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	Halogenâ€“Halogen Nonbonded Interactions. ACS Omega, 2021, 6, 15199-15204.	1.6	1
2	Re-Examination of Some Carbocations. Structures, Energies, and Charge Distributions. Journal of Organic Chemistry, 2020, 85, 11741-11749.	1.7	4
3	Increase in Strain Energy during Conversion of [4.4.4.5]Fenestrane to [4.4.4.4]Fenestrane: a Method for Estimating the Heats of Formation of Hydrocarbons and Their Derivatives from Ab Initio Energies. Journal of Organic Chemistry, 2020, 85, 4981-4987.	1.7	6
4	Total Synthesis of (Â±)â€Phyllantidine: Development and Mechanistic Evaluation of a Ring Expansion for Installation of Embedded Nitrogenâ€Oxygen Bonds. Angewandte Chemie, 2020, 132, 9844-9853.	1.6	5
5	Total Synthesis of (Â±)â€Phyllantidine: Development and Mechanistic Evaluation of a Ring Expansion for Installation of Embedded Nitrogenâ€Oxygen Bonds. Angewandte Chemie - International Edition, 2020, 59, 9757-9766.	7.2	25
6	Relationship between Rotational Barriers and Charge Shifts. Journal of Organic Chemistry, 2019, 84, 10938-10945.	1.7	2
7	Unrecognized Intramolecular and Intermolecular Attractive Interactions between Fluorine-Containing Motifs and Ether, Carbonyl, and Amino Moieties. Journal of Organic Chemistry, 2019, 84, 5783-5789.	1.7	4
8	The Anomeric Effect: Itâ€™s Complicated. Journal of Organic Chemistry, 2018, 83, 5242-5255.	1.7	65
9	Atomic Charges. Journal of Organic Chemistry, 2018, 83, 15463-15469.	1.7	63
10	Role of Intramolecular Electron Delocalization in the Câ€“X Bond Strength in CH_{4-n}X_n (n = 0â€“4, X = F, Cl, CN, OCH₃). Journal of Physical Chemistry A, 2018, 122, 7716-7722.	1.1	7
11	Methoxymethane Câ€“O Bond Strengths: Do Their Changes Result from Hyperconjugation or Polar Effects?. Journal of Physical Chemistry A, 2018, 122, 6021-6025.	1.1	8
12	Butadiene and Heterodienes Revisited. Journal of Organic Chemistry, 2018, 83, 8473-8482.	1.7	12
13	Dispersive Optical Activity of (R)-Methylene Norbornene: Intrinsic Response and Solvation Effects. Journal of Physical Chemistry A, 2017, 121, 8251-8266.	1.1	10
14	Experimental Demonstration of a Sizeable Nonclassical CHÂ·Â·Â·G Hydrogen Bond in Cyclohexane Derivatives: Stabilization of an Axial Cyano Group. Organic Letters, 2017, 19, 6408-6411.	2.4	6
15	Chiroptical Properties of Imines Derived from R-(+)-Norbornenone: The Role of Electronegativity Differences. Journal of Physical Chemistry A, 2017, 121, 8247-8250.	1.1	1
16	Chirality Induced by the Interaction of Câ•€ and Câ•Ÿ Bonds (Xâ•€H₂, NH,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 147 Td (N A, 2016, 120, 7771-7777.	1.1	4
17	Controlling the Conformational Energy of a Phenyl Group by Tuning the Strength of a Nonclassical CHÂ·Â·Â·O Hydrogen Bond: The Case of 5-Phenyl-1,3-dioxane. Journal of Organic Chemistry, 2016, 81, 12116-12127.	1.7	13
18	Electron Delocalization Range in Atoms and on Molecular Surfaces. Journal of Chemical Theory and Computation, 2016, 12, 3185-3194.	2.3	11

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19	Effect of Conjugation on Electron Distributions. Separation of Ïƒ and Ï€ Terms. Journal of Chemical Theory and Computation, 2016, 12, 1220-1227.	2.3	14
20	My Study of Optical Activity - From the Distant Past to the Present with Stops in-Between. ACS Symposium Series, 2015, , 23-47.	0.5	2
21	Rotamers of phenyl substituted 1,3-dioxanes and tetrahydropyrans: importance of CHâ‹¯O Coulombic interactions. Tetrahedron Letters, 2015, 56, 3438-3440.	0.7	1
22	The Role of CHÂ·Â·Â·O Coulombic Interactions in Determining Rotameric Conformations of Phenyl Substituted 1,3-Dioxanes and Tetrahydropyrans. Journal of Organic Chemistry, 2015, 80, 7884-7889.	1.7	9
23	Intrinsic Optical Activity and Large-Amplitude Displacement: Conformational Flexibility in (R)-Glycidyl Methyl Ether. Journal of Physical Chemistry A, 2015, 119, 8311-8327.	1.1	9
24	Effect of Remote Aryl Substituents on the Conformational Equilibria of 2,2-Diaryl-1,3-dioxanes: Importance of Electrostatic Interactions. Journal of Organic Chemistry, 2015, 80, 4108-4115.	1.7	5
25	Facile Oxidation of Primary Amines to Nitriles Using an Oxoammonium Salt. Organic Letters, 2014, 16, 6484-6487.	2.4	69
26	A Computational Study of RXHn Xâ€“H Bond Dissociation Enthalpies. Journal of Physical Chemistry A, 2014, 118, 2353-2359.	1.1	11
27	Large Solvation Effect in the Optical Rotatory Dispersion of Norbornenone. Angewandte Chemie - International Edition, 2014, 53, 1386-1389.	7.2	46
28	Calculations for the Properties and Reactions of the NH, PH, and AsH Counterparts of Dimethyl Ether and Acetone. Journal of Organic Chemistry, 2014, 79, 10849-10854.	1.7	2
29	Reactions of adamantanethione with Grignard reagents: there is no evidence of addition to the CS carbon. Tetrahedron Letters, 2014, 55, 4807-4809.	0.7	2
30	Insights on the Origin of the Unusually Large Specific Rotation of (1S,4S)-Norbornenone. Journal of Physical Chemistry A, 2014, 118, 4863-4871.	1.1	31
31	Correction to Accuracy of Calculations of Heats of Reduction/Hydrogenation: Application to Some Small Ring Systems. Journal of Organic Chemistry, 2013, 78, 11628-11628.	1.7	1
32	Substituent Effects on Oâ€“H Bond Dissociation Enthalpies: A Computational Study. Journal of Physical Chemistry A, 2013, 117, 213-218.	1.1	18
33	Proton Donor Acidity Controls Selectivity in Nonaromatic Nitrogen Heterocycle Synthesis. Science, 2013, 339, 678-682.	6.0	68
34	Computational Study of the Enantioselective Deprotonation of a Cyclopropanecarboxamide with an Alkyllithium in the Presence of Sparteine. Journal of Organic Chemistry, 2013, 78, 1742-1746.	1.7	2
35	Towards the Accurate and Efficient Calculation of Optical Rotatory Dispersion Using Augmented Minimal Basis Sets. Chirality, 2013, 25, 606-616.	1.3	26
36	Intrinsic Optical Activity and Conformational Flexibility: The Role of Size-Dependent Ring Morphology in Model Cycloketones. Journal of Physical Chemistry A, 2013, 117, 12382-12400.	1.1	20

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37	Contrasting Reactions of Ketones and Thioketones with Alkyllithiums: A Coordinated Experimental and Computational Investigation. Journal of the American Chemical Society, 2012, 134, 3199-3207.	6.6	12
38	A Tale of Two Carenes: Intrinsic Optical Activity and Large-Amplitude Nuclear Displacement. Journal of Physical Chemistry A, 2012, 116, 9516-9533.	1.1	28
39	Accuracy of Calculations of Heats of Reduction/Hydrogenation: Application to Some Small Ring Systems. Journal of Organic Chemistry, 2012, 77, 10393-10398.	1.7	14
40	Oscillator Strength: How Does TDDFT Compare to EOM-CCSD?. Journal of Chemical Theory and Computation, 2011, 7, 456-466.	2.3	123
41	Computational Study of the Properties and Reactions of Small Molecules Containing O, S, and Se. Journal of Physical Chemistry A, 2011, 115, 12624-12630.	1.1	8
42	Disparate behavior of ketones and thioketones on reaction with organolithiums. Tetrahedron Letters, 2011, 52, 2169-2171.	0.7	6
43	A comparison of some properties of C=O and C=S bonds. Arkivoc, 2011, 2011, 45-56.	0.3	13
44	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
45	Intramolecular Nonbonded Attractive Interactions: 1-Substituted Propenes. Journal of Chemical Theory and Computation, 2009, 5, 1033-1037.	2.3	21
46	Disparate Behavior of Carbonyl and Thiocarbonyl Compounds: Acyl Chlorides vs Thiocarbonyl Chlorides and Isocyanates vs Isothiocyanates. Journal of Organic Chemistry, 2009, 74, 3659-3664.	1.7	16
47	Excited States and Photochemistry of Bicyclo[1.1.0]butane. Journal of Physical Chemistry A, 2009, 113, 1686-1695.	1.1	7
48	The effects of conformation and solvation on optical rotation: Substituted epoxides. Chirality, 2008, 20, 357-369.	1.3	35
49	The dimer of phenylpropiolyl chloride. Tetrahedron Letters, 2008, 49, 2049-2051.	0.7	4
50	Optical Rotatory Dispersion of 2,3-Hexadiene and 2,3-Pentadiene. Journal of Physical Chemistry A, 2008, 112, 2415-2422.	1.1	41
51	Mechanism of the Oxidation of Alcohols by Oxoammonium Cations. Journal of Organic Chemistry, 2007, 72, 4504-4509.	1.7	203
52	Correlation Effects in EOM-CCSD for the Excited States:Â Evaluated by AIM Localization Index (LI) and Delocalization Index (DI). Journal of Physical Chemistry A, 2007, 111, 3592-3601.	1.1	33
53	Effect of Substituents and Conformations on the Optical Rotations of Cyclic Oxides and Related Compounds. Relationship between the Anomeric Effect and Optical Rotation1. Journal of Organic Chemistry, 2007, 72, 6206-6214.	1.7	14
54	Permanganate Oxidation of Alkenes. Substituent and Solvent Effects. Difficulties with MP2 Calculations. Journal of the American Chemical Society, 2006, 128, 11537-11544.	6.6	23

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55	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
56	Conformational studies of 3-hexyne. International Journal of Quantum Chemistry, 2006, 106, 3364-3370.	1.0	5
57	Application of the ONIOM method to enantioselective deprotonation in the presence of spartein. Computational and Theoretical Chemistry, 2006, 775, 93-99.	1.5	7
58	Conformational Preferences for 1,2- and 1,4-Difluorocyclohexane.. ChemInform, 2006, 37, no.	0.1	0
59	Conformational Preferences for 1,2- and 1,4-Difluorocyclohexane. Journal of Organic Chemistry, 2005, 70, 8381-8384.	1.7	19
60	Strained Hydrocarbons: Structures, Stability, and Reactivity. , 2005, , 717-740.		2
61	Photooxidation of Methylnaphthalenes. Journal of Organic Chemistry, 2005, 70, 105-109.	1.7	49
62	Comparison of CIS- and EOM-CCSD-Calculated Adiabatic Excited-State Structures. Changes in Charge Density on Going to Adiabatic Excited States. Journal of Physical Chemistry A, 2005, 109, 466-477.	1.1	35
63	Chiroptical Properties of 2-Chloropropionitrile. Journal of Physical Chemistry A, 2005, 109, 3448-3453.	1.1	30
64	Nonresonant Optical Activity of Isolated Organic Molecules. Journal of Physical Chemistry A, 2005, 109, 11752-11764.	1.1	110
65	Conformational Effects on Optical Rotation. 2-Substituted Butanes. Journal of Physical Chemistry A, 2005, 109, 3405-3410.	1.1	59
66	Deoxygenation of Alcohols Employing Water as the Hydrogen Atom Source. Journal of the American Chemical Society, 2005, 127, 12513-12515.	6.6	213
67	Strain, Structure, Stability and Reactivity. Foundations of Chemistry, 2004, 6, 65-80.	0.4	12
68	Conformational energies for 2-substituted butanes. Journal of Computational Chemistry, 2004, 25, 1127-1132.	1.5	5
69	Basis set effects on calculated geometries: 6-311++G** vs. aug-cc-pVDZ. Journal of Computational Chemistry, 2004, 25, 1342-1346.	1.5	213
70	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
71	Electronically Excited States of Methylenecycloalkanes. Journal of Physical Chemistry A, 2004, 108, 9417-9422.	1.1	4
72	NMR Chemical Shifts. Substituted Acetylenes. Journal of Organic Chemistry, 2004, 69, 1086-1096.	1.7	21

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73	Temperature Dependence of Optical Rotation:â€‰ Î±-Pinene, Î²-Pinene Pinane, Camphene, Camphor and Fenchone. Journal of Physical Chemistry A, 2004, 108, 5559-5563.	1.1	33
74	Optical Activity of 1-Butene, Butane, and Related Hydrocarbons. Journal of Physical Chemistry A, 2004, 108, 32-38.	1.1	59
75	Substituent Effects on the Acidity of Weak Acids. 4. Anilinium Ions. Collection of Czechoslovak Chemical Communications, 2004, 69, 2183-2192.	1.0	6
76	Conformational Effects on Optical Rotation. 3-Substituted 1-Butenes. Journal of the American Chemical Society, 2003, 125, 1888-1896.	6.6	110
77	2,6-Diaziadamantane:â€‰ A Single-Crystal X-ray Diffraction Study and Theoretical Calculations. Journal of Organic Chemistry, 2003, 68, 2129-2134.	1.7	7
78	The C7â^'C10 Cycloalkanes Revisited. Journal of Organic Chemistry, 2003, 68, 9322-9329.	1.7	86
79	Substituent Effects on the Acidity of Weak Acids. 3. Phenols and Benzyl Alcohols. Journal of Organic Chemistry, 2003, 68, 875-882.	1.7	29
80	An optical mounting system for cavity ring-down polarimetry. Review of Scientific Instruments, 2002, 73, 1340-1342.	0.6	10
81	Comparative Study of Anionic and Radical Cyclization for the Preparation of 1,3-Dimethylindans:â€‰ Highly Stereoselective Preparation ofcis-1,3-Disubstituted Indans via Intramolecular Carbolithiation. Organic Letters, 2002, 4, 791-794.	2.4	25
82	Dipole-Stabilized Carbanions:Â A Computational Study ofN-Methylformamide Anion and MethylN-Methylcarbamate Anion. Journal of Organic Chemistry, 2002, 67, 5365-5368.	1.7	11
83	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
84	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
85	Thermal Rearrangements of Spiro[2.4]hepta-1,4,6-trienes. Journal of Organic Chemistry, 2002, 67, 4436-4440.	1.7	12
86	Methyl Rotational Barriers in Amides and Thioamides. Journal of Organic Chemistry, 2002, 67, 826-830.	1.7	39
87	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
88	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
89	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
90	Antiaromaticity in Monocyclic Conjugated Carbon Rings. Chemical Reviews, 2001, 101, 1317-1332.	23.0	194

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91	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
92	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
93	Solvent Effects on Methyl Transfer Reactions. 2. The Reaction of Amines with Trimethylsulfonium Salts. Journal of the American Chemical Society, 2001, 123, 6092-6097.	6.6	34
94	Computational Study of 10-X-2 Ate Complexes Derived from Vinyllithiums and Vinyl Halides. Organometallics, 2001, 20, 771-774.	1.1	14
95	19F NMR Chemical Shifts. 1. Aliphatic Fluorides. Journal of Organic Chemistry, 2001, 66, 2809-2817.	1.7	28
96	A Transition State for the Enantioselective Deprotonation ofN-Boc-Pyrrolidine with Isopropyllithium/(â^')-Sparteine. Angewandte Chemie - International Edition, 2000, 39, 2127-2129.	7.2	43
97	Chiral diamines. 1. Relative energies of (â^')-sparteine conformers, interconversion barriers, and alkyllithium complexes. Journal of Molecular Structure, 2000, 556, 239-244.	1.8	28
98	Chiral diamines. Part 3: Effect of ligand structure on the enantioselective deprotonation of N-Boc-pyrrolidine with i-PrLi: a computational comparison of (â^')-sparteine and (S,S)-1,2-bis(N,N-dimethylamino)cyclohexane. Tetrahedron Letters, 2000, 41, 9365-9368.	0.7	25
99	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
100	Kinetics of the Base-Catalyzed Permanganate Oxidation of Benzaldehyde. Journal of Organic Chemistry, 2000, 65, 573-576.	1.7	23
101	Solvation and Structural Effects on the Stability of 10-X-2 Ate-Complexes:Â A Computational Study. Journal of Organic Chemistry, 2000, 65, 2014-2021.	1.7	32
102	Conformational Studies in the Cyclohexane Series. 2. Phenylcyclohexane and 1-Methyl-1-phenylcyclohexane. Journal of Organic Chemistry, 2000, 65, 1181-1187.	1.7	79
103	Vibrational Analysis of the Ground States of Trifluoroacetyl Fluoride and Trifluoroacetyl Chloride. Journal of Physical Chemistry A, 2000, 104, 370-379.	1.1	4
104	Origin of the Inversion of the Acidity Order for Haloacetic Acids on Going from the Gas Phase to Solution. Journal of Physical Chemistry A, 2000, 104, 7625-7628.	1.1	27
105	Stereochemistry of the Deamination of Spiropentylamine. Journal of Organic Chemistry, 1999, 64, 7763-7767.	1.7	15
106	Conformations of ethyl esters versus thiolesters. Theoretical Chemistry Accounts, 1999, 102, 272-278.	0.5	10
107	Comparison of density functional theory models' ability to reproduce experimental13C-NMR shielding values. Journal of Computational Chemistry, 1999, 20, 1299-1303.	1.5	73
108	The Interaction of Carbonyl Groups with Substituents. Accounts of Chemical Research, 1999, 32, 922-929.	7.6	121

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109	Conformational Studies in the Cyclohexane Series. 3. The Dihalocyclohexanes. Journal of Organic Chemistry, 1999, 64, 6387-6393.	1.7	49
110	NMR Chemical Shifts. 3. A Comparison of Acetylene, Allene, and the Higher Cumulenes. Journal of Organic Chemistry, 1999, 64, 6394-6400.	1.7	63
111	Conformational Composition of Gaseoustrans-1,4-Dichlorocyclohexane. Molecular Structures and Energy Differences of the aa and ee Components from Gas-Phase Electron Diffraction and ab Initio Calculations. Journal of Physical Chemistry A, 1999, 103, 7709-7714.	1.1	13
112	Solvent Effects on Methyl Transfer Reactions. 1. The Menshutkin Reaction. Journal of the American Chemical Society, 1999, 121, 2139-2146.	6.6	115
113	NMR Chemical Shifts. 2. Interpretation of the Carbon Chemical Shifts in Monocyclic Aromatic Compounds and Carbenes. Journal of Physical Chemistry A, 1999, 103, 21-27.	1.1	32
114	Rearrangements of Spiropentyl Cation. Journal of Organic Chemistry, 1999, 64, 7768-7772.	1.7	10
115	Deamination oftrans-2-Methyl- andtrans-2-Phenylcyclopropylamines. Journal of Organic Chemistry, 1999, 64, 7756-7762.	1.7	11
116	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
117	Aromaticity and its chemical manifestations. Theoretical and Computational Chemistry, 1999, 6, 519-536.	0.2	7
118	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
119	Internal hydrogen bonding in gaseous 3-aminoacrolein: an electron-diffraction investigation augmented by ab initio calculations of its molecular structure and conformational composition. Journal of Molecular Structure, 1998, 445, 1-11.	1.8	8
120	Effect of Fluorine Substitution on the Energies of Small Ring Compounds. Journal of the American Chemical Society, 1998, 120, 2932-2938.	6.6	53
121	Ring Expansion and Contraction of a Two-Carbon Bridged Spiropentane. Journal of Organic Chemistry, 1998, 63, 1390-1401.	1.7	33
122	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
123	Effect of Fluorine Substitution on the Carbon Acidity of Methane, Methyl Isocyanide, Acetonitrile, Acetaldehyde, and Nitromethane. Journal of Organic Chemistry, 1998, 63, 3937-3942.	1.7	32
124	Synthesis, Reactions, and Structural Studies of Two-Carbon Bridged Spiropentanes. Journal of Organic Chemistry, 1998, 63, 1402-1407.	1.7	15
125	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
126	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

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127	Substituent Effects. 7. Phenyl Derivatives. When Is a Fluorine a Ï€-Donor?. Journal of Organic Chemistry, 1998, 63, 3722-3730.	1.7	38
128	Ab Initio CBS-QCI Calculations of the Inversion Mode of Ammonia. Journal of Physical Chemistry A, 1997, 101, 3143-3151.	1.1	65
129	Properties of Some Condensed Aromatic Systems. Journal of Organic Chemistry, 1997, 62, 5720-5727.	1.7	144
130	13C NMR chemical shifts of methyl cation and anion: A relationship between chemical shift and charge?. Tetrahedron Letters, 1997, 38, 323-326.	0.7	11
131	Reactions of perfluoro-1-chloro-2-trimethylsilylcyclobutene. Tetrahedron Letters, 1997, 38, 1685-1688.	0.7	6
132	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
133	Origin of the Acidity of Enols and Carboxylic Acids. Journal of the American Chemical Society, 1996, 118, 8291-8299.	6.6	58
134	Carbonâ^'Carbon Rotational Barriers in Butane, 1-Butene, and 1,3-Butadiene. The Journal of Physical Chemistry, 1996, 100, 16162-16168.	2.9	130
135	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
136	The Role of Electrostatic Effects in Organic Chemistry. Journal of Chemical Education, 1996, 73, 1089.	1.1	31
137	Bent Bonds in Organic Compounds. Accounts of Chemical Research, 1996, 29, 229-234.	7.6	218
138	The role of hydrogens in stabilizing organic ions. Canadian Journal of Chemistry, 1996, 74, 892-900.	0.6	32
139	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
140	Solvent effects: 6. A comparison between gas phase and solution acidities. Journal of Computational Chemistry, 1996, 17, 185-190.	1.5	79
141	Ring contraction of a two-carbon bridged spiropentane. Tetrahedron Letters, 1996, 37, 8285-8288.	0.7	8
142	Solvent effects: 6. A comparison between gas phase and solution acidities. , 1996, 17, 185.		1
143	Solvent effects: 6. A comparison between gas phase and solution acidities. , 1996, 17, 185.		1
144	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

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145	Bridged spiropentanes: Ring expansion. Tetrahedron Letters, 1995, 36, 1171-1174.	0.7	11
146	A Comparison of Model Chemistries. Journal of the American Chemical Society, 1995, 117, 11299-11308.	6.6	315
147	Observation of the XY- abstraction products in the ion-molecule reactions X- + RY .fwdarw. XY- + R: an alternative to the SN2 mechanism at suprathermal collision energies. Journal of the American Chemical Society, 1995, 117, 1828-1832.	6.6	27
148	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
149	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
150	Why Does Thioformamide Have a Larger Rotational Barrier Than Formamide?. Journal of the American Chemical Society, 1995, 117, 2201-2209.	6.6	198
151	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
152	Solvent Effects on 1,2-Dihaloethane Gauche/Trans Ratios. The Journal of Physical Chemistry, 1995, 99, 9072-9079.	2.9	226
153	Thermochemistry of Carbonyl Reactions. 6. A Study of Hydration Equilibria. Journal of the American Chemical Society, 1994, 116, 11067-11077.	6.6	66
154	Formation and Reactions of Bicyclo[1.1.1]pentyl-1 Cations. Journal of the American Chemical Society, 1994, 116, 11990-11998.	6.6	50
155	Lone Pairs in Carbonyl Compounds and Ethers. Journal of Organic Chemistry, 1994, 59, 6817-6822.	1.7	58
156	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
157	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
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