# James T Hynes

## List of Publications by Citations



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|---|---|---|---|
| 246 papers | 19,950 citations | 79 h-index | 138 g-index |
| 264 ext. papers | 20,930 ext. citations | 6.3 avg, IF | 6.95 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 246 | The stable states picture of chemical reactions. II. Rate constants for condensed and gas phase reaction models. *Journal of Chemical Physics*, **1980**, 73, 2715-2732 | 3.9 | 1122 |
| 245 | A molecular jump mechanism of water reorientation. *Science*, **2006**, 311, 832-5 | 33.3 | 866 |
| 244 | Constrained reaction coordinate dynamics for the simulation of rare events. *Chemical Physics Letters*, **1989**, 156, 472-477 | 2.5 | 726 |
| 243 | Time-dependent fluorescence solvent shifts, dielectric friction, and nonequilibrium solvation in polar solvents. *The Journal of Physical Chemistry*, **1985**, 89, 4181-4188 | | 496 |
| 242 | Outer-sphere electron-transfer reactions and frequency-dependent friction. *The Journal of Physical Chemistry*, **1986**, 90, 3701-3706 | | 432 |
| 241 | Water Dynamics in the Hydration Shells of Biomolecules. *Chemical Reviews*, **2017**, 117, 10694-10725 | 68.1 | 410 |
| 240 | Solvation dynamics for an ion pair in a polar solvent: Time-dependent fluorescence and photochemical charge transfer. *Journal of Chemical Physics*, **1991**, 94, 5961-5979 | 3.9 | 379 |
| 239 | On the molecular mechanism of water reorientation. *Journal of Physical Chemistry B*, **2008**, 112, 14230-42 | 3.4 | 335 |
| 238 | Intramolecular vibrational relaxation and spectra of CH and CD overtones in benzene and perdeuterobenzene. *Journal of Chemical Physics*, **1984**, 81, 1115-1134 | 3.9 | 315 |
| 237 | Why water reorientation slows without iceberg formation around hydrophobic solutes. *Journal of Physical Chemistry B*, **2009**, 113, 2428-35 | 3.4 | 310 |
| 236 | A theoretical analysis of the sum frequency generation spectrum of the water surface. *Chemical Physics*, **2000**, 258, 371-390 | 2.3 | 310 |
| 235 | Hydrogen Bond Dynamics in Water and Ultrafast Infrared Spectroscopy. *Journal of Physical Chemistry A*, **2002**, 106, 11993-11996 | 2.8 | 309 |
| 234 | Molecular-dynamics simulation for a model nonadiabatic proton transfer reaction in solution. *Journal of Chemical Physics*, **1991**, 94, 3619-3628 | 3.9 | 299 |
| 233 | Molecular Mechanism of HCl Acid Ionization in Water: Ab Initio Potential Energy Surfaces and Monte Carlo Simulations. *Journal of Physical Chemistry B*, **1997**, 101, 10464-10478 | 3.4 | 283 |
| 232 | Reorientation and allied dynamics in water and aqueous solutions. *Annual Review of Physical Chemistry*, **2011**, 62, 395-416 | 15.7 | 268 |
| 231 | Nonequilibrium solvation effects on reaction rates for model SN2 reactions in water. *Journal of Chemical Physics*, **1989**, 90, 3537-3558 | 3.9 | 268 |
| 230 | Molecular dynamics of a model SN2 reaction in water. *Journal of Chemical Physics*, **1987**, 86, 1356-1376 | 3.9 | 258 |

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| 229 | Reorientional dynamics of water molecules in anionic hydration shells. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 11167-72 | 11.5 | 255 |
| 228 | Hydrogen Bond Dynamics in Water and Ultrafast Infrared Spectroscopy: A Theoretical Study. *Journal of Physical Chemistry A*, **2004**, 108, 1275-1289 | 2.8 | 236 |
| 227 | Vibrational energy relaxation of HOD in liquid D2O. *Journal of Chemical Physics*, **1996**, 104, 2356-2368 | 3.9 | 233 |
| 226 | Nonequilibrium solvation dynamics in solution reactions. *Journal of Chemical Physics*, **1983**, 78, 4174-4185 | 3.9 | 233 |
| 225 | Reactive modes in condensed phase reactions. *Journal of Chemical Physics*, **1981**, 74, 4465-4475 | 3.9 | 233 |
| 224 | Curve Crossing Formulation for Proton Transfer Reactions in Solution. *The Journal of Physical Chemistry*, **1996**, 100, 1118-1128 | | 232 |
| 223 | 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 | 3.4 | 223 |
| 222 | The stable states picture of chemical reactions. I. Formulation for rate constants and initial condition effects. *Journal of Chemical Physics*, **1980**, 73, 2700-2714 | 3.9 | 213 |
| 221 | Dynamical polar solvent effects on solution reactions: A simple continuum model. *Journal of Chemical Physics*, **1982**, 76, 2993-3001 | 3.9 | 213 |
| 220 | Dynamical theory of proton tunneling transfer rates in solution: general formulation. *Chemical Physics*, **1993**, 170, 315-346 | 2.3 | 211 |
| 219 | A dynamical theory of nonadiabatic proton and hydrogen atom transfer reaction rates in solution. *Chemical Physics Letters*, **1989**, 162, 19-26 | 2.5 | 207 |
| 218 | Classical dynamics of energy transfer between bonds in ABA triatomics. *Journal of Chemical Physics*, **1982**, 77, 3583-3594 | 3.9 | 195 |
| 217 | Vibrational relaxation of a dipolar molecule in water. *Journal of Chemical Physics*, **1992**, 96, 5354-5369 | 3.9 | 191 |
| 216 | Proton transfer in hydrogen-bonded acid□base complexes in polar solvents. *Journal of Chemical Physics*, **1995**, 102, 2487-2505 | 3.9 | 188 |
| 215 | Solute-dependent solvent force constants for ion pairs and neutral pairs in a polar solvent. *The Journal of Physical Chemistry*, **1989**, 93, 2184-2187 | | 177 |
| 214 | Vibrational phase and energy relaxation of CN□n water. *Journal of Chemical Physics*, **1998**, 108, 142-153 | 3.9 | 171 |
| 213 | Dynamics of ion pair interconversion in a polar solvent. *Journal of Chemical Physics*, **1990**, 93, 7137-7147 | 3.9 | 166 |
| 212 | Equilibrium and nonequilibrium solvation and solute electronic structure. III. Quantum theory. *Journal of Chemical Physics*, **1992**, 96, 5088-5110 | 3.9 | 162 |

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| 211 | Classical dynamics of highly excited CH and CD overtones in benzene and perdeuterobenzene. *Journal of Chemical Physics*, **1984**, 81, 1135-1144 | 3.9 | 160 |
| 210 | Nonadiabatic solvation model for SN2 reactions in polar solvents. *Journal of Chemical Physics*, **1987**, 86, 1377-1386 | 3.9 | 158 |
| 209 | Ultrafast vibrational population dynamics of water and related systems: a theoretical perspective. *Chemical Reviews*, **2004**, 104, 1915-28 | 68.1 | 152 |
| 208 | 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, 9747-55 | 16.4 | 151 |
| 207 | Solution reaction path Hamiltonian for reactions in polar solvents. I. Formulation. *Journal of Chemical Physics*, **1988**, 88, 6853-6862 | 3.9 | 146 |
| 206 | Equilibrium and nonequilibrium solvation and solute electronic structure. I. Formulation. *Journal of Chemical Physics*, **1990**, 93, 5194-5210 | 3.9 | 145 |
| 205 | Frequency Shifts in the Hydrogen-Bonded OH Stretch in Halide□Water Clusters. The Importance of Charge Transfer. *Journal of the American Chemical Society*, **2000**, 122, 6278-6286 | 16.4 | 144 |
| 204 | Short range caging effects for reactions in solution. I. Reaction rate constants and short range caging picture. *Journal of Chemical Physics*, **1979**, 71, 871-883 | 3.9 | 143 |
| 203 | Slow vibrational relaxation in picosecond iodine recombination in liquids. *Journal of Chemical Physics*, **1982**, 77, 2130-2143 | 3.9 | 143 |
| 202 | Fast vibrational relaxation for a dipolar molecule in a polar solvent. *The Journal of Physical Chemistry*, **1990**, 94, 8625-8628 | | 137 |
| 201 | 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 | 16.4 | 137 |
| 200 | On the residence time for water in a solute hydration shell: application to aqueous halide solutions. *Journal of Physical Chemistry B*, **2008**, 112, 7697-701 | 3.4 | 131 |
| 199 | Quantum mechanics of local mode ABA triatomic molecules. *Journal of Chemical Physics*, **1982**, 77, 3595-3604 | 3.9 | 128 |
| 198 | HCl acid ionization in water: A theoretical molecular modeling. *Journal of Molecular Liquids*, **1995**, 64, 25-37 | 6 | 127 |
| 197 | Molecular dynamics of the A+BC reaction in rare gas solution. *Journal of Chemical Physics*, **1986**, 85, 5625-5643 | 3.9 | 126 |
| 196 | Molecular dynamics simulation of electron-transfer reactions in solution. *The Journal of Physical Chemistry*, **1989**, 93, 6261-6265 | | 125 |
| 195 | Energy diffusion-controlled reactions in solution. *Journal of Chemical Physics*, **1982**, 77, 3736-3743 | 3.9 | 123 |
| 194 | A Theoretical Investigation of Excited-State Acidity of Phenol and Cyanophenols. *Journal of the American Chemical Society*, **2000**, 122, 12243-12253 | 16.4 | 122 |

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| 193 | Nonlinear resonances and vibrational energy flow in model hydrocarbon chains. *Journal of Chemical Physics*, **1983**, 79, 4247-4260 | 3.9 | 119 |
| 192 | Reduction of CO2 to methanol catalyzed by a biomimetic organo-hydride produced from pyridine. *Journal of the American Chemical Society*, **2014**, 136, 16081-95 | 16.4 | 113 |
| 191 | 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 | 16.4 | 108 |
| 190 | Do more strongly hydrogen-bonded water molecules reorient more slowly ?. *Chemical Physics Letters*, **2006**, 433, 80-85 | 2.5 | 106 |
| 189 | Intermolecular photochemical proton transfer in solution: new insights and perspectives. *Journal of Photochemistry and Photobiology A: Chemistry*, **2002**, 154, 3-11 | 4.7 | 102 |
| 188 | Water hydrogen-bond dynamics around amino acids: the key role of hydrophilic hydrogen-bond acceptor groups. *Journal of Physical Chemistry B*, **2010**, 114, 2083-9 | 3.4 | 100 |
| 187 | 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 | 2.8 | 100 |
| 186 | Molecular Mechanism of HF Acid Ionization in Water: An Electronic Structure Monte Carlo Study. *Journal of Physical Chemistry A*, **1999**, 103, 10398-10408 | 2.8 | 100 |
| 185 | Vibrational predissociation in hydrogen-bonded OHO complexes via OH stretch-OO stretch energy transfer. *Chemical Physics Letters*, **1993**, 204, 197-205 | 2.5 | 99 |
| 184 | Water hydrogen bond dynamics in aqueous solutions of amphiphiles. *Journal of Physical Chemistry B*, **2010**, 114, 3052-9 | 3.4 | 97 |
| 183 | Model molecular dynamics simulation of hydrochloric acid ionization at the surface of stratospheric ice. *Faraday Discussions*, **1998**, 110, 301-322 | 3.6 | 96 |
| 182 | Nonlinear Free Energy Relations for Adiabatic Proton Transfer Reactions in a Polar Environment. I. Fixed Proton Donor Acceptor Separation. *Journal of Physical Chemistry A*, **2002**, 106, 1834-1849 | 2.8 | 95 |
| 181 | Molecular dynamics of a model SN1 reaction in water. *Journal of Chemical Physics*, **1991**, 95, 5256-5267 | 3.9 | 95 |
| 180 | Nonequilibrium free energy surfaces for hydrogen-bonded proton-transfer complexes in solution. *The Journal of Physical Chemistry*, **1991**, 95, 10431-10442 | | 94 |
| 179 | Water reorientation, hydrogen-bond dynamics and 2D-IR spectroscopy next to an extended hydrophobic surface. *Faraday Discussions*, **2010**, 146, 263-81; discussion 283-98, 395-401 | 3.6 | 93 |
| 178 | Classical dynamics of intramolecular energy flow and overtone-induced dissociation in HO2H and HO2D. *Journal of Chemical Physics*, **1986**, 85, 5791-5804 | 3.9 | 93 |
| 177 | A simple dipole isomerization model for non-equilibrium solvation dynamics in reactions in polar solvents. *Chemical Physics*, **1984**, 90, 21-35 | 2.3 | 88 |
| 176 | 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 | | 85 |

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| 175 | Water jump reorientation: from theoretical prediction to experimental observation. *Accounts of Chemical Research*, **2012**, 45, 53-62 | 24.3 | 82 |
| 174 | Multiple time scales in solvation dynamics of DNA in aqueous solution: the role of water, counterions, and cross-correlations. *Journal of Physical Chemistry B*, **2006**, 110, 26396-402 | 3.4 | 82 |
| 173 | Chemical reaction rates and solvent friction. *Journal of Statistical Physics*, **1986**, 42, 149-168 | 1.5 | 82 |
| 172 | Stochastic trajectory simulation of iodine recombination in liquids. *Journal of Chemical Physics*, **1980**, 72, 177-188 | 3.9 | 82 |
| 171 | Biomolecular hydration dynamics: a jump model perspective. *Chemical Society Reviews*, **2013**, 42, 5672-83 | 38.5 | 81 |
| 170 | Dynamical Disorder in the DNA Hydration Shell. *Journal of the American Chemical Society*, **2016**, 138, 7610-20 | 16.4 | 80 |
| 169 | Environmental effects on a conical intersection: a model study. *Faraday Discussions*, **2004**, 127, 395-411 | 3.6 | 80 |
| 168 | Vibrational energy transfer from highly excited anharmonic oscillators. Dependence on quantum state and interaction potential. *Journal of Chemical Physics*, **1982**, 76, 6002-6014 | 3.9 | 78 |
| 167 | Excited-state charge transfer at a conical intersection: effects of an environment. *Journal of Physical Chemistry A*, **2006**, 110, 11411-23 | 2.8 | 77 |
| 166 | Saddle point model for atom transfer reactions in solution. *Journal of Chemical Physics*, **1981**, 75, 2191-2198 | 3.9 | 75 |
| 165 | Entropy of water in the hydration layer of major and minor grooves of DNA. *Journal of Physical Chemistry B*, **2006**, 110, 19611-8 | 3.4 | 71 |
| 164 | Electronic friction and electron transfer rates at metallic electrodes. *Journal of Chemical Physics*, **1993**, 99, 6517-6530 | 3.9 | 71 |
| 163 | Chemical reaction rates and solvation dynamics in electrolyte solutions: ion atmosphere friction. *Chemical Physics*, **1991**, 152, 169-183 | 2.3 | 70 |
| 162 | Multistep drug intercalation: molecular dynamics and free energy studies of the binding of daunomycin to DNA. *Journal of the American Chemical Society*, **2012**, 134, 8588-96 | 16.4 | 69 |
| 161 | Rate and Mechanisms for Water Exchange around Li+(aq) from MD Simulations. *Journal of Physical Chemistry B*, **2003**, 107, 4470-4477 | 3.4 | 69 |
| 160 | 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 | 2.8 | 69 |
| 159 | Pathways for H2O bend vibrational relaxation in liquid water. *Journal of Physical Chemistry A*, **2009**, 113, 8949-62 | 2.8 | 67 |
| 158 | Equilibrium and nonequilibrium solvation and solute electronic structure. II. Strong coupling limit. *Journal of Chemical Physics*, **1990**, 93, 5211-5223 | 3.9 | 66 |

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| 157 | Ab Initio Model Study of the Mechanism of Chlorine Nitrate Hydrolysis on Ice. *Journal of Physical Chemistry A*, **1998**, 102, 309-314 | 2.8 | 65 |
| 156 | Reactive dynamics for diffusive barrier crossing. *Journal of Chemical Physics*, **1978**, 69, 5246-5260 | 3.9 | 64 |
| 155 | Hydration Shell Exchange Kinetics: An MD Study for Na+(aq). *The Journal of Physical Chemistry*, **1996**, 100, 5611-5615 | | 63 |
| 154 | Well and barrier dynamics and electron transfer rates. A molecular dynamics study. *Chemical Physics*, **1993**, 176, 521-537 | 2.3 | 62 |
| 153 | Quantum dynamics of energy transfer between bonds in coupled Morse oscillator systems. *Journal of Chemical Physics*, **1984**, 81, 1314-1326 | 3.9 | 61 |
| 152 | On the ultrafast infrared spectroscopy of anion hydration shell hydrogen bond dynamics. *Journal of Physical Chemistry A*, **2006**, 110, 11237-43 | 2.8 | 60 |
| 151 | Kinetic Isotope Effects for Adiabatic Proton Transfer Reactions in a Polar Environment. *Journal of Physical Chemistry A*, **2003**, 107, 9022-9039 | 2.8 | 60 |
| 150 | Microscopic boundary layer effects and rough sphere rotation. *Journal of Chemical Physics*, **1977**, 67, 3256-3267 | 3.9 | 58 |
| 149 | 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, 7477-88 | 16.4 | 57 |
| 148 | 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 | 3.8 | 57 |
| 147 | Vibrational relaxation times for a model hydrogen-bonded complex in a polar solvent. *Chemical Physics*, **1993**, 175, 205-221 | 2.3 | 56 |
| 146 | Roles of the Lewis acid and base in the chemical reduction of CO2 catalyzed by frustrated Lewis pairs. *Inorganic Chemistry*, **2013**, 52, 10062-6 | 5.1 | 55 |
| 145 | A Theoretical Study of the Reaction of ClONO2 with HCl on Ice. *Journal of Physical Chemistry A*, **1999**, 103, 3797-3801 | 2.8 | 55 |
| 144 | Solution reaction path Hamiltonian for reactions in polar solvents. II. Applications. *Journal of Chemical Physics*, **1988**, 88, 6863-6869 | 3.9 | 54 |
| 143 | Coupling between protein and reaction dynamics in enzymatic processes: application of Grote-Hynes Theory to catechol O-methyltransferase. *Journal of the American Chemical Society*, **2006**, 128, 6186-93 | 16.4 | 53 |
| 142 | Non-adiabatic dynamics close to conical intersections and the surface hopping perspective. *Frontiers in Chemistry*, **2014**, 2, 97 | 5 | 52 |
| 141 | Charged PushPull Polyenes in Solution: Anomalous Solvatochromism and Nonlinear Optical Properties. *Journal of Physical Chemistry A*, **2003**, 107, 6032-6046 | 2.8 | 52 |
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| 139 | Reactive paths in the diffusion limit. *Journal of Chemical Physics*, **1982**, 77, 1295-1301 | 3.9 | 52 |
| 138 | Catalytic Reduction of CO2 by Renewable Organohydrides. *Journal of Physical Chemistry Letters*, **2015**, 6, 5078-92 | 6.4 | 51 |
| 137 | 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, 19911-7 | 3.6 | 51 |
| 136 | Depth-dependent dissociation of nitric acid at an aqueous surface: Car-Parrinello molecular dynamics. *Journal of Physical Chemistry A*, **2009**, 113, 1295-307 | 2.8 | 51 |
| 135 | Ultrafast energy transfer from the intramolecular bending vibration to librations in liquid water. *Journal of Physical Chemistry A*, **2009**, 113, 6657-65 | 2.8 | 50 |
| 134 | Water reorientation dynamics in the first hydration shells of F- and I-. *Physical Chemistry Chemical Physics*, **2011**, 13, 19895-901 | 3.6 | 49 |
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| 132 | 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 | 2.8 | 47 |
| 131 | A dynamical theory of unimolecular ionic dissociation reactions in polar solvents. *Journal of Chemical Physics*, **1988**, 88, 2513-2525 | 3.9 | 47 |
| 130 | Coupling of translational and reactive dynamics for a Fokker□Planck model. *Journal of Chemical Physics*, **1978**, 68, 3203-3216 | 3.9 | 47 |
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| 128 | Charge Transfer Reactions and Solvation Dynamics **1994**, 345-381 | | 46 |
| 127 | Theoretical aspects of tunneling proton transfer reactions in a polar environment. *Journal of Physical Organic Chemistry*, **2010**, 23, 632-646 | 2.1 | 45 |
| 126 | Dielectric friction and solvation dynamics: a molecular dynamics study. *The Journal of Physical Chemistry*, **1992**, 96, 4068-4074 | | 45 |
| 125 | Theoretical study of O--O single bond formation in the oxidation of water by the ruthenium blue dimer. *Journal of Physical Chemistry A*, **2011**, 115, 8003-16 | 2.8 | 43 |
| 124 | Dynamical friction effects on the photoisomerization of a model protonated Schiff base in solution. *Journal of Physical Chemistry A*, **2011**, 115, 3720-35 | 2.8 | 42 |
| 123 | Theoretical study of the dissociation of nitric acid at a model aqueous surface. *Journal of Physical Chemistry A*, **2007**, 111, 11033-42 | 2.8 | 42 |
| 122 | Nuclear Quantum Effects in Water Reorientation and Hydrogen-Bond Dynamics. *Journal of Physical Chemistry Letters*, **2017**, 8, 2602-2607 | 6.4 | 40 |

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| 121 | Conical intersections in solution: non-equilibrium versus equilibrium solvation. *Molecular Physics*, **2006**, 104, 903-914 | 1.7 | 40 |
| 120 | Benzimidazoles as Metal-Free and Recyclable Hydrides for CO Reduction to Formate. *Journal of the American Chemical Society*, **2019**, 141, 272-280 | 16.4 | 40 |
| 119 | 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 | 2.8 | 38 |
| 118 | Twisted intramolecular charge transfer dynamics in polar solvents. *Journal of Photochemistry and Photobiology A: Chemistry*, **1994**, 82, 67-79 | 4.7 | 37 |
| 117 | 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 | 2.8 | 35 |
| 116 | VB resonance theory in solution. I. Multistate formulation. *Journal of Chemical Physics*, **1995**, 102, 7864-7884 | 3.9 | 35 |
| 115 | How Acidic Is Carbonic Acid?. *Journal of Physical Chemistry B*, **2016**, 120, 2440-51 | 3.4 | 34 |
| 114 | Acid Ionization of HBr in a Small Water Cluster. *Israel Journal of Chemistry*, **1999**, 39, 273-281 | 3.4 | 32 |
| 113 | Bihalide ion combination reactions in solution: electronic structure and solvation aspects. *Chemical Physics*, **1994**, 183, 309-323 | 2.3 | 32 |
| 112 | Short range caging effects for reactions in solution. II. Escape probability and time dependent reactivity. *Journal of Chemical Physics*, **1979**, 71, 884-893 | 3.9 | 31 |
| 111 | On Hydrodynamic Models for Brownian Motion. *Journal of Chemical Physics*, **1972**, 57, 5612-5613 | 3.9 | 31 |
| 110 | Are there dynamical effects in enzyme catalysis? Some thoughts concerning the enzymatic chemical step. *Archives of Biochemistry and Biophysics*, **2015**, 582, 42-55 | 4.1 | 30 |
| 109 | Ultrafast librational relaxation of H2O in liquid water. *Journal of Physical Chemistry B*, **2013**, 117, 4541-52 | 3.4 | 30 |
| 108 | Transient initial condition effects for Brownian particle motion. *Journal of Chemical Physics*, **1973**, 59, 3459-3467 | 3.9 | 28 |
| 107 | Water Structure, Dynamics, and Sum-Frequency Generation Spectra at Electrified Graphene Interfaces. *Journal of Physical Chemistry Letters*, **2020**, 11, 624-631 | 6.4 | 28 |
| 106 | Tracking energy transfer from excited to accepting modes: application to water bend vibrational relaxation. *Physical Chemistry Chemical Physics*, **2012**, 14, 6332-42 | 3.6 | 27 |
| 105 | A theoretical study of the H2SO4+H2O -→HSO4 ⁻+H3O+ reaction at the surface of aqueous aerosols. *Theoretical Chemistry Accounts*, **2004**, 111, 182-187 | 1.9 | 25 |
| 104 | VB resonance theory in solution. II. I2⁻+I in acetonitrile. *Journal of Chemical Physics*, **1995**, 102, 7885-7904 | 3.9 | 25 |

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| 103 | Perspective: Structure and ultrafast dynamics of biomolecular hydration shells. *Structural Dynamics*, **2017**, 4, 044018 | 3.2 | 23 |
| 102 | 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, 2271-80 | 3.4 | 22 |
| 101 | Molecules in motion: chemical reaction and allied dynamics in solution and elsewhere. *Annual Review of Physical Chemistry*, **2015**, 66, 1-20 | 15.7 | 21 |
| 100 | Photoisomerization for a model protonated Schiff base in solution: sloped/peaked conical intersection perspective. *Journal of Chemical Physics*, **2012**, 137, 22A543 | 3.9 | 21 |
| 99 | Acid-Base Proton Transfer and Ion Pair Formation in Solution. *Advances in Chemical Physics*, **2007**, 381-430 | | 21 |
| 98 | 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 | 3.9 | 21 |
| 97 | Solvation Dynamics in Liquid Water. 1. Ultrafast Energy Fluxes. *Journal of Physical Chemistry B*, **2015** , 119, 7558-70 | 3.4 | 20 |
| 96 | Initial condition effects for diffusive barrier crossing. *Journal of Chemical Physics*, **1978**, 69, 5261-5266 | 3.9 | 20 |
| 95 | Equilibrium and nonequilibrium solvation and solute electronic structure. *International Journal of Quantum Chemistry*, **1990**, 38, 821-833 | 2.1 | 19 |
| 94 | On the Fokker-Planck equation for the linear chain. *Molecular Physics*, **1974**, 28, 997-1004 | 1.7 | 19 |
| 93 | Theoretical studies of heterogeneous reaction mechanisms relevant for stratospheric ozone depletion. *International Journal of Quantum Chemistry*, **1999**, 75, 683-692 | 2.1 | 18 |
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| 91 | Direct and indirect solvent coupling vibrational dephasing mechanisms in hydrogen-bonded molecules. *The Journal of Physical Chemistry*, **1991**, 95, 4651-4659 | | 17 |
| 90 | Vibrational symmetry breaking of NO3- in aqueous solution: NO asymmetric stretch frequency distribution and mean splitting. *Journal of Physical Chemistry A*, **2010**, 114, 1255-69 | 2.8 | 16 |
| 89 | Non-adiabatic transition probability dependence on conical intersection topography. *Journal of Chemical Physics*, **2016**, 145, 194104 | 3.9 | 16 |
| 88 | Proton relay and electron flow in the OO single bond formation in water oxidation by the ruthenium blue dimer. *Energy and Environmental Science*, **2012**, 5, 7741 | 35.4 | 15 |
| 87 | Hydration shell exchange dynamics for in water. *Journal of Physics Condensed Matter*, **1996**, 8, 9411-9416 | 1.8 | 15 |
| 86 | Nonlinear fluctuations in master equation systems. I. Velocity correlation function for the Rayleigh model. *Journal of Chemical Physics*, **1975**, 62, 2972-2981 | 3.9 | 14 |

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| 84 | Temperature-Dependent Solvent Polarity Effects on Adiabatic Proton Transfer Rate Constants and Kinetic Isotope Effects. *Israel Journal of Chemistry*, **2004**, 44, 171-184 | 3.4 | 13 |
| 83 | Ab Initio Study of Nitromethane Deprotonation by (OH)-·nH2O Clusters. *Journal of Physical Chemistry A*, **1998**, 102, 3977-3984 | 2.8 | 13 |
| 82 | A stochastic theory of chemical reaction rates. I. Formalism. *Journal of Statistical Physics*, **1989**, 56, 879-893 | 1.5 | 13 |
| 81 | Dihydropteridine/Pteridine as a 2H/2e Redox Mediator for the Reduction of CO to Methanol: A Computational Study. *Journal of Physical Chemistry B*, **2017**, 121, 4158-4167 | 3.4 | 12 |
| 80 | Confined Water'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 | 6.4 | 12 |
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