Frank Jensen

List of Publications by Year in Descending Order

189 papers	9,159 citations	53 h-index	90 g-index
217 ext. papers	9,968 ext. citations	5.6 avg, IF	6.8 L-index

#	Paper	IF	Citations
189	Geometry Dependence of Spin-Orbit Coupling in Complexes of Molecular Oxygen with Atoms, H, or Organic Molecules.. *Journal of Physical Chemistry A*, **2022**,	2.8	3
188	Using atomic charges to model molecular polarization.. *Physical Chemistry Chemical Physics*, **2022**,	3.6	2
187	Helicity-dependent dissociative tunneling ionization of CF in multicycle circularly polarized intense laser fields.. *Physical Chemistry Chemical Physics*, **2022**,	3.6	1
186	The oxygen-organic molecule photosystem: revisiting the past, recalibrating the present, and redefining the future.. *Photochemical and Photobiological Sciences*, **2022**, 1	4.2	2
185	Asymmetric Dissociative Tunneling Ionization of Tetrafluoromethane in - 2 Intense Laser Fields.. *Frontiers in Chemistry*, **2022**, 10, 857863	5	2
184	Probing Basis Set Requirements for Calculating Core Ionization and Core Excitation Spectra Using Correlated Wave Function Methods. *Journal of Chemical Theory and Computation*, **2021**, 17, 2832-2842	6.4	4
183	Representing Exact Electron Densities by a Single Slater Determinant in Finite Basis Sets. *Journal of Chemical Theory and Computation*, **2021**, 17, 269-276	6.4	0
182	The primary photo-dissociation dynamics of lactate in aqueous solution: decarboxylation prevents dehydroxylation. *Physical Chemistry Chemical Physics*, **2021**, 23, 4555-4568	3.6	1
181	The primary photolysis dynamics of oxalate in aqueous solution: decarboxylation. *Physical Chemistry Chemical Physics*, **2021**, 23, 10040-10050	3.6	0
180	The complex between molecular oxygen and an organic molecule: modeling optical transitions to the intermolecular charge-transfer state. *Physical Chemistry Chemical Physics*, **2021**, 23, 15038-15048	3.6	2
179	Interaction of Amyloid-Ξ(1-42) Peptide and Its Aggregates with Lipid/Water Interfaces Probed by Vibrational Sum-Frequency Generation Spectroscopy. *Journal of Physical Chemistry B*, **2021**, 125, 11208-11218	3.4	5
178	Gas-phase action and fluorescence spectroscopy of mass-selected fluorescein monoanions and two derivatives. *Physical Chemistry Chemical Physics*, **2020**, 22, 9210-9215	3.6	3
177	Modeling the Effect of Solvents on Nonradiative Singlet Oxygen Deactivation: Going beyond Weak Coupling in Intermolecular Electronic-to-Vibrational Energy Transfer. *Journal of Physical Chemistry B*, **2020**, 124, 2245-2254	3.4	14
176	Reactivity of ⌗Dihydrofluoropolyethers toward OH Predicted by Multiconformer Transition State Theory and the Interacting Quantum Atoms Approach. *Journal of Physical Chemistry A*, **2020**, 124, 3460-3470	2.8	2
175	Laser-induced Coulomb-explosion imaging of the CS2 dimer: The effect of non-Coulombic interactions. *Physical Review A*, **2020**, 102,	2.6	5
174	The primary photo-dissociation dynamics of amino acids in aqueous solution: breaking the C-bond. *Physical Chemistry Chemical Physics*, **2020**, 22, 2307-2318	3.6	3
173	Polarizable charges in a generalized Born reaction potential. *Journal of Chemical Physics*, **2020**, 153, 024119	3.6	4

172	Structure, DFT based investigations on vibrational and nonlinear optical behavior of a new guanidinium cobalt thiocyanate complex. *Structural Chemistry*, **2020**, 31, 103-114	1.8	2
171	Molecular Dynamics Using Nonvariational Polarizable Force Fields: Theory, Periodic Boundary Conditions Implementation, and Application to the Bond Capacity Model. *Journal of Chemical Theory and Computation*, **2019**, 15, 6213-6224	6.4	7
170	The primary photo-dissociation dynamics of carboxylate anions in aqueous solution: decarboxylation. *Physical Chemistry Chemical Physics*, **2019**, 21, 7358-7366	3.6	5
169	Describing Molecular Polarizability by a Bond Capacity Model. *Journal of Chemical Theory and Computation*, **2019**, 15, 3093-3107	6.4	16
168	Tungsten Iodide Clusters as Singlet Oxygen Photosensitizers: Exploring the Domain of Resonant Energy Transfer at 1 eV. *Journal of Physical Chemistry A*, **2019**, 123, 1730-1739	2.8	8
167	Including implicit solvation in the bond capacity polarization model. *Journal of Chemical Physics*, **2019**, 151, 114118	3.9	6
166	Torsional effects in strong-field ionization of molecules. *Physical Review Research*, **2019**, 1,	3.9	2
165	Probing basis set requirements for calculating hyperfine coupling constants. *Journal of Chemical Physics*, **2019**, 151, 174107	3.9	7
164	Probing Basis Set Requirements for Calculating Core Ionization and Core Excitation Spectroscopy by the Self-Consistent-Field Approach. *Journal of Chemical Theory and Computation*, **2019**, 15, 325-337	6.4	33
163	Method Calibration or Data Fitting?. *Journal of Chemical Theory and Computation*, **2018**, 14, 4651-4661	6.4	19
162	Accelerating Kohn-Sham response theory using density fitting and the auxiliary-density-matrix method. *International Journal of Quantum Chemistry*, **2018**, 118, e25639	2.1	8
161	Development of polarization consistent basis sets for spin-spin coupling constant calculations for the atoms Li, Be, Na, and Mg. *Journal of Chemical Physics*, **2018**, 149, 044117	3.9	14
160	Structure factors for tunneling ionization rates of molecules: General grid-based methodology and convergence studies. *Journal of Chemical Physics*, **2018**, 149, 164107	3.9	8
159	Structural Investigation of Ye□limite, Ca4Al6O12SO4, by 27Al MAS and MQMAS NMR at Different Magnetic Fields. *Journal of Physical Chemistry C*, **2018**, 122, 12077-12089	3.8	12
158	Attosecond transient absorption spectroscopy of molecular nitrogen: Vibrational coherences in the b? 1□u state. *Chemical Physics Letters*, **2017**, 683, 408-415	2.5	21
157	Basis Sets in Quantum Chemistry. *Reviews in Computational Chemistry*, **2017**, 93-149		29
156	Using valence bond methods to estimate intramolecular basis set superposition errors. *Journal of Chemical Physics*, **2017**, 146, 184109	3.9	5
155	Protonation of aqueous alanine by photoionization of water. *Physical Chemistry Chemical Physics*, **2017**, 19, 1560-1570	3.6	5

154	How Large is the Elephant in the Density Functional Theory Room?. *Journal of Physical Chemistry A*, **2017**, 121, 6104-6107	2.8	20
153	Local decomposition of imaginary polarizabilities and dispersion coefficients. *Physical Chemistry Chemical Physics*, **2017**, 19, 20241-20250	3.6	6
152	Experimental and Theoretical Studies on the Reduction of CO2 to CO with Chloro(methyl)disilane Components from the Direct Process. *Synlett*, **2017**, 28, 2439-2444	2.2	4
151	Structure factors for tunneling ionization rates of molecules: General Hartree-Fock-based integral representation. *Physical Review A*, **2017**, 96,	2.6	11
150	Probing the Importance of Charge Flux in Force Field Modeling. *Journal of Chemical Theory and Computation*, **2017**, 13, 3715-3721	6.4	10
149	Synthesis of ent-BE-43547A reveals a potent hypoxia-selective anticancer agent and uncovers the biosynthetic origin of the APD-CLD natural products. *Nature Chemistry*, **2017**, 9, 264-272	17.6	35
148	Solvent-dependent singlet oxygen lifetimes: temperature effects implicate tunneling and charge-transfer interactions. *Physical Chemistry Chemical Physics*, **2016**, 18, 22946-61	3.6	110
147	Conformational Interconversions of Amino Acid Derivatives. *Journal of Chemical Theory and Computation*, **2016**, 12, 694-705	6.4	10
146	Enantioselective Formal [4+2] Cycloadditions to 3-Nitroindoles by Trienamine Catalysis: Synthesis of Chiral Dihydrocarbazoles. *Angewandte Chemie*, **2016**, 128, 1032-1036	3.6	16
145	Enantioselective Formal [4+2] Cycloadditions to 3-Nitroindoles by Trienamine Catalysis: Synthesis of Chiral Dihydrocarbazoles. *Angewandte Chemie - International Edition*, **2016**, 55, 1020-4	16.4	76
144	Dynamic resolution of 2-cyclohexylidene acetaldehydes through organocatalytic dienamine [4+2] cycloaddition. *Chemical Communications*, **2016**, 52, 7153-6	5.8	18
143	Searching the Force Field Electrostatic Multipole Parameter Space. *Journal of Chemical Theory and Computation*, **2016**, 12, 1824-32	6.4	15
142	Enantioselective Organocatalytic Cascade Approach to Different Classes of Benzofused Acetals. *Chemistry - A European Journal*, **2016**, 22, 16810-16818	4.8	24
141	Synthesis and evaluation of galacto-noeurostegine and its 2-deoxy analogue as glycosidase inhibitors. *Organic and Biomolecular Chemistry*, **2015**, 13, 7979-92	3.9	7
140	Observation of laser-induced electronic structure in oriented polyatomic molecules. *Nature Communications*, **2015**, 6, 7039	17.4	55
139	Toward an Enhanced Sampling Molecular Dynamics Method for Studying Ligand-Induced Conformational Changes in Proteins. *Journal of Physical Chemistry B*, **2015**, 119, 14594-603	3.4	4
138	Measurement and laser control of attosecond charge migration in ionized iodoacetylene. *Science*, **2015**, 350, 790-5	33.3	352
137	The same number of optimized parameters scheme for determining intermolecular interaction energies. *Journal of Chemical Physics*, **2015**, 142, 114116	3.9	9

136	Role of Multi-Electron Effects in the Asymmetry of Strong-Field Ionization and Fragmentation of Polar Molecules: The Methyl Halide Series. *Journal of Physical Chemistry A*, **2015**, 119, 11772-82	2.8	36
135	Segmented contracted basis sets optimized for nuclear magnetic shielding. *Journal of Chemical Theory and Computation*, **2015**, 11, 132-8	6.4	146
134	Organocatalytic Asymmetric 1,6-Addition/1,4-Addition Sequence to 2,4-Dienals for the Synthesis of Chiral Chromans. *Angewandte Chemie*, **2015**, 127, 8321-8325	3.6	25
133	Attosecond charge migration and its laser control. *Journal of Physics: Conference Series*, **2015**, 635, 112136	0.3	1
132	Organocatalytic Asymmetric 1,6-Addition/1,4-Addition Sequence to 2,4-Dienals for the Synthesis of Chiral Chromans. *Angewandte Chemie - International Edition*, **2015**, 54, 8203-7	16.4	81
131	Primary photochemistry of peroxynitrite in aqueous solution. *Chemical Physics Letters*, **2015**, 641, 187-192	2.5	5
130	Spectroscopy and picosecond dynamics of aqueous NO. *Journal of Chemical Physics*, **2014**, 141, 064310	3.9	3
129	On the photostability of peptides after selective photoexcitation of the backbone: prompt versus slow dissociation. *Physical Chemistry Chemical Physics*, **2014**, 16, 15831-8	3.6	22
128	Unifying General and Segmented Contracted Basis Sets. Segmented Polarization Consistent Basis Sets. *Journal of Chemical Theory and Computation*, **2014**, 10, 1074-85	6.4	159
127	A novel class of bis- and tris-chelate diam(m)inebis(dicarboxylato)platinum(IV) complexes as potential anticancer prodrugs. *Journal of Medicinal Chemistry*, **2014**, 57, 6751-64	8.3	39
126	Comprehensive analysis of energy minima of the 20 natural amino acids. *Journal of Physical Chemistry A*, **2014**, 118, 7876-91	2.8	43
125	Application of the weak-field asymptotic theory to tunneling ionization of H2O. *Physical Review A*, **2014**, 89,	2.6	23
124	Systematic Improvement of Potential-Derived Atomic Multipoles and Redundancy of the Electrostatic Parameter Space. *Journal of Chemical Theory and Computation*, **2014**, 10, 5493-504	6.4	26
123	Analysis of energy-optimized Gaussian basis sets for condensed phase density functional calculations. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	8
122	Electrostatic Potential of Insulin: Exploring the Limitations of Density Functional Theory and Force Field Methods. *Journal of Chemical Theory and Computation*, **2013**, 9, 3978-85	6.4	35
121	Structure factors for tunneling ionization rates of molecules. *Physical Review A*, **2013**, 87,	2.6	64
120	Polarization consistent basis sets. VIII. The transition metals Sc-Zn. *Journal of Chemical Physics*, **2013**, 138, 014107	3.9	23
119	Atomic orbital basis sets. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 273-295	7.9	117

118	Theoretical investigations and density functional theory based quantitative structure-activity relationships model for novel cytotoxic platinum(IV) complexes. *Journal of Medicinal Chemistry*, **2013**, 56, 330-44	8.3	69
117	Decay rate measurement of the first vibrationally excited state of MgH+ in a cryogenic Paul trap. *Physical Review Letters*, **2013**, 111, 053002	7.4	11
116	Basis Set Recommendations for DFT Calculations of Gas-Phase Optical Rotation at Different Wavelengths. *Journal of Chemical Theory and Computation*, **2012**, 8, 4425-33	6.4	22
115	Cross-trienamines in asymmetric organocatalysis. *Journal of the American Chemical Society*, **2012**, 134, 12943-6	16.4	103
114	Polarization consistent basis sets. VII. The elements K, Ca, Ga, Ge, As, Se, Br, and Kr. *Journal of Chemical Physics*, **2012**, 136, 114107	3.9	38
113	Duplex and triplex formation of mixed pyrimidine oligonucleotides with stacking of phenyl-triazole moieties in the major groove. *Journal of Organic Chemistry*, **2011**, 76, 6177-87	4.2	30
112	Predicting large-scale conformational changes in proteins using energy-weighted normal modes. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 2778-93	4.2	6
111	Searching Peptide Conformational Space. *Journal of Chemical Theory and Computation*, **2011**, 7, 1783-90	6.4	8
110	Harmonic Vibrational Analysis in Delocalized Internal Coordinates. *Journal of Chemical Theory and Computation*, **2011**, 7, 223-30	6.4	19
109	Synthesis and Inhibiting Activity of Some 4-Hydroxycoumarin Derivatives on HIV-1 Protease. *ISRN Pharmaceutics*, **2011**, 2011, 137637		4
108	Accurate calculations of the hydration free energies of druglike molecules using the reference interaction site model. *Journal of Chemical Physics*, **2010**, 133, 044104	3.9	43
107	An Atomic Counterpoise Method for Estimating Inter- and Intramolecular Basis Set Superposition Errors. *Journal of Chemical Theory and Computation*, **2010**, 6, 100-6	6.4	57
106	Describing Anions by Density Functional Theory: Fractional Electron Affinity. *Journal of Chemical Theory and Computation*, **2010**, 6, 2726-35	6.4	95
105	The optimum contraction of basis sets for calculating spin–spin coupling constants. *Theoretical Chemistry Accounts*, **2010**, 126, 371-382	1.9	103
104	Efficient RNA-targeting by the introduction of aromatic stacking in the duplex major groove via 5-(1-phenyl-1,2,3-triazol-4-yl)-2'-deoxyuridines. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 4702-10	3.4	33
103	Photomagnetic switching of heterometallic complexes [M(dmf)4(H2O)3(mu-CN)Fe(CN)5].H2O (M=Nd, La, Gd, Y) analyzed by single-crystal X-ray diffraction and ab initio theory. *Chemistry - A European Journal*, **2010**, 16, 7215-23	4.8	22
102	Locating seam minima for macromolecular systems. *Theoretical Chemistry Accounts*, **2009**, 123, 477-485	1.9	5
101	Modeling enzymatic transition states by force field methods. *International Journal of Quantum Chemistry*, **2009**, 109, 373-383	2.1	2

100	DFT study of the structure and spectral behavior of new pt(II) complexes with 5-methyl-5(4-pyridyl)hydantoin. *International Journal of Quantum Chemistry*, **2009**, 109, 826-836	2.1	11
99	Alkoxy Isothiocyanates as Intermediates in the Flash Vacuum Pyrolysis of Alkoxythioureas. *Australian Journal of Chemistry*, **2009**, 62, 69	1.2	5
98	Basis Set Convergence of Nuclear Magnetic Shielding Constants Calculated by Density Functional Methods. *Journal of Chemical Theory and Computation*, **2008**, 4, 719-27	6.4	276
97	A click chemistry approach towards nucleic acid major groove functionalization. *Nucleic Acids Symposium Series*, **2008**, 149-50		5
96	The accuracy of local MP2 methods for conformational energies. *Molecular Physics*, **2008**, 106, 1899-1906	1.7	25
95	Optimization of augmentation functions for correlated calculations of spin-spin coupling constants and related properties. *Journal of Chemical Physics*, **2008**, 129, 064111	3.9	65
94	Synthesis and DFT study of the spectral behavior of new 4-hydroxycoumarins. *International Journal of Quantum Chemistry*, **2008**, 108, 1340-1351	2.1	4
93	Synthesis, computational study and cytotoxic activity of new 4-hydroxycoumarin derivatives. *European Journal of Medicinal Chemistry*, **2008**, 43, 694-706	6.8	98
92	Stability of the three tetracoordinated dianions , , and. *Chemical Physics*, **2008**, 353, 189-192	2.3	1
91	Two classes of alongside charge-transfer interactions defined in one [2]catenane. *Journal of the American Chemical Society*, **2007**, 129, 7354-63	16.4	49
90	Polarization consistent basis sets. 4: the elements He, Li, Be, B, Ne, Na, Mg, Al, and Ar. *Journal of Physical Chemistry A*, **2007**, 111, 11198-204	2.8	89
89	Synthesis of 5-(1,2,3-triazol-4-yl)-2'-deoxyuridines by a click chemistry approach: stacking of triazoles in the major groove gives increased nucleic acid duplex stability. *ChemBioChem*, **2007**, 8, 2106-16	3.8	75
88	Force field modeling of conformational energies: Importance of multipole moments and intramolecular polarization. *International Journal of Quantum Chemistry*, **2007**, 107, 1390-1395	2.1	75
87	Force Field Modeling of Amino Acid Conformational Energies. *Journal of Chemical Theory and Computation*, **2007**, 3, 1774-88	6.4	63
86	Supramolecular receptor design: anion-triggered binding of C60. *Angewandte Chemie - International Edition*, **2006**, 45, 6848-53	16.4	84
85	The Basis Set Convergence of Spin-Spin Coupling Constants Calculated by Density Functional Methods. *Journal of Chemical Theory and Computation*, **2006**, 2, 1360-9	6.4	192
84	Controlled formation and topologies of thiophenolate-based macrocycles: rings, cylinders and bowls. *Dalton Transactions*, **2006**, 108-20	4.3	21
83	Anticancer thiopyrano[2,3-d][1,3]thiazol-2-ones with norbornane moiety. Synthesis, cytotoxicity, physico-chemical properties, and computational studies. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 5230-40	3.4	77

82	Overview of theoretical and computational methods applied to the oxygen-organic molecule photosystem. *Photochemistry and Photobiology*, **2006**, 82, 1136-60	3.6	94
81	Contracted basis sets for density functional calculations: segmented versus general contraction. *Journal of Chemical Physics*, **2005**, 122, 074111	3.9	9
80	Squeezing the [Cu-OH...H2O-Cu]3+ bridge by cryptate encapsulation. *Inorganic Chemistry*, **2005**, 44, 5987-9	5.1	20
79	The effect of different density functional methods on basis set parameters. *Chemical Physics Letters*, **2005**, 402, 510-513	2.5	30
78	The magnitude of pseudo-potential errors for density functional calculations. *Chemical Physics Letters*, **2005**, 406, 501-503	2.5	6
77	The magnitude of pseudo-potential errors for bond distances and vibrational frequencies. *Chemical Physics Letters*, **2005**, 412, 12-15	2.5	5
76	On the accuracy of numerical Hartree□Fock energies. *Theoretical Chemistry Accounts*, **2005**, 113, 187-190	1.9	24
75	Estimating the Hartree□Fock limit from finite basis set calculations. *Theoretical Chemistry Accounts*, **2005**, 113, 267-273	1.9	128
74	Chapter 1 An Introduction to the State of the Art in Quantum Chemistry. *Annual Reports in Computational Chemistry*, **2005**, 1, 3-17	1.8	3
73	Force Field Modelling of Conformational Energies. *Molecular Simulation*, **2004**, 30, 801-806	2	7
72	Polarization consistent basis sets. V. The elements Si-Cl. *Journal of Chemical Physics*, **2004**, 121, 3463-70	3.9	164
71	A Novel Zeolite-Induced Population of a Planar Viologen Conformation. New Viologen Charge Transfer Complexes and Alkene/Viologen/Zeolite Arrays. *Journal of Physical Chemistry B*, **2004**, 108, 4673-4678	3.4	9
70	A comparison of polarization and bond functions for density functional calculations. *Molecular Physics*, **2004**, 102, 2559-2562	1.7	3
69	Donor strength of □extended tetrathiafulvalenes: ionisation energies vs. oxidation potentials. A joint theoretical and experimental study. *Journal of Materials Chemistry*, **2004**, 14, 1768-1773		17
68	Polarization consistent basis sets. IV. The basis set convergence of equilibrium geometries, harmonic vibrational frequencies, and intensities. *Journal of Chemical Physics*, **2003**, 118, 2459	3.9	87
67	Transition states from empirical force fields. *Theoretical Chemistry Accounts*, **2003**, 109, 1-7	1.9	64
66	The structure of higher homologues of 1,6,6a□4-trithiapentalenes the question of no-bond-single-bond-resonance in five sulfuratom homologues. *Tetrahedron*, **2003**, 59, 10255-10259	2.4	9
65	Modeling chemical reactions for conformationally mobile systems with force field methods. *Journal of Chemical Physics*, **2003**, 118, 3523-3531	3.9	16

64	The influence of isotopomers on calculated thermodynamics quantities. *Molecular Physics*, **2003**, 101, 2315-2318	1.7	
63	Using force fields methods for locating transition structures. *Journal of Chemical Physics*, **2003**, 119, 8804-8808	3.9	17
62	Electron capture dissociation of weakly bound polypeptide polycationic complexes. *Rapid Communications in Mass Spectrometry*, **2002**, 16, 2260-5	2.2	59
61	Dissociative capture of hot (3–13 eV) electrons by polypeptide polycations: an efficient process accompanied by secondary fragmentation. *Chemical Physics Letters*, **2002**, 356, 201-206	2.5	165
60	Polarization consistent basis sets. II. Estimating the Kohn–Sham basis set limit. *Journal of Chemical Physics*, **2002**, 116, 7372-7379	3.9	325
59	Polarization consistent basis sets. III. The importance of diffuse functions. *Journal of Chemical Physics*, **2002**, 117, 9234-9240	3.9	269
58	Towards An Understanding of the Mechanism of Electron-Capture Dissociation: A Historical Perspective and Modern Ideas. *European Journal of Mass Spectrometry*, **2002**, 8, 337-349	1.1	215
57	Polarization consistent basis sets: Principles. *Journal of Chemical Physics*, **2001**, 115, 9113-9125	3.9	486
56	Steric Effects in SN2 Reactions. The Influence of Microsolvation. *Journal of Physical Chemistry A*, **2001**, 105, 3259-3268	2.8	53
55	The basis set convergence of the density functional energy for H2. *Chemical Physics Letters*, **2000**, 317, 400-403	2.5	17
54	The basis set convergence of the Hartree–Fock energy for H3 +, Li2 and N2. *Theoretical Chemistry Accounts*, **2000**, 104, 484-490	1.9	37
53	Pyrrolo-annelated tetrathiafulvalenes: the parent systems. *Journal of Organic Chemistry*, **2000**, 65, 5794-5805	4.2	118
52	The basis set convergence of the Hartree–Fock energy for H2. *Journal of Chemical Physics*, **1999**, 110, 6601-6605	3.9	77
51	Pyrrolo Annelated Tetrathiafulvalenes: The Parent Systems. *Organic Letters*, **1999**, 1, 1291-1294	6.2	59
50	Stationary points on the H2CO potential energy surface: dependence on theoretical level. *Theoretical Chemistry Accounts*, **1998**, 99, 295-300	1.9	17
49	Reaction of Organic Sulfides with Singlet Oxygen. A Revised Mechanism. *Journal of the American Chemical Society*, **1998**, 120, 4439-4449	16.4	117
48	Experimental and Computational Evidence for the Formation of Iminopersulfinic Acids. *Journal of Organic Chemistry*, **1998**, 63, 3397-3402	4.2	11
47	C24: Ring or fullerene?. *Journal of Chemical Physics*, **1998**, 108, 3213-3217	3.9	26

46	Transition State Looseness and Secondary Kinetic Isotope Effects. *Journal of the American Chemical Society*, **1997**, 119, 227-232	16.4	49
45	Experimental and ab Initio Computational Evidence for New Peroxidic Intermediates (Iminopersulfinic Acids). Substituent Effects in the Photooxidations of Sulfenic Acid Derivatives. *Journal of the American Chemical Society*, **1997**, 119, 4380-4387	16.4	13
44	Phenyl Radical, Cation, and Anion. The Triplet Singlet Gap and Higher Excited States of the Phenyl Cation. *Journal of the American Chemical Society*, **1997**, 119, 8083-8088	16.4	95
43	Kinetic Isotope Effects and Transition State Geometries. A Theoretical Investigation of E2 Model Systems. *Journal of Organic Chemistry*, **1997**, 62, 253-260	4.2	32
42	Conformations of Glycolic Acid.. *Acta Chemica Scandinavica*, **1997**, 51, 439-441		9
41	Basis Set and Correlation Effects on Transition State Geometries and Kinetic Isotope Effects. *The Journal of Physical Chemistry*, **1996**, 100, 16892-16898		18
40	Influence of Substituents on Kinetic Isotope Effects. *Journal of the American Chemical Society*, **1996**, 118, 10577-10583	16.4	10
39	Ring Strain Effects on the Interconversion of Intermediates in the Reaction of Organic Sulfides with Singlet Oxygen. *Journal of Organic Chemistry*, **1996**, 61, 4107-4110	4.2	16
38	The magnitude of intramolecular basis set superposition error. *Chemical Physics Letters*, **1996**, 261, 633-636	2.5	68
37	Gradient extremal bifurcation and turning points: An application to the H2CO potential energy surface. *Journal of Chemical Physics*, **1996**, 104, 8025-8031	3.9	53
36	Locating transition structures by mode following: A comparison of six methods on the Ar8 Lennard-Jones potential. *Journal of Chemical Physics*, **1995**, 102, 6706-6718	3.9	69
35	A Theoretical Study of the Allene Effect in [1,n] Sigmatropic Hydrogen Shifts. *Journal of the American Chemical Society*, **1995**, 117, 7487-7492	16.4	39
34	Surface-enhanced Raman spectroscopic investigations of thiazole orange derivatives using visible and near-infrared excitation. *Journal of Raman Spectroscopy*, **1995**, 26, 1009-1017	2.3	3
33	Transition structure modeling by intersecting potential energy surfaces. *Journal of Computational Chemistry*, **1994**, 15, 1199-1216	3.5	26
32	Inference of Transition State Geometries from Kinetic Isotope Effects: An Ab Initio Study of an E2 Model System. *Journal of the American Chemical Society*, **1994**, 116, 9302-9310	16.4	26
31	Ab initio study of the nucleophilic ring opening of ethylene oxide. Connection between secondary kinetic isotope effects and transition structures. *Journal of the Chemical Society Perkin Transactions II*, **1994**, 871		12
30	Crown ether annelated tetrathiafulvalenes. 2. *Journal of Organic Chemistry*, **1993**, 58, 1359-1366	4.2	43
29	Influence of the chalcogenocarbonyl group on the structure of heterocyclic analogues of tricarbonyl compounds. Synthesis and structural features of Schiff bases derived from 3-formyl-4-thio(seleno)coumarin. *Journal of the Chemical Society Perkin Transactions II*, **1993**, 2423-2428		8

28	The stability of cage and ring isomers for carbon and boron nitride clusters. *Chemical Physics Letters* , **1993**, 209, 417-422	2.5	40
27	Structure and stability of C24 and B12N12 isomers. *Chemical Physics Letters*, **1993**, 201, 89-96	2.5	228
26	Structure and stability of complexes of glycine and glycine methyl analogs with H+, Li+, and Na+. *Journal of the American Chemical Society*, **1992**, 114, 9533-9537	16.4	140
25	Locating minima on seams of intersecting potential energy surfaces. An application to transition structure modeling. *Journal of the American Chemical Society*, **1992**, 114, 1596-1603	16.4	35
24	New extended .pi.-electron donors. Tetrathiafulvalene systems with heterocyclic spacer groups. *Journal of the American Chemical Society*, **1992**, 114, 5035-5039	16.4	74
23	Reaction of organic sulfides with singlet oxygen. A theoretical study including electron correlation. *Journal of Organic Chemistry*, **1992**, 57, 6478-6487	4.2	33
22	A theoretical study of steric effects in SN2 reactions. *Chemical Physics Letters*, **1992**, 196, 368-376	2.5	42
21	A general procedure for obtaining wave functions obeying the virial theorem. *Journal of Computational Chemistry*, **1991**, 12, 1089-1096	3.5	18
20	Do rotational barriers dictate the regioselectivity in the ene reactions of singlet oxygen and triazolinedione with alkenes?. *Journal of the American Chemical Society*, **1991**, 113, 3180-3181	16.4	43
19	Improved radical stabilization energies. *Journal of Organic Chemistry*, **1991**, 56, 884-885	4.2	17
18	The dipole moment of carbon monoxide. *Journal of Chemical Physics*, **1991**, 94, 6660-6663	3.9	115
17	Structure and spectra of chlorine oxide dimers. *The Journal of Physical Chemistry*, **1990**, 94, 2235-2237		40
16	A remarkable large effect of spin contamination on calculated vibrational frequencies. *Chemical Physics Letters*, **1990**, 169, 519-528	2.5	83
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