R Benny Gerber

List of Publications by Year in Descending Order

334 papers	12,785 citations	58 h-index	95 g-index
346 ext. papers	13,483 ext. citations	5 avg, IF	6.45 L-index

#	Paper	IF	Citations
334	Absorption Spectra and the Electronic Structure of Gallic Acid in Water at Different pH: Experimental Data and Theoretical Cluster Models.. *Journal of Physical Chemistry A*, **2022**, 126, 190-197	2.8	1
333	Preparation and Characterization of the Halogen-Bonding Motif in the Isolated Cl⋯OH Complex with Cryogenic Ion Vibrational Spectroscopy.. *Journal of Physical Chemistry Letters*, **2022**, 2750-2756	6.4	3
332	Electronic and mechanical anharmonicities in the vibrational spectra of the H-bonded, cryogenically cooled X⋯HOCl (X=Cl, Br, I) complexes: Characterization of the strong anionic H-bond to an acidic OH group.. *Journal of Chemical Physics*, **2022**, 156, 174303	3.9	3
331	Size-Dependent Onset of Nitric Acid Dissociation in Cs⁺(HNO)(HO) Clusters at 20 K. *Journal of Physical Chemistry Letters*, **2021**, 12, 3335-3342	6.4	3
330	My Trajectory in Molecular Reaction Dynamics and Spectroscopy. *Annual Review of Physical Chemistry*, **2021**, 72, 1-34	15.7	
329	Toward a microscopic model of light absorbing dissolved organic compounds in aqueous environments: theoretical and experimental study. *Physical Chemistry Chemical Physics*, **2021**, 23, 10487-10497	3.6	3
328	Absorption spectra of pyruvic acid in water: insights from calculations for small hydrates and comparison to experiment. *Physical Chemistry Chemical Physics*, **2020**, 22, 12658-12670	3.6	10
327	Gas phase dynamics, conformational transitions and spectroscopy of charged saccharides: the oxocarbenium ion, protonated anhydrogalactose and protonated methyl galactopyranoside. *Physical Chemistry Chemical Physics*, **2020**, 22, 4144-4157	3.6	6
326	Absorption spectra of benzoic acid in water at different pH and in the presence of salts: insights from the integration of experimental data and theoretical cluster models. *Physical Chemistry Chemical Physics*, **2020**, 22, 5046-5056	3.6	13
325	Isomer-specific cryogenic ion vibrational spectroscopy of the D tagged Cs(HNO)(HO) complexes: ion-driven enhancement of the acidic H-bond to water. *Physical Chemistry Chemical Physics*, **2020**, 22, 4501-4507	3.6	7
324	Integrated experimental and theoretical approach to probe the synergistic effect of ammonia in methanesulfonic acid reactions with small alkylamines. *Environmental Sciences: Processes and Impacts*, **2020**, 22, 305-328	4.3	10
323	Impact of pH and NaCl and CaCl Salts on the Speciation and Photochemistry of Pyruvic Acid in the Aqueous Phase. *Journal of Physical Chemistry A*, **2020**, 124, 5071-5080	2.8	9
322	S2 Reactions of NO with Ions in Water: Microscopic Mechanisms, Intermediates, and Products. *Journal of Physical Chemistry A*, **2020**, 124, 711-720	2.8	5
321	Microscopic Mechanisms of NO Hydrolysis on the Surface of Water Droplets. *Journal of Physical Chemistry A*, **2020**, 124, 224-228	2.8	4
320	Dual Basis Approach for Ab Initio Anharmonic Calculations of Vibrational Spectroscopy: Application to Microsolvated Biomolecules. *Journal of Chemical Theory and Computation*, **2020**, 16, 7005-7016	6.4	1
319	Experimental and Theoretical Studies of the Environmental Sensitivity of the Absorption Spectra and Photochemistry of Nitenpyram and Analogs. *ACS Earth and Space Chemistry*, **2019**, 3, 2063-2075	3.2	7
318	Hydrogenic Stretch Spectroscopy of Glycine-Water Complexes: Anharmonic Ab Initio Classical Separable Potential Calculations. *Journal of Physical Chemistry A*, **2019**, 123, 8377-8384	2.8	

317	Sulfate and Carboxylate Suppress the Formation of ClNO2 at Atmospheric Interfaces. *ACS Earth and Space Chemistry*, **2019**, 3, 1987-1997	3.2	11
316	Ion reactions in atmospherically-relevant clusters: mechanisms, dynamics and spectroscopic signatures. *Faraday Discussions*, **2019**, 217, 342-360	3.6	3
315	Mechanisms and competition of halide substitution and hydrolysis in reactions of NO with seawater. *Science Advances*, **2019**, 5, eaav6503	14.3	11
314	Structures, Stability, and Decomposition Dynamics of the Polynitrogen Molecule NB(N) and Its Dimer [N][B(N)]. *Journal of Physical Chemistry A*, **2019**, 123, 7384-7393	2.8	4
313	Conformers of Ubiquitin 6+ for Different Charge Distributions: Atomistic Structures and Ion Mobility Cross Sections. *Journal of Physical Chemistry B*, **2019**, 123, 6401-6409	3.4	2
312	Anharmonic vibrational spectroscopy calculations using the ab initio CSP method: Applications to H2CO3, (H2CO3)2, H2CO3-H2O and isotopologues. *Chemical Physics*, **2018**, 514, 44-54	2.3	1
311	Molecular Dynamics of Photoinduced Reactions of Acrylic Acid: Products, Mechanisms, and Comparison with Experiment. *Journal of Physical Chemistry Letters*, **2018**, 9, 527-533	6.4	12
310	Autocorrelation of electronic wave-functions: a new approach for describing the evolution of electronic structure in the course of dynamics. *Molecular Physics*, **2018**, 116, 2512-2523	1.7	1
309	Uptake of water by an acid-base nanoparticle: theoretical and experimental studies of the methanesulfonic acid-methylamine system. *Physical Chemistry Chemical Physics*, **2018**, 20, 22249-22259	3.6	12
308	NO at water surfaces: binding forces, charge separation, energy accommodation and atmospheric implications. *Physical Chemistry Chemical Physics*, **2018**, 20, 17961-17976	3.6	12
307	Understanding interactions of organic nitrates with the surface and bulk of organic films: implications for particle growth in the atmosphere. *Environmental Sciences: Processes and Impacts*, **2018**, 20, 1593-1610	4.3	11
306	Double Photodetachment of F□HO: Experimental and Theoretical Studies of [F□HO]. *Journal of Physical Chemistry Letters*, **2018**, 9, 6808-6813	6.4	4
305	Adjacent keto and enol groups in photochemistry of a cyclic molecule: Products, mechanisms and dynamics. *Chemical Physics*, **2018**, 515, 177-186	2.3	3
304	Intrinsic structure of pentapeptide Leu-enkephalin: geometry optimization and validation by comparison of VSCF-PT2 calculations with cold ion spectroscopy. *Physical Chemistry Chemical Physics*, **2018**, 20, 24894-24901	3.6	9
303	Ab initio molecular dynamics studies of formic acid dimer colliding with liquid water. *Physical Chemistry Chemical Physics*, **2018**, 20, 23717-23725	3.6	7
302	The Role of Oxalic Acid in New Particle Formation from Methanesulfonic Acid, Methylamine, and Water. *Environmental Science & Technology*, **2017**, 51, 2124-2130	10.3	38
301	Approximate Quantum Dynamics using Ab Initio Classical Separable Potentials: Spectroscopic Applications. *Journal of Chemical Theory and Computation*, **2017**, 13, 982-991	6.4	8
300	Proton Transfer in Mixed Clusters of Methanesulfonic Acid, Methylamine, and Oxalic Acid: Implications for Atmospheric Particle Formation. *Journal of Physical Chemistry A*, **2017**, 121, 2377-2385	2.8	29

299	Photochemistry of Thin Solid Films of the Neonicotinoid Imidacloprid on Surfaces. *Environmental Science & Technology*, **2017**, 51, 2660-2668	10.3	26
298	Particle formation and growth from oxalic acid, methanesulfonic acid, trimethylamine and water: a combined experimental and theoretical study. *Physical Chemistry Chemical Physics*, **2017**, 19, 28286-28301	3.6	30
297	Trapping and Structural Characterization of the XNO□NO (X = Cl, Br, I) Exit Channel Complexes in the Water-Mediated X + NO Reactions with Cryogenic Vibrational Spectroscopy. *Journal of Physical Chemistry Letters*, **2017**, 8, 4710-4715	6.4	7
296	Concerted transfer of multiple protons in acid-water clusters: [(HCl)(HO)] and [(HF)(HO)]. *Physical Chemistry Chemical Physics*, **2017**, 19, 20641-20646	3.6	1
295	Nanoparticles grown from methanesulfonic acid and methylamine: microscopic structures and formation mechanism. *Physical Chemistry Chemical Physics*, **2017**, 19, 31949-31957	3.6	8
294	A Decapeptide Hydrated by Two Waters: Conformers Determined by Theory and Validated by Cold Ion Spectroscopy. *Journal of Physical Chemistry A*, **2017**, 121, 9401-9408	2.8	11
293	DMAP-assisted sulfonylation as an efficient step for the methylation of primary amine motifs on solid support. *Beilstein Journal of Organic Chemistry*, **2017**, 13, 806-816	2.5	7
292	Mean-Field Methods for Time-Dependent Quantum Dynamics of Many-Atom Systems. *Advances in Quantum Chemistry*, **2017**, 1-26	1.4	1
291	Photochemical Reactions of Cyclohexanone: Mechanisms and Dynamics. *Journal of Physical Chemistry A*, **2016**, 120, 7112-20	2.8	9
290	Dynamics and spectroscopy of CH□O excited electronic states. *Physical Chemistry Chemical Physics* , **2016**, 18, 10941-6	3.6	14
289	Formation of Carbonic Acid in Impact of CO2 on Ice and Water. *Journal of Physical Chemistry Letters*, **2016**, 7, 2905-9	6.4	13
288	Temperature and collision energy effects on dissociation of hydrochloric acid on water surfaces. *Physical Chemistry Chemical Physics*, **2016**, 18, 13432-42	3.6	12
287	Reactions of Methanesulfonic Acid with Amines and Ammonia as a Source of New Particles in Air. *Journal of Physical Chemistry B*, **2016**, 120, 1526-36	3.4	86
286	A Noble-Gas Hydride in a Nitrogen Medium: Structure, Spectroscopy, and Intermolecular Vibrations of HXeBr@(N2)22. *Journal of Physical Chemistry A*, **2016**, 120, 3372-9	2.8	2
285	First-principles anharmonic quantum calculations for peptide spectroscopy: VSCF calculations and comparison with experiments. *Physical Chemistry Chemical Physics*, **2016**, 18, 1607-14	3.6	23
284	Deprotonation of formic acid in collisions with a liquid water surface studied by molecular dynamics and metadynamics simulations. *Physical Chemistry Chemical Physics*, **2016**, 18, 29756-29770	3.6	16
283	Dynamics of Photochemical Reactions of Organic Carbonyls and their Clusters. *Advances in Chemical Physics*, **2016**, 1-22		
282	Infrared Spectrum of Toluene: Comparison of Anharmonic Isolated-Molecule Calculations and Experiments in Liquid Phase and in a Ne Matrix. *Journal of Physical Chemistry A*, **2016**, 120, 3380-9	2.8	12

281	Mechanism for formation of atmospheric Cl atom precursors in the reaction of dinitrogen oxides with HCl/Cl(-) on aqueous films. *Physical Chemistry Chemical Physics*, **2015**, 17, 19360-70	3.6	18
280	New particle formation and growth from methanesulfonic acid, trimethylamine and water. *Physical Chemistry Chemical Physics*, **2015**, 17, 13699-709	3.6	67
279	Mechanistic studies of malonic acid-mediated in situ acylation. *Biopolymers*, **2015**, 104, 495-505	2.2	2
278	Conformational structures of a decapeptide validated by first principles calculations and cold ion spectroscopy. *ChemPhysChem*, **2015**, 16, 1374-8	3.2	25
277	Absorption spectra and aqueous photochemistry of -hydroxyalkyl nitrates of atmospheric interest. *Molecular Physics*, **2015**, 113, 2179-2190	1.7	17
276	The future of airborne sulfur-containing particles in the absence of fossil fuel sulfur dioxide emissions. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 13514-9	11.5	57
275	High resolution absolute absorption cross sections of the B (1)A-X (1)Atransition of the CH2OO biradical. *Physical Chemistry Chemical Physics*, **2015**, 17, 32539-46	3.6	33
274	Computational studies of atmospherically-relevant chemical reactions in water clusters and on liquid water and ice surfaces. *Accounts of Chemical Research*, **2015**, 48, 399-406	24.3	68
273	Stability of Criegee intermediates formed by ozonolysis of different double bonds. *Journal of Physical Chemistry A*, **2015**, 119, 2318-25	2.8	13
272	Infrared identification of proton-bound rare-gas dimers (XeHXe)+, (KrHKr)+, and (KrHXe)+ and their deuterated species in solid hydrogen. *Journal of Physical Chemistry A*, **2015**, 119, 2651-60	2.8	19
271	Calculations predict a stable molecular crystal of N8. *Nature Chemistry*, **2014**, 6, 52-6	17.6	107
270	Hybrid MP2/MP4 potential surfaces in VSCF calculations of IR spectra: applications for organic molecules. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 119, 2-11	4.4	8
269	Reaction of a charge-separated ONONO2 species with water in the formation of HONO: an MP2 Molecular Dynamics study. *Physical Chemistry Chemical Physics*, **2014**, 16, 4483-7	3.6	24
268	Photochemistry of aldehyde clusters: cross-molecular versus unimolecular reaction dynamics. *Physical Chemistry Chemical Physics*, **2014**, 16, 23861-8	3.6	21
267	First and second deprotonation of H SO on wet hydroxylated (0001) quartz. *Physical Chemistry Chemical Physics*, **2014**, 16, 22287-98	3.6	9
266	Ionization of acids on the quasi-liquid layer of ice. *Journal of Physical Chemistry A*, **2014**, 118, 5029-37	2.8	14
265	Approximate first-principles anharmonic calculations of polyatomic spectra using MP2 and B3LYP potentials: comparisons with experiment. *Journal of Physical Chemistry A*, **2014**, 118, 6730-9	2.8	22
264	Chemically-bound xenon in fibrous silica. *Physical Chemistry Chemical Physics*, **2014**, 16, 11658-61	3.6	11

263	Isomerization and decomposition of a Criegee intermediate in the ozonolysis of alkenes: dynamics using a multireference potential. *Angewandte Chemie - International Edition*, **2014**, 53, 265-8	16.4	32
262	Ab initio and semi-empirical Molecular Dynamics simulations of chemical reactions in isolated molecules and in clusters. *Physical Chemistry Chemical Physics*, **2014**, 16, 9760-75	3.6	32
261	Modeling of HXeBr in CO2 and Xe environments: Structure, energetics and vibrational spectra. *Chemical Physics Letters*, **2014**, 594, 18-22	2.5	19
260	A highly efficient in situ N-acetylation approach for solid phase synthesis. *Organic and Biomolecular Chemistry*, **2014**, 12, 1879-84	3.9	11
259	Isomerization and Decomposition of a Criegee Intermediate in the Ozonolysis of Alkenes: Dynamics Using a Multireference Potential. *Angewandte Chemie*, **2014**, 126, 269-272	3.6	4
258	Amine–Amine Exchange in Aminium–Methanesulfonate Aerosols. *Journal of Physical Chemistry C*, **2014**, 118, 29431-29440	3.8	26
257	A Tandem In Situ Peptide Cyclization through Trifluoroacetic Acid Cleavage. *Angewandte Chemie*, **2014**, 126, 9604-9609	3.6	2
256	Raman spectroscopy of solutions and interfaces containing nitrogen dioxide, water, and 1,4 dioxane: evidence for repulsion of surface water by NO2 gas. *Journal of Chemical Physics*, **2014**, 140, 184702	3.0	3
255	Matrix effect on vibrational frequencies: experiments and simulations for HCl and HNgCl (Ng = Kr and Xe). *Journal of Chemical Physics*, **2014**, 140, 094303	3.9	20
254	An atomistic structure of ubiquitin +13 relevant in mass spectrometry: Theoretical prediction and comparison with experimental cross sections. *International Journal of Mass Spectrometry*, **2014**, 367, 10-15	1.9	11
253	Dissociation of HCl into Ions on Wet Hydroxylated (0001) α-Quartz. *Journal of Physical Chemistry Letters*, **2013**, 4, 3500-3507	6.4	19
252	When a proton attacks cellobiose in the gas phase: ab initio molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2013**, 15, 15382-91	3.6	3
251	Nitrogen dioxide at the air-water interface: trapping, absorption, and solvation in the bulk and at the surface. *Physical Chemistry Chemical Physics*, **2013**, 15, 204-12	3.6	30
250	Destabilization of noble-gas hydrides by a water environment: calculations for HXeOH@(H2O)n, HXeOXeH@(H2O)n, HXeBr@(H2O)n, HXeCCH@(H2O)n. *Physical Chemistry Chemical Physics*, **2013**, 15, 12610-6	3.6	7
249	Spectroscopy of the C-H stretching vibrational band in selected organic molecules. *Journal of Physical Chemistry A*, **2013**, 117, 7442-52	2.8	15
248	On the crystallographic accuracy of structure prediction by implicit water models: Tests for cyclic peptides. *Chemical Physics*, **2013**, 415, 168-172	2.3	13
247	Vibrational self-consistent field calculations for spectroscopy of biological molecules: new algorithmic developments and applications. *Physical Chemistry Chemical Physics*, **2013**, 15, 9468-92	3.6	143
246	Dynamics of triplet-state photochemistry of pentanal: mechanisms of Norrish I, Norrish II, and H abstraction reactions. *Journal of Physical Chemistry A*, **2013**, 117, 11711-24	2.8	21

245	Ionization of Nitric Acid on Crystalline Ice: The Role of Defects and Collective Proton Movement. *Journal of Physical Chemistry Letters*, **2013**, 4, 1850-5	6.4	25
244	Photooxidation of ammonia on TiO2 as a source of NO and NO2 under atmospheric conditions. *Journal of the American Chemical Society*, **2013**, 135, 8606-15	16.4	54
243	Decomposition mechanisms and dynamics of N6: Bond orders and partial charges along classical trajectories. *Chemical Physics Letters*, **2012**, 531, 46-51	2.5	21
242	Hydration of cellobiose: Structure and dynamics of cellobiose (H2O)n, n=5–25. *Chemical Physics Letters*, **2012**, 531, 52-58	2.5	15
241	Mechanism and electronic transition in the reaction: On the fly dynamics simulations with multi-reference potentials. *Chemical Physics Letters*, **2012**, 535, 44-48	2.5	9
240	Isomerization and ionization of N2O4 on model ice and silica surfaces. *Chemical Physics*, **2012**, 405, 52-59	2.3	11
239	Migration and chemical reaction of H+ in protonated β-galactose. *Physical Chemistry Chemical Physics*, **2012**, 14, 13522-6	3.6	3
238	Interaction and reaction of the hydroxyl ion with β-D-galactose and its hydrated complex: an ab initio molecular dynamics study. *Physical Chemistry Chemical Physics*, **2012**, 14, 12086-9	3.6	4
237	Monosaccharide-water complexes: vibrational spectroscopy and anharmonic potentials. *Journal of Physical Chemistry A*, **2012**, 116, 11088-94	2.8	11
236	Intrinsic lifetimes and kinetic stability in media of noble-gas hydrides. *Chemical Physics Letters*, **2012**, 545, 1-8	2.5	20
235	NOx Reactions on Aqueous Surfaces with Gaseous HCl: Formation of a Potential Precursor to Atmospheric Cl Atoms. *Journal of Physical Chemistry Letters*, **2012**, 3, 3405-10	6.4	30
234	Absorption spectra and photolysis of methyl peroxide in liquid and frozen water. *Journal of Physical Chemistry A*, **2012**, 116, 6068-77	2.8	40
233	Computational studies of protonated β-D-galactose and its hydrated complex: structures, interactions, proton transfer dynamics, and spectroscopy. *Journal of Physical Chemistry B*, **2012**, 116, 4851-9	3.4	15
232	Femtosecond timescale deactivation of electronically excited peroxides at ice surfaces. *Molecular Physics*, **2012**, 110, 605-617	1.7	19
231	Simplified mechanism for new particle formation from methanesulfonic acid, amines, and water via experiments and ab initio calculations. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 18719-24	11.5	131
230	Protonated sugars: vibrational spectroscopy and conformational structure of protonated O-methyl β-D-galactopyranoside. *Molecular Physics*, **2012**, 110, 1609-1615	1.7	16
229	Vibrational spectra of α-glucose, β-glucose, and sucrose: anharmonic calculations and experiment. *Journal of Physical Chemistry A*, **2011**, 115, 5859-72	2.8	54
228	Conformational transitions of glycine induced by vibrational excitation of the O-H stretch. *Physical Chemistry Chemical Physics*, **2011**, 13, 8715-22	3.6	17

227	Proton transfer and dissociation of GlyLysH+ following O-H and N-H stretching mode excitations: dynamics simulations. *Journal of the American Chemical Society*, **2011**, 133, 16510-7	16.4	11
226	Raman and infrared spectra of cellobiose in the solid state: What can be learned from single-molecule calculations?. *Chemical Physics Letters*, **2011**, 514, 284-290	2.5	12
225	Raman and IR spectra of butane: Anharmonic calculations and interpretation of room temperature spectra. *Chemical Physics Letters*, **2011**, 515, 7-12	2.5	26
224	Structures of the xylose–water complex: Energetics, transitions between conformers and spectroscopy. *Chemical Physics Letters*, **2011**, 518, 49-54	2.5	9
223	A new hybrid algorithm for finding the lowest minima of potential surfaces: approach and application to peptides. *Journal of Computational Chemistry*, **2011**, 32, 1785-800	3.5	15
222	Stability of noble-gas hydrocarbons in an organic liquid-like environment: HXeCCH in acetylene. *Physical Chemistry Chemical Physics*, **2011**, 13, 19601-6	3.6	26
221	Raman spectra of long chain hydrocarbons: anharmonic calculations, experiment and implications for imaging of biomembranes. *Physical Chemistry Chemical Physics*, **2011**, 13, 12724-33	3.6	37
220	Isotopic hydration of cellobiose: vibrational spectroscopy and dynamical simulations. *Journal of Physical Chemistry A*, **2011**, 115, 9498-509	2.8	25
219	Tributes to Victoria Buch. *Journal of Physical Chemistry A*, **2011**, 115, 5709-14	2.8	
218	Ultrafast photochemistry of methyl hydroperoxide on ice particles. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 6600-4	11.5	18
217	On the Mean Accuracy of the Separable VSCF Approximation for Large Molecules. *Journal of Physical Chemistry C*, **2010**, 114, 20603-20608	3.8	9
216	Catalytic role for water in the atmospheric production of ClNO. *Journal of Physical Chemistry A*, **2010**, 114, 4609-18	2.8	38
215	Hygroscopic growth and deliquescence of NaCl nanoparticles mixed with surfactant SDS. *Journal of Physical Chemistry B*, **2010**, 114, 2435-49	3.4	31
214	Sugar-salt and sugar-salt-water complexes: structure and dynamics of glucose-KNO3-(H2O)n. *Physical Chemistry Chemical Physics*, **2010**, 12, 3550-8	3.6	16
213	Predicted compounds of radon with acetylene and water. *Physical Chemistry Chemical Physics*, **2010**, 12, 11791-4	3.6	18
212	Chlorine activation indoors and outdoors via surface-mediated reactions of nitrogen oxides with hydrogen chloride. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 13647-54	11.5	96
211	Direct visualization of the H-Xe bond in xenon hydrides: xenon isotopic shift in the IR spectra. *Journal of Chemical Physics*, **2009**, 131, 151101	3.9	27
210	Matrix-isolation and ab initio study of HXeCCH complexed with acetylene. *Chemical Physics Letters*, **2009**, 481, 83-87	2.5	31

209	Lifetimes of compounds made of noble-gas atoms with water. *Chemical Physics Letters*, **2009**, 482, 30-33	2.5	38
208	Ultrafast nonadiabatic photodissociation dynamics of F2 in solid Ar. *Laser Physics*, **2009**, 19, 1651-1659	1.2	4
207	Autobiography of Robert Benny Gerber. *Journal of Physical Chemistry A*, **2009**, 113, 7163-70	2.8	
206	Anharmonic vibrational spectroscopy calculations for proton-bound amino acid dimers. *Journal of Physical Chemistry A*, **2009**, 113, 1905-12	2.8	24
205	Structure of large nitrate-water clusters at ambient temperatures: simulations with effective fragment potentials and force fields with implications for atmospheric chemistry. *Journal of Physical Chemistry A*, **2009**, 113, 12805-14	2.8	44
204	Dynamics simulations of atmospherically relevant molecular reactions. *International Reviews in Physical Chemistry*, **2009**, 28, 207-222	7	33
203	Ionization of N2O4 in contact with water: mechanism, time scales and atmospheric implications. *Journal of the American Chemical Society*, **2009**, 131, 12180-5	16.4	67
202	Noble-gas hydrides: new chemistry at low temperatures. *Accounts of Chemical Research*, **2009**, 42, 183-91	24.3	219
201	Ultrafast phase transitions in metastable water near liquid interfaces. *Faraday Discussions*, **2009**, 141, 67-79; discussion 81-98	3.6	22
200	Complexes of HNO3 and NO3 - with NO2 and N2O4, and their potential role in atmospheric HONO formation. *Physical Chemistry Chemical Physics*, **2008**, 10, 6019-32	3.6	36
199	A small neutral molecule with two noble-gas atoms: HXeOXeH. *Journal of the American Chemical Society*, **2008**, 130, 6114-8	16.4	97
198	Raman spectra of complexes of HNO3 and NO3- with NO2 at surfaces and with N2O4 in solution. *Physical Chemistry Chemical Physics*, **2008**, 10, 4748-53	3.6	12
197	Calculation of vibrational transition frequencies and intensities in water dimer: comparison of different vibrational approaches. *Journal of Physical Chemistry A*, **2008**, 112, 4324-35	2.8	149
196	Conformational evolution of ubiquitin ions in electrospray mass spectrometry: molecular dynamics simulations at gradually increasing temperatures. *Physical Chemistry Chemical Physics*, **2008**, 10, 3077-82	3.6	48
195	Mid-IR spectra of different conformers of phenylalanine in the gas phase. *Physical Chemistry Chemical Physics*, **2008**, 10, 1248-56	3.6	48
194	Dynamics of proton recombination with NO3- anion in water clusters. *Physical Chemistry Chemical Physics*, **2008**, 10, 1091-3	3.6	26
193	On the number of significant mode-mode anharmonic couplings in vibrational calculations: Correlation-corrected vibrational self-consistent field treatment of di-, tri-, and tetrapeptides. *Journal of Chemical Physics*, **2008**, 128, 165105	3.9	54
192	Anharmonic vibrational spectroscopy calculations with electronic structure potentials: comparison of MP2 and DFT for organic molecules. *Theoretical Chemistry Accounts*, **2008**, 120, 273-279	1.9	49

191	Early structural evolution of native cytochrome c after solvent removal. *ChemBioChem*, **2008**, 9, 2417-23	3.8	57
190	Critical size for intracluster proton transfer from water to an anion. *Angewandte Chemie - International Edition*, **2008**, 47, 6272-4	16.4	14
189	Vibrational spectroscopy of triacetone triperoxide (TATP): anharmonic fundamentals, overtones and combination bands. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2008**, 71, 1438-45	4.4	25
188	Predicted stability of the organo-xenon compound HXeCCH above the cryogenic range. *Chemical Physics Letters*, **2008**, 460, 23-26	2.5	32
187	Vibrational spectroscopy for glycine adsorbed on silicon clusters: Harmonic and anharmonic calculations for models of the Si(1 0 0)-2 □1 surface. *Chemical Physics*, **2008**, 347, 218-228	2.3	21
186	Anharmonic vibrational calculations modeling the raman spectra of intermediates in the photoactive yellow protein (PYP) photocycle. *Journal of the American Chemical Society*, **2007**, 129, 4584-94	16.4	21
185	Vibrational spectroscopy of protonated imidazole and its complexes with water molecules: ab initio anharmonic calculations and experiments. *Journal of Physical Chemistry A*, **2007**, 111, 7374-81	2.8	28
184	Dynamics of electronic states and spin-flip for photodissociation of dihalogens in matrices: experiment and semiclassical surface-hopping and quantum model simulations for F2 and ClF in solid Ar. *Journal of Physical Chemistry A*, **2007**, 111, 9573-85	2.8	28
183	Photodissociation yields for vibrationally excited states of sulfuric acid under atmospheric conditions. *Geophysical Research Letters*, **2007**, 34,	4.9	20
182	The dynamics of water evaporation from partially solvated cytochrome c in the gas phase. *Physical Chemistry Chemical Physics*, **2007**, 9, 4690-7	3.6	54
181	Self-Consistent-Field Methods for Vibrational Excitations in Polyatomic Systems. *Advances in Chemical Physics*, **2007**, 97-132		168
180	Coherence and control of molecular dynamics in rare gas matrices **2007**, 257-385		6
179	Vibrational spectroscopy of (SO4(2-)).(H2O)n clusters, n=1-5: harmonic and anharmonic calculations and experiment. *Journal of Chemical Physics*, **2007**, 127, 094305	3.9	50
178	Predicted stability and structure of (HXeCCH)n (n=2 or 4) clusters and of crystalline HXeCCH. *Journal of Chemical Physics*, **2007**, 126, 021108	3.9	26
177	Acceleration of Correlation-corrected Vibrational Self-consistent Field Calculation Times for Large Polyatomic Molecules. *Theoretical Chemistry Accounts*, **2006**, 117, 69-72	1.9	37
176	High coordination chemically bound compounds of noble gases with hydrocarbons: Ng(CCH)4 and Ng(CCH)6, (Ng=Xe or Kr). *Journal of Chemical Physics*, **2006**, 124, 231103	3.9	12
175	Stability and structure of oligomers and polymers made of xenon and hydrocarbons: theoretical predictions. *Journal of Chemical Physics*, **2006**, 125, 201101	3.9	10
174	Evolution of conformational changes in the dynamics of small biological molecules: a hybrid MD/RRK approach. *Physical Chemistry Chemical Physics*, **2006**, 8, 4915-23	3.6	3

173	New organic noble gas molecules: energetics, stability and potential energy surfaces of HCCXeCCH and HCCKrCCH. *Physical Chemistry Chemical Physics*, **2006**, 8, 4175-81	3.6	21
172	Dynamical Simulations of Photoionization of Small Biological Molecules **2006**, 213-237		
171	Theoretical prediction of chemically bound compounds made of argon and hydrocarbons. *Journal of the American Chemical Society*, **2006**, 128, 7156-7	16.4	27
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