Kenneth B Wiberg

List of Publications by Year
in descending order

441	30,615	6233 80	6454 157
papers	citations	h-index	g-index

447	447	447	16636
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Determining atom-centered monopoles from molecular electrostatic potentials. The need for high sampling density in formamide conformational analysis. Journal of Computational Chemistry, 1990, 11, 361-373.	1.5	4,216
2	Solvent Effects. 5. Influence of Cavity Shape, Truncation of Electrostatics, and Electron Correlation on ab Initio Reaction Field Calculations. The Journal of Physical Chemistry, 1996, 100, 16098-16104.	2.9	1,211
3	Solvent effects. 1. The mediation of electrostatic effects by solvents. Journal of the American Chemical Society, 1991, 113, 4776-4782.	6.6	971
4	The Deuterium Isotope Effect. Chemical Reviews, 1955, 55, 713-743.	23.0	643
5	Comparison of atomic charges derived via different procedures. Journal of Computational Chemistry, 1993, 14, 1504-1518.	1.5	623
6	The Concept of Strain in Organic Chemistry. Angewandte Chemie International Edition in English, 1986, 25, 312-322.	4.4	578
7	Solvent effects. 3. Tautomeric equilibria of formamide and 2-pyridone in the gas phase and solution: an ab initio SCRF study. Journal of the American Chemical Society, 1992, 114, 1645-1652.	6.6	531
8	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. Journal of the American Chemical Society, 1987, 109, 5935-5943.	6.6	452
9	Solvent effects. 2. Medium effect on the structure, energy, charge density, and vibrational frequencies of sulfamic acid. Journal of the American Chemical Society, 1992, 114, 523-529.	6.6	367
10	Hartreeâ€“Fock second derivatives and electric field properties in a solvent reaction field: Theory and application. Journal of Chemical Physics, 1991, 95, 8991-8998.	1.2	365
11	A Comparison of Model Chemistries. Journal of the American Chemical Society, 1995, 117, 11299-11308.	6.6	315
12	Amides. 3. Experimental and Theoretical Studies of the Effect of the Medium on the Rotational Barriers for N,N-Dimethylformamide and N,N-Dimethylacetamide. Journal of the American Chemical Society, 1995, 117, 4261-4270.	6.6	310
13	Theoretical analysis of hydrocarbon properties. 1. Bonds, structures, charge concentrations, and charge relaxations. Journal of the American Chemical Society, 1987, 109, 985-1001.	6.6	298
14	[1.1.1]Propellane. Journal of the American Chemical Society, 1982, 104, 5239-5240.	6.6	274
15	Theoretical analysis of hydrocarbon properties. 2. Additivity of group properties and the origin of strain energy. Journal of the American Chemical Society, 1987, 109, 1001-1012.	6.6	248
16	A time-dependent density functional theory study of the electronically excited states of formaldehyde, acetaldehyde and acetone. Chemical Physics Letters, 1998, 297, 60-64.	1.2	237
17	Resonance interactions in acyclic systems. 3. Formamide internal rotation revisited. Charge and energy redistribution along the C-N bond rotational pathway. Journal of the American Chemical Society, 1992, 114, 831-840.	6.6	228
18	Solvent Effects on 1,2-Dihaloethane Gauche/Trans Ratios. The Journal of Physical Chemistry, 1995, 99, 9072-9079.	2.9	226

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19	A Scheme for Strain Energy Minimization. Application to the Cycloalkanes1. Journal of the American Chemical Society, 1965, 87, 1070-1078.	6.6	218
20	Bent Bonds in Organic Compounds. Accounts of Chemical Research, 1996, 29, 229-234.	7.6	218
21	Small ring propellanes. Chemical Reviews, 1989, 89, 975-983.	23.0	213
22	Basis set effects on calculated geometries: 6-311++G** vs. aug-cc-pVDZ. Journal of Computational Chemistry, 2004, 25, 1342-1346.	1.5	213
23	Deoxygenation of Alcohols Employing Water as the Hydrogen Atom Source. Journal of the American Chemical Society, 2005, 127, 12513-12515.	6.6	213
24	Mechanism of the Oxidation of Alcohols by Oxoammonium Cations. Journal of Organic Chemistry, 2007, 72, 4504-4509.	1.7	203
25	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. Journal of Chemical Theory and Computation, 2010, 6, 370-383.	2.3	202
26	Cyclopropene. V. Some Reactions of Cyclopropene1. Journal of the American Chemical Society, 1960, 82, 6375-6380.	6.6	200
27	Why Does Thioformamide Have a Larger Rotational Barrier Than Formamide?. Journal of the American Chemical Society, 1995, 117, 2201-2209.	6.6	198
28	Cavity Ring-Down Polarimetry (CRDP):â€‰ A New Scheme for Probing Circular Birefringence and Circular Dichroism in the Gas Phase. Journal of Physical Chemistry A, 2000, 104, 5959-5968.	1.1	197
29	Antiaromaticity in Monocyclic Conjugated Carbon Rings. Chemical Reviews, 2001, 101, 1317-1332.	23.0	194
30	The Mechanisms of Permanganate Oxidation. IV. Hydroxylation of Olefins and Related Reactions. Journal of the American Chemical Society, 1957, 79, 2822-2824.	6.6	177
31	Reactions of [1.1.1]propellane. Journal of the American Chemical Society, 1990, 112, 2194-2216.	6.6	172
32	Thermochemical studies of carbonyl compounds. 5. Enthalpies of reduction of carbonyl groups. Journal of the American Chemical Society, 1991, 113, 3447-3450.	6.6	162
33	Rotational barriers. 2. Energies of alkane rotamers. An examination of gauche interactions. Journal of the American Chemical Society, 1988, 110, 8029-8038.	6.6	161
34	Origin of the Gauche Effect in substituted ethanes and ethenes. The Journal of Physical Chemistry, 1990, 94, 6956-6959.	2.9	156
35	Heats of formation of C4H6 hydrocarbons. Journal of the American Chemical Society, 1968, 90, 3395-3397.	6.6	154
36	Das Konzept der Spannung in der Organischen Chemie. Angewandte Chemie, 1986, 98, 312-322.	1.6	151

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37	Group equivalents for convertingab initio energies to enthalpies of formation. Journal of Computational Chemistry, 1984, 5, 197-199.	1.5	145
38	Electronically excited states of ethylene. The Journal of Physical Chemistry, 1992, 96, 10756-10768.	2.9	144
39	Properties of Some Condensed Aromatic Systems. Journal of Organic Chemistry, 1997, 62, 5720-5727.	1.7	144
40	Rotational barriers. 4. Dimethoxymethane. The anomeric effect revisited. Journal of the American Chemical Society, 1989, 111, 4821-4828.	6.6	141
41	Cyclopropene. IV. The Infrared, Ultraviolet and N.m.r. Spectra of Cyclopropene and Some Related Compounds1. Journal of the American Chemical Society, 1961, 83, 1226-1230.	6.6	139
42	Lactones. 2. Enthalpies of hydrolysis, reduction, and formation of the C4-C13 monocyclic lactones. Strain energies and conformations. Journal of the American Chemical Society, 1991, 113, 7697-7705.	6.6	139
43	Barriers to rotation adjacent to double bonds. Journal of the American Chemical Society, 1985, 107, 5035-5041.	6.6	134
44	Polarographic reduction of the azines. Journal of the American Chemical Society, 1970, 92, 7154-7160.	6.6	132
45	Substituent effects. 4. Nature of substituent effects at carbonyl groups. Journal of the American Chemical Society, 1992, 114, 8644-8654.	6.6	132
46	Stereoselectivity of cyclization of substituted 5-hexen-1-yllithiums: regiospecific and highly stereoselective insertion of an unactivated alkene into a carbon-lithium bond. Journal of the American Chemical Society, 1991, 113, 5720-5727.	6.6	131
47	Conformational Studies in the Cyclohexane Series. 1. Experimental and Computational Investigation of Methyl, Ethyl, Isopropyl, andtert-Butylcyclohexanes. Journal of Organic Chemistry, 1999, 64, 2085-2095.	1.7	131
48	Carbonâ^'Carbon Rotational Barriers in Butane, 1-Butene, and 1,3-Butadiene. The Journal of Physical Chemistry, 1996, 100, 16162-16168.	2.9	130
49	Application of strain energy minimization to the dynamics of conformational changes. Journal of the American Chemical Society, 1972, 94, 8426-8430.	6.6	126
50	Inverted geometries at carbon. Accounts of Chemical Research, 1984, 17, 379-386.	7.6	125
51	Oscillator Strength: How Does TDDFT Compare to EOM-CCSD?. Journal of Chemical Theory and Computation, 2011, 7, 456-466.	2.3	123
52	Origin of the stability of carbon tetrafluoride: negative hyperconjugation reexamined. Journal of the American Chemical Society, 1993, 115, 614-625.	6.6	122
53	The Interaction of Carbonyl Groups with Substituents. Accounts of Chemical Research, 1999, 32, 922-929.	7.6	121
54	Solvent Effects on Methyl Transfer Reactions. 1. The Menshutkin Reaction. Journal of the American Chemical Society, 1999, 121, 2139-2146.	6.6	115

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55	Microwave Spectrum, Structure, and Dipole Moment of Cyclopropene. Journal of Chemical Physics, 1959, 30, 512-516.	1.2	113
56	Vibrational spectrum, structure, and energy of [1.1.1]propellane. Journal of the American Chemical Society, 1985, 107, 7247-7257.	6.6	113
57	A vibrational study of cyclohexane and some of its isotopic derivatives-III. A vibrational analysis of cyclohexane, cyclohexane-d12, cyclohexane-1,1,4,4-d4 and cyclohexane-1,1,2,2,4,4,5,5-d8. Spectrochimica Acta Part A: Molecular Spectroscopy, 1973, 29, 583-594.	0.1	110
58	Solvent Effects on the Thioamide Rotational Barrier:â€‰ An Experimental and Theoretical Study. Journal of the American Chemical Society, 2001, 123, 2038-2046.	6.6	110
59	A Comparison of the Electronic Transition Energies for Ethene, Isobutene, Formaldehyde, and Acetone Calculated Using RPA, TDDFT, and EOM-CCSD. Effect of Basis Sets. Journal of Physical Chemistry A, 2002, 106, 4192-4199.	1.1	110
60	Conformational Effects on Optical Rotation. 3-Substituted 1-Butenes. Journal of the American Chemical Society, 2003, 125, 1888-1896.	6.6	110
61	Nonresonant Optical Activity of Isolated Organic Molecules. Journal of Physical Chemistry A, 2005, 109, 11752-11764.	1.1	110
62	The Mechanisms of Hydrogen Peroxide Reactions. I. The Conversion of Benzonitrile to Benzamide. Journal of the American Chemical Society, 1953, 75, 3961-3964.	6.6	109
63	Nature of substituent effects in nuclear magnetic resonance spectroscopy. 1. Factor analysis of carbon-13 chemical shifts in aliphatic halides. Journal of Organic Chemistry, 1980, 45, 4936-4947.	1.7	109
64	Assignment of the ~A state in bicyclobutane. The multiphoton ionization spectrum and calculations of transition energies. Journal of the American Chemical Society, 1991, 113, 4782-4791.	6.6	109
65	Strain energies of small ring propellanes. Journal of the American Chemical Society, 1983, 105, 1227-1233.	6.6	108
66	Some Observations on Allylic Oxidation1. Journal of Organic Chemistry, 1964, 29, 3353-3361.	1.7	105
67	An Experimental and Computational Investigation of the Enantioselective Deprotonation of Boc-piperidine. Journal of the American Chemical Society, 2002, 124, 1889-1896.	6.6	102
68	Rotational barriers in aldehydes and ketones coordinated to neutral Lewis acids. Journal of the American Chemical Society, 1988, 110, 6642-6650.	6.6	97
69	The N.m.r. Spectra of Bicyclo [2.1.1]hexane Derivatives. Journal of the American Chemical Society, 1962, 84, 1594-1597.	6.6	94
70	Butadiene. 1. A normal coordinate analysis and infrared intensities. Structure of the second rotamer. Journal of the American Chemical Society, 1990, 112, 1509-1519.	6.6	91
71	Ab initio calculation of molar volumes: Comparison with experiment and use in solvation models. Journal of Computational Chemistry, 1995, 16, 385-394.	1.5	90
72	Bicyclo [2.1.1.]hexane Derivatives1. Journal of the American Chemical Society, 1961, 83, 3998-4006.	6.6	88

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73	Structures, energies, and modes of interconversion of C4H7+ ions. Journal of the American Chemical Society, 1988, 110, 7652-7659.	6.6	88
74	Cavity ring-down polarimetry (CRDP): theoretical and experimental characterization. Journal of the Optical Society of America B: Optical Physics, 2002, 19, 125.	0.9	88
75	The C7â^'C10 Cycloalkanes Revisited. Journal of Organic Chemistry, 2003, 68, 9322-9329.	1.7	86
76	Acidity of (Z)- and (E)-methyl acetates: relationship to Meldrum's acid. Journal of the American Chemical Society, 1988, 110, 1872-1874.	6.6	85
77	Azines. A theoretical study of .pi.-electron delocalization. Journal of the American Chemical Society, 1989, 111, 4178-4190.	6.6	85
78	Solvent effects. 4. Effect of solvent on the E/Z energy difference for methyl formate and methyl acetate. Journal of the American Chemical Society, 1993, 115, 1078-1084.	6.6	85
79	Substituent Effects on the Acidity of Weak Acids. 2. Calculated Gas-Phase Acidities of Substituted Benzoic Acids. Journal of Organic Chemistry, 2002, 67, 4787-4794.	1.7	84
80	Acid-catalyzed solvolyses of bicyclobutane derivatives. Stereochemistry of the cyclopropylcarbinyl-cyclopropylcarbinyl and related rearrangements. Journal of the American Chemical Society, 1970, 92, 571-579.	6.6	82
81	Lactones. 1. X-ray crystallographic studies of nonanolactone and tridecanolactone: nature of CH.cntdot..cntdot..cntdot.O nonbonded interactions. Journal of the American Chemical Society, 1991, 113, 971-977.	6.6	81
82	Resonance interactions in acyclic systems. 1. Energies and charge distributions in allyl anions and related compounds. Journal of the American Chemical Society, 1990, 112, 61-72.	6.6	80
83	The Mechanisms of Permanganate Oxidation. I. The Oxidation of Some Aromatic Aldehydes1. Journal of the American Chemical Society, 1955, 77, 1786-1795.	6.6	79
84	A vibrational study of cyclohexane and some of its isotopic derivativesâ€"I. Spectrochimica Acta Part A: Molecular Spectroscopy, 1971, 27, 1139-1151.	0.1	79
85	Solvent effects: 6. A comparison between gas phase and solution acidities. Journal of Computational Chemistry, 1996, 17, 185-190.	1.5	79
86	Conformational Studies in the Cyclohexane Series. 2. Phenylcyclohexane and 1-Methyl-1-phenylcyclohexane. Journal of Organic Chemistry, 2000, 65, 1181-1187.	1.7	79
87	Application of the Pople-Snatry-Segal complete neglect of differential overlap method to some hydrocarbons and their cations. Journal of the American Chemical Society, 1968, 90, 59-63.	6.6	78
88	Bicyclo[1.1.1]pentane1. Journal of the American Chemical Society, 1966, 88, 4437-4441.	6.6	77
89	Resonance interactions in acyclic systems. 5. Structures, charge distributions, and energies of some heterobutadiene rotamers. Journal of the American Chemical Society, 1992, 114, 8654-8668.	6.6	76
90	Stabilization of Carbanions. 1. Origin of the Increased Acidity of Dimethyl Sulfide As Compared to Dimethyl Ether. Journal of the American Chemical Society, 1994, 116, 10489-10497.	6.6	76

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91	Comparison of differentab initio theoretical models for calculating isodesmic reaction energies for small ring and related compounds. Journal of Computational Chemistry, 1997, 18, 108-114.	1.5	74
92	[1.1.1]Propellane: Reaction with free radicals. Tetrahedron Letters, 1986, 27, 1553-1556.	0.7	73
93	Comparison of density functional theory models' ability to reproduce experimental13C-NMR shielding values. Journal of Computational Chemistry, 1999, 20, 1299-1303.	1.5	73
94	Chiral Diamines 4:Â A Computational Study of the Enantioselective Deprotonation of Boc-pyrrolidine with an Alkyllithium in the Presence of a Chiral Diamine. Journal of the American Chemical Society, 2001, 123, 8231-8238.	6.6	73
95	Bicyclo[2.2.0]hex-1(4)-ene. Tetrahedron, 1986, 42, 1895-1902.	1.0	72
96	The Mechanisms of Hydrogen Peroxide Reactions. II. A Comparison of the Reactivity of Hydroxyl Ion and Hydroperoxide Ion toward Benzonitrile. Journal of the American Chemical Society, 1955, 77, 2519-2522.	6.6	71
97	The Stereochemistry of the Chromic Acid Oxidation of Tertiary Hydrogens1. Journal of the American Chemical Society, 1961, 83, 423-429.	6.6	69
98	Facile Oxidation of Primary Amines to Nitriles Using an Oxoammonium Salt. Organic Letters, 2014, 16, 6484-6487.	2.4	69
99	Proton Donor Acidity Controls Selectivity in Nonaromatic Nitrogen Heterocycle Synthesis. Science, 2013, 339, 678-682.	6.0	68
100	The Kinetics of the Chromic Acid Oxidation of Benzaldehyde. Journal of the American Chemical Society, 1958, 80, 3022-3029.	6.6	67
101	Substituent effects. 5. Vinyl and ethynyl derivatives. An examination of the interaction of amino and hydroxy groups with carbon-carbon double and triple bonds. Journal of the American Chemical Society, 1993, 115, 9234-9242.	6.6	67
102	Resonance interactions in acyclic systems. 2. Y-Conjugated anions and cations. Journal of the American Chemical Society, 1990, 112, 4177-4182.	6.6	66
103	Thermochemistry of Carbonyl Reactions. 6. A Study of Hydration Equilibria. Journal of the American Chemical Society, 1994, 116, 11067-11077.	6.6	66
104	6-Substituted Bicyclo[3.1.1]heptanes1. Journal of Organic Chemistry, 1966, 31, 2250-2254.	1.7	65
105	Ab Initio CBS-QCI Calculations of the Inversion Mode of Ammonia. Journal of Physical Chemistry A, 1997, 101, 3143-3151.	1.1	65
106	Câ”O and Câ”S Bonds:Â Stability, Bond Dissociation Energies, and Resonance Stabilization. Journal of Organic Chemistry, 1998, 63, 8668-8681.	1.7	65
107	The Anomeric Effect: Itâ€™s Complicated. Journal of Organic Chemistry, 2018, 83, 5242-5255.	1.7	65
108	The Nuclear Magnetic Resonance Spectra of Cyclopropane Derivatives. Journal of the American Chemical Society, 1963, 85, 2788-2790.	6.6	64

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109	Electronic states of organic molecules. 3. Photoelectron spectra of cycloalkenes and methylenecycloalkanes. Journal of the American Chemical Society, 1976, 98, 7179-7182.	6.6	64
110	Structures and energies of the tricyclo[4.1.0.01,3]heptanes and the tetracyclo[4.2.1.02,905,9]nonanes. Extended group equivalents for converting ab initio energies to heats of formation. Journal of Organic Chemistry, 1985, 50, 5285-5291.	1.7	64
111	Stereochemistry of the intramolecular enamine/enal (enone) cycloaddition reaction and subsequent transformations. Journal of the American Chemical Society, 1986, 108, 8274-8277.	6.6	64
112	Cyclopropene. I. The Reaction of 2-Bromocyclopropanecarboxylates with Potassium t-Butoxide. Journal of the American Chemical Society, 1957, 79, 4994-4999.	6.6	63
113	NMR Chemical Shifts. 3. A Comparison of Acetylene, Allene, and the Higher Cumulenes. Journal of Organic Chemistry, 1999, 64, 6394-6400.	1.7	63
114	Atomic Charges. Journal of Organic Chemistry, 2018, 83, 15463-15469.	1.7	63
115	sâ€Tetrazine. II. Infrared Spectra. Journal of Chemical Physics, 1961, 35, 1939-1945.	1.2	61
116	Tricyclo[4.2.2.22,5]dodeca-1,5-diene. Journal of the American Chemical Society, 1984, 106, 2194-2200.	6.6	61
117	Substituent Effects on the Acidity of Weak Acids. 1. Bicyclo[2.2.2]octane-1-carboxylic Acids and Bicyclo[1.1.1]pentane-1-carboxylic Acids. Journal of Organic Chemistry, 2002, 67, 1613-1617.	1.7	61
118	Bicyclo[1.1.1]pentane derivatives. Journal of Organic Chemistry, 1970, 35, 369-373.	1.7	60
119	Charge redistribution in the molecular vibrations of acetylene, ethylene, ethane, methane, silane and the ammonium ion. Signs of the M-H bond moments. The Journal of Physical Chemistry, 1984, 88, 586-593.	2.9	60
120	Rotational cooling in a supersonic expansion of ammonia. Journal of Chemical Physics, 1981, 74, 6975-6976.	1.2	59
121	Enthalpies of formation of fused cyclobutane derivatives. Journal of the American Chemical Society, 1982, 104, 5679-5686.	6.6	59
122	Ab Initio Study of the Stability of the Ylide-like Intermediate Methyleneoxonium in the Reaction between Singlet Methylene and Water. Journal of the American Chemical Society, 1996, 118, 5408-5411.	6.6	59
123	Optical Activity of 1-Butene, Butane, and Related Hydrocarbons. Journal of Physical Chemistry A, 2004, 108, 32-38.	1.1	59
124	Conformational Effects on Optical Rotation. 2-Substituted Butanes. Journal of Physical Chemistry A, 2005, 109, 3405-3410.	1.1	59
125	The Deuterium Isotope Effect of Some Ionic Reactions of Benzaldehyde. Journal of the American Chemical Society, 1954, 76, 5371-5375.	6.6	58
126	Lone Pairs in Carbonyl Compounds and Ethers. Journal of Organic Chemistry, 1994, 59, 6817-6822.	1.7	58

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127	Origin of the Acidity of Enols and Carboxylic Acids. Journal of the American Chemical Society, 1996, 118, 8291-8299.	6.6	58
128	ETHYL BICYCLO[1.1.0]BUTANE-1-CARBOXYLATE1. Journal of the American Chemical Society, 1959, 81, 5261-5262.	6.6	57
129	Isotopic perturbation of resonance. Carbon-13 nuclear magnetic resonance of 2-deuterio-2-bicyclo[2.1.1]hexyl cation. Journal of the American Chemical Society, 1977, 99, 8072-8073.	6.6	57
130	Butadiene. 2. Examination of the energetic preference for coplanarity of double bonds. Comparison of butadiene, acrolein, and vinylamine. Journal of the American Chemical Society, 1991, 113, 2890-2898.	6.6	57
131	An Experimental and Computational Study of the Enantioselective Lithiation ofN-Boc-pyrrolidine Using Sparteine-like Chiral Diamines. Journal of the American Chemical Society, 2004, 126, 15480-15489.	6.6	56
132	Substituent effects. 1. Methyl derivatives. Journal of the American Chemical Society, 1990, 112, 8765-8775.	6.6	54
133	Structures and charge distributions in alkoxide ions. Journal of the American Chemical Society, 1990, 112, 3379-3385.	6.6	53
134	Effect of Fluorine Substitution on the Energies of Small Ring Compounds. Journal of the American Chemical Society, 1998, 120, 2932-2938.	6.6	53
135	Chromic acid oxidation of isopropyl alcohol. Preoxidation equilibria. Journal of the American Chemical Society, 1969, 91, 927-932.	6.6	52
136	Permanganate oxidation of crotonic acid. Spectrometric detection of an intermediate. Journal of the American Chemical Society, 1973, 95, 3034-3035.	6.6	52
137	The PE spectrum of [1.1.1]propellane: evidence for a non-bonding MO?. Journal of the American Chemical Society, 1985, 107, 7172-7174.	6.6	52
138	The Energy Components of the Anomeric Effect for 2-Methoxytetrahydropyran. An Experimental Comparison of the Gas Phase and Solutions. Journal of the American Chemical Society, 1994, 116, 2197-2198.	6.6	52
139	The Kinetics of the Permanganate Oxidation of Alkenes1. Journal of the American Chemical Society, 1966, 88, 5827-5832.	6.6	51
140	.DELTA.1,4-Bicyclo[2.2.0]hexene. Journal of the American Chemical Society, 1971, 93, 246-247.	6.6	51
141	Carbanions 2. Intramolecular Interactions in Carbanions Stabilized by Carbonyl, Cyano, Isocyano, and Nitro Groups. Journal of Organic Chemistry, 1995, 60, 6327-6334.	1.7	51
142	The Deuterium Isotope Effect in the Side Chain Halogenation of Toluene1. Journal of the American Chemical Society, 1958, 80, 3033-3039.	6.6	50
143	Formation and Reactions of Bicyclo[1.1.1]pentyl-1 Cations. Journal of the American Chemical Society, 1994, 116, 11990-11998.	6.6	50
144	1,3-Shifts. III. The Kinetics of the Thermal Rearrangement of Phenyl Benzanilimino Ethers1. Journal of the American Chemical Society, 1955, 77, 2205-2209.	6.6	49

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145	Strained Small Ring Compounds: Bridgehead Substituted Bicyclo [2.1.1]hexanes. Journal of the American Chemical Society, 1963, 85, 3188-3193.	6.6	49
146	Nuclear magnetic resonance spectra of cyclopropyl derivatives. Journal of Organic Chemistry, 1973, 38, 378-381.	1.7	49
147	Structures, bonding, and absorption spectra of amine-sulfur dioxide charge-transfer complexes. Journal of the American Chemical Society, 1992, 114, 7527-7535.	6.6	49
148	Conformational Studies in the Cyclohexane Series. 3. The Dihalocyclohexanes. Journal of Organic Chemistry, 1999, 64, 6387-6393.	1.7	49
149	Photooxidation of Methylnaphthalenes. Journal of Organic Chemistry, 2005, 70, 105-109.	1.7	49
150	Substituent Effects. 6. Heterosubstituted Allyl Radicals. Comparison with Substituted Allyl Cations and Anions. Journal of the American Chemical Society, 1995, 117, 6535-6543.	6.6	48
151	NMR Chemical Shifts. 1. The Role of Relative Atomic Orbital Phase in Determining the Sign of the Paramagnetic Terms:Â ClF, CH3F, CH3NH3+, FNH3+, and HCâ‹®CF. Journal of Physical Chemistry A, 1998, 102, 8766-8773.	1.1	48
152	The Stereochemistry of the Wolff Rearrangement. Journal of the American Chemical Society, 1956, 78, 1640-1645.	6.6	47
153	sâ€Tetrazine. I. Highâ€Resolution Vaporâ€Phase Study of the Visiblenâ†'Ï€ Vibronic Absorption Band Systems. Journal of Chemical Physics, 1961, 35, 1925-1938.	1.2	47
154	Electronic states of organic molecules. I. Potential functions for the deformation of methane. Journal of the American Chemical Society, 1976, 98, 1212-1218.	6.6	47
155	Barriers to rotation adjacent to double bonds. 2. n-Propyl versus isopropyl groups. Journal of the American Chemical Society, 1986, 108, 5817-5822.	6.6	47
156	The Photolysis of Diazomethyl t-Butyl Ketone. Journal of the American Chemical Society, 1954, 76, 5367-5371.	6.6	46
157	Tricyclo[3.2.1.01.5]octane. 3,2,1-Propellane. Journal of the American Chemical Society, 1972, 94, 7396-7401.	6.6	46
158	Ab Initio Study of the Solvent Effects on the Singletâ^'Triplet Gap of Nitrenium Ions and Carbenes. Journal of Physical Chemistry A, 1998, 102, 2732-2738.	1.1	46
159	Large Solvation Effect in the Optical Rotatory Dispersion of Norbornenone. Angewandte Chemie - International Edition, 2014, 53, 1386-1389.	7.2	46
160	Sum-over-States Calculation of the Specific Rotations of Some Substituted Oxiranes, Chloropropionitrile, Ethane, and Norbornenone. Journal of Physical Chemistry A, 2006, 110, 13995-14002.	1.1	45
161	Enthalpy of the metal catalyzed isomerizations of quadricyclane and of tricyclo[4.1.0.02,7]heptane. Journal of the American Chemical Society, 1976, 98, 5411-5412.	6.6	44
162	Enthalpies of hydration of alkenes. 4. Formation of acyclic tert-alcohols. Journal of Organic Chemistry, 1991, 56, 5108-5110.	1.7	44

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