Journal of Physical Chemistry A*, **2010**, 114, 1996-2000	2.8	25
261	Quantum Mechanical Approaches to Selenium Biochemistry **2010**, 585-603		

260	A localized electrons detector for atomic and molecular systems. *Theoretical Chemistry Accounts*, **2010**, 127, 393-400	1.9	34
259	A simple representation of energy matrix elements in terms of symmetry-invariant bases. *Journal of Computational Chemistry*, **2010**, 31, 492-6	3.5	
258	The localized electrons detector as an ab initio representation of molecular structures. *International Journal of Quantum Chemistry*, **2010**, 110, n/a-n/a	2.1	7
257	Can correlation bring electrons closer together?. *Molecular Physics*, **2009**, 107, 1089-1093	1.7	28
256	Is the size of an atom determined by its ionization energy?. *Chemical Physics Letters*, **2009**, 480, 127-131	2.5	19
255	QTAIM study of an alpha-helix hydrogen bond network. *Journal of Physical Chemistry B*, **2009**, 113, 10957-64	3.4	46
254	Homolytic bond-dissociation enthalpies of tin bonds and tin□ligand bond strengths □ A□computational study. *Canadian Journal of Chemistry*, **2009**, 87, 974-983	0.9	8
253	On the local representation of the electronic momentum operator in atomic systems. *Journal of Chemical Physics*, **2008**, 129, 024110	3.9	28
252	Gas-Phase Interaction of Calcium (Ca(2+)) with Seleno Derivatives of Uracil. *Journal of Chemical Theory and Computation*, **2008**, 4, 1002-11	6.4	14
251	Characterization of the bond between hydrogen and the non-nuclear attractor in anionic water clusters. *Physical Chemistry Chemical Physics*, **2008**, 10, 6814-9	3.6	8
250	Effect of substituents on the GPx-like activity of ebselen: steric versus electronic. *Journal of Physical Chemistry A*, **2008**, 112, 1013-7	2.8	35
249	Bond length and the electron density at the bond critical point: X--X, Z--Z, and C--Z bonds (X = Li-F, Z = Na-Cl). *Journal of Computational Chemistry*, **2008**, 29, 367-79	3.5	17
248	Factors controlling extremely strong AAA-DDD triply hydrogen-bonded complexes. *Chemical Physics Letters*, **2008**, 450, 210-213	2.5	10
247	The Hydrated Electron as a Pseudo-Atom in Cavity-Bound Water Clusters. *Journal of Chemical Theory and Computation*, **2007**, 3, 1054-63	6.4	31
246	A Density Functional Study of Methanol Clusters. *Journal of Chemical Theory and Computation*, **2007**, 3, 54-61	6.4	118
245	A density functional theory study of the mechanism of the Paal□Knorr pyrrole synthesis. *Computational and Theoretical Chemistry*, **2007**, 811, 97-107		22
244	Modeling the reaction mechanisms for redox regulation of protein tyrosine phosphatase 1B activity. *Theoretical Chemistry Accounts*, **2007**, 118, 573-578	1.9	2
243	A Non-Born□Oppenheimer Self-consistent Field Method. *Journal of Mathematical Chemistry*, **2007**, 42, 353-365	2.1	3

242	The Development of Computational Chemistry in Canada. *Reviews in Computational Chemistry*, **2007**, 213-299		2
241	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, 3152-60	2.8	44
240	Atomic contributions to bond dissociation energies in aliphatic hydrocarbons. *Journal of Chemical Physics*, **2006**, 125, 204103	3.9	49
239	Modeling the reduction of hydrogen peroxide by glutathione peroxidase mimics. *Journal of Physical Chemistry A*, **2006**, 110, 8979-85	2.8	31
238	Theoretical study of the thermolysis of beta-hydroxyl aldehydes. *Journal of Physical Chemistry A*, **2006**, 110, 8710-8	2.8	3
237	Modeling competitive reaction mechanisms of peroxynitrite oxidation of guanine. *Journal of Physical Chemistry A*, **2006**, 110, 9908-14	2.8	18
236	An Atoms in Molecules Study of the Halogen Resonance Effect. *Journal of Chemical Theory and Computation*, **2006**, 2, 271-80	6.4	7
235	Evaluation of effective core potentials and basis sets for the prediction of the geometries of alkyltin halides. *Journal of Physical Chemistry A*, **2006**, 110, 5893-6	2.8	25
234	Calibration of a computational scheme for solvation studies: halide ions bound to water X(H2O)□ (X = F, Cl, Br). *Molecular Physics*, **2006**, 104, 389-394	1.7	1
233	Preparation and evaluation of novel stationary phases for improved chromatographic purification of pneumocandin B0. *Journal of Chromatography A*, **2006**, 1101, 204-13	4.5	2
232	Extended weak bonding interactions in DNA: pi-stacking (base-base), base-backbone, and backbone-backbone interactions. *Journal of Physical Chemistry B*, **2006**, 110, 563-78	3.4	199
231	An evaluation of various computational methods for the treatment of organoselenium compounds. *Journal of Physical Chemistry A*, **2005**, 109, 10373-9	2.8	27
230	Characterization of a closed-shell fluorine-fluorine bonding interaction in aromatic compounds on the basis of the electron density. *Journal of Physical Chemistry A*, **2005**, 109, 3669-81	2.8	149
229	Fluorine-fluorine spin-spin coupling constants in aromatic compounds: correlations with the delocalization index and with the internuclear separation. *Journal of Chemical Information and Modeling*, **2005**, 45, 354-9	6.1	36
228	Validation of a computational scheme to study 15N and 13C nuclear shielding constants. *Chemical Physics Letters*, **2005**, 401, 7-12	2.5	20
227	A theoretical study of the fluorine valence shell in methyl fluoride. *Chemical Physics Letters*, **2005**, 403, 47-54	2.5	8
226	The first example of a cage critical point in a single ring: A novel twisted □-helical ring topology. *Chemical Physics Letters*, **2005**, 409, 265-269	2.5	43
225	The host□guest inclusion complex of p-chlorophenol inside □-cyclodextrin: An atoms in molecules study. *Chemical Physics Letters*, **2005**, 416, 70-74	2.5	3

224	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	1.7	9
223	The effect of electron-withdrawing groups on 15N and 13C chemical shifts: a density functional study on a series of pyrroles. *Molecular Physics*, **2005**, 103, 1113-1129	1.7	10
222	Computation of Hyperfine Coupling Tensors to Complement EPR Experiments **2004**, 565-580		
221	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	2.8	36
220	Stereoselective synthesis of a potent thrombin inhibitor by a novel P2-P3 lactone ring opening. *Journal of Organic Chemistry*, **2004**, 69, 3620-7	4.2	46
219	Alkoxy radicals in the gaseous phase: ß-scission reactions and formation by radical addition to carbonyl compounds. *Canadian Journal of Chemistry*, **2003**, 81, 431-442	0.9	55
218	Coming to Grips with N□□□N Bonds. 2. Homocorrelations between Parameters Deriving from the Electron Density at the Bond Critical Point 1. *Journal of Physical Chemistry A*, **2003**, 107, 272-284	2.8	82
217	Modeling the reaction mechanisms of the amide hydrolysis in an N-(o-carboxybenzoyl)-L-amino acid. *Journal of the American Chemical Society*, **2003**, 125, 6994-7000	16.4	35
216	Modeling the reaction mechanisms of the imide formation in an N-(o-carboxybenzoyl)-L-amino acid. *Journal of the American Chemical Society*, **2003**, 125, 3642-8	16.4	16
215	The Calculation of the Hyperfine Coupling Tensors of Biological Radicals. *Progress in Theoretical Chemistry and Physics*, **2003**, 239-265	0.6	
214	Recent applications of density functional theory calculations to biomolecules. *Theoretical Chemistry Accounts*, **2002**, 108, 1-11	1.9	40
213	ELECTRON CORRELATION STUDIES BY MEANS OF ELECTRON-PAIR DENSITY FUNCTIONS **2002**, 577-611		1
212	HYDROXYL RADICAL REACTIONS IN BIOLOGICAL MEDIA. *Recent Advances in Computational*, **2002**, 387-415		5
211	Molecular structures and excited states of CpM(CO)(2) (Cp = eta(5)-C(5)H(5); M = Rh, Ir) and [Cl(2)Rh(CO)(2)](-). Theoretical evidence for a competitive charge transfer mechanism. *Journal of the American Chemical Society*, **2002**, 124, 2664-71	16.4	22
210	Theoretical studies of the cross-linking mechanisms between cytosine and tyrosine. *Journal of the American Chemical Society*, **2002**, 124, 2753-61	16.4	34
209	Density Functional Study of the Proline-Catalyzed Direct Aldol Reaction. *Journal of Physical Chemistry A*, **2002**, 106, 5155-5159	2.8	172
208	A Computational Study of the Kinetics of the NO3Hydrogen-Abstraction Reaction from a Series of Aldehydes (XCHO:□X = F, Cl, H, CH3). *Journal of Physical Chemistry A*, **2002**, 106, 384-394	2.8	27
207	A Computational Study of the Isomerization of Prolyl Amides As Catalyzed by Intramolecular Hydrogen Bonding. *Journal of Physical Chemistry A*, **2002**, 106, 11168-11172	2.8	23

206	Crystal chemistry of tetraradial species. Part 10. Tilting at windmills: conformations of the tetraphenyl species ZPh40, 1 (Z = B, C, N). *Canadian Journal of Chemistry*, **2002**, 80, 1351-1366	0.9	13
205	Efficient synthesis of the optically active dihydropyrimidinone of a potent 1A- selective adrenoceptor antagonist. *Canadian Journal of Chemistry*, **2002**, 80, 646-652	0.9	17
204	A multi-component model for radiation damage to DNA from its constituents. *Theoretical and Computational Chemistry*, **2001**, 9, 409-466		3
203	A density functional theory study of the dimers of HX (X = F, Cl, and Br). *Journal of Computational Chemistry*, **2001**, 22, 1590-1597	3.5	23
202	A theoretical study of 5-halouracils: electron affinities, ionization potentials and dissociation of the related anions. *Chemical Physics Letters*, **2001**, 343, 151-158	2.5	110
201	On the importance of prereactive complexes in molecule-radical reactions: hydrogen abstraction from aldehydes by OH. *Journal of the American Chemical Society*, **2001**, 123, 2018-24	16.4	211
200	Coming to Grips with NHN Bonds. 1. Distance Relationships and Electron Density at the Bond Critical Point. *Journal of Physical Chemistry A*, **2001**, 105, 6552-6566	2.8	95
199	Addition vs Abstraction Reactions of the Methyl Radical with Nitrones, Alkenes, Aldehydes, and Imines. *Journal of Physical Chemistry A*, **2001**, 105, 7096-7105	2.8	20
198	Modeling the action of an antitumor drug: a density functional theory study of the mechanism of tirapazamine. *Journal of the American Chemical Society*, **2001**, 123, 7320-5	16.4	23
197	Hydrogen-bond mediated catalysis: the aminolysis of 6-chloropyrimidine as catalyzed by derivatives of uracil. *Journal of the American Chemical Society*, **2001**, 123, 2047-52	16.4	7
196	A Quantum Chemical and TST Study of the OH Hydrogen-Abstraction Reaction from Substituted Aldehydes: FCHO and ClCHO. *Journal of Physical Chemistry A*, **2001**, 105, 9034-9039	2.8	38
195	Electron affinities and ionization potentials of nucleotide bases. *Chemical Physics Letters*, **2000**, 322, 129-135	2.5	213
194	Cusp conditions for non-Coulombic interactions. *Computational and Theoretical Chemistry*, **2000**, 527, 27-33		8
193	An assessment of theoretical methods for the study of transition metal carbonyl complexes: [Cl2Rh(CO)2] and [Cl2Rh(CO)] as case studies. *Journal of Chemical Physics*, **2000**, 113, 9393-9401	3.9	22
192	Effects of Alkyl Substituents on the Excited States of Naphthalene: Semiempirical Study. *Journal of Physical Chemistry A*, **2000**, 104, 1020-1029	2.8	10
191	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	3.9	35
190	Radial moments of the electron density: Gas phase results and the effects of solvation. *Journal of Chemical Physics*, **2000**, 112, 1113-1121	3.9	4
189	Catalysis Mediated by Hydrogen Bonding: A Computational Study of the Aminolysis of 6-Chloropyrimidine. *Journal of the American Chemical Society*, **2000**, 122, 5384-5386	16.4	7

188	Theoretical Studies of the Radiation Products of Hydroxyproline. *Journal of Physical Chemistry A*, **2000**, 104, 8583-8592	2.8	19
187	A Density Functional Theory Study of the Radiation Products of Glycine. *Journal of Physical Chemistry A*, **2000**, 104, 5080-5086	2.8	35
186	Intracule and Extracule Densities: Historical Perspectives and Future Prospects. *Mathematical and Computational Chemistry*, **2000**, 231-248		13
185	Electronic structures of the bound excited quartet states of the helium anion. *Physical Review A*, **1999**, 60, 4375-4378	2.6	7
184	The topological features of the intracule density of the uniform electron gas. *Chemical Physics Letters*, **1999**, 304, 393-398	2.5	14
183	A combined quantum mechanics and molecular dynamics study of small Jahn□Teller distorted hydrocarbons: Another difficult test for density-functional theory. *Journal of Chemical Physics*, **1999**, 110, 12059-12069	3.9	16
182	Protonation and Deprotonation Effects on the Chemistry of the Third-Row Elements: Homolytic versus Heterolytic Cleavage. *Journal of Physical Chemistry A*, **1999**, 103, 7087-7093	2.8	10
181	Reply to □Comment on Effects of Ionizing Radiation on Crystalline Cytosine Monohydrate□*Journal of Physical Chemistry B*, **1999**, 103, 3051-3052	3.4	9
180	A Density-Functional Theory Investigation of the Radiation Products of l-□-Alanine. *Journal of Physical Chemistry A*, **1999**, 103, 4303-4308	2.8	40
179	Theoretical Investigation of Adenine Radicals Generated in Irradiated DNA Components. *Journal of Physical Chemistry B*, **1998**, 102, 10602-10614	3.4	66
178	Effects of Ionizing Radiation on Crystalline Cytosine Monohydrate. *Journal of Physical Chemistry B*, **1998**, 102, 7484-7491	3.4	62
177	Ab Initio Studies of the Contrasting Butadiene Cheletropic and Diels□Alder Cycloaddition Reactivities Observed for □arbenic□Phosphorus (Phosphenium) and Arsenic (Arsenium) Cations□ *Organometallics*, **1998**, 17, 4014-4029	3.8	10
176	A Comprehensive Study of Sugar Radicals in Irradiated DNA. *Journal of Physical Chemistry B*, **1998**, 102, 7674-7686	3.4	44
175	van der Waals Complexes of Water with Oxygen and Nitrogen: Infrared Spectra and Atmospheric Implications. *Journal of Physical Chemistry A*, **1998**, 102, 7294-7296	2.8	44
174	Comparison of Experimental and Calculated Hyperfine Coupling Constants. Which Radicals Are Formed in Irradiated Guanine?. *Journal of Physical Chemistry B*, **1998**, 102, 9332-9343	3.4	78
173	Radiation Products of Thymine, 1-Methylthymine, and Uracil Investigated by Density Functional Theory. *Journal of Physical Chemistry B*, **1998**, 102, 5369-5377	3.4	76
172	A spin-density polarization index. *Journal of Chemical Physics*, **1998**, 108, 2824-2830	3.9	3
171	The calculation of accurate 17O hyperfine coupling constants in the hydroxyl radical: A difficult problem for current quantum chemical methods. *Journal of Chemical Physics*, **1998**, 109, 9451-9462	3.9	9

170	The convergence of basis set contractions: A case study of the molecular hyperfine structure of NH214. *Journal of Chemical Physics*, **1997**, 107, 6270-6274	3.9	6
169	Density functional theory investigation of hyperfine coupling constants in peroxyl radicals. *Journal of Chemical Physics*, **1997**, 106, 7738-7748	3.9	39
168	Calculation of Quadrupole Moments of Polycyclic Aromatic Hydrocarbons: Applications to Chromatography. *Journal of Physical Chemistry A*, **1997**, 101, 5374-5377	2.8	18
167	Theoretical Study of the Effects of Protonation and Deprotonation on Bond Dissociation Energies of Second-Row Elements: Comparison with First-Row Elements. *Journal of the American Chemical Society*, **1997**, 119, 4214-4219	16.4	20
166	An orbital-based density difference index for the comparison of electron density distributions. *Journal of Chemical Physics*, **1997**, 107, 6693-6698	3.9	3
165	Density functional theory studies of the quadrupole moments of benzene and naphthalene. *Chemical Physics Letters*, **1997**, 277, 252-256	2.5	14
164	Electronegativity and Hardness of Disjoint and Transferable Molecular Fragments. *The Journal of Physical Chemistry*, **1996**, 100, 3448-3453		16
163	The 28-Electron Tetraatomic Molecules: N4, CN2O, BFN2, C2O2, B2F2, CBFO, C2FN, and BNO2. Challenges for Computational and Experimental Chemistry. *The Journal of Physical Chemistry*, **1996**, 100, 5702-5714		96
162	Electron Densities of Homonuclear Diatomic Molecules As Calculated from Density Functional Theory. *The Journal of Physical Chemistry*, **1996**, 100, 5274-5280		20
161	Tautomeric Equilibria of Hydroxypyridines in Different Solvents: An ab Initio Study. *The Journal of Physical Chemistry*, **1996**, 100, 16141-16146		73
160	Topological properties of the electronic structures of the reactants, transition states, and products of the reactions of the hydroxyl radical with the series C2HnF6−n, n = 1−6. *Canadian Journal of Chemistry*, **1996**, 74, 786-800	0.9	4
159	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	3.9	48
158	Mechanism of C2H4 dehydrogenation to C2H2 on the Ni(111) surface. *Chemical Physics Letters*, **1996**, 253, 129-134	2.5	3
157	A theoretical study of proton transfers in aqueous para-, ortho-hydroxypyridine and para-, ortho-hydroxyquinoline. *Chemical Physics Letters*, **1996**, 259, 647-653	2.5	15
156	Electron Densities of Several Small Molecules As Calculated from Density Functional Theory. *The Journal of Physical Chemistry*, **1996**, 100, 6317-6324		33
155	The 2Σ states of HBeO, HMgO, and HCaO. *Journal of Chemical Physics*, **1996**, 104, 4055-4060	3.9	13
154	Polarizable point-charge model for water: Results under normal and extreme conditions. *Journal of Chemical Physics*, **1996**, 105, 4742-4750	3.9	162
153	CaOH has a second linear structure HCaO. *Journal of Chemical Physics*, **1995**, 103, 10070-10073	3.9	10

152	Re-examination of the hyperfine structure of 14NH2. *Journal of Chemical Physics*, **1995**, 102, 3674-3678	3.9	8
151	Internal motion and the tunneling rates of CH+4 and CD+4. *Journal of Chemical Physics*, **1995**, 103, 8166-8173	3.9	7
150	Trans-stilbene in methanol solution On the effect of flexible atomic charges in computer simulations. *Molecular Physics*, **1995**, 86, 327-346	1.7	
149	Ab initio studies of reactions of hydroxyl radicals with fluorinated ethanes. *The Journal of Physical Chemistry*, **1995**, 99, 13402-13411		48
148	A Theoretical Study of the Effects of Protonation and Deprotonation on Bond Dissociation Energies. *Journal of the American Chemical Society*, **1995**, 117, 8816-8822	16.4	35
147	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		24
146	Hyperfine Structures of the Series C2HnF5-n, n = 0-5: A Density Functional Theory Study. *The Journal of Physical Chemistry*, **1995**, 99, 623-629		18
145	The Electron Density as Calculated From Density Functional Theory. *Recent Advances in Computational*, **1995**, 369-401		7
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