James T Hynes

List of Publications by Year in descending order

247 papers	22,161 citations	5896 81 h-index	8866 145 g-index
264 all docs	264 docs citations	264 times ranked	9221 citing authors

#	Article	IF	Citations
1	Confined Waterâ€™s Dielectric Constant Reduction Is Due to the Surrounding Low Dielectric Media and Not to Interfacial Molecular Ordering. Journal of Physical Chemistry Letters, 2021, 12, 4319-4326.	4.6	53
2	A Model Electron Transfer Reaction in Confined Aqueous Solution. ChemPhysChem, 2021, 22, 2247-2255.	2.1	2
3	Electron Flow Characterization of Charge Transfer for Carbonic Acid to Strong Base Proton Transfer in Aqueous Solution. Journal of Physical Chemistry B, 2021, 125, 11473-11490.	2.6	2
4	Ultrafast Rotational and Translational Energy Relaxation in Neat Liquids. Journal of Physical Chemistry B, 2021, 125, 12806-12819.	2.6	1
5	Water Structure, Dynamics, and Sum-Frequency Generation Spectra at Electrified Graphene Interfaces. Journal of Physical Chemistry Letters, 2020, 11, 624-631.	4.6	45
6	Solvation Dynamics in Water. 4. On the Initial Regime of Solvation Relaxation. Journal of Physical Chemistry B, 2020, 124, 7668-7681.	2.6	8
7	Water dynamics at electrified graphene interfaces: a jump model perspective. Physical Chemistry Chemical Physics, 2020, 22, 10581-10591.	2.8	19
8	Intact carbonic acid is a viable protonating agent for biological bases. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 20837-20843.	7.1	8
9	Dynamical Recrossing in the Intercalation Process of the Anticancer Agent Proflavine into DNA. Journal of Physical Chemistry B, 2019, 123, 10904-10914.	2.6	9
10	Benzimidazoles as Metal-Free and Recyclable Hydrides for CO₂ Reduction to Formate. Journal of the American Chemical Society, 2019, 141, 272-280.	13.7	67
11	Predicting Hydride Donor Strength via Quantum Chemical Calculations of Hydride Transfer Activation Free Energy. Journal of Physical Chemistry B, 2018, 122, 1278-1288.	2.6	15
12	Renewable Hydride Donors for the Catalytic Reduction of CO₂: A Thermodynamic and Kinetic Study. Journal of Physical Chemistry B, 2018, 122, 10179-10189.	2.6	13
13	Solvation Dynamics in Liquid Water. III. Energy Fluxes and Structural Changes. Journal of Physical Chemistry B, 2017, 121, 1377-1385.	2.6	14
14	Water Dynamics in the Hydration Shells of Biomolecules. Chemical Reviews, 2017, 117, 10694-10725.	47.7	574
15	Perspective: Structure and ultrafast dynamics of biomolecular hydration shells. Structural Dynamics, 2017, 4, 044018.	2.3	34
16	Nuclear Quantum Effects in Water Reorientation and Hydrogen-Bond Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 2602-2607.	4.6	51
17	Translational versus rotational energy flow in water solvation dynamics. Chemical Physics Letters, 2017, 683, 483-487.	2.6	6
18	Dihydropteridine/Pteridine as a 2H⁺/2e^{â€“} Redox Mediator for the Reduction of CO₂ to Methanol: A Computational Study. Journal of Physical Chemistry B, 2017, 121, 4158-4167.	2.6	13

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19	Non-adiabatic transition probability dependence on conical intersection topography. Journal of Chemical Physics, 2016, 145, 194104.	3.0	24
20	How Acidic Is Carbonic Acid?. Journal of Physical Chemistry B, 2016, 120, 2440-2451.	2.6	63
21	Solvation Dynamics in Water: 2. Energy Fluxes on Excited- and Ground-State Surfaces. Journal of Physical Chemistry B, 2016, 120, 11287-11297.	2.6	12
22	Dynamical Disorder in the DNA Hydration Shell. Journal of the American Chemical Society, 2016, 138, 7610-7620.	13.7	103
23	Reaction Mechanism for Direct Proton Transfer from Carbonic Acid to a Strong Base in Aqueous Solution II: Solvent Coordinate-Dependent Reaction Path. Journal of Physical Chemistry B, 2016, 120, 2281-2290.	2.6	12
24	Reaction Mechanism for Direct Proton Transfer from Carbonic Acid to a Strong Base in Aqueous Solution I: Acid and Base Coordinate and Charge Dynamics. Journal of Physical Chemistry B, 2016, 120, 2271-2280.	2.6	24
25	Solvation Dynamics in Liquid Water. 1. Ultrafast Energy Fluxes. Journal of Physical Chemistry B, 2015, 119, 7558-7570.	2.6	26
26	Effect of Solvent Dielectric Constant and Acidity on the OH Vibration Frequency in Hydrogen-Bonded Complexes of Fluorinated Ethanols. Journal of Physical Chemistry B, 2015, 119, 9278-9286.	2.6	11
27	Are there dynamical effects in enzyme catalysis? Some thoughts concerning the enzymatic chemical step. Archives of Biochemistry and Biophysics, 2015, 582, 42-55.	3.0	36
28	Catalytic Reduction of CO₂ by Renewable Organohydrides. Journal of Physical Chemistry Letters, 2015, 6, 5078-5092.	4.6	59
29	Molecules in Motion: Chemical Reaction and Allied Dynamics in Solution and Elsewhere. Annual Review of Physical Chemistry, 2015, 66, 1-20.	10.8	25
30	Non-adiabatic dynamics close to conical intersections and the surface hopping perspective. Frontiers in Chemistry, 2014, 2, 97.	3.6	64
31	Reduction of CO₂ to Methanol Catalyzed by a Biomimetic Organo-Hydride Produced from Pyridine. Journal of the American Chemical Society, 2014, 136, 16081-16095.	13.7	131
32	Conical intersection structure and dynamics for a model protonated schiff base photoisomerization in solution. International Journal of Quantum Chemistry, 2013, 113, 296-305.	2.0	7
33	Roles of the Lewis Acid and Base in the Chemical Reduction of CO₂ Catalyzed by Frustrated Lewis Pairs. Inorganic Chemistry, 2013, 52, 10062-10066.	4.0	58
34	Biomolecular hydration dynamics: a jump model perspective. Chemical Society Reviews, 2013, 42, 5672.	38.1	100
35	Ultrafast Librational Relaxation of H₂O in Liquid Water. Journal of Physical Chemistry B, 2013, 117, 4541-4552.	2.6	35
36	Theoretical Study of Water Oxidation by the Ruthenium Blue Dimer. II. Proton Relay Chain Mechanism for the Step [bpy₂(HOO)Ru^{IV}ORu^{IV}(OH)bpy₂]⁴⁺ â†' [bpy₂(O₂^{â€“})Ru^{IV}ORu^{III}(OH₂)bpy₂]<sup>4 Journal of Physical Chemistry B, 2013, 117, 15761-15773.	2.6	10

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37	Water Jump Reorientation: From Theoretical Prediction to Experimental Observation. Accounts of Chemical Research, 2012, 45, 53-62.	15.6	90
38	Tracking energy transfer from excited to accepting modes: application to water bend vibrational relaxation. Physical Chemistry Chemical Physics, 2012, 14, 6332.	2.8	29
39	Photoisomerization for a model protonated Schiff base in solution: Sloped/peaked conical intersection perspective. Journal of Chemical Physics, 2012, 137, 22A543.	3.0	26
40	Multistep Drug Intercalation: Molecular Dynamics and Free Energy Studies of the Binding of Daunomycin to DNA. Journal of the American Chemical Society, 2012, 134, 8588-8596.	13.7	78
41	Proton relay and electron flow in the Oâ€“O single bond formation in water oxidation by the ruthenium blue dimer. Energy and Environmental Science, 2012, 5, 7741.	30.8	16
42	Non-monotonic dependence of water reorientation dynamics on surface hydrophilicity: competing effects of the hydration structure and hydrogen-bond strength. Physical Chemistry Chemical Physics, 2011, 13, 19911.	2.8	60
43	Dynamical Friction Effects on the Photoisomerization of a Model Protonated Schiff Base in Solution. Journal of Physical Chemistry A, 2011, 115, 3720-3735.	2.5	43
44	Theoretical Study of Oâ€“O Single Bond Formation in the Oxidation of Water by the Ruthenium Blue Dimer. Journal of Physical Chemistry A, 2011, 115, 8003-8016.	2.5	46
45	Water reorientation dynamics in the first hydration shells of Fâ^' and Iâ^'. Physical Chemistry Chemical Physics, 2011, 13, 19895.	2.8	52
46	Reorientation and Allied Dynamics in Water and Aqueous Solutions. Annual Review of Physical Chemistry, 2011, 62, 395-416.	10.8	310
47	Water reorientation in the hydration shells of hydrophilic and hydrophobic solutes. Science China: Physics, Mechanics and Astronomy, 2010, 53, 1068-1072.	5.1	11
48	Theoretical aspects of tunneling proton transfer reactions in a polar environment. Journal of Physical Organic Chemistry, 2010, 23, 632-646.	1.9	49
49	Vibrational Symmetry Breaking of NO₃^{â^'} in Aqueous Solution: NO Asymmetric Stretch Frequency Distribution and Mean Splitting. Journal of Physical Chemistry A, 2010, 114, 1255-1269.	2.5	18
50	Water Hydrogen-Bond Dynamics around Amino Acids: The Key Role of Hydrophilic Hydrogen-Bond Acceptor Groups. Journal of Physical Chemistry B, 2010, 114, 2083-2089.	2.6	113
51	Water reorientation, hydrogen-bond dynamics and 2D-IR spectroscopy next to an extended hydrophobic surface. Faraday Discussions, 2010, 146, 263.	3.2	98
52	Water Hydrogen Bond Dynamics in Aqueous Solutions of Amphiphiles. Journal of Physical Chemistry B, 2010, 114, 3052-3059.	2.6	106
53	Editorial: Pushing Through Interdisciplinary Boundaries. ChemPhysChem, 2009, 10, 4-4.	2.1	0
54	Ultrafast Energy Transfer from the Intramolecular Bending Vibration to Librations in Liquid Water. Journal of Physical Chemistry A, 2009, 113, 6657-6665.	2.5	52

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55	Pathways for H₂O Bend Vibrational Relaxation in Liquid Water. Journal of Physical Chemistry A, 2009, 113, 8949-8962.	2.5	73
56	Why Water Reorientation Slows without Iceberg Formation around Hydrophobic Solutes. Journal of Physical Chemistry B, 2009, 113, 2428-2435.	2.6	338
57	Nitric Acid Dissociation at an Aqueous Surface: Occurrence and Mechanism. Israel Journal of Chemistry, 2009, 49, 251-259.	2.3	5
58	Depth-Dependent Dissociation of Nitric Acid at an Aqueous Surface: Carâ^'Parrinello Molecular Dynamics. Journal of Physical Chemistry A, 2009, 113, 1295-1307.	2.5	54
59	Dynamic Effects on Reaction Rates in a Michael Addition Catalyzed by Chalcone Isomerase. Beyond the Frozen Environment Approach. Journal of the American Chemical Society, 2008, 130, 7477-7488.	13.7	61
60	On the Residence Time for Water in a Solute Hydration Shell: Application to Aqueous Halide Solutions. Journal of Physical Chemistry B, 2008, 112, 7697-7701.	2.6	143
61	On the Molecular Mechanism of Drug Intercalation into DNA: A Simulation Study of the Intercalation Pathway, Free Energy, and DNA Structural Changes. Journal of the American Chemical Society, 2008, 130, 9747-9755.	13.7	176
62	On the Molecular Mechanism of Water Reorientation. Journal of Physical Chemistry B, 2008, 112, 14230-14242.	2.6	380
63	A Theoretical Study of the Formation of the Aminoacetonitrile Precursor of Glycine on Icy Grain Mantles in the Interstellar Medium. Journal of Physical Chemistry C, 2008, 112, 2972-2980.	3.1	64
64	Reorientional dynamics of water molecules in anionic hydration shells. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 11167-11172.	7.1	279
65	Acid-Base Proton Transfer and Ion Pair Formation in Solution. Advances in Chemical Physics, 2007, , 381-430.	0.3	33
66	Theoretical Study of the Dissociation of Nitric Acid at a Model Aqueous Surface. Journal of Physical Chemistry A, 2007, 111, 11033-11042.	2.5	45
67	Concerted Proton-Transfer Mechanism and Solvation Effects in the HNC/HCN Isomerization on the Surface of Icy Grain Mantles in the Interstellar Medium. Journal of Physical Chemistry C, 2007, 111, 15026-15033.	3.1	20
68	A Molecular Jump Mechanism of Water Reorientation. Science, 2006, 311, 832-835.	12.6	988
69	Multiple Time Scales in Solvation Dynamics of DNA in Aqueous Solution:Â The Role of Water, Counterions, and Cross-Correlations. Journal of Physical Chemistry B, 2006, 110, 26396-26402.	2.6	92
70	Coupling between Protein and Reaction Dynamics in Enzymatic Processes:Â Application of Groteâ^'Hynes Theory to CatecholO-Methyltransferase. Journal of the American Chemical Society, 2006, 128, 6186-6193.	13.7	57
71	Excited-State Charge Transfer at a Conical Intersection:â€‰ Effects of an Environment. Journal of Physical Chemistry A, 2006, 110, 11411-11423.	2.5	82
72	On the Ultrafast Infrared Spectroscopy of Anion Hydration Shell Hydrogen Bond Dynamics. Journal of Physical Chemistry A, 2006, 110, 11237-11243.	2.5	63

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73	Entropy of Water in the Hydration Layer of Major and Minor Grooves of DNA. Journal of Physical Chemistry B, 2006, 110, 19611-19618.	2.6	85
74	Do more strongly hydrogen-bonded water molecules reorient more slowly ?. Chemical Physics Letters, 2006, 433, 80-85.	2.6	115
75	Conical intersections in solution: non-equilibrium versus equilibrium solvation. Molecular Physics, 2006, 104, 903-914.	1.7	40
76	A theoretical study of the H2SO4+H2O â†' HSO4 â^'+H3O+ reaction at the surface of aqueous aerosols. Theoretical Chemistry Accounts, 2004, 111, 182-187.	1.4	28
77	Environmental effects on a conical intersection: A model study. Faraday Discussions, 2004, 127, 395.	3.2	85
78	Kinetic Isotope Effects for Nonadiabatic Proton Transfer Reactions in a Polar Environment. 2. Comparison with an Electronically Diabatic Description. Journal of Physical Chemistry A, 2004, 108, 11809-11818.	2.5	51
79	Ultrafast Vibrational Population Dynamics of Water and Related Systems:Â A Theoretical Perspective. Chemical Reviews, 2004, 104, 1915-1928.	47.7	163
80	Temperature-Dependent Solvent Polarity Effects on Adiabatic Proton Transfer Rate Constants and Kinetic Isotope Effects. Israel Journal of Chemistry, 2004, 44, 171-184.	2.3	15
81	Hydrogen Bond Dynamics in Water and Ultrafast Infrared Spectroscopy:â€‰ A Theoretical Study. Journal of Physical Chemistry A, 2004, 108, 1275-1289.	2.5	252
82	Kinetic Isotope Effects for Nonadiabatic Proton Transfer Reactions in a Polar Environment. 1. Interpretation of Tunneling Kinetic Isotopic Effects. Journal of Physical Chemistry A, 2004, 108, 11793-11808.	2.5	115
83	On the Dissociation of Aromatic Radical Anions in Solution. 1. Formulation and Application top-Cyanochlorobenzene Radical Anion. Journal of Physical Chemistry A, 2003, 107, 11271-11291.	2.5	40
84	Rate and Mechanisms for Water Exchange around Li+(aq) from MD Simulations. Journal of Physical Chemistry B, 2003, 107, 4470-4477.	2.6	70
85	Charged Pushâ^'Pull Polyenes in Solution:â€‰ Anomalous Solvatochromism and Nonlinear Optical Properties. Journal of Physical Chemistry A, 2003, 107, 6032-6046.	2.5	63
86	Kinetic Isotope Effects for Adiabatic Proton Transfer Reactions in a Polar Environment. Journal of Physical Chemistry A, 2003, 107, 9022-9039.	2.5	63
87	On the Dissociation of Aromatic Radical Anions in Solution. 2. Reaction Path and Rate Constant Analysis. Journal of Physical Chemistry A, 2003, 107, 11292-11306.	2.5	40
88	Adsorption of HF and HCl molecules on ice at 190 and 235 K from molecular dynamics simulations: Free energy profiles and residence times. Journal of Chemical Physics, 2003, 118, 9814-9823.	3.0	24
89	Nonlinear Free Energy Relations for Adiabatic Proton Transfer Reactions in a Polar Environment. II. Inclusion of the Hydrogen Bond Vibration. Journal of Physical Chemistry A, 2002, 106, 1850-1861.	2.5	78
90	Nonlinear Free Energy Relations for Adiabatic Proton Transfer Reactions in a Polar Environment. I. Fixed Proton Donorâ^'Acceptor Separation. Journal of Physical Chemistry A, 2002, 106, 1834-1849.	2.5	106

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91	A Theoretical Analysis of the Sum Frequency Generation Spectrum of the Water Surface. II. Time-Dependent Approach. Journal of Physical Chemistry B, 2002, 106, 673-685.	2.6	251
92	Hydrogen Bond Dynamics in Water and Ultrafast Infrared Spectroscopy. Journal of Physical Chemistry A, 2002, 106, 11993-11996.	2.5	325
93	Intermolecular photochemical proton transfer in solution: new insights and perspectives. Journal of Photochemistry and Photobiology A: Chemistry, 2002, 154, 3-11.	3.9	113
94	Crossing the Transition State in Solution. , 2002, , 231-258.		6
95	A theoretical analysis of the sum frequency generation spectrum of the water surface. Chemical Physics, 2000, 258, 371-390.	1.9	340
96	A Theoretical Investigation of Excited-State Acidity of Phenol and Cyanophenols. Journal of the American Chemical Society, 2000, 122, 12243-12253.	13.7	145
97	Frequency Shifts in the Hydrogen-Bonded OH Stretch in Halideâ^'Water Clusters. The Importance of Charge Transfer. Journal of the American Chemical Society, 2000, 122, 6278-6286.	13.7	150
98	Molecular Mechanism of HF Acid Ionization in Water:Â An Electronic Structureâ^'Monte Carlo Study. Journal of Physical Chemistry A, 1999, 103, 10398-10408.	2.5	111
99	The protean proton in water. Nature, 1999, 397, 565-567.	27.8	94
100	Theoretical studies of heterogeneous reaction mechanisms relevant for stratospheric ozone depletion. International Journal of Quantum Chemistry, 1999, 75, 683-692.	2.0	20
101	A Theoretical Study of the Reaction of ClONO2 with HCl on Ice. Journal of Physical Chemistry A, 1999, 103, 3797-3801.	2.5	63
102	Acid Ionization of HBr in a Small Water Cluster. Israel Journal of Chemistry, 1999, 39, 273-281.	2.3	37
103	Ab Initio Model Study of the Mechanism of Chlorine Nitrate Hydrolysis on Ice. Journal of Physical Chemistry A, 1998, 102, 309-314.	2.5	73
104	Ab Initio Study of Nitromethane Deprotonation by (OH)-Â·nH2O Clusters. Journal of Physical Chemistry A, 1998, 102, 3977-3984.	2.5	14
105	Two Valence Bond State Model for Molecular Nonlinear Optical Properties. Nonequilibrium Solvation Formulation. Journal of Physical Chemistry A, 1998, 102, 7712-7722.	2.5	58
106	Model molecular dynamics simulation of hydrochloric acid ionization at the surface of stratospheric ice. Faraday Discussions, 1998, 110, 301-322.	3.2	102
107	Vibrational phase and energy relaxation of CNâ^' in water. Journal of Chemical Physics, 1998, 108, 142-153.	3.0	173
108	On the photodissociation of alkali-metal halides in solution. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 977-988.	1.7	52

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109	Molecular Mechanism of HCl Acid Ionization in Water:â€‰ Ab Initio Potential Energy Surfaces and Monte Carlo Simulations. Journal of Physical Chemistry B, 1997, 101, 10464-10478.	2.6	299
110	Excited state intramolecular charge transfer rates of p-dirnethylaminobenzonitrile (DMABN) in solution: a two-dimensional dynamics perspective. Journal of Photochemistry and Photobiology A: Chemistry, 1997, 105, 337-343.	3.9	51
111	Adiabatic acid-base proton transfer in solution. AIP Conference Proceedings, 1996, , .	0.4	2
112	Vibrational energy relaxation of HOD in liquid D2O. Journal of Chemical Physics, 1996, 104, 2356-2368.	3.0	248
113	Curve Crossing Formulation for Proton Transfer Reactions in Solution. The Journal of Physical Chemistry, 1996, 100, 1118-1128.	2.9	246
114	Hydration Shell Exchange Kinetics:Â An MD Study for Na+(aq). The Journal of Physical Chemistry, 1996, 100, 5611-5615.	2.9	66
115	Hydration shell exchange dynamics for in water. Journal of Physics Condensed Matter, 1996, 8, 9411-9416.	1.8	17
116	HCl acid ionization in water: A theoretical molecular modeling. Journal of Molecular Liquids, 1995, 64, 25-37.	4.9	142
117	VB resonance theory in solution. I. Multistate formulation. Journal of Chemical Physics, 1995, 102, 7864-7884.	3.0	40
118	VB resonance theory in solution. II. I2â^'â–I+Iâ^' in acetonitrile. Journal of Chemical Physics, 1995, 102, 7885-7901.	3.0	28
119	Nonequilibrium Free Energy Functions, Recombination Dynamics, and Vibrational Relaxation of I2- in Acetonitrile: Molecular Dynamics of Charge Flow in the Electronically Adiabatic Limit. The Journal of Physical Chemistry, 1995, 99, 7557-7567.	2.9	90
120	Proton transfer in hydrogenâ€bonded acidâ€“base complexes in polar solvents. Journal of Chemical Physics, 1995, 102, 2487-2505.	3.0	202
121	Ultrafast vibrational predissociation and relaxation in hydrogen-bonded systems. AIP Conference Proceedings, 1994, , .	0.4	0
122	Ionization of Acids in Water. ACS Symposium Series, 1994, , 143-153.	0.5	11
123	Twisted intramolecular charge transfer dynamics in polar solvents. Journal of Photochemistry and Photobiology A: Chemistry, 1994, 82, 67-79.	3.9	39
124	Bihalide ion combination reactions in solution: electronic structure and solvation aspects. Chemical Physics, 1994, 183, 309-323.	1.9	38
125	Wet chemistry. Nature, 1994, 369, 439-440.	27.8	14
126	Charge Transfer Reactions and Solvation Dynamics. , 1994, , 345-381.		54

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127	Vibrational predissociation in hydrogen-bonded OHâ€¦O complexes via OH stretch-OO stretch energy transfer. Chemical Physics Letters, 1993, 204, 197-205.	2.6	104
128	Vibrational relaxation times for a model hydrogen-bonded complex in a polar solvent. Chemical Physics, 1993, 175, 205-221.	1.9	58
129	Well and barrier dynamics and electron transfer rates. A molecular dynamics study. Chemical Physics, 1993, 176, 521-537.	1.9	65
130	Dynamical theory of proton tunneling transfer rates in solution: general formulation. Chemical Physics, 1993, 170, 315-346.	1.9	228
131	Electronic friction and electron transfer rates at metallic electrodes. Journal of Chemical Physics, 1993, 99, 6517-6530.	3.0	80
132	Dielectric friction and solvation dynamics: a molecular dynamics study. The Journal of Physical Chemistry, 1992, 96, 4068-4074.	2.9	48
133	Vibrational relaxation of a dipolar molecule in water. Journal of Chemical Physics, 1992, 96, 5354-5369.	3.0	202
134	A theoretical model for SN1 ionic dissociation in solution. 1. Activation free energetics and transition-state structure. Journal of the American Chemical Society, 1992, 114, 10508-10528.	13.7	117
135	Equilibrium and nonequilibrium solvation and solute electronic structure. III. Quantum theory. Journal of Chemical Physics, 1992, 96, 5088-5110.	3.0	166
136	Molecularâ€dynamics simulation for a model nonadiabatic proton transfer reaction in solution. Journal of Chemical Physics, 1991, 94, 3619-3628.	3.0	323
137	Activation to the transition state: reactant and solvent energy flow for a model SN2 reaction in water. Journal of the American Chemical Society, 1991, 113, 74-87.	13.7	149
138	Direct and indirect solvent coupling vibrational dephasing mechanisms in hydrogen-bonded molecules. The Journal of Physical Chemistry, 1991, 95, 4651-4659.	2.9	18
139	Nonequilibrium free energy surfaces for hydrogen-bonded proton-transfer complexes in solution. The Journal of Physical Chemistry, 1991, 95, 10431-10442.	2.9	105
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141	Solvation dynamics for an ion pair in a polar solvent: Timeâ€dependent fluorescence and photochemical charge transfer. Journal of Chemical Physics, 1991, 94, 5961-5979.	3.0	396
142	Molecular dynamics of a modelSN1 reaction in water. Journal of Chemical Physics, 1991, 95, 5256-5267.	3.0	103
143	Fast vibrational relaxation for a dipolar molecule in a polar solvent. The Journal of Physical Chemistry, 1990, 94, 8625-8628.	2.9	147
144	Equilibrium and nonequilibrium solvation and solute electronic structure. I. Formulation. Journal of Chemical Physics, 1990, 93, 5194-5210.	3.0	154

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146	Equilibrium and nonequilibrium solvation and solute electronic structure. International Journal of Quantum Chemistry, 1990, 38, 821-833.	2.0	20
147	Dynamics of ion pair interconversion in a polar solvent. Journal of Chemical Physics, 1990, 93, 7137-7147.	3.0	179
148	Environmental Dynamics and Electron Transfer Reactions. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1990, , 133-148.	0.2	3
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150	Nonequilibrium solvation effects on reaction rates for model SN2 reactions in water. Journal of Chemical Physics, 1989, 90, 3537-3558.	3.0	289
151	A dynamical theory of nonadiabatic proton and hydrogen atom transfer reaction rates in solution. Chemical Physics Letters, 1989, 162, 19-26.	2.6	223
152	Constrained reaction coordinate dynamics for the simulation of rare events. Chemical Physics Letters, 1989, 156, 472-477.	2.6	840
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154	A stochastic theory of chemical reaction rates. II. Applications. Journal of Statistical Physics, 1989, 56, 895-910.	1.2	11
155	Molecular dynamics simulation of electron-transfer reactions in solution. The Journal of Physical Chemistry, 1989, 93, 6261-6265.	2.9	138
156	Solute-dependent solvent force constants for ion pairs and neutral pairs in a polar solvent. The Journal of Physical Chemistry, 1989, 93, 2184-2187.	2.9	188
157	Solution reaction path Hamiltonian for reactions in polar solvents. I. Formulation. Journal of Chemical Physics, 1988, 88, 6853-6862.	3.0	156
158	A dynamical theory of unimolecular ionic dissociation reactions in polar solvents. Journal of Chemical Physics, 1988, 88, 2513-2525.	3.0	49
159	Solution reaction path Hamiltonian for reactions in polar solvents. II. Applications. Journal of Chemical Physics, 1988, 88, 6863-6869.	3.0	66
160	Nonadiabatic solvation model for SN2 reactions in polar solvents. Journal of Chemical Physics, 1987, 86, 1377-1386.	3.0	166
161	Molecular dynamics of a modelSN2 reaction in water. Journal of Chemical Physics, 1987, 86, 1356-1376.	3.0	277
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164	Chemical reaction rates and solvent friction. Journal of Statistical Physics, 1986, 42, 149-168.	1.2	91
165	Probability oscillations in single pass curve crossings: Semiclassical predictions of nonmonotonic dependence on crossing velocity. Journal of Chemical Physics, 1986, 84, 1554-1564.	3.0	6
166	Classical dynamics of intramolecular energy flow and overtoneâ€induced dissociation in HO2H and HO2D. Journal of Chemical Physics, 1986, 85, 5791-5804.	3.0	99
167	Time-dependent fluorescence solvent shifts, dielectric friction, and nonequilibrium solvation in polar solvents. The Journal of Physical Chemistry, 1985, 89, 4181-4188.	2.9	522
168	Intramolecular vibrational relaxation and spectra of CH and CD overtones in benzene and perdeuterobenzene. Journal of Chemical Physics, 1984, 81, 1115-1134.	3.0	330
169	Classical dynamics of highly excited CH and CD overtones in benzene and perdeuterobenzene. Journal of Chemical Physics, 1984, 81, 1135-1144.	3.0	170
170	A simple dipole isomerization model for non-equilibrium solvation dynamics in reactions in polar solvents. Chemical Physics, 1984, 90, 21-35.	1.9	91
171	Quantum dynamics of energy transfer between bonds in coupled Morse oscillator systems. Journal of Chemical Physics, 1984, 81, 1314-1326.	3.0	63
172	Nonequilibrium solvation dynamics in solution reactions. Journal of Chemical Physics, 1983, 78, 4174-4185.	3.0	241
173	Nonlinear resonances and vibrational energy flow in model hydrocarbon chains. Journal of Chemical Physics, 1983, 79, 4247-4260.	3.0	122
174	Slow vibrational relaxation in picosecond iodine recombination in liquids. Journal of Chemical Physics, 1982, 77, 2130-2143.	3.0	154
175	Hydrodynamic interaction effects on isomerization rates in chain molecules. Journal of Chemical Physics, 1982, 77, 4739-4746.	3.0	8
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178	Dynamical polar solvent effects on solution reactions: A simple continuum model. Journal of Chemical Physics, 1982, 76, 2993-3001.	3.0	224
179	Classical dynamics of energy transfer between bonds in ABA triatomics. Journal of Chemical Physics, 1982, 77, 3583-3594.	3.0	202
180	Quantum mechanics of local mode ABA triatomic molecules. Journal of Chemical Physics, 1982, 77, 3595-3604.	3.0	143

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