Leo Radom

List of Publications by Year in Descending Order

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	Glossary of terms used in physical organic chemistry (IUPAC Recommendations 2021). *Pure and Applied Chemistry*, **2022**, 94, 353-534	2.1	4
461	Carnosine and Carcinine Derivatives Rapidly React with Hypochlorous Acid to Form Chloramines and Dichloramines. *Chemical Research in Toxicology*, **2019**, 32, 513-525	4	6
460	An ONIOM investigation of the effect of conformation on bond dissociation energies in peptides. *Journal of Computational Chemistry*, **2019**, 40, 82-88	3.5	4
459	Effect of Hydrogen Bonding and Partial Deprotonation on the Oxidation of Peptides. *Journal of Physical Chemistry A*, **2018**, 122, 1741-1746	2.8	13
458	David Parker Craig AO FAA. 23 December 1919 – 1 July 2015. *Biographical Memoirs of Fellows of the Royal Society*, **2018**, 64, 107-129	0.1	1
457	Modelling the Effect of Conformation on Hydrogen-Atom Abstraction from Peptides. *Australian Journal of Chemistry*, **2018**, 71, 257	1.2	4
456	Computational Tale of Two Enzymes: Glycerol Dehydration With or Without B. *Journal of the American Chemical Society*, **2018**, 140, 8487-8496	16.4	16
455	Solvation of the Glycyl Radical. *Journal of Physical Chemistry A*, **2018**, 122, 7212-7217	2.8	1
454	Accelerated Protein Synthesis via One-Pot Ligation-Deselenization Chemistry. *CheM*, **2017**, 2, 703-715	16.2	45
453	Impact of Hydrogen Bonding on the Susceptibility of Peptides to Oxidation. *Chemistry - an Asian Journal*, **2017**, 12, 1485-1489	4.5	6
452	Watson-Crick Base Pair Radical Cation as a Model for Oxidative Damage in DNA. *Journal of Physical Chemistry Letters*, **2017**, 8, 3159-3165	6.4	15
451	Hydrogen-adduction to open-shell graphene fragments: spectroscopy, thermochemistry and astrochemistry. *Chemical Science*, **2017**, 8, 1186-1194	9.4	4
450	Restricted-Open-Shell G4(MP2)-Type Procedures. *Journal of Physical Chemistry A*, **2016**, 120, 9299-9304	2.8	11
449	On the inclusion of post-MP2 contributions to double-hybrid density functionals. *Journal of Computational Chemistry*, **2016**, 37, 183-93	3.5	25
448	Preparation of an ion with the highest calculated proton affinity: -diethynylbenzene dianion. *Chemical Science*, **2016**, 7, 6245-6250	9.4	14
447	Beyond the Halogen Bond: Examining the Limits of Extended Polybromide Networks through Quantum-Chemical Investigations. *Chemistry - an Asian Journal*, **2016**, 11, 682-6	4.5	8
446	Factors influencing the formation of polybromide monoanions in solutions of ionic liquid bromide salts. *Physical Chemistry Chemical Physics*, **2016**, 18, 7251-60	3.6	32

445	Hydrogen-atom attack on phenol and toluene is ortho-directed. *Physical Chemistry Chemical Physics* , **2016**, 18, 8625-36	3.6	8
444	Hydrogen Abstraction by OH and SH Radicals from Amino Acids and Their Peptide Derivatives. *Journal of Chemical Theory and Computation*, **2016**, 12, 1606-13	6.4	14
443	Reactivity of disulfide bonds is markedly affected by structure and environment: implications for protein modification and stability. *Scientific Reports*, **2016**, 6, 38572	4.9	68
442	Seventh Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC7). *Australian Journal of Chemistry*, **2016**, 69, 931	1.2	0
441	Role of Hydrogen Bonding on the Reactivity of Thiyl Radicals: A Mass Spectrometric and Computational Study Using the Distonic Radical Ion Approach. *Journal of Physical Chemistry A*, **2016** , 120, 8184-8189	2.8	9
440	Frequency Scale Factors for Some Double-Hybrid Density Functional Theory Procedures: Accurate Thermochemical Components for High-Level Composite Protocols. *Journal of Chemical Theory and Computation*, **2016**, 12, 3774-80	6.4	31
439	Hydrogen from Formic Acid via Its Selective Disproportionation over Nanodomain-Modified Zeolites. *ACS Catalysis*, **2015**, 5, 4353-4362	13.1	14
438	Gas-phase structure and reactivity of the keto tautomer of the deoxyguanosine radical cation. *Physical Chemistry Chemical Physics*, **2015**, 17, 25837-44	3.6	12
437	H and D attachment to naphthalene: spectra and thermochemistry of cold gas-phase 1-C10H9 and 1-C10H8D radicals and cations. *Journal of Physical Chemistry A*, **2015**, 119, 3225-32	2.8	6
436	Outcome-changing effect of polarity reversal in hydrogen-atom-abstraction reactions. *Journal of Physical Chemistry A*, **2015**, 119, 3843-7	2.8	16
435	W2X and W3X-L: Cost-Effective Approximations to W2 and W4 with kJ mol(-1) Accuracy. *Journal of Chemical Theory and Computation*, **2015**, 11, 2109-19	6.4	80
434	Rapid additive-free selenocystine-selenoester peptide ligation. *Journal of the American Chemical Society*, **2015**, 137, 14011-4	16.4	131
433	Hydrogen-atom abstraction from a model amino acid: dependence on the attacking radical. *Journal of Physical Chemistry B*, **2015**, 119, 783-8	3.4	29
432	Accurate quadruple-basis-set approximation for double-hybrid density functional theory with an order of magnitude reduction in computational cost. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	18
431	Effect of protonation state and interposed connector groups on bond dissociation enthalpies of alcohols and related systems. *Journal of Physical Chemistry A*, **2014**, 118, 2810-9	2.8	26
430	Performance of Density Functional Theory Procedures for the Calculation of Proton-Exchange Barriers: Unusual Behavior of M06-Type Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 3777-83	6.4	37
429	Hydrogen from formic acid through its selective disproportionation over sodium germanate--a non-transition-metal catalysis system. *Angewandte Chemie - International Edition*, **2014**, 53, 11275-9	16.4	9
428	Hydrogen from Formic Acid through Its Selective Disproportionation over Sodium Germanate—A Non-Transition-Metal Catalysis System. *Angewandte Chemie*, **2014**, 126, 11457-11461	3.6	2

427	W3X: A Cost-Effective Post-CCSD(T) Composite Procedure. *Journal of Chemical Theory and Computation*, **2013**, 9, 4769-78	6.4	47
426	Evaluation of the heats of formation of corannulene and C60 by means of high-level theoretical procedures. *Journal of Physical Chemistry A*, **2013**, 117, 1834-42	2.8	42
425	Gas-phase infrared spectrum and acidity of the radical cation of 9-methylguanine. *Chemical Communications*, **2013**, 49, 7343-5	5.8	25
424	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, 7028-31	3.6	57
423	Hierarchy of relative bond dissociation enthalpies and their use to efficiently compute accurate absolute bond dissociation enthalpies for C-H, C-C, and C-F bonds. *Journal of Physical Chemistry A*, **2013**, 117, 3666-75	2.8	26
422	Effect of substituents on the preferred modes of one-electron reductive cleavage of N-Cl and N-Br bonds. *Journal of Physical Chemistry A*, **2013**, 117, 460-72	2.8	20
421	Chemoselective Peptide Ligation□Desulfurization at Aspartate. *Angewandte Chemie*, **2013**, 125, 9905-9909	3.6	19
420	Chemoselective peptide ligation-desulfurization at aspartate. *Angewandte Chemie - International Edition*, **2013**, 52, 9723-7	16.4	98
419	Proton-bound homodimers involving second-row atoms. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	3
418	Performance of Gradient-Corrected and Hybrid Density Functional Theory: Role of the Underlying Local Density Approximation and the Gradient Correction. *Journal of Chemical Theory and Computation*, **2012**, 8, 4899-906	6.4	12
417	Heteroatomic deprotonation of substituted methanes and methyl radicals: theoretical insights into structure, stability, and thermochemistry. *Journal of Physical Chemistry A*, **2012**, 116, 12381-7	2.8	19
416	Reactivities of amino acid derivatives toward hydrogen abstraction by Cl□and OH□*Journal of Organic Chemistry*, **2012**, 77, 9807-12	4.2	39
415	The elusive 5'-deoxyadenosyl radical in coenzyme-B12-mediated reactions. *Journal of the American Chemical Society*, **2012**, 134, 1591-9	16.4	48
414	Computational design of effective, bioinspired HOCl antioxidants: the role of intramolecular Cl+ and H+ shifts. *Journal of the American Chemical Society*, **2012**, 134, 19240-5	16.4	15
413	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, 4259-69	6.4	59
412	Influence of connector groups on the interactions of substituents with carbon-centered radicals. *Journal of Physical Chemistry A*, **2012**, 116, 10203-8	2.8	8
411	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, 4211-21	2.8	65
410	BDE261: a comprehensive set of high-level theoretical bond dissociation enthalpies. *Journal of Physical Chemistry A*, **2012**, 116, 4975-86	2.8	58

409	Heats of Formation for CrO, CrO2, and CrO3: An Extreme Challenge for Black-Box Composite Procedures. *Journal of Chemical Theory and Computation*, **2012**, 8, 3159-66	6.4	22
408	Determination of Barrier Heights for Proton Exchange in Small Water, Ammonia, and Hydrogen Fluoride Clusters with G4(MP2)-Type, MPn, and SCS-MPn Procedures-A Caveat. *Journal of Chemical Theory and Computation*, **2012**, 8, 3128-36	6.4	50
407	Approaches for obtaining accurate rate constants for hydrogen abstraction by a chlorine atom. *Journal of Physical Chemistry A*, **2012**, 116, 3745-52	2.8	24
406	Comment on the ionization energy of B2F4. *Journal of Physical Chemistry A*, **2012**, 116, 9214-5	2.8	3
405	N?H and N?Cl homolytic bond dissociation energies and radical stabilization energies: An assessment of theoretical procedures through comparison with benchmark-quality W2w data. *International Journal of Quantum Chemistry*, **2012**, 112, 1862-1878	2.1	37
404	Proton-bound homodimers involving second-row atoms. *Highlights in Theoretical Chemistry*, **2012**, 15-22		
403	Hydrogen abstraction by chlorine atom from amino acids: remarkable influence of polar effects on regioselectivity. *Journal of the American Chemical Society*, **2011**, 133, 16553-9	16.4	43
402	Obtaining Good Performance With Triple-Type Basis Sets in Double-Hybrid Density Functional Theory Procedures. *Journal of Chemical Theory and Computation*, **2011**, 7, 2852-63	6.4	52
401	Model for the exceptional reactivity of peroxiredoxins 2 and 3 with hydrogen peroxide: a kinetic and computational study. *Journal of Biological Chemistry*, **2011**, 286, 18048-55	5.4	92
400	Effect of substituents on the stabilities of multiply-substituted carbon-centered radicals. *Organic and Biomolecular Chemistry*, **2011**, 9, 3636-57	3.9	55
399	One-electron reduction of N-chlorinated and N-brominated species is a source of radicals and bromine atom formation. *Chemical Research in Toxicology*, **2011**, 24, 371-82	4	26
398	Effect of substituents on the strength of N-X (X = H, F, and Cl) bond dissociation energies: a high-level quantum chemical study. *Journal of Physical Chemistry A*, **2011**, 115, 5496-504	2.8	26
397	Assessment of theoretical procedures for hydrogen-atom abstraction by chlorine, and related reactions. *Theoretical Chemistry Accounts*, **2011**, 130, 251-260	1.9	34
396	The spectroscopy and thermochemistry of phenylallyl radical chromophores. *Chemical Science*, **2011**, 2, 1755	9.4	25
395	G4(MP2)-6X: A Cost-Effective Improvement to G4(MP2). *Journal of Chemical Theory and Computation*, **2011**, 7, 112-20	6.4	119
394	O - H Bond Dissociation Energies. *Australian Journal of Chemistry*, **2011**, 64, 394	1.2	18
393	Spectroscopy and thermochemistry of a jet-cooled open-shell polyene: 1,4-pentadienyl radical. *Journal of Chemical Physics*, **2011**, 135, 124306	3.9	11
392	Modeling the reactions catalyzed by coenzyme B12-dependent enzymes. *Accounts of Chemical Research*, **2010**, 43, 642-51	24.3	46

391	G4-SP, G4(MP2)-SP, G4-sc, and G4(MP2)-sc: Modifications to G4 and G4(MP2) for the Treatment of Medium-Sized Radicals. *Journal of Chemical Theory and Computation*, **2010**, 6, 2647-53	6.4	34
390	A computational study of methanol-to-hydrocarbon conversion Towards the design of a low-barrier process. *Canadian Journal of Chemistry*, **2010**, 88, 866-876	0.9	15
389	Gas-Phase Synthesis and Reactivity of Lithium Acetylide Ion, Li?C?C *Angewandte Chemie*, **2010**, 122, 5287-5290	3.6	1
388	Gas-phase synthesis and reactivity of lithium acetylide ion, Li-C[triple bond]C-. *Angewandte Chemie - International Edition*, **2010**, 49, 5161-4	16.4	8
387	On the reaction of glycerol dehydratase with but-3-ene-1,2-diol. *Chemistry - A European Journal*, **2009**, 15, 4865-73	4.8	7
386	On the importance of ribose orientation in the substrate activation of the coenzyme B12-dependent mutases. *Chemistry - A European Journal*, **2009**, 15, 8578-85	4.8	18
385	Low barrier hydrogenolysis of the carbon-heteroatom bond as catalyzed by HAlF(4). *Organic Letters* , **2009**, 11, 749-51	6.2	17
384	What factors determine whether a proton-bound homodimer has a symmetric or an asymmetric hydrogen bond?. *Molecular Physics*, **2009**, 107, 1095-1105	1.7	22
383	Hydrogen abstraction by chlorine atom from small organic molecules containing amino acid functionalities: an assessment of theoretical procedures. *Journal of Physical Chemistry A*, **2009**, 113, 11817-32	2.8	15
382	Structures and thermochemistry of the alkali metal monoxide anions, monoxide radicals, and hydroxides. *Journal of Physical Chemistry A*, **2009**, 113, 9501-10	2.8	12
381	Ab initio investigation of the fragmentation of 5,5-diamino-substituted 1,4,2-oxathiazoles. *Organic Letters*, **2009**, 11, 1325-8	6.2	10
380	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, 9861-73	2.8	70
379	Consequences of spin contamination in unrestricted calculations on open-shell species: effect of Hartree-Fock and M ller-Plesset contributions in hybrid and double-hybrid density functional theory approaches. *Journal of Physical Chemistry A*, **2008**, 112, 13225-30	2.8	112
378	The carbon-skeleton rearrangement in tropane alkaloid biosynthesis. *Journal of the American Chemical Society*, **2008**, 130, 10684-90	16.4	18
377	Nature of Glycine and Its Carbon Radical in Aqueous Solution: A Theoretical Investigation. *Journal of Chemical Theory and Computation*, **2008**, 4, 1788-94	6.4	23
376	Zeolite-catalyzed hydrogenation of carbon dioxide and ethene. *Journal of the American Chemical Society*, **2008**, 130, 9790-9	16.4	63
375	Lithium monoxide anion: a ground-state triplet with the strongest base to date. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 7647-51	11.5	34
374	Toward an improved understanding of the glutamate mutase system. *Journal of the American Chemical Society*, **2007**, 129, 1623-33	16.4	19

373	Proton-bound homodimers: how are the binding energies related to proton affinities?. *Journal of the American Chemical Society*, **2007**, 129, 12197-9	16.4	38
372	Uncatalyzed transfer hydrogenation of quinones and related systems: a theoretical mechanistic study. *Journal of Physical Chemistry A*, **2007**, 111, 6456-67	2.8	16
371	An evaluation of harmonic vibrational frequency scale factors. *Journal of Physical Chemistry A*, **2007**, 111, 11683-700	2.8	1987
370	Uncatalyzed 1,4-hydrogenation of polycyclic aromatic hydrocarbons: A computational study. *Computational and Theoretical Chemistry*, **2007**, 811, 13-17		10
369	A Theoretical Approach to Substituent Interactions in Substituted Benzenes. *Progress in Physical Organic Chemistry*, **2007**, 1-61		37
368	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
367	Hydrogenation of simple aromatic molecules: a computational study of the mechanism. *Journal of the American Chemical Society*, **2007**, 129, 924-33	16.4	40
366	An experimental and theoretical investigation of gas-phase reactions of Ca2+ with glycine. *Chemistry - A European Journal*, **2006**, 12, 6787-96	4.8	55
365	Rearrangements in Model Peptide-Type Radicals via Intramolecular Hydrogen-Atom Transfer. *Helvetica Chimica Acta*, **2006**, 89, 2254-2272	2	35
364	A restricted-open-shell complete-basis-set model chemistry. *Journal of Chemical Physics*, **2006**, 125, 094106	3.9	173
363	Thermochemistry and kinetics of hydrogen abstraction by methyl radical from polycyclic aromatic hydrocarbons. *Journal of Physical Chemistry A*, **2006**, 110, 13624-31	2.8	39
362	Metal-mediated formation of gas-phase amino acid radical cations. *Journal of Physical Chemistry A*, **2006**, 110, 8304-15	2.8	62
361	Gas-phase regiocontrolled generation of charged amino acid and peptide radicals. *Chemical Communications*, **2006**, 4233-5	5.8	51
360	Effect of side chains on competing pathways for beta-scission reactions of peptide-backbone alkoxyl radicals. *Journal of Physical Chemistry A*, **2006**, 110, 10316-23	2.8	17
359	Design of effective zeolite catalysts for the complete hydrogenation of CO2. *Journal of the American Chemical Society*, **2006**, 128, 5322-3	16.4	57
358	In search of radical intermediates in the reactions catalyzed by lysine 2,3-aminomutase and lysine 5,6-aminomutase. *Journal of the American Chemical Society*, **2006**, 128, 16004-5	16.4	20
357	Insights into the hydrogen-abstraction reactions of diol dehydratase: relevance to the catalytic mechanism and suicide inactivation. *Journal of the American Chemical Society*, **2006**, 128, 3433-44	16.4	25
356	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, 8942-51	2.8	67

355	Base-catalyzed hydrogenation: rationalizing the effects of catalyst and substrate structures and solvation. *Journal of the American Chemical Society*, **2005**, 127, 2443-54	16.4	43
354	On the relationship between the preferred site of hydrogen bonding and protonation. *Journal of Physical Chemistry A*, **2005**, 109, 5509-17	2.8	50
353	Structures and thermochemistry of calcium-containing molecules. *Journal of Physical Chemistry A*, **2005**, 109, 9156-68	2.8	15
352	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
351	Why are the Ca2+ and K+ binding energies of formaldehyde and ammonia reversed with respect to their proton affinities?. *Journal of Physical Chemistry A*, **2005**, 109, 6735-42	2.8	14
350	Bond dissociation energies and radical stabilization energies associated with model peptide-backbone radicals. *Journal of Physical Chemistry A*, **2005**, 109, 6318-25	2.8	67
349	Modeling Scission Reactions of Peptide Backbone Alkoxy Radicals: Backbone C-C Bond Fission. *Journal of Chemical Theory and Computation*, **2005**, 1, 889-99	6.4	6
348	Divergent mechanisms of suicide inactivation for ethanolamine ammonia-lyase. *Journal of the American Chemical Society*, **2005**, 127, 8856-64	16.4	24
347	Understanding Metal-Free Catalytic Hydrogenation: A Systematic Theoretical Study of the Hydrogenation of Ethene. *Australian Journal of Chemistry*, **2004**, 57, 659	1.2	16
346	Reliable Theoretical Procedures for Calculating the Rate of Methyl Radical Addition to CarbonCarbon Double and Triple Bonds. *Journal of Physical Chemistry A*, **2004**, 108, 2874-2883	2.8	115
345	Comparison of the kinetics and thermodynamics for methyl radical addition to C=C, C=O, and C=S double bonds. *Journal of the American Chemical Society*, **2004**, 126, 1732-40	16.4	63
344	Gas-Phase Reactions between Urea and Ca2+: The Importance of Coulomb Explosions. *Journal of Physical Chemistry A*, **2004**, 108, 10080-10088	2.8	45
343	Remembrance: John A. Pople (19252004). *Journal of Chemical Physics*, **2004**, 120, 9445-9445	3.9	2
342	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
341	Suicide inactivation of dioldehydratase by glycolaldehyde and chloroacetaldehyde: an examination of the reaction mechanism. *Journal of the American Chemical Society*, **2004**, 126, 12206-7	16.4	15
340	Inhibition of peptidylglycine alpha-amidating monooxygenase by exploitation of factors affecting the stability and ease of formation of glycyl radicals. *Journal of the American Chemical Society*, **2004**, 126, 13306-11	16.4	16
339	Understanding Alkyl Substituent Effects in R-O Bond Dissociation Reactions in Open- and Closed-Shell Systems **2004**, 563-579		7
338	The unusual bifunctional catalysis of epimerization and desaturation by carbapenem synthase. *Journal of the American Chemical Society*, **2004**, 126, 9932-3	16.4	24

337	Alkoxy radicals in the gaseous phase: β-scission reactions and formation by radical addition to carbonyl compounds. *Canadian Journal of Chemistry*, **2003**, 81, 431-442	0.9	55
336	What Is the Origin of the Contrathermodynamic Behavior in Methyl Radical Addition to Alkynes versus Alkenes?. *Journal of Physical Chemistry A*, **2003**, 107, 6082-6090	2.8	38
335	Strategic use of amino acid N-substituents to limit α-carbon-centered radical formation and consequent loss of stereochemical integrity. *Tetrahedron: Asymmetry*, **2003**, 14, 2919-2926		20
334	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
333	Homoanomeric Effect in the 1,2-Dimethoxyethyl Radical. *Australian Journal of Chemistry*, **2003**, 56, 429	1.2	4
332	Performance of the RB3-LYP, RMP2, and UCCSD(T) Procedures in Calculating Radical Stabilization Energies for NHX Radicals. *Journal of Physical Chemistry A*, **2003**, 107, 7985-7990	2.8	32
331	Heats of Formation of Alkali Metal and Alkaline Earth Metal Oxides and Hydroxides: Surprisingly Demanding Targets for High-Level ab Initio Procedures. *Journal of Physical Chemistry A*, **2003**, 107, 5617-5630	2.8	70
330	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
329	Variable trends in R-X bond dissociation energies (R = Me, Et, i-Pr, t-Bu). *Organic Letters*, **2003**, 5, 4689-92	6.2	70
328	Interactions between Neutral Molecules and Ca2+: An Assessment of Theoretical Procedures. *Journal of Physical Chemistry A*, **2003**, 107, 10456-10461	2.8	41
327	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
326	Ab initio evidence for slow fragmentation in RAFT polymerization. *Journal of the American Chemical Society*, **2003**, 125, 1490-1	16.4	142
325	Calculation of accurate imaginary frequencies and tunnelling coefficients for hydrogen abstraction reactions using IRCmax. *Molecular Physics*, **2003**, 101, 1329-1338	1.7	35
324	Proton-transport catalysis, proton abstraction, and proton exchange in HF+HOC+ and H2O+HOC+ and analogous deuterated reactions. *Journal of Chemical Physics*, **2003**, 118, 6222-6229	3.9	22
323	Factors controlling the addition of carbon-centered radicals to alkenes. *Macromolecular Symposia*, **2002**, 182, 1-14	0.8	20
322	Understanding the mechanism of action of B12-dependent ethanolamine ammonia-lyase: synergistic interactions at play. *Journal of the American Chemical Society*, **2002**, 124, 14054-65	16.4	50
321	Methyl Radical Addition to CS Double Bonds: Kinetic versus Thermodynamic Preferences. *Journal of Physical Chemistry A*, **2002**, 106, 12124-12138	2.8	76
320	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

319	Substituent effects in isoxazoles: identification of 4-substituted isoxazoles as Michael acceptors. *Perkin Transactions II RSC*, **2002**, 2031-2038		9
318	Theoretical studies of coenzyme B12-dependent carbon-skeleton rearrangements. *Theoretical and Computational Chemistry*, **2001**, 183-214		1
317	Catalysis by mutants of methylmalonyl-CoA mutase: a theoretical rationalization for a change in the rate-determining step. *ChemBioChem*, **2001**, 2, 919-22	3.8	14
316	Was steuert die Additionen kohlenstoffzentrierter Radikale an Alkene? Antworten auf experimenteller und theoretischer Grundlage. *Angewandte Chemie*, **2001**, 113, 1380-1414	3.6	63
315	A G2 study of SH+ exchange reactions involving lone-pair donors and unsaturated hydrocarbons. *Chemistry - A European Journal*, **2001**, 7, 1516-24	4.8	13
314	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
313	Towards multireference equivalents of the G2 and G3 methods. *Journal of Chemical Physics*, **2001**, 115, 8758-8772	3.9	19
312	CH···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
311	A Theoretical Investigation of the Effects of Electronegative Substitution on the Strength of CH···N Hydrogen Bonds. *Journal of Physical Chemistry A*, **2001**, 105, 8718-8726	2.8	55
310	Bond Dissociation Energies and Radical Stabilization Energies Associated with Substituted Methyl Radicals. *Journal of Physical Chemistry A*, **2001**, 105, 6750-6756	2.8	241
309	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
308	Enzyme catalysis of 1,2-amino shifts: the cooperative action of B6, B12, and aminomutases. *Journal of the American Chemical Society*, **2001**, 123, 8678-89	16.4	60
307	Singlet-triplet splittings and barriers to Wolff rearrangement for carbonyl carbenes. *Journal of the American Chemical Society*, **2001**, 123, 6069-76	16.4	63
306	Understanding the mechanism of B(12)-dependent diol dehydratase: a synergistic retro-push--pull proposal. *Journal of the American Chemical Society*, **2001**, 123, 1664-75	16.4	71
305	Theoretical Thermochemistry of Radicals **2001**, 161-197		1
304	Exchange of Cl+ between Lone-Pair Donors and Donors: A Computational Study. *European Journal of Mass Spectrometry*, **2000**, 6, 153-160	1.1	7
303	Are the Approach Directions of and Nucleophiles to the Sulfur Atom of Thiiranium and Thiirenium Ions Different?. *Chemistry - A European Journal*, **2000**, 6, 590-591	4.8	7
302	Hemispiroalkaplanes: hydrocarbon cage systems with a pyramidal-tetracoordinate carbon atom and remarkable basicity. *Chemistry - A European Journal*, **2000**, 6, 2470-83	4.8	32

301	The involvement of ion□neutral complexes in ethylene loss from [PhC(CH3)2]+ and its isomers. *International Journal of Mass Spectrometry*, **2000**, 199, 29-40	1.9	5
300	Formation of three-membered phosphorus heterocycles via ligand-exchange reactions in mono-adducts of the phosphenium ion: an ab initio investigation. *International Journal of Mass Spectrometry*, **2000**, 201, 205-213	1.9	2
299	Rearrangement and fragmentation pathways of [C3H7Z]+ ions (Z = NH and S): are ion□neutral complexes important?. *International Journal of Mass Spectrometry*, **2000**, 194, 181-196	1.9	7
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