David M Smith

List of Publications by Year
in descending order

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72 papers	1,929 citations	279487 23 h-index	276539 41 g-index
80 all docs	80 docs citations	80 times ranked	1612 citing authors

#	Article	IF	Citations
1	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
2	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
3	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
4	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
5	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
6	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
7	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
8	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
9	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
10	Modeling the Reactions Catalyzed by Coenzyme B₁₂-Dependent Enzymes. Accounts of Chemical Research, 2010, 43, 642-651.	7.6	58
11	The Elusive 5â€²-Deoxyadenosyl Radical in Coenzyme-B₁₂-Mediated Reactions. Journal of the American Chemical Society, 2012, 134, 1591-1599.	6.6	57
12	Deprotonation of Enoxy Radicals: Theoretical Validation of a 50-Year-Old Mechanistic Proposal. Angewandte Chemie - International Edition, 2003, 42, 1867-1870.	7.2	56
13	Toward a Consistent Mechanism for Diol Dehydratase Catalyzed Reactions:Â An Application of the Partial-Proton-Transfer Concept. Journal of the American Chemical Society, 1999, 121, 5700-5704.	6.6	54
14	Facilitation of Enzyme-Catalyzed Reactions by Partial Proton Transfer:Â Application to Coenzyme-B12-Dependent Methylmalonyl-CoA Mutase. Journal of the American Chemical Society, 1999, 121, 1383-1384.	6.6	48
15	Complementary Molecular Dynamics and X-ray Reflectivity Study of an Imidazolium-Based Ionic Liquid at a Neutral Sapphire Interface. Journal of Physical Chemistry Letters, 2015, 6, 549-555.	2.1	37
16	The Unusual Bifunctional Catalysis of Epimerization and Desaturation by Carbapenem Synthase. Journal of the American Chemical Society, 2004, 126, 9932-9933.	6.6	29
17	On the Mechanism of Action of Vitamin B12:Â Theoretical Studies of the 2-Methyleneglutarate Mutase Catalyzed Rearrangement. Journal of the American Chemical Society, 1999, 121, 1037-1044.	6.6	27
18	Insights into the Hydrogen-Abstraction Reactions of Diol Dehydratase:Â Relevance to the Catalytic Mechanism and Suicide Inactivation. Journal of the American Chemical Society, 2006, 128, 3433-3444.	6.6	27

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19	Mechanism of the Waterâ€“Gas Shift Reaction Catalyzed by Efficient Rutheniumâ€Based Catalysts: A Computational and Experimental Study. Angewandte Chemie - International Edition, 2019, 58, 741-745.	7.2	27
20	Divergent Mechanisms of Suicide Inactivation for Ethanolamine Ammonia-Lyase. Journal of the American Chemical Society, 2005, 127, 8856-8864.	6.6	26
21	How B6Helps B12:Â The Roles of B6, B12, and the Enzymes in Aminomutase-Catalyzed Reactions. Journal of the American Chemical Society, 2000, 122, 10208-10209.	6.6	25
22	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, 16004-16005.	6.6	25
23	Nature of Glycine and Its Î±-Carbon Radical in Aqueous Solution: A Theoretical Investigation. Journal of Chemical Theory and Computation, 2008, 4, 1788-1794.	2.3	24
24	On the thermodynamic equilibrium between (R)â€2â€hydroxyacylâ€CoA and 2â€enoylâ€CoA. FEBS Journal, 2010, 277, 1738-1746.	2.2	24
25	Computational Tale of Two Enzymes: Glycerol Dehydration With or Without B₁₂. Journal of the American Chemical Society, 2018, 140, 8487-8496.	6.6	24
26	On the Importance of Ribose Orientation in the Substrate Activation of the Coenzyme B₁₂â€Dependent Mutases. Chemistry - A European Journal, 2009, 15, 8578-8585.	1.7	23
27	A computational study of the chlorination and hydroxylation of amines by hypochlorous acid. Organic and Biomolecular Chemistry, 2015, 13, 11740-11752.	1.5	23
28	Dynamic equilibria in supported ionic liquid phase (SILP) catalysis: in situ IR spectroscopy identifies [Ru(CO)_xCl_y]_n species in water gas shift catalysis. Catalysis Science and Technology, 2018, 8, 344-357.	2.1	23
29	Insights from molecular dynamics simulations on structural organization and diffusive dynamics of an ionic liquid at solid and vacuum interfaces. Journal of Colloid and Interface Science, 2019, 553, 350-363.	5.0	23
30	Human dipeptidyl peptidase III: insights into ligand binding from a combined experimental and computational approach. Journal of Molecular Recognition, 2011, 24, 804-814.	1.1	21
31	Towards multireference equivalents of the G2 and G3 methods. Journal of Chemical Physics, 2001, 115, 8758-8772.	1.2	20
32	Toward an Improved Understanding of the Glutamate Mutase System. Journal of the American Chemical Society, 2007, 129, 1623-1633.	6.6	20
33	The Protonation States of the Active-Site Histidines in (6â€“4) Photolyase. Journal of Chemical Theory and Computation, 2012, 8, 1078-1091.	2.3	20
34	The Carbon-Skeleton Rearrangement in Tropane Alkaloid Biosynthesis. Journal of the American Chemical Society, 2008, 130, 10684-10690.	6.6	19
35	Calculating CD Spectra of Flexible Peptides: An Assessment of TD-DFT Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3270-3279.	2.3	18
36	Suicide Inactivation of Dioldehydratase by Glycolaldehyde and Chloroacetaldehyde:Â an Examination of the Reaction Mechanism. Journal of the American Chemical Society, 2004, 126, 12206-12207.	6.6	17

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37	Dissociation energies of CÎ±â€“H bonds in amino acids â€“ a re-examination. RSC Advances, 2013, 3, 12403.	1.7	17
38	Water in an electric field does not dance alone: The relation between equilibrium structure, time dependent viscosity and molecular motions. Journal of Molecular Liquids, 2019, 282, 303-315.	2.3	17
39	The ring-puckering motion in perfluorocyclobutane. Journal of Molecular Structure, 1997, 405, 159-167.	1.8	16
40	Catalysis by Mutants of Methylmalonyl-CoA Mutase: A Theoretical Rationalization for a Change in the Rate-Determining Step. ChemBioChem, 2001, 2, 919-922.	1.3	16
41	Improving the performance of supported ionic liquid phase (SILP) catalysts for the ultra-low-temperature waterâ€“gas shift reaction using metal salt additives. Green Chemistry, 2019, 21, 5008-5018.	4.6	16
42	The additivity of the Ï€-electron correlation energy in planar heteroatomic molecules. Chemical Physics, 2001, 269, 11-28.	0.9	15
43	Rhodomyrtals Aâ€“D, four unusual phloroglucinol-sesquiterpene adducts from Rhodomyrtus psidioides. RSC Advances, 2014, 4, 13514-13517.	1.7	15
44	The electronic spectroscopy of 1,2,3-triazine. Chemical Physics, 1997, 221, 11-21.	0.9	14
45	Calculation of the CD Spectrum of a Peptide from Its Conformational Phase Space: The Case of Met-enkephalin and Its Unnatural Analogue. Journal of Chemical Theory and Computation, 2012, 8, 1694-1705.	2.3	14
46	Computational study of the cyclopalladation mechanism of azobenzene with PdCl2 in N,N-dimethylformamide. Journal of Organometallic Chemistry, 2011, 696, 661-669.	0.8	13
47	On the correlation energy features in planar heteroatomic molecular systems. Journal of Chemical Physics, 2001, 115, 3474-3483.	1.2	12
48	Transfer hydrogenation between ethane and ethene: a critical assessment of theoretical procedures. Molecular Physics, 2006, 104, 777-794.	0.8	12
49	On the modeling of arginineâ€bound carboxylates: A case study with Pyruvate Formateâ€Lyase. Journal of Computational Chemistry, 2008, 29, 2425-2433.	1.5	11
50	Modeling the Reactions Catalyzed by Coenzyme B₁₂ Dependent Enzymes: Accuracy and Cost-Quality Balance. Journal of Physical Chemistry A, 2018, 122, 1747-1755.	1.1	11
51	On the Reaction of Glycerol Dehydratase with Butâ€3â€eneâ€1,2â€diol. Chemistry - A European Journal, 2009, 15, 4865-4873.	1.7	10
52	Adsorption of Aspartate Derivatives to Calcite Surfaces in Aqueous Environment. Crystal Growth and Design, 2020, 20, 2853-2859.	1.4	10
53	Designing aryl cations for direct observation in solution: ab initio MO calculations of UV spectra. Perkin Transactions II RSC, 2002, , 906-913.	1.1	8
54	In Pursuit of the Elusive Bond-Stretch Isomers by ab Initio MethodsBenzocyclobutene, Benzo[1,2:4,5]dicyclobutadiene, and Some Related Substituted Systems. Journal of Physical Chemistry A, 2003, 107, 10396-10405.	1.1	8

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55	Mechanism of the Waterâ€“Gas Shift Reaction Catalyzed by Efficient Ruthenium Based Catalysts: A Computational and Experimental Study. Angewandte Chemie, 2018, 131, 751.	1.6	8
56	An Exact Algorithm to Detect the Percolation Transition in Molecular Dynamics Simulations of Cross-Linking Polymer Networks. Journal of Chemical Theory and Computation, 2021, 17, 6449-6457.	2.3	8
57	Nonâ€enzymatic Ribonucleotide Reduction in the Prebiotic Context. Chemistry - A European Journal, 2015, 21, 6132-6143.	1.7	7
58	Cu carbonyls enhance the performance of Ru-based SILP waterâ€“gas shift catalysts: a combinedin situDRIFTS and DFT study. Catalysis Science and Technology, 2020, 10, 252-262.	2.1	7
59	Improving the Performance of Supported Ionic Liquid Phase Catalysts for the Ultra-Low-Temperature Water Gas Shift Reaction Using Organic Salt Additives. ACS Catalysis, 2022, 12, 5661-5672.	5.5	7
60	Estimating the Ï€-bond energies and the stabilities of oxy-substituted carbocations. Computational and Theoretical Chemistry, 2007, 811, 355-359.	1.5	6
61	Computational Study of Glycerol Binding within the Active Site of Coenzyme B₁₂-Dependent Diol Dehydratase. Journal of Physical Chemistry B, 2019, 123, 6178-6187.	1.2	6
62	A compound QM/MM procedure: Comparative performance on a pyruvate formateâ€lyase model system. Journal of Computational Chemistry, 2010, 31, 1024-1035.	1.5	5
63	Resolution of protein hydrogen/deuterium exchange by fitting amide exchange probabilities to the peptide isotopic envelopes. Rapid Communications in Mass Spectrometry, 2019, 33, 1248-1257.	0.7	5
64	Exploring Reactive Conformations of Coenzyme A during Binding and Unbinding to Pyruvate Formateâ€“Lyase. Journal of Physical Chemistry A, 2019, 123, 9345-9356.	1.1	4
65	Glycerol as a Substrate and Inactivator of Coenzyme B₁₂â€Dependent Diol Dehydratase. Chemistry - A European Journal, 2021, 27, 7930-7941.	1.7	4
66	Localization improvement of deuterium uptake in hydrogen/deuterium exchange in proteins. Journal of Chemometrics, 2017, 31, e2876.	0.7	3
67	The Influence of Chemical Change on Protein Dynamics: A Case Study with Pyruvate Formateâ€Lyase. Chemistry - A European Journal, 2019, 25, 8741-8753.	1.7	3
68	Structural characterization of an ionic liquid in bulk and in nano-confined environment using data from MD simulations. Data in Brief, 2020, 28, 104794.	0.5	3
69	Establishing conditions for simulating hydrophobic solutes in electric fields by molecular dynamics. Journal of Molecular Modeling, 2014, 20, 2359.	0.8	2
70	Theoretical studies of coenzyme B12-dependent carbon-skeleton rearrangements. Theoretical and Computational Chemistry, 2001, , 183-214.	0.2	1
71	Mechanism of the Waterâ€“Gas Shift Reaction Catalyzed by Efficient Rutheniumâ€Based Catalysts: A Computational and Experimental Study. Angewandte Chemie, 2018, 131, 650.	1.6	0
72	The Influence of Chemical Change on Protein Dynamics: A Case Study with Pyruvate Formateâ€Lyase. Chemistry - A European Journal, 2019, 25, 8653.	1.7	0