Ã€ngels GonzÃ¡lez-Lafont

List of Publications by Year
in descending order

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140 papers	3,903 citations	147726 31 h-index	155592 55 g-index
143 all docs	143 docs citations	143 times ranked	3072 citing authors

#	Article	IF	Citations
1	N-Substituted 5-(1H-Indol-2-yl)-2-methoxyanilines Are Allosteric Inhibitors of the Linoleate Oxygenase Activity of Selected Mammalian ALOX15 Orthologs: Mechanism of Action. Journal of Medicinal Chemistry, 2022, 65, 1979-1995.	2.9	4
2	The role of acetylated cyclooxygenase-2 in the biosynthesis of resolvin precursors derived from eicosapentaenoic acid. Organic and Biomolecular Chemistry, 2022, 20, 1260-1274.	1.5	3
3	Theoretical Characterization of the Step-by-Step Mechanism of Conversion of Leukotriene A4 to Leukotriene B4 Catalysed by the Enzyme Leukotriene A4 Hydrolase. International Journal of Molecular Sciences, 2022, 23, 3140.	1.8	3
4	Molecular Insights into the Regulation of 3-Phosphoinositide-Dependent Protein Kinase 1: Modeling the Interaction between the Kinase and the Pleckstrin Homology Domains. ACS Omega, 2022, 7, 25186-25199.	1.6	4
5	Conformational Heterogeneity and Cooperative Effects of Mammalian ALOX15. International Journal of Molecular Sciences, 2021, 22, 3285.	1.8	5
6	Accounting for the instantaneous disorder in the enzymeâ€“substrate Michaelis complex to calculate the Gibbs free energy barrier of an enzyme reaction. Physical Chemistry Chemical Physics, 2021, 23, 13042-13054.	1.3	5
7	Understanding the Molecular Details of the Mechanism That Governs the Oxidation of Arachidonic Acid Catalyzed by Aspirin-Acetylated Cyclooxygenase-2. ACS Catalysis, 2020, 10, 138-153.	5.5	6
8	A protocol to obtain multidimensional quantum tunneling corrections derived from QM(DFT)/MM calculations for an enzyme reaction. Physical Chemistry Chemical Physics, 2020, 22, 27385-27393.	1.3	2
9	Deciphering the Molecular Details of the Lipoxin Formation Mechanism in the 5(S),15(S)-DiHpETE Biosynthetic Pathway Catalyzed by Reticulocyte 15-Lipoxygenase-1. Journal of Physical Chemistry B, 2020, 124, 11406-11418.	1.2	1
10	A role of Gln596 in fine-tuning mammalian ALOX15 specificity, protein stability and allosteric properties. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2020, 1865, 158680.	1.2	6
11	Unraveling how the Gly526Ser mutation arrests prostaglandin formation from arachidonic acid catalyzed by cyclooxygenase-2: a combined molecular dynamics and QM/MM study. RSC Advances, 2020, 10, 986-997.	1.7	4
12	Mutations of Triad Determinants Changes the Substrate Alignment at the Catalytic Center of Human ALOX5. ACS Chemical Biology, 2019, 14, 2768-2782.	1.6	13
13	Unraveling the Molecular Details of the Complete Mechanism That Governs the Synthesis of Prostaglandin G2 Catalyzed by Cyclooxygenase-2. ACS Omega, 2019, 4, 2063-2074.	1.6	6
14	Synthetic Photoswitchable Neurotransmitters Based on Bridged Azobenzenes. Organic Letters, 2019, 21, 3780-3784.	2.4	42
15	Comparing Hydrolysis and Transglycosylation Reactions Catalyzed by Thermus thermophilus Î²-Glycosidase. A Combined MD and QM/MM Study. Frontiers in Chemistry, 2019, 7, 200.	1.8	18
16	Mutagenesis of Sequence Determinants of Truncated Porcine ALOX15 Induces Changes in the Reaction Specificity by Altering the Catalytic Mechanism of Initial Hydrogen Abstraction. Chemistry - A European Journal, 2018, 24, 962-973.	1.7	13
17	Understanding the Molecular Mechanism of the Ala-versus-Gly Concept Controlling the Product Specificity in Reactions Catalyzed by Lipoxygenases: A Combined Molecular Dynamics and QM/MM Study of Coral 8R-Lipoxygenase. ACS Catalysis, 2017, 7, 4854-4866.	5.5	17
18	Understanding how cAMP-dependent protein kinase can catalyze phosphoryl transfer in the presence of Ca2+and Sr2+: a QM/MM study. Physical Chemistry Chemical Physics, 2017, 19, 10377-10394.	1.3	6

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19	Inhibition of Mammalian 15-Lipoxygenase by Three Ebselen-like Drugs. A QM/MM and MM/PBSA Comparative Study. Journal of Physical Chemistry A, 2017, 121, 9752-9763.	1.1	19
20	Kinetic isotope effects in chemical and biochemical reactions: physical basis and theoretical methods of calculation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 584-603.	6.2	21
21	Understanding the Mechanism of the Hydrogen Abstraction from Arachidonic Acid Catalyzed by the Human Enzyme 15-Lipoxygenase-2. A Quantum Mechanics/Molecular Mechanics Free Energy Simulation. Journal of Chemical Theory and Computation, 2016, 12, 2079-2090.	2.3	33
22	Computational insight into the catalytic implication of head/tail-first orientation of arachidonic acid in human 5-lipoxygenase: consequences for the positional specificity of oxygenation. Physical Chemistry Chemical Physics, 2016, 18, 23017-23035.	1.3	22
23	Is Regioselectivity in the Enzymeâ€Catalyzed Hydroperoxidation of Arachidonic Acid Necessarily Determined by Hydrogen Abstraction? The Case of Rabbit Leu597Ala/Ile663Ala ALOX15 Mutant. ChemPhysChem, 2016, 17, 3321-3332.	1.0	4
24	Evolutionary alteration of ALOX15 specificity optimizes the biosynthesis of antiinflammatory and proresolving lipoxins. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E4266-75.	3.3	54
25	How Can Linoleic Acid Be the Preferential Substrate of the Enzyme 15-Lipoxygenase-1? A QM/MM Approach. Journal of Physical Chemistry B, 2016, 120, 1950-1960.	1.2	18
26	A QM/MM study of Kemptide phosphorylation catalyzed by protein kinase A. The role of Asp166 as a general acid/base catalyst. Physical Chemistry Chemical Physics, 2015, 17, 3497-3511.	1.3	18
27	SP20 Phosphorylation Reaction Catalyzed by Protein Kinase A: QM/MM Calculations Based on Recently Determined Crystallographic Structures. ACS Catalysis, 2015, 5, 4897-4912.	5.5	19
28	Regioâ€•and Stereospecificity in the Oxygenation of Arachidonic Acid Catalyzed by Leu597 Mutants of Rabbit 15â€Lipoxygenase: A QM/MM Study. ChemPhysChem, 2014, 15, 2303-2310.	1.0	11
29	Unraveling How Enzymes Can Use Bulky Residues To Drive Site-Selective Câ€“H Activation: The Case of Mammalian Lipoxygenases Catalyzing Arachidonic Acid Oxidation. ACS Catalysis, 2014, 4, 4351-4363.	5.5	39
30	Introducing Mutations to Modify the C13/C9 Ratio in Linoleic Acid Oxygenations Catalyzed by Rabbit 15â€Lipoxygenase: A QM/MM and MD Study. ChemPhysChem, 2014, 15, 4049-4054.	1.0	7
31	A QM/MM study of the associative mechanism for the phosphorylation reaction catalyzed by protein kinase A and its D166A mutant. Journal of Computer-Aided Molecular Design, 2014, 28, 1077-1091.	1.3	11
32	An Insight into the Regiospecificity of Linoleic Acid Peroxidation Catalyzed by Mammalian 15-Lipoxygenases. Journal of Physical Chemistry B, 2013, 117, 3747-3754.	1.2	17
33	On the Regioâ€•and Stereospecificity of Arachidonic Acid Peroxidation Catalyzed by Mammalian 15â€Lypoxygenases: A Combined Molecular Dynamics and QM/MM Study. ChemPhysChem, 2013, 14, 3777-3787.	1.0	11
34	Role of Arg403 for thermostability and catalytic activity of rabbit 12/15-lipoxygenase. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2013, 1831, 1079-1088.	1.2	17
35	Theoretical Analysis of the Catalytic Mechanism of Helicobacter pylori Glutamate Racemase. Journal of Physical Chemistry B, 2012, 116, 12406-12414.	1.2	12
36	Theoretical Study of the Mechanism of the Hydride Transfer between Ferredoxinâ€“NADP⁺ Reductase and NADP⁺: The Role of Tyr303. Journal of the American Chemical Society, 2012, 134, 20544-20553.	6.6	40

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37	Ligandâ€induced formation of transient dimers of mammalian 12/15â€lipoxygenase: A key to allosteric behavior of this class of enzymes?. Proteins: Structure, Function and Bioinformatics, 2012, 80, 703-712.	1.5	33
38	Influence of the enzyme phosphorylation state and the substrate on PKA enzyme dynamics. Biophysical Chemistry, 2012, 161, 17-28.	1.5	9
39	A QM/MM study of the phosphoryl transfer to the Kemptide substrate catalyzed by protein kinase A. The effect of the phosphorylation state of the protein on the mechanism. Physical Chemistry Chemical Physics, 2011, 13, 530-539.	1.3	25
40	Substrate binding to mammalian 15-lipoxygenase. Journal of Computer-Aided Molecular Design, 2011, 25, 825-835.	1.3	15
41	A variational transition state theory description of periselectivity effects on cycloadditions of ketenes with cyclopentadiene. Theoretical Chemistry Accounts, 2011, 128, 569-577.	0.5	7
42	Variational transitionâ€state theory study of the rate constant of the DMSÂ·OH scavenging reaction by O₂. Journal of Computational Chemistry, 2011, 32, 2104-2118.	1.5	2
43	A theoretical study of the DMSÂ·OH scavenging reaction by OH. Its relevance in DMSO formation. Computational and Theoretical Chemistry, 2011, 965, 249-258.	1.1	5
44	Insights into the Mechanism of Binding of Arachidonic Acid to Mammalian 15-Lipoxygenases. Journal of Physical Chemistry B, 2010, 114, 7037-7046.	1.2	30
45	Mechanism of the Hydride Transfer between Anabaena Tyr303Ser FNR_{rd}/FNR_{ox} and NADP⁺/H. A Combined Pre-Steady-State Kinetic/Ensemble-Averaged Transition-State Theory with Multidimensional Tunneling Study. Journal of Physical Chemistry B, 2010, 114, 3368-3379.	1.2	27
46	Canonical Variational Transition-State Theory Study of the CF3CHFCH2F + OH Reaction. Journal of Physical Chemistry A, 2010, 114, 2768-2777.	1.1	2
47	Formation pathways of DMSO from DMSâ€OH in the presence of O₂ and NO_x: A theoretical study. Journal of Computational Chemistry, 2009, 30, 173-182.	1.5	9
48	Formation pathways of DMSO₂ in the addition channel of the OHâ€initiated DMS oxidation: A theoretical study. Journal of Computational Chemistry, 2009, 30, 1477-1489.	1.5	5
49	Formation pathways of CH3SOH from CH3S(OH)CH3 in the presence of O2: a theoretical study. Theoretical Chemistry Accounts, 2009, 123, 93-103.	0.5	6
50	Benchmark calculations on models of the phosphoryl transfer reaction catalyzed by protein kinase A. Theoretical Chemistry Accounts, 2009, 124, 197-215.	0.5	4
51	The effect of electron-withdrawing groups in the fragmentation of the radical anions of benzyl phenyl ethers. Computational and Theoretical Chemistry, 2009, 913, 228-235.	1.5	3
52	How the Substrate d-Glutamate Drives the Catalytic Action of Bacillus subtilis Glutamate Racemase. Journal of the American Chemical Society, 2009, 131, 3509-3521.	6.6	23
53	Canonical Variational Transition-State Theory Study of the CF3CH2CH3 + OH Reaction. Journal of Physical Chemistry B, 2008, 112, 328-335.	1.2	16
54	Tunneling in Green Tea:Â Understanding the Antioxidant Activity of Catechol-Containing Compounds. A Variational Transition-State Theory Study. Journal of the American Chemical Society, 2007, 129, 5846-5854.	6.6	96

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55	Methanesulfinic Acid Reaction with OH:â€‰ Mechanism, Rate Constants, and Atmospheric Implications. Journal of Physical Chemistry A, 2007, 111, 7825-7832.	1.1	9
56	Theoretical Modeling of Hydroxyl-Radical-Induced Lipid Peroxidation Reactions. Journal of Physical Chemistry B, 2007, 111, 5684-5693.	1.2	46
57	New Insights into the Reaction Mechanism Catalyzed by the Glutamate Racemase Enzyme:Â pH Titration Curves and Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 2385-2397.	1.2	13
58	Methyl Vinyl Ketone+OH and Methacrolein+OH Oxidation Reactions: A Master Equation Analysis of the Pressure- and Temperature-Dependent Rate Constants. Chemistry - A European Journal, 2007, 13, 1180-1190.	1.7	8
59	A PM3/d specific reaction parameterization for iron atom in the hydrogen abstraction catalyzed by soybean lipoxygenase-1. Journal of Computational Chemistry, 2007, 28, 997-1005.	1.5	15
60	Kinetic Study on the Reaction of OH Radical with Dimethyl Sulfide in the Absence of Oxygen. ChemPhysChem, 2007, 8, 255-263.	1.0	11
61	Comparative study of the prereactive protein kinase A Michaelis complex with Kemptide substrate. Journal of Computer-Aided Molecular Design, 2007, 21, 603-615.	1.3	7
62	Enzyme Dynamics and Tunneling Enhanced by Compression in the Hydrogen Abstraction Catalyzed by Soybean Lipoxygenase-1. Journal of Physical Chemistry B, 2006, 110, 24708-24719.	1.2	51
63	Variational Transition-State Theory Study of the Dimethyl Sulfoxide (DMSO) and OH Reactionâ€. Journal of Physical Chemistry A, 2006, 110, 798-808.	1.1	23
64	On the Ionization State of the Substrate in the Active Site of Glutamate Racemase. A QM/MM Study about the Importance of Being Zwitterionicâ€. Journal of Physical Chemistry A, 2006, 110, 717-725.	1.1	33
65	Searching for Saddle Points by Using the Nudged Elastic Band Method:â€‰ An Implementation for Gas-Phase Systems. Journal of Chemical Theory and Computation, 2006, 2, 895-904.	2.3	33
66	A Theoretical Analysis of Rate Constants and Kinetic Isotope Effects Corresponding to Different Reactant Valleys in Lactate Dehydrogenase. Journal of the American Chemical Society, 2006, 128, 16851-16863.	6.6	52
67	Enthalpies of formation of isopreneâ€™s major oxidation byproducts. Chemical Physics Letters, 2005, 409, 255-259.	1.2	1
68	Electronic structure study of the initiation routes of the dimethyl sulfide oxidation by OH. Journal of Computational Chemistry, 2005, 26, 569-583.	1.5	27
69	Pressure Dependence in the Methyl Vinyl Ketone+OH and Methacrolein+OH Oxidation Reactions: An Electronic Structure Study. ChemPhysChem, 2005, 6, 1567-1573.	1.0	7
70	A Molecular Dynamics Simulation of the Binding Modes of d-Glutamate and d-Glutamine to Glutamate Racemase. Journal of Chemical Theory and Computation, 2005, 1, 737-749.	2.3	9
71	Reaction Mechanism of the Mandelate Anion Racemization Catalyzed by Mandelate Racemase Enzyme:Â A QM/MM Molecular Dynamics Free Energy Study. Journal of Physical Chemistry B, 2005, 109, 21089-21101.	1.2	10
72	A Theoretical Study of the Competitive Homolytic/Heterolytic Aniomesolytic Cleavages of Câ^'O Alkyl Ether Bonds. Journal of Organic Chemistry, 2005, 70, 540-548.	1.7	10

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73	A Fast Radical Chain Mechanism in the Polyfluoroalkoxylation of Aromatics through NO2 Group Displacement. Mechanistic and Theoretical Studies. Journal of Organic Chemistry, 2005, 70, 1718-1727.	1.7	29
74	A QM/MM Exploration of the Potential Energy Surface of Pyruvate to Lactate Transformation Catalyzed by LDH. Improving the Accuracy of Semiempirical Descriptions. Journal of Chemical Theory and Computation, 2005, 1, 750-761.	2.3	22
75	Hydrogen Abstraction by Soybean Lipoxygenase-1. Density Functional Theory Study on Active Site Models in Terms of Gibbs Free Energies. Journal of Physical Chemistry B, 2004, 108, 13831-13838.	1.2	20
76	Geometry optimization and transition state search in enzymes: Different options in the microiterative method. International Journal of Quantum Chemistry, 2004, 98, 367-377.	1.0	26
77	Testing electronic structure methods for describing intermolecular H Â· Â· Â· H interactions in supramolecular chemistry. Journal of Computational Chemistry, 2004, 25, 99-105.	1.5	35
78	Rate constants of gas-phase hydrogen abstraction reactions: a balance between the association and the abstraction dynamical bottlenecks. Computational and Theoretical Chemistry, 2004, 709, 35-43.	1.5	12
79	Photo-oxidation of lipids by singlet oxygen: a theoretical study. Chemical Physics Letters, 2004, 398, 336-342.	1.2	23
80	Variational Transition State Theory as a Tool To Determine Kinetic Selectivity in Reactions Involving a Valley-Ridge Inflection Point. Journal of the American Chemical Society, 2004, 126, 13089-13094.	6.6	40
81	Rate Constants for the Hydrogen Abstractions in the OH-Initiated Oxidation of Glycolaldehyde. A Variational Transition-state Theory Calculation. Journal of Physical Chemistry A, 2004, 108, 5117-5125.	1.1	12
82	The curvature of the Arrhenius plots predicted by conventional canonical transition-state theory in the absence of tunneling. Theoretical Chemistry Accounts, 2003, 110, 352-357.	0.5	25
83	Dependence of the rate constants on the treatment of internal rotation modes: The reaction OH + CH3SH â†' CH3S + H2O as an example. Journal of Computational Chemistry, 2003, 24, 701-706.	1.5	9
84	How important is the refinement of transition state structures in enzymatic reactions?. Computational and Theoretical Chemistry, 2003, 632, 297-307.	1.5	14
85	Determination of enzymatic reaction pathways using QM/MM methods. International Journal of Quantum Chemistry, 2003, 93, 229-244.	1.0	52
86	Variational Transition-State Theory Rate Constant Calculations of the OH + CH3SH Reaction and Several Isotopic Variants. Journal of Physical Chemistry A, 2003, 107, 4490-4496.	1.1	30
87	Variational Transition-State Theory Rate Constant Calculations with Multidimensional Tunneling Corrections of the Reaction of Acetone with OH. Journal of Physical Chemistry A, 2002, 106, 11760-11770.	1.1	40
88	Thermodynamics, Kinetics, and Dynamics of the Two Alternative Aniomesolytic Fragmentations of Câ^'O Bonds:â€‰ An Electrochemical and Theoretical Study. Journal of the American Chemical Society, 2002, 124, 4708-4715.	6.6	28
89	On the modulation of the substrate activity for the racemization catalyzed by mandelate racemase enzyme. A QM/MM study. Physical Chemistry Chemical Physics, 2002, 4, 5365-5371.	1.3	9
90	The search for stationary points on a quantum mechanical/molecular mechanical potential-energy surface. Theoretical Chemistry Accounts, 2002, 107, 147-153.	0.5	16

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91	Test of variational transition state theory with multidimensional tunneling contributions against experimental kinetic isotope effects for the CH n D 4â^'n + OHâ†'P (n=0, 4) reactions. Theoretical Chemistry Accounts, 2002, 108, 38-40.	0.5	11
92	On the evaluation of quasi-thermodynamic magnitudes from rate constant values. Influence of the variational and tunnelling contributions. Chemical Physics Letters, 2002, 353, 154-162.	1.2	8
93	Monte Carlo Simulations of Chemical Reactions in Solution. , 2002, , 125-177.		0
94	The1H NMR Chemical Shift for the Hydroxy Proton of 4-(Dimethylamino)-2â€˜-hydroxychalcone in Chloroform:â€‰ A Theoretical Approach to Its Inverse Dependence on the Temperature. Organic Letters, 2001, 3, 589-592.	2.4	11
95	A QM/MM Study of the Racemization of Vinylglycolate Catalyzed by Mandelate Racemase Enzyme. Journal of the American Chemical Society, 2001, 123, 709-721.	6.6	38
96	Variational Transition State Calculations of the CH2F2 + OH Hydrogen Abstraction Reaction. Journal of Physical Chemistry A, 2001, 105, 10553-10561.	1.1	21
97	The reactions CHnD4â^'n+OHâ†'P and CH4+ODâ†'CH3+HOD as a test of current direct dynamics computational methods to determine variational transition-state rate constants. I.. Journal of Chemical Physics, 2001, 114, 2154-2165.	1.2	44
98	The reactions CHnD4â^'n+OHâ†'P and CH4+ODâ†'CH3+HOD as a test of current direct dynamics multicoefficient methods to determine variational transition state rate constants. II. Journal of Chemical Physics, 2001, 115, 4515-4526.	1.2	29
99	Effective way of modeling chemical catalysis: Empirical valence bond picture of role of solvent and catalyst in alkylation reactions. Journal of Computational Chemistry, 2000, 21, 607-625.	1.5	17
100	Effect of a complex formation on the calculated low-pressure rate constant of a bimolecular gas-phase reaction governed by tunneling. Journal of Computational Chemistry, 1999, 20, 1685-1692.	1.5	17
101	Mechanism of the Gas-Phase HO + H2O â†' H2O + OH Reaction and Several Associated Isotope Exchange Reactions:â€‰ A Canonical Variational Transition State Theory Plus Multidimensional Tunneling Calculation. Journal of Physical Chemistry A, 1999, 103, 1044-1053.	1.1	34
102	Variational Transition-State Theory with Optimized Orientation of the Dividing Surface and Semiclassical Tunneling Calculations for Deuterium and Muonium Kinetic Isotope Effects in the Free Radical Association Reaction H + C2H4 â†' C2H5. Journal of Physical Chemistry A, 1999, 103, 5061-5074.	1.1	50
103	Asymmetry of the Hydrogen Bond of Hydrogen Phthalate Anion in Solution. A QM/MM Study. Journal of the American Chemical Society, 1999, 121, 9198-9207.	6.6	51
104	Effect of the hydrogen bond network in carbonic anhydrase II zinc binding site. A theoretical study. Canadian Journal of Chemistry, 1998, 76, 1027-1032.	0.6	3
105	Theoretical study of the role of arginine 127 in the water-promoted mechanism of peptide cleavage by carboxypeptidase A. New Journal of Chemistry, 1998, 22, 319-326.	1.4	21
106	Temperature Dependence of Proton NMR Chemical Shift As a Criterion To Identify Low-Barrier Hydrogen Bonds. Journal of the American Chemical Society, 1998, 120, 10203-10209.	6.6	53
107	Explanation of Deuterium and Muonium Kinetic Isotope Effects for Hydrogen Atom Addition to an Olefin. Journal of the American Chemical Society, 1998, 120, 12141-12142.	6.6	20
108	Reaction-Path and Dual-Level Dynamics Calculations of the CH3F + OH Reaction. Journal of Physical Chemistry A, 1998, 102, 10715-10722.	1.1	23

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109	Variational Transition State Theory and Tunneling Calculations with Reorientation of the Generalized Transition States for Methyl Cation Transfer. Journal of Physical Chemistry A, 1998, 102, 3420-3428.	1.1	48
110	Entropic Effects on the Dynamical Bottleneck Location and Tunneling Contributions for C2H4 + H â†' C2H5:â€‰ Variable Scaling of External Correlation Energy for Association Reactions. Journal of the American Chemical Society, 1998, 120, 5559-5567.	6.6	30
111	Theoretical study of the unimolecular dissociation of the acetone cation radical. Molecular Physics, 1997, 92, 393-398.	0.8	6
112	Is an Extremely Low-Field Proton Signal in the NMR Spectrum Conclusive Evidence for a Low-Barrier Hydrogen Bond?. Journal of Physical Chemistry A, 1997, 101, 8727-8733.	1.1	55
113	On pKaMatching as a Requirement To Form a Low-Barrier Hydrogen Bond. A Theoretical Study in Gas Phase. Journal of Physical Chemistry A, 1997, 101, 3880-3886.	1.1	48
114	Theoretical Study of the Low-Barrier Hydrogen Bond in the Hydrogen Maleate Anion in the Gas Phase. Comparison with Normal Hydrogen Bonds. Journal of the American Chemical Society, 1997, 119, 1081-1086.	6.6	151
115	Understanding the activation energy trends for the C2H4+OHâ†'C2H4OH reaction by using canonical variational transition state theory. Journal of Chemical Physics, 1997, 107, 7266-7274.	1.2	50
116	On the interpolation of the frequencies of vibrational modes in variational transition state calculations: an adiabatic or diabatic scheme?. Molecular Physics, 1996, 89, 633-644.	0.8	9
117	Kinetic Isotope Effects as Tools To Reveal Solvation Changes Accompanying a Proton Transfer. A Canonical Unified Statistical Theory Calculation. The Journal of Physical Chemistry, 1996, 100, 19389-19397.	2.9	10
118	Choice of the reaction coordinate in electron-transfer reactions in solution. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 1451-1455.	1.7	1
119	On the water-promoted mechanism of peptide cleavage by carboxypeptidase A. A theoretical study. Canadian Journal of Chemistry, 1994, 72, 2077-2083.	0.6	18
120	MORATE: a program for direct dynamics calculations of chemical reaction rates by semiempirical molecular orbital theory. Computer Physics Communications, 1993, 75, 143-159.	3.0	107
121	Direct dynamics calculation of the kinetic isotope effect for an organic hydrogen-transfer reaction, including corner-cutting tunneling in 21 dimensions. Journal of the American Chemical Society, 1993, 115, 7806-7817.	6.6	348
122	The mechanism of exchange of intramolecularly hydrogen-bonded protons in a diamide. Journal of the Chemical Society Perkin Transactions II, 1992, , 1621-1624.	0.9	1
123	Variational Transition-State Theory with Multidimensional, Semiclassical, Ground-State Transmission Coefficients. ACS Symposium Series, 1992, , 16-36.	0.5	18
124	Temperature dependence of the kinetic isotope effect for a gas-phase SN2 reaction: Cl- + CH3Br. Journal of the American Chemical Society, 1991, 113, 9404-9405.	6.6	88
125	Direct dynamics calculations with NDDO (neglect of diatomic differential overlap) molecular orbital theory with specific reaction parameters. The Journal of Physical Chemistry, 1991, 95, 4618-4627.	2.9	285
126	Interpolated variational transitionâ€štate theory: Practical methods for estimating variational transitionâ€štate properties and tunneling contributions to chemical reaction rates from electronic structure calculations. Journal of Chemical Physics, 1991, 95, 8875-8894.	1.2	296

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127	A Monte Carlo simulation of free energy relationships for the electron transfer reaction between Fe+and Fe2+in water. Journal of Computational Chemistry, 1991, 12, 1165-1171.	1.5	11
128	Molecular modeling of solvation. Clâ^'(D2O). Journal of Chemical Physics, 1991, 94, 5544-5558.	1.2	42
129	The role of many-body interactions in the stability of hydrated Cu2+ clusters. Chemical Physics, 1990, 141, 379-392.	0.9	23
130	The regioselectivity of 4-nitroanisole photosubstitution with primary amines. A mechanistic and theoretical study. Journal of Organic Chemistry, 1990, 55, 3303-3310.	1.7	33
131	Effect of solvent fluctuations in the electron-transfer process between two Fe+ ions. Journal of the Chemical Society Faraday Transactions I, 1989, 85, 1207.	1.0	2
132	On constraining solvent molecule displacements in electron-transfer reactions: a critical discussion. The Journal of Physical Chemistry, 1989, 93, 4677-4682.	2.9	3
133	Hydration of Fe+: A Monte Carlo simulation of water clusters and of a dilute aqueous solution. Journal of Computational Chemistry, 1988, 9, 819-826.	1.5	3
134	Analytical potential from ab initio calculations for the Fe+-H2O and Feo-H2O systems. International Journal of Quantum Chemistry, 1988, 33, 77-85.	1.0	4
135	Excited states and electronic spectra of monosubstituted benzenes. An AM1 study. Spectrochimica Acta Part A: Molecular Spectroscopy, 1988, 44, 1427-1434.	0.1	15
136	The Cu+â€“H2O interaction potential and its application to the study of [Cu(H2O)n]+clusters at different temperatures. Journal of the Chemical Society, Faraday Transactions 2, 1988, 84, 693-704.	1.1	9
137	The nucleophilic aromatic photosubstitutions of 4,5-dinitroveratrole with amines. Tetrahedron, 1987, 43, 351-360.	1.0	28
138	A Monte Carlo simulation of Fe2+ aqueous solvation. Chemical Physics, 1987, 111, 241-247.	0.9	30
139	Theoretical study of several Fe(H2o)n2+clusters at different temperatures. International Journal of Quantum Chemistry, 1986, 29, 1373-1382.	1.0	14
140	An intermolecular potential function for the Fe(II)-H2O system from ab initio calculations. International Journal of Quantum Chemistry, 1986, 30, 663-670.	1.0	9