

Kenneth B Wiberg

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440
papers

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75
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147
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447
ext. papers

28,323
ext. citations

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L-index

#	Paper	IF	Citations
440	Determining atom-centered monopoles from molecular electrostatic potentials. The need for high sampling density in formamide conformational analysis. <i>Journal of Computational Chemistry</i> , 1990 , 11, 361-373	3.5	3726
439	Solvent Effects. 5. Influence of Cavity Shape, Truncation of Electrostatics, and Electron Correlation on ab Initio Reaction Field Calculations. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 16098-16104		1127
438	Solvent effects. 1. The mediation of electrostatic effects by solvents. <i>Journal of the American Chemical Society</i> , 1991 , 113, 4776-4782	16.4	880
437	Comparison of atomic charges derived via different procedures. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1504-1518	3.5	569
436	The Deuterium Isotope Effect. <i>Chemical Reviews</i> , 1955 , 55, 713-743	68.1	537
435	Solvent effects. 3. Tautomeric equilibria of formamide and 2-pyridone in the gas phase and solution: an ab initio SCRF study. <i>Journal of the American Chemical Society</i> , 1992 , 114, 1645-1652	16.4	484
434	The Concept of Strain in Organic Chemistry. <i>Angewandte Chemie International Edition in English</i> , 1986 , 25, 312-322		461
433	Barriers to rotation adjacent to double bonds. 3. The carbon-oxygen barrier in formic acid, methyl formate, acetic acid, and methyl acetate. The origin of ester and amide resonance. <i>Journal of the American Chemical Society</i> , 1987 , 109, 5935-5943	16.4	400
432	Hartree-Fock second derivatives and electric field properties in a solvent reaction field: Theory and application. <i>Journal of Chemical Physics</i> , 1991 , 95, 8991-8998	3.9	342
431	Solvent effects. 2. Medium effect on the structure, energy, charge density, and vibrational frequencies of sulfamic acid. <i>Journal of the American Chemical Society</i> , 1992 , 114, 523-529	16.4	335
430	A Comparison of Model Chemistries. <i>Journal of the American Chemical Society</i> , 1995 , 117, 11299-11308	16.4	288
429	Amides. 3. Experimental and Theoretical Studies of the Effect of the Medium on the Rotational Barriers for N,N-Dimethylformamide and N,N-Dimethylacetamide. <i>Journal of the American Chemical Society</i> , 1995 , 117, 4261-4270	16.4	284
428	Theoretical analysis of hydrocarbon properties. 1. Bonds, structures, charge concentrations, and charge relaxations. <i>Journal of the American Chemical Society</i> , 1987 , 109, 985-1001	16.4	260
427	Theoretical analysis of hydrocarbon properties. 2. Additivity of group properties and the origin of strain energy. <i>Journal of the American Chemical Society</i> , 1987 , 109, 1001-1012	16.4	221
426	[1.1.1]Propellane. <i>Journal of the American Chemical Society</i> , 1982 , 104, 5239-5240	16.4	219
425	A time-dependent density functional theory study of the electronically excited states of formaldehyde, acetaldehyde and acetone. <i>Chemical Physics Letters</i> , 1998 , 297, 60-64	2.5	216
424	Resonance interactions in acyclic systems. 3. Formamide internal rotation revisited. Charge and energy redistribution along the C-N bond rotational pathway. <i>Journal of the American Chemical Society</i> , 1992 , 114, 831-840	16.4	211

423	Solvent Effects on 1,2-Dihaloethane Gauche/Trans Ratios. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 9072-9079		210
422	A Scheme for Strain Energy Minimization. Application to the Cycloalkanes ¹ . <i>Journal of the American Chemical Society</i> , 1965 , 87, 1070-1078	16.4	194
421	Bent Bonds in Organic Compounds. <i>Accounts of Chemical Research</i> , 1996 , 29, 229-234	24.3	189
420	Electronic Transition Energies: A Study of the Performance of a Large Range of Single Reference Density Functional and Wave Function Methods on Valence and Rydberg States Compared to Experiment. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 370-83	6.4	181
419	Cavity Ring-Down Polarimetry (CRDP): A New Scheme for Probing Circular Birefringence and Circular Dichroism in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 5959-5968	2.8	181
418	Small ring propellanes. <i>Chemical Reviews</i> , 1989 , 89, 975-983	68.1	181
417	Why Does Thioformamide Have a Larger Rotational Barrier Than Formamide?. <i>Journal of the American Chemical Society</i> , 1995 , 117, 2201-2209	16.4	178
416	Deoxygenation of alcohols employing water as the hydrogen atom source. <i>Journal of the American Chemical Society</i> , 2005 , 127, 12513-5	16.4	175
415	Mechanism of the oxidation of alcohols by oxoammonium cations. <i>Journal of Organic Chemistry</i> , 2007 , 72, 4504-9	4.2	170
414	Cyclopropene. V. Some Reactions of Cyclopropene ¹ . <i>Journal of the American Chemical Society</i> , 1960 , 82, 6375-6380	16.4	169
413	Antiaromaticity in monocyclic conjugated carbon rings. <i>Chemical Reviews</i> , 2001 , 101, 1317-31	68.1	165
412	The Mechanisms of Permanganate Oxidation. IV. Hydroxylation of Olefins and Related Reactions. <i>Journal of the American Chemical Society</i> , 1957 , 79, 2822-2824	16.4	152
411	Basis set effects on calculated geometries: 6-311++G** vs. aug-cc-pVDZ. <i>Journal of Computational Chemistry</i> , 2004 , 25, 1342-6	3.5	149
410	Origin of the Gauche Effect in substituted ethanes and ethenes. <i>The Journal of Physical Chemistry</i> , 1990 , 94, 6956-6959		147
409	Thermochemical studies of carbonyl compounds. 5. Enthalpies of reduction of carbonyl groups. <i>Journal of the American Chemical Society</i> , 1991 , 113, 3447-3450	16.4	140
408	Rotational barriers. 2. Energies of alkane rotamers. An examination of gauche interactions. <i>Journal of the American Chemical Society</i> , 1988 , 110, 8029-8038	16.4	140
407	Electronically excited states of ethylene. <i>The Journal of Physical Chemistry</i> , 1992 , 96, 10756-10768		139
406	Heats of formation of C ₄ H ₆ hydrocarbons. <i>Journal of the American Chemical Society</i> , 1968 , 90, 3395-3397	16.4	138

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- 402 Rotational barriers. 4. Dimethoxymethane. The anomeric effect revisited. *Journal of the American Chemical Society*, **1989**, 111, 4821-4828 16.4 128
- 401 Reactions of [1.1.1]propellane. *Journal of the American Chemical Society*, **1990**, 112, 2194-2216 16.4 125
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- 399 Cyclopropene. IV. The Infrared, Ultraviolet and N.m.r. Spectra of Cyclopropene and Some Related Compounds. *Journal of the American Chemical Society*, **1961**, 83, 1226-1230 16.4 122
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- 397 Barriers to rotation adjacent to double bonds. *Journal of the American Chemical Society*, **1985**, 107, 5035-5041 119
- 396 Substituent effects. 4. Nature of substituent effects at carbonyl groups. *Journal of the American Chemical Society*, **1992**, 114, 8644-8654 16.4 118
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381	Solvent effects on the thioamide rotational barrier: an experimental and theoretical study. <i>Journal of the American Chemical Society</i> , 2001 , 123, 2038-46	16.4	101
380	Assignment of the \tilde{A} state in bicyclobutane. The multiphoton ionization spectrum and calculations of transition energies. <i>Journal of the American Chemical Society</i> , 1991 , 113, 4782-4791	16.4	101
379	Nonresonant optical activity of isolated organic molecules. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 11752-64	2.8	100
378	Some Observations on Allylic Oxidation ¹ . <i>Journal of Organic Chemistry</i> , 1964 , 29, 3353-3361	4.2	94
377	Vibrational spectrum, structure, and energy of [1.1.1]propellane. <i>Journal of the American Chemical Society</i> , 1985 , 107, 7247-7257	16.4	91
376	An experimental and computational investigation of the enantioselective deprotonation of Boc-piperidine. <i>Journal of the American Chemical Society</i> , 2002 , 124, 1889-96	16.4	88
375	Strain energies of small ring propellanes. <i>Journal of the American Chemical Society</i> , 1983 , 105, 1227-1233	16.4	88
374	Rotational barriers in aldehydes and ketones coordinated to neutral Lewis acids. <i>Journal of the American Chemical Society</i> , 1988 , 110, 6642-6650	16.4	86
373	Ab initio calculation of molar volumes: Comparison with experiment and use in solvation models. <i>Journal of Computational Chemistry</i> , 1995 , 16, 385-394	3.5	83
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