R Benny Gerber

List of Publications by Year
in descending order

338 papers	14,242 citations	18436 62 h-index	33814 99 g-index
346 all docs	346 docs citations	346 times ranked	6470 citing authors

#	Article	IF	Citations
1	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.	1.1	4
2	Preparation and Characterization of the Halogen-Bonding Motif in the Isolated Cl^{â€“}Â·IOH Complex with Cryogenic Ion Vibrational Spectroscopy. Journal of Physical Chemistry Letters, 2022, 13, 2750-2756.	2.1	9
3	Electronic and mechanical anharmonicities in the vibrational spectra of the H-bonded, cryogenically cooled Xâ¯â€‰Â·â€‰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.	1.2	11
4	Energy transfer, pre-reactive complex formation and recombination reactions during the collision of peroxy radicals. Physical Chemistry Chemical Physics, 2022, 24, 10033-10043.	1.3	6
5	My Trajectory in Molecular Reaction Dynamics and Spectroscopy. Annual Review of Physical Chemistry, 2021, 72, 1-34.	4.8	7
6	Size-Dependent Onset of Nitric Acid Dissociation in Cs⁺Â·(HNO₃)(H₂O)_{n=0â€“11} Clusters at 20 K. Journal of Physical Chemistry Letters, 2021, 12, 3335-3342.	2.1	7
7	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.	1.3	7
8	S_N2 Reactions of N₂O₅ with Ions in Water: Microscopic Mechanisms, Intermediates, and Products. Journal of Physical Chemistry A, 2020, 124, 711-720.	1.1	8
9	Microscopic Mechanisms of N₂O₅ Hydrolysis on the Surface of Water Droplets. Journal of Physical Chemistry A, 2020, 124, 224-228.	1.1	9
10	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.	2.3	8
11	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.	1.3	19
12	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.	1.3	8
13	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.	1.3	28
14	Isomer-specific cryogenic ion vibrational spectroscopy of the D₂ tagged Cs⁺(HNO₃)(H₂O)_{n=0â€“2} complexes: ion-driven enhancement of the acidic H-bond to water. Physical Chemistry Chemical Physics, 2020, 22, 4501-4507.	1.3	9
15	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.	1.7	18
16	Impact of pH and NaCl and CaCl₂ Salts on the Speciation and Photochemistry of Pyruvic Acid in the Aqueous Phase. Journal of Physical Chemistry A, 2020, 124, 5071-5080.	1.1	18
17	Structures, Stability, and Decomposition Dynamics of the Polynitrogen Molecule N₅⁺B(N₃)₄^{â€“} and Its Dimer [N₅⁺]₂[B(N₃)₄^{â€“}]₂. Journal of Physical Chemistry A, 2019, 123, 7384-7393.	1.1	6
18	Conformers of Ubiquitin 6+ for Different Charge Distributions: Atomistic Structures and Ion Mobility Cross Sections. Journal of Physical Chemistry B, 2019, 123, 6401-6409.	1.2	2

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19	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.	1.2	8
20	Hydrogenic Stretch Spectroscopy of Glycineâ€“Water Complexes: Anharmonic Ab Initio Classical Separable Potential Calculations. Journal of Physical Chemistry A, 2019, 123, 8377-8384.	1.1	0
21	Sulfate and Carboxylate Suppress the Formation of ClNO2 at Atmospheric Interfaces. ACS Earth and Space Chemistry, 2019, 3, 1987-1997.	1.2	18
22	Ion reactions in atmospherically-relevant clusters: mechanisms, dynamics and spectroscopic signatures. Faraday Discussions, 2019, 217, 342-360.	1.6	3
23	Mechanisms and competition of halide substitution and hydrolysis in reactions of N ₂ O ₅ with seawater. Science Advances, 2019, 5, eaav6503.	4.7	16
24	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.	0.9	4
25	Molecular Dynamics of Photoinduced Reactions of Acrylic Acid: Products, Mechanisms, and Comparison with Experiment. Journal of Physical Chemistry Letters, 2018, 9, 527-533.	2.1	15
26	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.	0.8	2
27	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.	1.7	12
28	Double Photodetachment of F^{â€“}Â·H₂O: Experimental and Theoretical Studies of [FÂ·H₂O]⁺. Journal of Physical Chemistry Letters, 2018, 9, 6808-6813.	2.1	5
29	Adjacent keto and enol groups in photochemistry of a cyclic molecule: Products, mechanisms and dynamics. Chemical Physics, 2018, 515, 177-186.	0.9	3
30	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.	1.3	18
31	Ab initio molecular dynamics studies of formic acid dimer colliding with liquid water. Physical Chemistry Chemical Physics, 2018, 20, 23717-23725.	1.3	15
32	Uptake of water by an acidâ€“base nanoparticle: theoretical and experimental studies of the methanesulfonic acidâ€“methylamine system. Physical Chemistry Chemical Physics, 2018, 20, 22249-22259.	1.3	15
33	N₂O₅at water surfaces: binding forces, charge separation, energy accommodation and atmospheric implications. Physical Chemistry Chemical Physics, 2018, 20, 17961-17976.	1.3	18
34	The Role of Oxalic Acid in New Particle Formation from Methanesulfonic Acid, Methylamine, and Water. Environmental Science & Technology, 2017, 51, 2124-2130.	4.6	53
35	Approximate Quantum Dynamics using Ab Initio Classical Separable Potentials: Spectroscopic Applications. Journal of Chemical Theory and Computation, 2017, 13, 982-991.	2.3	8
36	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.	1.1	42

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37	Photochemistry of Thin Solid Films of the Neonicotinoid Imidacloprid on Surfaces. Environmental Science & Technology, 2017, 51, 2660-2668.	4.6	37
38	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.	1.3	42
39	Trapping and Structural Characterization of the XNO₂Â·NO₃^{â€“} (X =) Tj ETQq1 1 0.784314 rgBT Reactions with Cryogenic Vibrational Spectroscopy. Journal of Physical Chemistry Letters, 2017, 8, 4710-4715.	2.1	11
40	Concerted transfer of multiple protons in acidâ€“water clusters: [(HCl)(H₂O)]₂ and [(HF)(H₂O)]₄. Physical Chemistry Chemical Physics, 2017, 19, 20641-20646.	1.3	3
41	Nanoparticles grown from methanesulfonic acid and methylamine: microscopic structures and formation mechanism. Physical Chemistry Chemical Physics, 2017, 19, 31949-31957.	1.3	11
42	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.	1.1	16
43	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.	1.3	9
44	Mean-Field Methods for Time-Dependent Quantum Dynamics of Many-Atom Systems. Advances in Quantum Chemistry, 2017, , 1-26.	0.4	2
45	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.	1.3	22
46	Dynamics of Photochemical Reactions of Organic Carbonyls and their Clusters. Advances in Chemical Physics, 2016, , 1-22.	0.3	0
47	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, 3380-3389.	1.1	16
48	Photochemical Reactions of Cyclohexanone: Mechanisms and Dynamics. Journal of Physical Chemistry A, 2016, 120, 7112-7120.	1.1	17
49	Dynamics and spectroscopy of CH2OO excited electronic states. Physical Chemistry Chemical Physics, 2016, 18, 10941-10946.	1.3	19
50	Formation of Carbonic Acid in Impact of CO2 on Ice and Water. Journal of Physical Chemistry Letters, 2016, 7, 2905-2909.	2.1	16
51	Temperature and collision energy effects on dissociation of hydrochloric acid on water surfaces. Physical Chemistry Chemical Physics, 2016, 18, 13432-13442.	1.3	13
52	Reactions of Methanesulfonic Acid with Amines and Ammonia as a Source of New Particles in Air. Journal of Physical Chemistry B, 2016, 120, 1526-1536.	1.2	115
53	A Noble-Gas Hydride in a Nitrogen Medium: Structure, Spectroscopy, and Intermolecular Vibrations of HXeBr@(N₂)₂₂. Journal of Physical Chemistry A, 2016, 120, 3372-3379.	1.1	4
54	First-principles anharmonic quantum calculations for peptide spectroscopy: VSCF calculations and comparison with experiments. Physical Chemistry Chemical Physics, 2016, 18, 1607-1614.	1.3	32

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55	Mechanistic studies of malonic acidâ€mediated in situ acylation. Biopolymers, 2015, 104, 495-505.	1.2	3
56	Conformational Structures of a Decapeptide Validated by First Principles Calculations and Cold Ion Spectroscopy. ChemPhysChem, 2015, 16, 1374-1378.	1.0	28
57	Absorption spectra and aqueous photochemistry of Î²-hydroxyalkyl nitrates of atmospheric interest. Molecular Physics, 2015, 113, 2179-2190.	0.8	22
58	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, 13514-13519.	3.3	76
59	High resolution absolute absorption cross sections of the BÌƒ ¹Aâ€²â€“XÌƒ ¹Aâ€² transition of the CH₂OO biradical. Physical Chemistry Chemical Physics, 2015, 17, 32539-32546.	1.3	42
60	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.	7.6	89
61	Stability of Criegee Intermediates Formed by Ozonolysis of Different Double Bonds. Journal of Physical Chemistry A, 2015, 119, 2318-2325.	1.1	18
62	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, 2651-2660.	1.1	23
63	Mechanism for formation of atmospheric Cl atom precursors in the reaction of dinitrogen oxides with HCl/Cl^{â^'}on aqueous films. Physical Chemistry Chemical Physics, 2015, 17, 19360-19370.	1.3	20
64	Tribute to Markku O. RÃsÃnen. Journal of Physical Chemistry A, 2015, 119, 2187-2190.	1.1	1
65	New particle formation and growth from methanesulfonic acid, trimethylamine and water. Physical Chemistry Chemical Physics, 2015, 17, 13699-13709.	1.3	88
66	Amineâ€“Amine Exchange in Aminiumâ€“Methanesulfonate Aerosols. Journal of Physical Chemistry C, 2014, 118, 29431-29440.	1.5	31
67	Frontispiz: A Tandem In Situ Peptide Cyclization through Trifluoroacetic Acid Cleavage. Angewandte Chemie, 2014, 126, n/a-n/a.	1.6	0
68	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.	1.2	3
69	Matrix effect on vibrational frequencies: Experiments and simulations for HCl and HNgCl (Ng = Kr and) Tj ETQq1 1 0.784314 rgBT /Ov	1.2	21
70	Frontispiece: A Tandem In Situ Peptide Cyclization through Trifluoroacetic Acid Cleavage. Angewandte Chemie - International Edition, 2014, 53, n/a-n/a.	7.2	0
71	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.	0.7	12
72	Calculations predict a stable molecular crystal of N8. Nature Chemistry, 2014, 6, 52-56.	6.6	152

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73	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.	2.0	8
74	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.	1.3	31
75	Photochemistry of aldehyde clusters: cross-molecular versus unimolecular reaction dynamics. Physical Chemistry Chemical Physics, 2014, 16, 23861-23868.	1.3	21
76	First and second deprotonation of H₂SO₄on wet hydroxylated (0001) Î±-quartz. Physical Chemistry Chemical Physics, 2014, 16, 22287-22298.	1.3	12
77	Ionization of Acids on the Quasi-Liquid Layer of Ice. Journal of Physical Chemistry A, 2014, 118, 5029-5037.	1.1	17
78	Approximate First-Principles Anharmonic Calculations of Polyatomic Spectra Using MP2 and B3LYP Potentials: Comparisons with Experiment. Journal of Physical Chemistry A, 2014, 118, 6730-6739.	1.1	32
79	Chemically-bound xenon in fibrous silica. Physical Chemistry Chemical Physics, 2014, 16, 11658-11661.	1.3	13
80	Isomerization and Decomposition of a Criegee Intermediate in the Ozonolysis of Alkenes: Dynamics Using a Multireference Potential. Angewandte Chemie - International Edition, 2014, 53, 265-268.	7.2	33
81	Ab initio and semi-empirical Molecular Dynamics simulations of chemical reactions in isolated molecules and in clusters. Physical Chemistry Chemical Physics, 2014, 16, 9760-9775.	1.3	35
82	Modeling of HXeBr in CO2 and Xe environments: Structure, energetics and vibrational spectra. Chemical Physics Letters, 2014, 594, 18-22.	1.2	20
83	A highly efficient in situ N-acetylation approach for solid phase synthesis. Organic and Biomolecular Chemistry, 2014, 12, 1879-1884.	1.5	14
84	Dissociation of HCl into Ions on Wet Hydroxylated (0001) Î±-Quartz. Journal of Physical Chemistry Letters, 2013, 4, 3500-3507.	2.1	19
85	When a proton attacks cellobiose in the gas phase: ab initio molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 15382.	1.3	4
86	Nitrogen dioxide at the airâ€“water interface: trapping, absorption, and solvation in the bulk and at the surface. Physical Chemistry Chemical Physics, 2013, 15, 204-212.	1.3	33
87	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.	1.3	8
88	Spectroscopy of the Câ€“H Stretching Vibrational Band in Selected Organic Molecules. Journal of Physical Chemistry A, 2013, 117, 7442-7452.	1.1	22
89	On the crystallographic accuracy of structure prediction by implicit water models: Tests for cyclic peptides. Chemical Physics, 2013, 415, 168-172.	0.9	13
90	Vibrational self-consistent field calculations for spectroscopy of biological molecules: new algorithmic developments and applications. Physical Chemistry Chemical Physics, 2013, 15, 9468.	1.3	163

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91	Dynamics of Triplet-State Photochemistry of Pentanal: Mechanisms of Norrish I, Norrish II, and H Abstraction Reactions. Journal of Physical Chemistry A, 2013, 117, 11711-11724.	1.1	26
92	Ionization of Nitric Acid on Crystalline Ice: The Role of Defects and Collective Proton Movement. Journal of Physical Chemistry Letters, 2013, 4, 1850-1855.	2.1	25
93	Photooxidation of Ammonia on TiO₂ as a Source of NO and NO₂ under Atmospheric Conditions. Journal of the American Chemical Society, 2013, 135, 8606-8615.	6.6	72
94	Femtosecond timescale deactivation of electronically excited peroxides at ice surfaces. Molecular Physics, 2012, 110, 605-617.	0.8	21
95	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, 18719-18724.	3.3	173
96	Protonated sugars: vibrational spectroscopy and conformational structure of protonatedO-methyl Î±-D-galactopyranoside. Molecular Physics, 2012, 110, 1609-1615.	0.8	17
97	Isomerization and ionization of N2O4 on model ice and silica surfaces. Chemical Physics, 2012, 405, 52-59.	0.9	13
98	Migration and chemical reaction of H+ in protonated Î²-galactose. Physical Chemistry Chemical Physics, 2012, 14, 13522.	1.3	4
99	Interaction and reaction of the hydroxyl ion with Î²-d-galactose and its hydrated complex: an ab initio molecular dynamics study. Physical Chemistry Chemical Physics, 2012, 14, 12086.	1.3	5
100	Monosaccharide-Water Complexes: Vibrational Spectroscopy and Anharmonic Potentials. Journal of Physical Chemistry A, 2012, 116, 11088-11094.	1.1	13
101	Intrinsic lifetimes and kinetic stability in media of noble-gas hydrides. Chemical Physics Letters, 2012, 545, 1-8.	1.2	23
102	NO_x Reactions on Aqueous Surfaces with Gaseous HCl: Formation of a Potential Precursor to Atmospheric Cl Atoms. Journal of Physical Chemistry Letters, 2012, 3, 3405-3410.	2.1	34
103	Absorption Spectra and Photolysis of Methyl Peroxide in Liquid and Frozen Water. Journal of Physical Chemistry A, 2012, 116, 6068-6077.	1.1	49
104	Computational Studies of Protonated Î²-d-Galactose and Its Hydrated Complex: Structures, Interactions, Proton Transfer Dynamics, and Spectroscopy. Journal of Physical Chemistry B, 2012, 116, 4851-4859.	1.2	17
105	Decomposition mechanisms and dynamics of N6: Bond orders and partial charges along classical trajectories. Chemical Physics Letters, 2012, 531, 46-51.	1.2	25
106	Hydration of cellobiose: Structure and dynamics of cellobiose â€“(H2O)n, n=5â€“25. Chemical Physics Letters, 2012, 531, 52-58.	1.2	15
107	Mechanism and electronic transition in the reaction: On the fly dynamics simulations with multi-reference potentials. Chemical Physics Letters, 2012, 535, 44-48.	1.2	10
108	Stability of noble-gas hydrocarbons in an organic liquid-like environment: HXeCCH in acetylene. Physical Chemistry Chemical Physics, 2011, 13, 19601.	1.3	26

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109	Raman spectra of long chain hydrocarbons: anharmonic calculations, experiment and implications for imaging of biomembranes. Physical Chemistry Chemical Physics, 2011, 13, 12724.	1.3	41
110	Isotopic Hydration of Cellobiose: Vibrational Spectroscopy and Dynamical Simulations. Journal of Physical Chemistry A, 2011, 115, 9498-9509.	1.1	27
111	Tributes to Victoria Buch. Journal of Physical Chemistry A, 2011, 115, 5709-5714.	1.1	0
112	Vibrational Spectra of Î±-Glucose, Î²-Glucose, and Sucrose: Anharmonic Calculations and Experiment. Journal of Physical Chemistry A, 2011, 115, 5859-5872.	1.1	63
113	Conformational transitions of glycine induced by vibrational excitation of the Oâ€“H stretch. Physical Chemistry Chemical Physics, 2011, 13, 8715-8722.	1.3	19
114	Proton Transfer and Dissociation of GlyLysH⁺ following Oâ€“H and Nâ€“H Stretching Mode Excitations: Dynamics Simulations. Journal of the American Chemical Society, 2011, 133, 16510-16517.	6.6	11
115	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.	1.2	14
116	Raman and IR spectra of butane: Anharmonic calculations and interpretation of room temperature spectra. Chemical Physics Letters, 2011, 515, 7-12.	1.2	29
117	Structures of the xyloseâ€“water complex: Energetics, transitions between conformers and spectroscopy. Chemical Physics Letters, 2011, 518, 49-54.	1.2	10
118	A new hybrid algorithm for finding the lowest minima of potential surfaces: Approach and application to peptides. Journal of Computational Chemistry, 2011, 32, 1785-1800.	1.5	19
119	Ultrafast photochemistry of methyl hydroperoxide on ice particles. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 6600-6604.	3.3	19
120	On the Mean Accuracy of the Separable VSCF Approximation for Large Molecules. Journal of Physical Chemistry C, 2010, 114, 20603-20608.	1.5	9
121	Catalytic Role for Water in the Atmospheric Production of ClNO. Journal of Physical Chemistry A, 2010, 114, 4609-4618.	1.1	40
122	Hygroscopic Growth and Deliquescence of NaCl Nanoparticles Mixed with Surfactant SDS. Journal of Physical Chemistry B, 2010, 114, 2435-2449.	1.2	42
123	Sugarâ€“salt and sugarâ€“saltâ€“water complexes: structure and dynamics of glucoseâ€“KNO3â€“(H2O)n. Physical Chemistry Chemical Physics, 2010, 12, 3550.	1.3	16
124	Predicted compounds of radon with acetylene and water. Physical Chemistry Chemical Physics, 2010, 12, 11791.	1.3	22
125	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, 13647-13654.	3.3	107
126	Direct visualization of the Hâ€“Xe bond in xenon hydrides: Xenon isotopic shift in the IR spectra. Journal of Chemical Physics, 2009, 131, 151101.	1.2	30

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127	Matrix-isolation and ab initio study of HXeCCH complexed with acetylene. Chemical Physics Letters, 2009, 481, 83-87.	1.2	32
128	Lifetimes of compounds made of noble-gas atoms with water. Chemical Physics Letters, 2009, 482, 30-33.	1.2	42
129	Ultrafast nonadiabatic photodissociation dynamics of F2 in solid Ar. Laser Physics, 2009, 19, 1651-1659.	0.6	4
130	Autobiography of Robert Benny Gerber. Journal of Physical Chemistry A, 2009, 113, 7163-7170.	1.1	0
131	Anharmonic Vibrational Spectroscopy Calculations for Proton-Bound Amino Acid Dimers. Journal of Physical Chemistry A, 2009, 113, 1905-1912.	1.1	24
132	Structure of Large Nitrateâˆ'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, 12805-12814.	1.1	47
133	Dynamics simulations of atmospherically relevant molecular reactions. International Reviews in Physical Chemistry, 2009, 28, 207-222.	0.9	36
134	Ionization of N₂O₄ in Contact with Water: Mechanism, Time Scales and Atmospheric Implications. Journal of the American Chemical Society, 2009, 131, 12180-12185.	6.6	72
135	Noble-Gas Hydrides: New Chemistry at Low Temperatures. Accounts of Chemical Research, 2009, 42, 183-191.	7.6	241
136	Ultrafast phase transitions in metastable water near liquid interfaces. Faraday Discussions, 2009, 141, 67-79.	1.6	24
137	Anharmonic vibrational spectroscopy calculations with electronic structure potentials: comparison of MP2 and DFT for organic molecules. Theoretical Chemistry Accounts, 2008, 120, 273-279.	0.5	51
138	Early Structural Evolution of Native Cytochrome c after Solvent Removal. ChemBioChem, 2008, 9, 2417-2423.	1.3	66
139	Critical Size for Intracluster Proton Transfer from Water to an Anion. Angewandte Chemie - International Edition, 2008, 47, 6272-6274.	7.2	14
140	Vibrational spectroscopy of triacetone triperoxide (TATP): Anharmonic fundamentals, overtones and combination bands. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1438-1445.	2.0	30
141	Predicted stability of the organo-xenon compound HXeCCH above the cryogenic range. Chemical Physics Letters, 2008, 460, 23-26.	1.2	34
142	Vibrational spectroscopy for glycine adsorbed on silicon clusters: Harmonic and anharmonic calculations for models of the Si(100)-2Ã—1 surface. Chemical Physics, 2008, 347, 218-228.	0.9	26
143	Complexes of HNO3 and NO3âˆ' with NO2 and N2O4, and their potential role in atmospheric HONO formation. Physical Chemistry Chemical Physics, 2008, 10, 6019.	1.3	39
144	A Small Neutral Molecule with Two Noble-Gas Atoms: HXeOXeH. Journal of the American Chemical Society, 2008, 130, 6114-6118.	6.6	111

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145	Raman spectra of complexes of HNO3 and NO3â˜ with NO2 at surfaces and with N2O4 in solution. Physical Chemistry Chemical Physics, 2008, 10, 4748.	1.3	13
146	Calculation of Vibrational Transition Frequencies and Intensities in Water Dimer:â€‰ Comparison of Different Vibrational Approaches. Journal of Physical Chemistry A, 2008, 112, 4324-4335.	1.1	165
147	Conformational evolution of ubiquitin ions in electrospray mass spectrometry: molecular dynamics simulations at gradually increasing temperatures. Physical Chemistry Chemical Physics, 2008, 10, 3077.	1.3	54
148	Mid-IRspectra of different conformers of phenylalanine in the gas phase. Physical Chemistry Chemical Physics, 2008, 10, 1248-1256.	1.3	53
149	Dynamics of proton recombination with NO3â˜ anion in water clusters. Physical Chemistry Chemical Physics, 2008, 10, 1091.	1.3	26
150	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.	1.2	58
151	The dynamics of water evaporation from partially solvated cytochrome c in the gas phase. Physical Chemistry Chemical Physics, 2007, 9, 4690.	1.3	60
152	Self-Consistent-Field Methods for Vibrational Excitations in Polyatomic Systems. Advances in Chemical Physics, 2007, , 97-132.	0.3	189
153	Coherence and control of molecular dynamics in rare gas matrices. , 2007, , 257-385.		7
154	Vibrational spectroscopy of (SO42â˜)â˜™(H2O)n clusters, n=1â€“5: Harmonic and anharmonic calculations and experiment. Journal of Chemical Physics, 2007, 127, 094305.	1.2	51
155	Predicted stability and structure of (HXeCCH)n(n=2or4) clusters and of crystalline HXeCCH. Journal of Chemical Physics, 2007, 126, 021108.	1.2	26
156	Anharmonic Vibrational Calculations Modeling the Raman Spectra of Intermediates in the Photoactive Yellow Protein (PYP) Photocycle. Journal of the American Chemical Society, 2007, 129, 4584-4594.	6.6	22
157	Vibrational Spectroscopy of Protonated Imidazole and its Complexes with Water Molecules:Â Ab Initio Anharmonic Calculations and Experimentsâ€. Journal of Physical Chemistry A, 2007, 111, 7374-7381.	1.1	30
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