David C Chatfield

List of Publications by Year
in descending order

29 papers	1,137 citations	516215 16 h-index	476904 29 g-index
29 all docs	29 docs citations	29 times ranked	1091 citing authors

#	Article	IF	Citations
1	Enzyme mechanisms with hybrid quantum and molecular mechanical potentials. I. Theoretical considerations. International Journal of Quantum Chemistry, 1996, 60, 1189-1200.	1.0	185
2	Optimization of quantum mechanical molecular mechanical partitioning schemes: Gaussian delocalization of molecular mechanical charges and the double link atom method. Journal of Chemical Physics, 2002, 117, 10534-10547.	1.2	173
3	Molecular Dynamics of Staphylococcal Nuclease:Â Comparison of Simulation with15N and13C NMR Relaxation Data. Journal of the American Chemical Society, 1998, 120, 5301-5311.	6.6	121
4	Global control of suprathreshold reactivity by quantized transition states. Journal of the American Chemical Society, 1991, 113, 486-494.	6.6	95
5	Quantum-dynamical characterization of reactive transition states. Faraday Discussions of the Chemical Society, 1991, 91, 289.	2.2	71
6	HIV-1 Protease Cleavage Mechanism Elucidated with Molecular Dynamics Simulation. Journal of the American Chemical Society, 1995, 117, 5561-5572.	6.6	64
7	The nature and role of quantized transition states in the accurate quantum dynamics of the reaction O+H2â†'OH+H. Journal of Chemical Physics, 1993, 98, 342-362.	1.2	58
8	HIV-1 protease cleavage mechanism: A theoretical investigation based on classical MD simulation and reaction path calculations using a hybrid QM/MM potential. Computational and Theoretical Chemistry, 1998, 423, 79-92.	1.5	52
9	Quantized dynamical bottlenecks and transition state control of the reaction of D with H2: Effect of varying the total angular momentum. Journal of Chemical Physics, 2000, 112, 8387-8408.	1.2	38
10	1,3-Dipolar Cycloadditions of Trimethylsilyldiazomethane Revisited:â€‰ Steric Demand of the Dipolarophile and the Influence on Product Distribution. Journal of Organic Chemistry, 2007, 72, 650-653.	1.7	28
11	Methyl Motional Parameters in Crystallinel-Alanine:Â Molecular Dynamics Simulation and NMR. Journal of Physical Chemistry B, 2000, 104, 11342-11348.	1.2	27
12	Correlation Times and Adiabatic Barriers for Methyl Rotation in SNase. Journal of Biomolecular NMR, 2004, 29, 377-385.	1.6	20
13	Regioselectivity of Michael Additions to 3-(Pyridin-3-yl or Pyrimidin-2-yl)propenoates and TheirN-Oxides - Experimental and Theoretical Studies. European Journal of Organic Chemistry, 2005, 2005, 3297-3303.	1.2	18
14	Paramagnetic Nuclear Magnetic Resonance Relaxation and Molecular Mechanics Studies of the Chloroperoxidaseâ€"Indole Complex: Insights into the Mechanism of Chloroperoxidase-Catalyzed Regioselective Oxidation of Indole. Biochemistry, 2013, 52, 3688-3701.	1.2	18
15	Iterative methods for solving the non-sparse equations of quantum mechanical reactive scattering. Computer Physics Communications, 1989, 53, 357-379.	3.0	17
16	Benchmark calculations of thermal reaction rates. I. Quantal scattering theory. Journal of Chemical Physics, 1991, 94, 2040-2044.	1.2	17
17	Chloroperoxidase-Catalyzed Epoxidation of cis-Î²-Methylstyrene: Distal Pocket Flexibility Tunes Catalytic Reactivity. Journal of Physical Chemistry B, 2012, 116, 12905-12914.	1.2	16
18	Complex generalized minimal residual algorithm for iterative solution of quantumâ€mechanical reactive scattering equations. Journal of Chemical Physics, 1992, 97, 8322-8333.	1.2	14

#	Article	IF	Citations
19	Enantiospecificity of Chloroperoxidase-Catalyzed Epoxidation: Biased Molecular Dynamics Study of a Cis-Î²-Methylstyrene/Chloroperoxidase-Compound I Complex. Biophysical Journal, 2011, 100, 1066-1075.	0.2	14
20	Theoretical Study of HOCl-Catalyzed Ketoâ€“Enol Tautomerization of Î²-Cyclopentanedione in an Explicit Water Environment. Journal of Physical Chemistry A, 2013, 117, 8437-8448.	1.1	13
21	Preconditioned complex generalized minimal residual algorithm for dense algebraic variational equations in quantum reactive scattering. Journal of Chemical Physics, 1993, 99, 2739-2751.	1.2	12
22	The conformation of end-groups is one determinant of carotenoid topology suitable for high fidelity molecular recognition: A study of Î²- and Îµ-end-groups. Archives of Biochemistry and Biophysics, 2010, 493, 169-174.	1.4	11
23	A Possible Mechanism for Redox Control of Human Neuroglobin Activity. Journal of Chemical Information and Modeling, 2014, 54, 1997-2003.	2.5	11
24	Methyl dynamics in crystalline amino acids: MD and NMR. Journal of Computational Chemistry, 2003, 24, 1052-1058.	1.5	10
25	Stateâ€selected chemical reaction dynamics at the S matrix level: Finalâ€state specificities of nearâ€threshold processes at low and high energies. Journal of Chemical Physics, 1992, 96, 4313-4323.	1.2	8
26	Chloroperoxidase-Catalyzed Epoxidation of Cis-Î²-Methylstyrene: NHâ€“S Hydrogen Bonds and Proximal Helix Dipole Change the Catalytic Mechanism and Significantly Lower the Reaction Barrier. Journal of Physical Chemistry B, 2015, 119, 14350-14363.	1.2	8
27	Proximal Pocket Controls Alkene Oxidation Selectivity of Cytochrome P450 and Chloroperoxidase toward Small, Nonpolar Substrates. Journal of Physical Chemistry B, 2018, 122, 7828-7838.	1.2	7
28	Proximal Pocket Hydrogen Bonds Significantly Influence the Mechanism of Chloroperoxidase Compound I Formation. Journal of Physical Chemistry B, 2015, 119, 12590-12602.	1.2	6
29	How the Proximal Pocket May Influence the Enantiospecificities of Chloroperoxidase-Catalyzed Epoxidations of Olefins. International Journal of Molecular Sciences, 2016, 17, 1297.	1.8	5