Leo Radom

List of Publications by Citations

462 papers	32,778 citations	78 h-index	164 g-index
492 ext. papers	34,442 ext. citations	8 avg, IF	7.22 L-index

#	Paper	IF	Citations
462	Harmonic Vibrational Frequencies: An Evaluation of Hartree–Fock, Møller–Plesset, Quadratic Configuration Interaction, Density Functional Theory, and Semiempirical Scale Factors. *The Journal of Physical Chemistry*, **1996**, 100, 16502-16513		6154
461	An evaluation of harmonic vibrational frequency scale factors. *Journal of Physical Chemistry A*, **2007**, 111, 11683-700	2.8	1987
460	Extension of Gaussian-2 theory to molecules containing third-row atoms Ga–Kr. *Journal of Chemical Physics*, **1995**, 103, 6104-6113	3.9	847
459	Scaling Factors for Obtaining Fundamental Vibrational Frequencies and Zero-Point Energies from HF/6–31G* and MP2/6–31G* Harmonic Frequencies. *Israel Journal of Chemistry*, **1993**, 33, 345-350	3.4	743
458	Extension of Gaussian-2 (G2) theory to molecules containing third-row atoms K and Ca. *Journal of Chemical Physics*, **1997**, 107, 5016-5021	3.9	712
457	Factors Controlling the Addition of Carbon-Centered Radicals to Alkenes-An Experimental and Theoretical Perspective. *Angewandte Chemie - International Edition*, **2001**, 40, 1340-1371	16.4	565
456	Extension of Gaussian-1 (G1) theory to bromine-containing molecules. *Journal of Chemical Physics*, **1991**, 94, 511-516	3.9	461
455	Extension of Gaussian-2 (G2) theory to bromine- and iodine-containing molecules: Use of effective core potentials. *Journal of Chemical Physics*, **1995**, 103, 1878-1885	3.9	441
454	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	16.4	376
453	Heats of Formation from G2, G2(MP2), and G2(MP2,SVP) Total Energies. *The Journal of Physical Chemistry*, **1996**, 100, 17460-17464		302
452	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	16.4	279
451	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	3.9	264
450	Bond Dissociation Energies and Radical Stabilization Energies Associated with Substituted Methyl Radicals. *Journal of Physical Chemistry A*, **2001**, 105, 6750-6756	2.8	241
449	Assigning absolute values to proton affinities: a differentiation between competing scales. *Journal of the American Chemical Society*, **1993**, 115, 4885-4888	16.4	229
448	Ab initio statistical thermodynamical models for the computation of third-law entropies. *Journal of Chemical Physics*, **1997**, 106, 6655-6674	3.9	227
447	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	16.4	227
446	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	16.4	219

445	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	16.4	211
444	Transition structures for the interchange of hydrogen atoms within the water dimer. *Journal of Chemical Physics*, **1990**, 92, 1240-1247	3.9	208
443	Trends in R-X bond dissociation energies (R = Me, Et, i-Pr, t-Bu; X = H, CH3, OCH3, OH, F): a surprising shortcoming of density functional theory. *Journal of Physical Chemistry A*, **2005**, 109, 7558-66	2.8	203
442	Strong conformational consequences of hyperconjugation. *Journal of the American Chemical Society*, **1972**, 94, 6221-6223	16.4	202
441	Gaussian-2 (G2) theory: Reduced basis set requirements. *Journal of Chemical Physics*, **1996**, 104, 5148-5152	3.9	197
440	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	3.9	193
439	A Priori Prediction of Propagation Rate Coefficients in Free-Radical Polymerizations: Propagation of Ethylene. *Macromolecules*, **1995**, 28, 8771-8781	5.5	182
438	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	16.4	177
437	A restricted-open-shell complete-basis-set model chemistry. *Journal of Chemical Physics*, **2006**, 125, 094106	3.9	173
436	Calculation of Proton Affinities Using the G2(MP2,SVP) Procedure. *The Journal of Physical Chemistry*, **1995**, 99, 6468-6471		164
435	Distonic radical cations. *Tetrahedron*, **1986**, 42, 6225-6234	2.4	157
434	Theoretical approach to substituent effects. Phenols and phenoxide ions. *Journal of Organic Chemistry*, **1980**, 45, 818-826	4.2	149
433	Ab initio evidence for slow fragmentation in RAFT polymerization. *Journal of the American Chemical Society*, **2003**, 125, 1490-1	16.4	142
432	Radical Addition to Alkenes:Further Assessment of Theoretical Procedures. *Journal of Physical Chemistry A*, **1998**, 102, 2237-2245	2.8	142
431	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	139
430	The weakly exothermic rearrangement of methoxy radical (CH3O?) to the hydroxymethyl radical (CH2OH?). *Journal of Chemical Physics*, **1983**, 78, 845-853	3.9	137
429	Rapid additive-free selenocystine-selenoester peptide ligation. *Journal of the American Chemical Society*, **2015**, 137, 14011-4	16.4	131
428	C–H···X Hydrogen Bonds of Acetylene, Ethylene, and Ethane with First- and Second-Row Hydrides. *Journal of Physical Chemistry A*, **2001**, 105, 4470-4479	2.8	128

427	Radical Addition to Alkenes: An Assessment of Theoretical Procedures. *The Journal of Physical Chemistry*, **1995**, 99, 8582-8588		125
426	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	2.5	124
425	Slow convergence of the møller-plesset perturbation series: the dissociation energy of hydrogen cyanide and the electron affinity of the cyano radical. *Chemical Physics Letters*, **1987**, 138, 481-485	2.5	122
424	G4(MP2)-6X: A Cost-Effective Improvement to G4(MP2). *Journal of Chemical Theory and Computation*, **2011**, 7, 112-20	6.4	119
423	Ylides and ylidions: a comparative study of unusual gas-phase structures. *Journal of the American Chemical Society*, **1987**, 109, 2250-2263	16.4	119
422	Reliable Theoretical Procedures for Calculating the Rate of Methyl Radical Addition to Carbon□Carbon Double and Triple Bonds. *Journal of Physical Chemistry A*, **2004**, 108, 2874-2883	2.8	115
421	On the mechanism of action of adenosylcobalamin. *Journal of the American Chemical Society*, **1976**, 98, 6331-8	16.4	115
420	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	16.4	115
419	Substituent Effects in Xanthate-Mediated Polymerization of Vinyl Acetate: Ab Initio Evidence for an Alternative Fragmentation Pathway. *Macromolecules*, **2004**, 37, 590-596	5.5	114
418	An assessment of theoretical procedures for the calculation of reliable radical stabilization energies□*Journal of the Chemical Society Perkin Transactions II*, **1999**, 2305-2313		114
417	Gas-Phase Non-Identity SN2 Reactions of Halide Anions with Methyl Halides: A High-Level Computational Study. *Journal of the American Chemical Society*, **1996**, 118, 6273-6284	16.4	114
416	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	16.4	114
415	A theoretical study of the CHNO isomers. *Journal of the American Chemical Society*, **1977**, 99, 7806-7816	16.4	114
414	Consequences of spin contamination in unrestricted calculations on open-shell species: effect of Hartree-Fock and Møller-Plesset contributions in hybrid and double-hybrid density functional theory approaches. *Journal of Physical Chemistry A*, **2008**, 112, 13225-30	2.8	112
413	The performance of B3-LYP density functional theory in describing SN2 reactions at saturated carbon. *Chemical Physics Letters*, **1996**, 260, 558-564	2.5	111
412	The application of ab initio molecular orbital theory to structural moieties of carbohydrates. *Carbohydrate Research*, **1974**, 38, 81-95	2.9	110
411	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	16.4	107
410	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	16.4	103

409	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	2.8	102
408	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	16.4	100
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406	Structures and stabilities of gas-phase C2H3O+ ions: an ab initio molecular orbital study. *Journal of the American Chemical Society*, **1983**, 105, 309-314	16.4	98
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401	Zeolites as Transition-Metal-Free Hydrogenation Catalysts: A Theoretical Mechanistic Study. *Journal of the American Chemical Society*, **2000**, 122, 2613-2620	16.4	92
400	Deceptive convergence in mller-plesset perturbation energies. *Chemical Physics Letters*, **1986**, 132, 16-22	2.5	92
399	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	16.4	92
398	Bond dissociation energies and radical stabilization energies: an assessment of contemporary theoretical procedures. *Journal of Physical Chemistry A*, **2007**, 111, 13638-44	2.8	91
397	Fulvalenes, Fulvenes, and Related Molecules: An ab Initio Study. *Journal of Organic Chemistry*, **1997**, 62, 2026-2038	4.2	90
396	Determination of Arrhenius Parameters for Propagation in Free-Radical Polymerizations: An Assessment of ab Initio Procedures. *The Journal of Physical Chemistry*, **1996**, 100, 18997-19006		90
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394	Ring Opening of the Cyclopropylcarbinyl Radical and Its N- and O-Substituted Analogues: A Theoretical Examination of Very Fast Unimolecular Reactions. *Journal of the American Chemical Society*, **1998**, 120, 10223-10233	16.4	89
393	A theoretical study of substituted CHNO isomers. *Journal of the American Chemical Society*, **1978**, 100, 3674-3685	16.4	87
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390	The Ionization of Alkanes. *Israel Journal of Chemistry*, **1983**, 23, 21-36	3.4	84
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388	Design of radical-resistant amino acid residues: a combined theoretical and experimental investigation. *Journal of the American Chemical Society*, **2003**, 125, 4119-24	16.4	82
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386	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	16.4	79
385	Theoretical study of the organosulfur systems CSHn (n=0□4) and CSHn+ (n=0□5): Dissociation energies, ionization energies, and enthalpies of formationa). *Journal of Chemical Physics*, **1992**, 97, 6766-6773	3.9	78
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379	The evaluation of molecular electron affinities. *Journal of Computational Chemistry*, **1986**, 7, 349-358	3.5	74
378	Theoretical approach to substituent effects. Structures and stabilities of carbanions XCH2. *Journal of Organic Chemistry*, **1981**, 46, 1693-1699	4.2	74
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345	Evaluation of accurate gas-phase acidities. *The Journal of Physical Chemistry*, **1991**, 95, 10549-10551		60
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314	Interconversion of (S)-glutamate and (2S,3S)-3-methylaspartate: a distinctive B(12)-dependent carbon-skeleton rearrangement. *Journal of the American Chemical Society*, **2001**, 123, 7963-72	16.4	50
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