Leo Radom

List of Publications by Year
in descending order

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467	36,502	5248	4419
papers	citations	83 h-index	172 g-index

492	492	492	17713
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Harmonic Vibrational Frequencies:Â An Evaluation of Hartreeâ^'Fock, MÃ¸llerâ^'Plesset, Quadratic Configuration Interaction, Density Functional Theory, and Semiempirical Scale Factors. The Journal of Physical Chemistry, 1996, 100, 16502-16513.	2.9	6,586
2	An Evaluation of Harmonic Vibrational Frequency Scale Factors. Journal of Physical Chemistry A, 2007, 111, 11683-11700.	1.1	2,264
3	Extension of Gaussianâ€2 theory to molecules containing thirdâ€row atoms Gaâ€“Kr. Journal of Chemical Physics, 1995, 103, 6104-6113.	1.2	958
4	Extension of Gaussian-2 (G2) theory to molecules containing third-row atoms K and Ca. Journal of Chemical Physics, 1997, 107, 5016-5021.	1.2	807
5	Scaling Factors for Obtaining Fundamental Vibrational Frequencies and Zeroâ€Point Energies from HF/6â€“31G* and MP2/6â€“31G* Harmonic Frequencies. Israel Journal of Chemistry, 1993, 33, 345-350.	1.0	791
6	Factors Controlling the Addition of Carbon-Centered Radicals to Alkenesâ€”An Experimental and Theoretical Perspective. Angewandte Chemie - International Edition, 2001, 40, 1340-1371.	7.2	640
7	Extension of Gaussianâ€1 (G1) theory to bromineâ€containing molecules. Journal of Chemical Physics, 1991, 94, 511-516.	1.2	518
8	Extension of Gaussianâ€2 (G2) theory to bromineâ€and iodineâ€containing molecules: Use of effective core potentials. Journal of Chemical Physics, 1995, 103, 1878-1885.	1.2	481
9	Molecular orbital theory of the electronic structure of organic compounds. XIII. Fourier component analysis of internal rotation potential functions in saturated molecules. Journal of the American Chemical Society, 1972, 94, 2371-2381.	6.6	405
10	Heats of Formation from G2, G2(MP2), and G2(MP2,SVP) Total Energies. The Journal of Physical Chemistry, 1996, 100, 17460-17464.	2.9	327
11	Molecular orbital theory of the electronic structure of organic compounds. XII. Conformations, stabilities, and charge distributions in monosubstituted benzenes. Journal of the American Chemical Society, 1972, 94, 1496-1504.	6.6	304
12	G3-RAD and G3X-RAD: Modified Gaussian-3 (G3) and Gaussian-3X (G3X) procedures for radical thermochemistry. Journal of Chemical Physics, 2003, 118, 4849-4860.	1.2	276
13	Bond Dissociation Energies and Radical Stabilization Energies Associated with Substituted Methyl Radicals. Journal of Physical Chemistry A, 2001, 105, 6750-6756.	1.1	265
14	Detection of the prototype phosphonium (CH2PH3), sulfonium (CH2SH2) and chloronium (CH2ClH) ylides by neutralization-reionization mass spectrometry: a theoretical prediction. Journal of the American Chemical Society, 1984, 106, 5805-5808.	6.6	261
15	Ab initiostatistical thermodynamical models for the computation of third-law entropies. Journal of Chemical Physics, 1997, 106, 6655-6674.	1.2	253
16	Assigning absolute values to proton affinities: a differentiation between competing scales. Journal of the American Chemical Society, 1993, 115, 4885-4888.	6.6	244
17	Molecular orbital theory of the electronic structure of organic compounds. XVII. Internal rotation in 1,2-disubstituted ethanes. Journal of the American Chemical Society, 1973, 95, 693-698.	6.6	235
18	Transition structures for the interchange of hydrogen atoms within the water dimer. Journal of Chemical Physics, 1990, 92, 1240-1247.	1.2	230

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19	Gas-Phase Identity SN2 Reactions of Halide Anions with Methyl Halides: A High-Level Computational Study. Journal of the American Chemical Society, 1995, 117, 2024-2032.	6.6	230
20	Strong conformational consequences of hyperconjugation. Journal of the American Chemical Society, 1972, 94, 6221-6223.	6.6	224
21	Gaussianâ€2 (G2) theory: Reduced basis set requirements. Journal of Chemical Physics, 1996, 104, 5148-5152.	1.2	216
22	Trends in Râ˜X Bond Dissociation Energies (R = Me, Et,i-Pr,t-Bu; X = H, CH3, OCH3, OH, F):Â A Surprising Shortcoming of Density Functional Theory. Journal of Physical Chemistry A, 2005, 109, 7558-7566.	1.1	210
23	A restricted-open-shell complete-basis-set model chemistry. Journal of Chemical Physics, 2006, 125, 094106.	1.2	208
24	An assessment of theoretical procedures for the calculation of reliable free radical thermochemistry: A recommended new procedure. Journal of Chemical Physics, 1998, 108, 604-615.	1.2	206
25	A Priori Prediction of Propagation Rate Coefficients in Free-Radical Polymerizations: Propagation of Ethylene. Macromolecules, 1995, 28, 8771-8781.	2.2	205
26	Structures and stabilities of singly charged three-electron hemibonded systems and their hydrogen-bonded isomers. Journal of the American Chemical Society, 1988, 110, 4931-4941.	6.6	194
27	Rapid Additive-Free Selenocysteineâ€“Selenoester Peptide Ligation. Journal of the American Chemical Society, 2015, 137, 14011-14014.	6.6	181
28	Calculation of Proton Affinities Using the G2(MP2,SVP) Procedure. The Journal of Physical Chemistry, 1995, 99, 6468-6471.	2.9	179
29	Molecular orbital theory of the electronic structure of organic compounds. VII. Systematic study of energies, conformations, and bond interactions. Journal of the American Chemical Society, 1971, 93, 289-300.	6.6	172
30	Distonic radical cations. Tetrahedron, 1986, 42, 6225-6234.	1.0	170
31	Theoretical approach to substituent effects. Phenols and phenoxide ions. Journal of Organic Chemistry, 1980, 45, 818-826.	1.7	165
32	Ab Initio Evidence for Slow Fragmentation in RAFT Polymerization. Journal of the American Chemical Society, 2003, 125, 1490-1491.	6.6	148
33	The weakly exothermic rearrangement of methoxy radical (CH3Oâ‹…) to the hydroxymethyl radical (CH2OHâ‹…). Journal of Chemical Physics, 1983, 78, 845-853.	1.2	147
34	Gas-Phase Non-Identity SN2 Reactions of Halide Anions with Methyl Halides:Â A High-Level Computational Study. Journal of the American Chemical Society, 1996, 118, 6273-6284.	6.6	147
35	Radical Addition to Alkenes:Â Further Assessment of Theoretical Procedures. Journal of Physical Chemistry A, 1998, 102, 2237-2245.	1.1	147
36	G4(MP2)-6X: A Cost-Effective Improvement to G4(MP2). Journal of Chemical Theory and Computation, 2011, 7, 112-120.	2.3	145

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37	The reversible addition-fragmentation chain transfer process and the strength and limitations of modeling: Comment on ?the magnitude of the fragmentation rate coefficient?. Journal of Polymer Science Part A, 2003, 41, 2828-2832.	2.5	143
38	Ylides and ylidions: a comparative study of unusual gas-phase structures. Journal of the American Chemical Society, 1987, 109, 2250-2263.	6.6	137
39	Consequences of Spin Contamination in Unrestricted Calculations on Open-Shell Species: Effect of Hartreeâ^'Fock and MÃ¸llerâ^'Plesset Contributions in Hybrid and Double-Hybrid Density Functional Theory Approaches. Journal of Physical Chemistry A, 2008, 112, 13225-13230.	1.1	137
40	Radical Addition to Alkenes: An Assessment of Theoretical Procedures. The Journal of Physical Chemistry, 1995, 99, 8582-8588.	2.9	135
41	Câ^'HÂ·Â·Â·X Hydrogen Bonds of Acetylene, Ethylene, and Ethane with First- and Second-Row Hydrides. Journal of Physical Chemistry A, 2001, 105, 4470-4479.	1.1	135
42	An evaluation of the performance of density functional theory, MP2, MP4, F4, G2(MP2) and G2 procedures in predicting gas-phase proton affinities. Chemical Physics Letters, 1994, 231, 345-351.	1.2	133
43	Slow convergence of the mÃ¸ller-plesset perturbation series: the dissociation energy of hydrogen cyanide and the electron affinity of the cyano radical. Chemical Physics Letters, 1987, 138, 481-485.	1.2	130
44	Molecular orbital theory of the electronic structure of organic compounds. XVI. Conformations and stabilities of substituted ethyl, propyl, and butyl cations. Journal of the American Chemical Society, 1972, 94, 5935-5945.	6.6	127
45	The mechanism of action of adenosylcobalamin. Journal of the American Chemical Society, 1976, 98, 6331-6338.	6.6	126
46	A theoretical study of the CHNO isomers. Journal of the American Chemical Society, 1977, 99, 7806-7816.	6.6	124
47	Substituent Effects in Xanthate-Mediated Polymerization of Vinyl Acetate:â€‰ Ab Initio Evidence for an Alternative Fragmentation Pathway. Macromolecules, 2004, 37, 590-596.	2.2	124
48	Reliable Theoretical Procedures for Calculating the Rate of Methyl Radical Addition to Carbonâ^'Carbon Double and Triple Bonds. Journal of Physical Chemistry A, 2004, 108, 2874-2883.	1.1	122
49	Unimolecular rearrangements connecting hydroxyethylidene (CH3-C-OH), acetaldehyde (CH3-CH:O), and vinyl alcohol (CH2:CH-OH). Journal of the American Chemical Society, 1991, 113, 6452-6458.	6.6	121
50	An assessment of theoretical procedures for the calculation of reliable radical stabilization energiesâ€Šâ€â€¡. Journal of the Chemical Society Perkin Transactions II, 1999, , 2305-2313.	0.9	121
51	The application of ab initio molecular orbital theory to structural moieties of carbohydrates. Carbohydrate Research, 1974, 38, 81-95.	1.1	119
52	The performance of B3-LYP density functional theory in describing SN2 reactions at saturated carbon. Chemical Physics Letters, 1996, 260, 558-564.	1.2	118
53	Comparison of the Addition of CH3.bul., CH2OH.bul., and CH2CN.bul. Radicals to Substituted Alkenes: A Theoretical Study of the Reaction Mechanism. Journal of the American Chemical Society, 1994, 116, 6284-6292.	6.6	114
54	Molecular orbital theory of the electronic structure of organic compounds. XXII. Structures and stabilities of C3H3+ and C3H+ cations. Journal of the American Chemical Society, 1976, 98, 10-14.	6.6	113

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55	Zeolites as Transition-Metal-Free Hydrogenation Catalysts:â€‰ A Theoretical Mechanistic Study. Journal of the American Chemical Society, 2000, 122, 2613-2620.	6.6	113
56	Structures and stabilities of gas-phase C2H3O+ ions: an ab initio molecular orbital study. Journal of the American Chemical Society, 1983, 105, 309-314.	6.6	110
57	Chemoselective Peptide Ligationâ€“Desulfurization at Aspartate. Angewandte Chemie - International Edition, 2013, 52, 9723-9727.	7.2	110
58	Why does unrestricted Mo/llerâ€“Plesset perturbation theory converge so slowly for spinâ€contaminated wave functions?. Journal of Chemical Physics, 1988, 89, 7307-7314.	1.2	109
59	An Assessment of the Performance of High-Level Theoretical Procedures in the Computation of the Heats of Formation of Small Open-Shell Molecules. Journal of Physical Chemistry A, 2002, 106, 7927-7936.	1.1	109
60	Gas-Phase Identity SN2 Reactions of Halide Anions and Methyl Halides with Retention of Configuration. Journal of the American Chemical Society, 1996, 118, 11258-11264.	6.6	108
61	Planar-Tetracoordinate Carbon in a Neutral Saturated Hydrocarbon: Theoretical Design and Characterization. Angewandte Chemie - International Edition, 1999, 38, 2875-2878.	7.2	106
62	W2X and W3X-L: Cost-Effective Approximations to W2 and W4 with kJ mol^{â€“1} Accuracy. Journal of Chemical Theory and Computation, 2015, 11, 2109-2119.	2.3	106
63	Phenyl Radical, Cation, and Anion. The Tripletâ^'Singlet Gap and Higher Excited States of the Phenyl Cation. Journal of the American Chemical Society, 1997, 119, 8083-8088.	6.6	103
64	Deceptive convergence in mÃ¸ller-plesset perturbation energies. Chemical Physics Letters, 1986, 132, 16-22.	1.2	101
65	Fulvalenes, Fulvenes, and Related Molecules:â€‰ An ab Initio Study. Journal of Organic Chemistry, 1997, 62, 2026-2038.	1.7	101
66	Bond Dissociation Energies and Radical Stabilization Energies:â€‰ An Assessment of Contemporary Theoretical Procedures. Journal of Physical Chemistry A, 2007, 111, 13638-13644.	1.1	101
67	Reactivity of disulfide bonds is markedly affected by structure and environment: implications for protein modification and stability. Scientific Reports, 2016, 6, 38572.	1.6	101
68	A theoretical study of substituted CHNO isomers. Journal of the American Chemical Society, 1978, 100, 3674-3685.	6.6	100
69	A theoretical approach to substituent effects. Structural consequences of methyl hyperconjugation. Methyl tilt angles and carbon-hydrogen bond lengths. Journal of the American Chemical Society, 1980, 102, 2253-2259.	6.6	98
70	Model for the Exceptional Reactivity of Peroxiredoxins 2 and 3 with Hydrogen Peroxide. Journal of Biological Chemistry, 2011, 286, 18048-18055.	1.6	97
71	Ring Opening of the Cyclopropylcarbinyl Radical and ItsN- andO-Substituted Analogues:Â A Theoretical Examination of Very Fast Unimolecular Reactions. Journal of the American Chemical Society, 1998, 120, 10223-10233.	6.6	96
72	Determination of Arrhenius Parameters for Propagation in Free-Radical Polymerizations:â€‰ An Assessment of ab Initio Procedures. The Journal of Physical Chemistry, 1996, 100, 18997-19006.	2.9	95

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73	Proton-Transport Catalysis:Â A Systematic Study of the Rearrangement of the Isoformyl Cation to the Formyl Cation. Journal of the American Chemical Society, 1997, 119, 7573-7578.	6.6	95
74	The Ionization of Alkanes. Israel Journal of Chemistry, 1983, 23, 21-36.	1.0	92
75	Assessment of Theoretical Procedures for Calculating Barrier Heights for a Diverse Set of Water-Catalyzed Proton-Transfer Reactions. Journal of Physical Chemistry A, 2012, 116, 4211-4221.	1.1	92
76	Water-Catalyzed Interconversion of Conventional and Distonic Radical Cations:Â Methanol and Methyleneoxonium Radical Cations. Journal of the American Chemical Society, 1996, 118, 6299-6300.	6.6	90
77	An ab initio molecular orbital study of the structures and stabilities of the C2H4O+.cntdot. isomers. Journal of the American Chemical Society, 1979, 101, 5540-5545.	6.6	88
78	Existence of stable structural isomers of ketene. A theoretical study of the C2H2O potential energy surface. Journal of Organic Chemistry, 1982, 47, 1869-1875.	1.7	88
79	Entropies and Free Energies of Protonation and Proton-Transfer Reactions. Journal of the American Chemical Society, 1997, 119, 9014-9020.	6.6	86
80	Design of Radical-Resistant Amino Acid Residues:Â A Combined Theoretical and Experimental Investigation. Journal of the American Chemical Society, 2003, 125, 4119-4124.	6.6	86
81	Methylenoxonium radical cation (CH2OH2+.bul.): a surprisingly stable isomer of the methanol radical cation. Journal of the American Chemical Society, 1982, 104, 2929-2930.	6.6	85
82	Theoretical study of the organosulfur systems CSHn (n=0â€“4) and CSHn+ (n=0â€“5): Dissociation 6766-6773.	1.2	85
83	HOC+: An observable interstellar species? A comparison with the isomeric and isoelectronic HCO+, HCN and HNC. Chemical Physics, 1981, 60, 1-10.	0.9	84
84	Theoretical approach to substituent effects. Structures and stabilities of carbanions XCH2. Journal of Organic Chemistry, 1981, 46, 1693-1699.	1.7	83
85	Methyl Radical Addition to CS Double Bonds:â€‰ Kinetic versus Thermodynamic Preferences. Journal of Physical Chemistry A, 2002, 106, 12124-12138.	1.1	82
86	The Wolff Rearrangement: The Relevant Portion of the Oxirene-Ketene Potential Energy Hypersurface. Journal of the American Chemical Society, 1994, 116, 10159-10164.	6.6	80
87	Effects of Neutral Bases on the Isomerization of Conventional Radical Cations CH3Xâ€¢+to Their Distonic Isomersâ€¢CH2X+H (X = F, OH, NH2):Â Proton-Transport Catalysis and Other Mechanisms. Journal of the American Chemical Society, 1997, 119, 9831-9839.	6.6	80
88	Understanding the Mechanism of B12-Dependent Diol Dehydratase:Â A Synergistic Retro-Pushâ^'Pull Proposal. Journal of the American Chemical Society, 2001, 123, 1664-1675.	6.6	80
89	Structural predictions for open-shell systems: a comparative assessment of ab initio procedures. The Journal of Physical Chemistry, 1983, 87, 79-82.	2.9	79
90	Variable Trends in Râ^'X Bond Dissociation Energies (R = Me, Et,i-Pr,t-Bu). Organic Letters, 2003, 5, 4689-4692.	2.4	79

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91	W1X-1 and W1X-2: W1-Quality Accuracy with an Order of Magnitude Reduction in Computational Cost. Journal of Chemical Theory and Computation, 2012, 8, 4259-4269.	2.3	79
92	The evaluation of molecular electron affinities. Journal of Computational Chemistry, 1986, 7, 349-358.	1.5	78
93	6-311G(MC)(d,p): a second-row analogue of the 6-311G(d,p) basis set: calculated heats of formation for second-row hydrides. The Journal of Physical Chemistry, 1988, 92, 4875-4880.	2.9	78
94	The structure and stability of the O2+2 dication: a dramatic failure of MÃ¸llerâ€"Plesset perturbation theory. Chemical Physics Letters, 1991, 182, 216-224.	1.2	78
95	The oxygen analog of the protonated cyclopropane problem. A theoretical study of the C2H5O+ potential energy surface. Journal of the American Chemical Society, 1981, 103, 1913-1922.	6.6	77
96	Understanding the Mechanism of B12-Dependent Methylmalonyl-CoA Mutase:Â Partial Proton Transfer in Action. Journal of the American Chemical Society, 1999, 121, 9388-9399.	6.6	77
97	Optimization and Basis-Set Dependence of a Restricted-Open-Shell Form of B2-PLYP Double-Hybrid Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 9861-9873.	1.1	77
98	Experimental evidence for the existence of a stable isomer of CH3OH+.cntdot.: the methylenoxonium radical cation, CH2OH2+.cntdot.. Journal of the American Chemical Society, 1982, 104, 2930-2931.	6.6	76
99	Heats of Formation of Alkali Metal and Alkaline Earth Metal Oxides and Hydroxides:â€‰ Surprisingly Demanding Targets for High-Level ab Initio Procedures. Journal of Physical Chemistry A, 2003, 107, 5617-5630.	1.1	76
100	Is SN2 Substitution with Inversion of Configuration at Vinylic Carbon Feasible?. Journal of the American Chemical Society, 1994, 116, 5961-5962.	6.6	75
101	Gas-Phase Identity SN2 Reactions of Halide Ions at Neutral Nitrogen: A High-Level Computational Study. Journal of the American Chemical Society, 1995, 117, 9012-9018.	6.6	75
102	Assessment of Procedures for Calculating Radical Hyperfine Structures. Journal of Physical Chemistry A, 1997, 101, 1352-1359.	1.1	75
103	Structures and stabilities of C3H6O+. isomers. An ab initio molecular orbital study. Journal of the American Chemical Society, 1980, 102, 2246-2252.	6.6	74
104	Alkaplanes: a class of neutral hydrocarbons containing a potentially planar tetracoordinate carbon. Journal of the American Chemical Society, 1993, 115, 3320-3321.	6.6	74
105	Gas-phase acidities: a comparison of density functional, MP2, MP4, F4, G2(MP2, SVP), G2(MP2) and G2 procedures. Chemical Physics Letters, 1995, 245, 123-128.	1.2	74
106	The additivity of polarization function and electron correlation effects in ab initio molecular-orbital calculations. Chemical Physics Letters, 1982, 89, 497-500.	1.2	73
107	Bond Dissociation Energies and Radical Stabilization Energies Associated with Model Peptide-Backbone Radicals. Journal of Physical Chemistry A, 2005, 109, 6318-6325.	1.1	72
108	Is formamide planar or nonplanar?. Journal of the American Chemical Society, 1979, 101, 2233-2234.	6.6	71

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109	Methane dication: planar but not square. Journal of the American Chemical Society, 1989, 111, 1155-1156.	6.6	71
110	Zeolite-Catalyzed Hydrogenation of Carbon Dioxide and Ethene. Journal of the American Chemical Society, 2008, 130, 9790-9799.	6.6	71
111	Determination of Barrier Heights for Proton Exchange in Small Water, Ammonia, and Hydrogen Fluoride Clusters with G4(MP2)-Type, MPn, and SCS-MPn Proceduresâ€”A Caveat. Journal of Chemical Theory and Computation, 2012, 8, 3128-3136.	2.3	71
112	Comparison of the Kinetics and Thermodynamics for Methyl Radical Addition to CC, CO, and CS Double Bonds. Journal of the American Chemical Society, 2004, 126, 1732-1740.	6.6	70
113	An Assessment of Theoretical Procedures for Predicting the Thermochemistry and Kinetics of Hydrogen Abstraction by Methyl Radical from Benzene. Journal of Physical Chemistry A, 2006, 110, 8942-8951.	1.1	70
114	Isoelectronic analogs of molecular nitrogen: Tightly bound multiply charged species. Journal of Chemical Physics, 1989, 91, 2971-2979.	1.2	69
115	Nitrosomethane and its nitrone and oxime isomers. A theoretical study of 1,2- and 1,3-intramolecular hydrogen shifts. Journal of the American Chemical Society, 1980, 102, 4069-4074.	6.6	68
116	Rearrangement and dissociative reactions of the methanol radical cation (CH3OH.bul.+): a comparison of theory and experiment. Journal of the American Chemical Society, 1991, 113, 7903-7912.	6.6	68
117	Singletâ^'Triplet Splittings and Barriers to Wolff Rearrangement for Carbonyl Carbenes. Journal of the American Chemical Society, 2001, 123, 6069-6076.	6.6	68
118	Vinyl alcohol. A stable molecule. Journal of the American Chemical Society, 1977, 99, 6443-6444.	6.6	67
119	Are polar interactions important in the addition of methyl radical to alkenes?. Journal of the American Chemical Society, 1993, 115, 11050-11051.	6.6	67
120	Enzyme Catalysis of 1,2-Amino Shifts:â€‰ The Cooperative Action of B6, B12, and Aminomutases. Journal of the American Chemical Society, 2001, 123, 8678-8689.	6.6	67
121	Accurate quantum chemical energies for tetrapeptide conformations: why MP2 data with an insufficient basis set should be handled with caution. Physical Chemistry Chemical Physics, 2013, 15, 7028.	1.3	67
122	Ethynol: a theoretical prediction of remarkably high gas-phase acidity. Journal of the American Chemical Society, 1989, 111, 8297-8299.	6.6	66
123	Evaluation of accurate gas-phase acidities. The Journal of Physical Chemistry, 1991, 95, 10549-10551.	2.9	66
124	Addition of tert-Butyl Radical to Substituted Alkenes: A Theoretical Study of the Reaction Mechanism. Journal of the American Chemical Society, 1994, 116, 11938-11943.	6.6	66
125	An evaluation of the performance of G2, G2(MP2) and G2(MP2,SVP) theories for heats of formation and heats of reaction in the case of 'large' hydrocarbons. Molecular Physics, 1996, 88, 759-765.	0.8	66
126	Metal-Mediated Formation of Gas-Phase Amino Acid Radical Cationsâ€,#. Journal of Physical Chemistry A, 2006, 110, 8304-8315.	1.1	64

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127	Accelerated Protein Synthesis via One-Pot Ligation-Deselenization Chemistry. CheM, 2017, 2, 703-715.	5.8	64
128	Ab initio molecular orbital studies of sigmatropic rearrangements. International Journal of Quantum Chemistry, 1978, 14, 767-777.	1.0	63
129	Conformations, stabilities, and charge distributions in 2- and 3-monosubstituted furans. An ab initio molecular orbital study. Journal of the American Chemical Society, 1978, 100, 3981-3991.	6.6	63
130	A theoretical approach to the Birch reduction. Structures and stabilities of the radical anions of substituted benzenes. Journal of the American Chemical Society, 1980, 102, 3370-3376.	6.6	63
131	Intramolecular hydrogen migration in ionized amines: a theoretical study of the gas-phase analogs of the Hofmann-Loeffler and related rearrangements. Journal of the American Chemical Society, 1987, 109, 2910-2915.	6.6	63
132	New Theoretical and Experimental Proton Affinities for Methyl Halides and Diazomethane: A Revision of the Methyl Cation Affinity Scale. The Journal of Physical Chemistry, 1994, 98, 13099-13101.	2.9	63
133	Effect of substituents on the stabilities of multiply-substituted carbon-centered radicals. Organic and Biomolecular Chemistry, 2011, 9, 3636.	1.5	63
134	BDE261: A Comprehensive Set of High-Level Theoretical Bond Dissociation Enthalpies. Journal of Physical Chemistry A, 2012, 116, 4975-4986.	1.1	62
135	Oxirene: To Be or Not To Be?. The Journal of Physical Chemistry, 1994, 98, 8660-8665.	2.9	61
136	Effect of the Penultimate Unit on Radical Stability and Reactivity in Free-Radical Polymerization. Macromolecules, 1999, 32, 2935-2940.	2.2	61
137	The Effects of Protonation on the Structure, Stability, and Thermochemistry of Carbon-Centered Organic Radicals. Journal of the American Chemical Society, 1997, 119, 12889-12895.	6.6	60
138	Cyanovinyl radical: an illustration of the poor performance of unrestricted perturbation theory and density functional theory procedures in calculating radical stabilization energies. Theoretical Chemistry Accounts, 1999, 102, 92-96.	0.5	60
139	A Theoretical Investigation of the Effects of Electronegative Substitution on the Strength of Câ˜HÂ·Â·Â·N Hydrogen Bonds. Journal of Physical Chemistry A, 2001, 105, 8718-8726.	1.1	60
140	Interconversion of (S)-Glutamate and (2S,3S)-3-Methylaspartate:Â A Distinctive B12-Dependent Carbon-Skeleton Rearrangement. Journal of the American Chemical Society, 2001, 123, 7963-7972.	6.6	60
141	Understanding the Mechanism of Action of B12-Dependent Ethanolamine Ammonia-Lyase:Â Synergistic Interactions at Play. Journal of the American Chemical Society, 2002, 124, 14054-14065.	6.6	60
142	Design of Effective Zeolite Catalysts for the Complete Hydrogenation of CO2. Journal of the American Chemical Society, 2006, 128, 5322-5323.	6.6	60
143	On the nature of the â€˜methoxyâ€™ cation. Organic Mass Spectrometry, 1982, 17, 315-317.	1.3	59
144	Acidities, Proton Affinities, and Other Thermochemical Properties of Hypohalous Acids HOX (X = Fâ˜I):Â A High-Level Computational Study. The Journal of Physical Chemistry, 1996, 100, 3498-3503.	2.9	59

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145	Obtaining Good Performance With Triple-Î¶-Type Basis Sets in Double-Hybrid Density Functional Theory Procedures. Journal of Chemical Theory and Computation, 2011, 7, 2852-2863.	2.3	59
146	Heats of Formation of Alkali and Alkaline Earth Oxides and Hydroxides:Â Some Dramatic Failures of the G2 Method. Journal of Physical Chemistry A, 1999, 103, 7522-7527.	1.1	58
147	Alkoxy radicals in the gaseous phase: Î²-scission reactions and formation by radical addition to carbonyl compounds. Canadian Journal of Chemistry, 2003, 81, 431-442.	0.6	58
148	Modeling the Reactions Catalyzed by Coenzyme B₁₂-Dependent Enzymes. Accounts of Chemical Research, 2010, 43, 642-651.	7.6	58
149	An Experimental and Theoretical Investigation of Gas-Phase Reactions of Ca2+ with Glycine. Chemistry - A European Journal, 2006, 12, 6787-6796.	1.7	57
150	The Elusive 5â€²-Deoxyadenosyl Radical in Coenzyme-B₁₂-Mediated Reactions. Journal of the American Chemical Society, 2012, 134, 1591-1599.	6.6	57
151	Ab initio study of the benzene radical anion. Journal of the American Chemical Society, 1978, 100, 4681-4685.	6.6	55
152	A theoretical approach to the Birch reduction. Structures and stabilities of cyclohexadienes. Journal of the American Chemical Society, 1981, 103, 284-289.	6.6	55
153	Theoretical study of the structure and unimolecular decomposition pathways of ethyloxonium, [CH3CH2OH2]+. Organic Mass Spectrometry, 1991, 26, 227-234.	1.3	54
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