Henrik G Kjaergaard

List of Publications by Year in Descending Order

223 papers	13,059 citations	54 h-index	107 g-index
239 ext. papers	14,616 ext. citations	5 avg, IF	6.46 L-index

#	Paper	IF	Citations
223	Vibrational Spectroscopy of the Water Dimer at Jet-Cooled and Atmospheric Temperatures.. *Annual Review of Physical Chemistry*, **2022**,	15.7	1
222	Reduced-dimensional vibrational models of the water dimer.. *Journal of Chemical Physics*, **2022**, 156, 164304	3.9	
221	Hydrotrioxide (ROOOH) formation in the atmosphere. *Science*, **2022**, 376, 979-982	33.3	4
220	Effect of Freezing out Vibrational Modes on Gas-Phase Fluorescence Spectra of Small Ionic Dyes. *Journal of Physical Chemistry Letters*, **2021**, 12, 11346-11352	6.4	1
219	Atmospheric Fate of the CHSOO Radical from the CHS + O Equilibrium. *Journal of Physical Chemistry A*, **2021**, 125, 8933-8941	2.8	4
218	Coupling of torsion and OH-stretching in tert-butyl hydroperoxide. I. The cold and warm first OH-stretching overtone spectrum. *Journal of Chemical Physics*, **2021**, 154, 164306	3.9	5
217	Coupling of torsion and OH-stretching in tert-butyl hydroperoxide. II. The OH-stretching fundamental and overtone spectra. *Journal of Chemical Physics*, **2021**, 154, 164307	3.9	5
216	Trimethylamine Outruns Terpenes and Aromatics in Atmospheric Autoxidation. *Journal of Physical Chemistry A*, **2021**, 125, 4454-4466	2.8	4
215	Unimolecular Reactions Following Indoor and Outdoor Limonene Ozonolysis. *Journal of Physical Chemistry A*, **2021**, 125, 669-680	2.8	10
214	A new setup for low-temperature gas-phase ion fluorescence spectroscopy. *Review of Scientific Instruments*, **2021**, 92, 033105	1.7	4
213	Atmospheric Chemistry of CHOCFCHF.. *Journal of Physical Chemistry A*, **2021**, 125, 10640-10648	2.8	0
212	Oxidation kinetics of n-pentanol: A theoretical study of the reactivity of the 1-hydroxy-1-peroxypentyl radical. *Combustion and Flame*, **2020**, 219, 20-32	5.3	11
211	Double Bonds Are Key to Fast Unimolecular Reactivity in First-Generation Monoterpene Hydroxy Peroxy Radicals. *Journal of Physical Chemistry A*, **2020**, 124, 2885-2896	2.8	18
210	Attenuated Deuterium Stabilization of Hydrogen-Bound Complexes at Room Temperature. *Journal of Physical Chemistry A*, **2020**, 124, 1763-1774	2.8	3
209	Conformer-Specific Photolysis of Pyruvic Acid and the Effect of Water. *Journal of Physical Chemistry A*, **2020**, 124, 1240-1252	2.8	9
208	Accurate Calculations of OH-Stretching Intensities with a Reduced-Dimensional Local Mode Model Including Eckart Axis Embedding. *Journal of Physical Chemistry A*, **2020**, 124, 932-942	2.8	9
207	Global airborne sampling reveals a previously unobserved dimethyl sulfide oxidation mechanism in the marine atmosphere. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 4505-4510	11.5	61

206	Acetonyl Peroxy and Hydro Peroxy Self- and Cross-Reactions: Kinetics, Mechanism, and Chaperone Enhancement from the Perspective of the Hydroxyl Radical Product. *Journal of Physical Chemistry A* , **2020**, 124, 8128-8143	2.8	2
205	SO formation and peroxy radical isomerization in the atmospheric reaction of OH radicals with dimethyl disulfide. *Chemical Communications*, **2020**, 56, 13634-13637	5.8	3
204	Spectroscopy of OSSO and Other Sulfur Compounds Thought to be Present in the Venus Atmosphere. *Journal of Physical Chemistry A*, **2020**, 124, 7047-7059	2.8	10
203	New Insights into the Radical Chemistry and Product Distribution in the OH-Initiated Oxidation of Benzene. *Environmental Science & Technology*, **2020**, 54, 13467-13477	10.3	14
202	Atmospheric Autoxidation of Amines. *Environmental Science & Technology*, **2020**, 54, 11087-11099	10.3	15
201	Room Temperature Gas-Phase Detection and Gibbs Energies of Water Amine Bimolecular Complex Formation. *Journal of Physical Chemistry A*, **2020**, 124, 7113-7122	2.8	8
200	Room Temperature Gibbs Energies of Hydrogen-Bonded Alcohol Dimethylselenide Complexes. *Journal of Physical Chemistry A*, **2019**, 123, 8427-8434	2.8	5
199	Stereoselectivity in Atmospheric Autoxidation. *Journal of Physical Chemistry Letters*, **2019**, 10, 6260-6266	6.4	14
198	Unimolecular Reactions of Peroxy Radicals Formed in the Oxidation of □Pinene and □Pinene by Hydroxyl Radicals. *Journal of Physical Chemistry A*, **2019**, 123, 1661-1674	2.8	43
197	Gibbs energy of complex formation □ombining infrared spectroscopy and vibrational theory. *International Reviews in Physical Chemistry*, **2019**, 38, 115-148	7	17
196	Local Modes of Vibration: The Effect of Low-Frequency Vibrations **2019**, 389-424		0
195	Highly Oxygenated Organic Molecules (HOM) from Gas-Phase Autoxidation Involving Peroxy Radicals: A Key Contributor to Atmospheric Aerosol. *Chemical Reviews*, **2019**, 119, 3472-3509	68.1	262
194	Simulated Electronic Absorption Spectra of Sulfur-Containing Molecules Present in Earth□ Atmosphere. *Journal of Physical Chemistry A*, **2019**, 123, 6605-6617	2.8	7
193	Formation of Highly Oxidized Molecules from NO3 Radical Initiated Oxidation of □-Carene: A Mechanistic Study. *ACS Earth and Space Chemistry*, **2019**, 3, 1460-1470	3.2	13
192	Thermalized Epoxide Formation in the Atmosphere. *Journal of Physical Chemistry A*, **2019**, 123, 10620-10630	2.8	9
191	Accuracy of XH-stretching intensities with the Deng□an potential. *Molecular Physics*, **2019**, 117, 1629-1639	1.7	5
190	Intramolecular Hydrogen Shift Chemistry of Hydroperoxy-Substituted Peroxy Radicals. *Journal of Physical Chemistry A*, **2019**, 123, 590-600	2.8	22
189	The Importance of Peroxy Radical Hydrogen-Shift Reactions in Atmospheric Isoprene Oxidation. *Journal of Physical Chemistry A*, **2019**, 123, 920-932	2.8	41

188	Absolute fundamental and overtone OH and OD stretching intensities of alcohols. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2019**, 208, 315-324	4.4	7
187	Computational and Experimental Evidence of Two Competing Thermal Electrocyclization Pathways for Vinylheptafulvene. *Chemistry - an Asian Journal*, **2019**, 14, 1111-1116	4.5	6
186	Atmospheric Hydroxyl Radical Source: Reaction of Triplet SO and Water. *Journal of Physical Chemistry A*, **2018**, 122, 4465-4469	2.8	22
185	Fundamental FH-stretching transition frequencies and oscillator strengths in hydrogen bonded FH complexes. *Chemical Physics Letters*, **2018**, 692, 291-297	2.5	3
184	Computational Comparison of Different Reagent Ions in the Chemical Ionization of Oxidized Multifunctional Compounds. *Journal of Physical Chemistry A*, **2018**, 122, 269-279	2.8	31
183	Atmospheric autoxidation is increasingly important in urban and suburban North America. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 64-69	11.5	101
182	Quantum Effects for a Proton in a Low-Barrier, Double-Well Potential: Core Level Photoemission Spectroscopy of Acetylacetone. *Journal of Physical Chemistry Letters*, **2018**, 9, 521-526	6.4	13
181	Hybridization of Nitrogen Determines Hydrogen-Bond Acceptor Strength: Gas-Phase Comparison of Redshifts and Equilibrium Constants. *Journal of Physical Chemistry A*, **2018**, 122, 3899-3908	2.8	7
180	Kinetics and Product Yields of the OH Initiated Oxidation of Hydroxymethyl Hydroperoxide. *Journal of Physical Chemistry A*, **2018**, 122, 6292-6302	2.8	19
179	Atmospheric chemistry of hexa- and penta-fluorobenzene: UV photolysis and kinetics and mechanisms of the reactions of Cl atoms and OH radicals. *Physical Chemistry Chemical Physics*, **2018**, 20, 28796-28809	3.6	4
178	Computational Investigation of RO + HO and RO + RO Reactions of Monoterpene Derived First-Generation Peroxy Radicals Leading to Radical Recycling. *Journal of Physical Chemistry A*, **2018**, 122, 9542-9552	2.8	9
177	Calculated Hydrogen Shift Rate Constants in Substituted Alkyl Peroxy Radicals. *Journal of Physical Chemistry A*, **2018**, 122, 8665-8673	2.8	37
176	Reactivity of Electronically Excited SO with Alkanes. *Journal of Physical Chemistry A*, **2018**, 122, 7782-7788	2.8	3
175	Vibrational transitions in hydrogen bonded bimolecular complexes □A local mode perturbation theory approach to transition frequencies and intensities. *Journal of Molecular Spectroscopy*, **2017**, 334, 1-9	1.3	18
174	Kinetic Energy Density as a Predictor of Hydrogen-Bonded OH-Stretching Frequencies. *Journal of Physical Chemistry A*, **2017**, 121, 3452-3460	2.8	20
173	Alkoxy Radical Bond Scissions Explain the Anomalously Low Secondary Organic Aerosol and Organonitrate Yields From □Pinene + NO. *Journal of Physical Chemistry Letters*, **2017**, 8, 2826-2834	6.4	26
172	Side-by-Side Comparison of Hydroperoxide and Corresponding Alcohol as Hydrogen-Bond Donors. *Journal of Physical Chemistry A*, **2017**, 121, 2951-2959	2.8	20
171	Isomerization of Second-Generation Isoprene Peroxy Radicals: Epoxide Formation and Implications for Secondary Organic Aerosol Yields. *Environmental Science & Technology*, **2017**, 51, 4978-4987	10.3	39

170	Subtle differences in the hydrogen bonding of alcohol to divalent oxygen and sulfur. *Chemical Physics Letters*, **2017**, 667, 146-153	2.5	28
169	Towards Storage of Solar Energy in Photochromic Molecules: Benzannulation of the Dihydroazulene/Vinylheptafulvene Couple. *ChemPhotoChem*, **2017**, 1, 206-212	3.3	19
168	Photoswitchable Dihydroazulene Macrocycles for Solar Energy Storage: The Effects of Ring Strain. *Journal of Organic Chemistry*, **2017**, 82, 10398-10407	4.2	23
167	Dimethyl Sulfoxide Complexes Detected at Ambient Conditions. *Journal of Physical Chemistry A*, **2017**, 121, 6046-6053	2.8	5
166	Ultraviolet Spectroscopy of the Gas Phase Hydration of Methylglyoxal. *ACS Earth and Space Chemistry*, **2017**, 1, 345-352	3.2	16
165	The weak fundamental NH-stretching transition in amines. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2017**, 173, 201-206	4.4	7
164	Kinetics and Products of the Reaction of the First-Generation Isoprene Hydroxy Hydroperoxide (ISOPOOH) with OH. *Journal of Physical Chemistry A*, **2016**, 120, 1441-51	2.8	84
163	Spectroscopy and dynamics of double proton transfer in formic acid dimer. *Physical Chemistry Chemical Physics*, **2016**, 18, 24654-62	3.6	36
162	Theoretical Investigation of Substituent Effects on the Dihydroazulene/Vinylheptafulvene Photoswitch: Increasing the Energy Storage Capacity. *Journal of Physical Chemistry A*, **2016**, 120, 9782-9793	2.8	28
161	Intramolecular Hydrogen Bonding in Substituted Aminoalcohols. *Journal of Physical Chemistry A*, **2016**, 120, 6371-8	2.8	34
160	Accurate thermodynamic properties of gas phase hydrogen bonded complexes. *Physical Chemistry Chemical Physics*, **2016**, 18, 23831-9	3.6	17
159	Identification of OSSO as a near-UV absorber in the Venusian atmosphere. *Geophysical Research Letters*, **2016**, 43, 11,146	4.9	45
158	Characterisation of dihydroazulene and vinylheptafulvene derivatives using Raman spectroscopy: The CN-stretching region. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2016**, 161, 70-6	4.4	3
157	On the association of neutral and cationic tris(tetrathiafulvaleno)dodecadehydro[18]annulenes. *Organic and Biomolecular Chemistry*, **2016**, 14, 425-429	3.9	6
156	Rapid Hydrogen Shift Scrambling in Hydroperoxy-Substituted Organic Peroxy Radicals. *Journal of Physical Chemistry A*, **2016**, 120, 266-75	2.8	49
155	Production and Fate of C4 Dihydroxycarbonyl Compounds from Isoprene Oxidation. *Journal of Physical Chemistry A*, **2016**, 120, 106-17	2.8	30
154	Solar Thermal Energy Storage in a Photochromic Macrocycle. *Chemistry - A European Journal*, **2016**, 22, 10796-800	4.8	30
153	Cost-Effective Implementation of Multiconformer Transition State Theory for Peroxy Radical Hydrogen Shift Reactions. *Journal of Physical Chemistry A*, **2016**, 120, 10072-10087	2.8	55

152	Hydroxyl radical-induced formation of highly oxidized organic compounds. *Nature Communications*, **2016**, 7, 13677	17.4	124
151	Infrared spectroscopic probing of dimethylamine clusters in an Ar matrix. *Journal of Environmental Sciences*, **2016**, 40, 51-9	6.4	16
150	Unimolecular HO2 Loss from Peroxy Radicals Formed in Autoxidation Is Unlikely under Atmospheric Conditions. *Journal of Physical Chemistry A*, **2016**, 120, 3588-95	2.8	14
149	Competition between chloride and sulphate during the reformation of calcined hydrotalcite. *Applied Clay Science*, **2016**, 132-133, 650-659	5.2	12
148	Computational methodology study of the optical and thermochemical properties of a molecular photoswitch. *Journal of Physical Chemistry A*, **2015**, 119, 896-904	2.8	45
147	The effect of large amplitude motions on the vibrational intensities in hydrogen bonded complexes. *Journal of Chemical Physics*, **2015**, 142, 094304	3.9	34
146	Mechanism of the hydroxyl radical oxidation of methacryloyl peroxynitrate (MPAN) and its pathway toward secondary organic aerosol formation in the atmosphere. *Physical Chemistry Chemical Physics* , **2015**, 17, 17914-26	3.6	88
145	Theoretical investigation of the hydrogen shift reactions in peroxy radicals derived from the atmospheric decomposition of 3-methyl-3-buten-1-ol (MBO331). *Chemical Physics Letters*, **2015**, 619, 236-240	2.5	16
144	Chemical properties of HULIS from three different environments. *Journal of Atmospheric Chemistry*, **2015**, 72, 65-80	3.2	25
143	Infrared and Near-Infrared Spectroscopy of Acetylacetone and Hexafluoroacetylacetone. *Journal of Physical Chemistry A*, **2015**, 119, 7980-90	2.8	32
142	Unusual Low-Energy Near-Infrared Bands for Ferrocenyl–Naphthalimide Donor–Acceptor Dyads with Aromatic Spacer Groups: Prediction by Time-Dependent DFT and Observation by OTTLE Spectroscopy. *Organometallics*, **2015**, 34, 2662-2666	3.8	11
141	Gas Phase Detection of the NH-P Hydrogen Bond and Importance of Secondary Interactions. *Journal of Physical Chemistry A*, **2015**, 119, 10988-98	2.8	47
140	Intramolecular Hydrogen Bonding in Methyl Lactate. *Journal of Physical Chemistry A*, **2015**, 119, 9692-702	2.8	28
139	Controlling two-step multimode switching of dihydroazulene photoswitches. *Chemistry - A European Journal*, **2015**, 21, 3968-77	4.8	28
138	Interactions between tetrathiafulvalene units in dimeric structures - the influence of cyclic cores. *Beilstein Journal of Organic Chemistry*, **2015**, 11, 930-48	2.5	7
137	Photoabsorption cross-section measurements of 32S, 33S, 34S, and 36S sulfur dioxide from 190 to 220 nm. *Journal of Geophysical Research D: Atmospheres*, **2015**, 120, 2546-2557	4.4	31
136	Towards solar energy storage in the photochromic dihydroazulene-vinylheptafulvene system. *Chemistry - A European Journal*, **2015**, 21, 7454-61	4.8	64
135	Computational Study of Hydrogen Shifts and Ring-Opening Mechanisms in α-Pinene Ozonolysis Products. *Journal of Physical Chemistry A*, **2015**, 119, 11366-75	2.8	66

134	Effects of chemical complexity on the autoxidation mechanisms of endocyclic alkene ozonolysis products: from methylcyclohexenes toward understanding α-pinene. *Journal of Physical Chemistry A*, **2015**, 119, 4633-50	2.8	83
133	Atmospheric fate of methyl vinyl ketone: peroxy radical reactions with NO and HO2. *Journal of Physical Chemistry A*, **2015**, 119, 4562-72	2.8	60
132	Theoretical study, and infrared and Raman spectra of copper(II) chelated complex with dibenzoylmethane. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 128, 272-9	4.4	17
131	The effect of large amplitude motions on the transition frequency redshift in hydrogen bonded complexes: a physical picture. *Journal of Chemical Physics*, **2014**, 140, 184309	3.9	41
130	Identification and characterization of the HCl-DMS gas phase molecular complex via infrared spectroscopy and electronic structure calculations. *Journal of Physical Chemistry A*, **2014**, 118, 1384-9	2.8	47
129	The formation of highly oxidized multifunctional products in the ozonolysis of cyclohexene. *Journal of the American Chemical Society*, **2014**, 136, 15596-606	16.4	187
128	Benchmarking ab initio binding energies of hydrogen-bonded molecular clusters based on FTIR spectroscopy. *Journal of Physical Chemistry A*, **2014**, 118, 5316-22	2.8	48
127	The effect of fluorine substitution in alcohol-amine complexes. *Physical Chemistry Chemical Physics*, **2014**, 16, 22882-91	3.6	57
126	A large source of low-volatility secondary organic aerosol. *Nature*, **2014**, 506, 476-9	50.4	1078
125	Resolving the anomalous infrared spectrum of the MeCN-HCl molecular cluster using ab initio molecular dynamics. *Physical Chemistry Chemical Physics*, **2014**, 16, 24685-90	3.6	7
124	Similar strength of the NH···O and NH···S hydrogen bonds in binary complexes. *Journal of Physical Chemistry A*, **2014**, 118, 11074-82	2.8	47
123	Positively Charged Phosphorus as a Hydrogen Bond Acceptor. *Journal of Physical Chemistry Letters*, **2014**, 5, 4225-31	6.4	82
122	Are Bond Critical Points Really Critical for Hydrogen Bonding?. *Journal of Chemical Theory and Computation*, **2013**, 9, 3263-6	6.4	348
121	Intramolecular interactions in 2-aminoethanol and 3-aminopropanol. *Journal of Physical Chemistry A* , **2013**, 117, 10260-73	2.8	33
120	Criegee Intermediates React with Ozone. *Journal of Physical Chemistry Letters*, **2013**, 4, 2525-2529	6.4	67
119	Autoxidation of Organic Compounds in the Atmosphere. *Journal of Physical Chemistry Letters*, **2013**, 4, 3513-3520	6.4	347
118	Methyl chavicol reactions with ozone, OH and NO3 radicals: Rate constants and gas-phase products. *Atmospheric Environment*, **2013**, 77, 696-702	5.3	14
117	The gas-phase reaction of methane sulfonic acid with the hydroxyl radical without and with water vapor. *Physical Chemistry Chemical Physics*, **2013**, 15, 5140-50	3.6	22

116	Weak intramolecular OH?hydrogen bonding in methallyl- and allyl-carbinol. *Chemical Physics Letters*, **2013**, 582, 31-37	2.5	9
115	Ultrathin reduced graphene oxide films as transparent top-contacts for light switchable solid-state molecular junctions. *Advanced Materials*, **2013**, 25, 4164-70	24	68
114	Fundamental and overtone vibrational spectroscopy, enthalpy of hydrogen bond formation and equilibrium constant determination of the methanol-dimethylamine complex. *Physical Chemistry Chemical Physics*, **2013**, 15, 10194-206	3.6	65
113	Atmospheric fate of methacrolein. 2. Formation of lactone and implications for organic aerosol production. *Journal of Physical Chemistry A*, **2012**, 116, 5763-8	2.8	51
112	Absolute intensities of NH-stretching transitions in dimethylamine and pyrrole. *Journal of Physical Chemistry A*, **2012**, 116, 290-6	2.8	41
111	Atmospheric fate of methacrolein. 1. Peroxy radical isomerization following addition of OH and O2. *Journal of Physical Chemistry A*, **2012**, 116, 5756-62	2.8	145
110	Design aspects of bright red emissive silver nanoclusters/DNA probes for microRNA detection. *ACS Nano*, **2012**, 6, 8803-14	16.7	163
109	On the possible catalysis by single water molecules of gas-phase hydrogen abstraction reactions by OH radicals. *Physical Chemistry Chemical Physics*, **2012**, 14, 12992-9	3.6	28
108	Peroxy radical chemistry and OH radical production during the NO₃-initiated oxidation of isoprene. *Atmospheric Chemistry and Physics*, **2012**, 12, 7499-7515	6.8	57
107	Identification of the dimethylamine-trimethylamine complex in the gas phase. *Journal of Chemical Physics*, **2012**, 136, 184305	3.9	54
106	Intramolecular OH interactions in alkenols and alkynols. *Physical Chemistry Chemical Physics*, **2011**, 13, 14183-93	3.6	43
105	A computational study of the oxidation of SO2 to SO3 by gas-phase organic oxidants. *Journal of Physical Chemistry A*, **2011**, 115, 8669-81	2.8	77
104	Definition of the hydrogen bond (IUPAC Recommendations 2011). *Pure and Applied Chemistry*, **2011**, 83, 1637-1641	2.1	1111
103	Defining the hydrogen bond: An account (IUPAC Technical Report). *Pure and Applied Chemistry*, **2011**, 83, 1619-1636	2.1	738
102	Fourier transform infrared spectroscopy and theoretical study of dimethylamine dimer in the gas phase. *Journal of Physical Chemistry A*, **2011**, 115, 12097-104	2.8	57
101	Ultraviolet absorption cross sections of carbonyl sulfide isotopologues OC³²S, OC³³S, OC³⁴S and O¹³CS: isotopic fractionation in photolysis and atmospheric implications. *Atmospheric Chemistry and Physics*, **2011**, 11, 10293-10303	6.8	41
100	Widening of the hydrogen bonded OH-streching bands due to the wagging and OO-stretching modes in H2OH2O. *Chemical Physics Letters*, **2011**, 513, 167-172	2.5	12
99	Peroxy radical isomerization in the oxidation of isoprene. *Physical Chemistry Chemical Physics*, **2011**, 13, 13607-13	3.6	267

98	XH-stretching overtone transitions calculated using explicitly correlated coupled cluster methods. *Journal of Chemical Physics*, **2010**, 132, 174304	3.9	37
97	Comment on "Unexpected epoxide formation in the gas-phase photooxidation of isoprene". *Science*, **2010**, 327, 644; author reply 644	33.3	1
96	Calculated spectroscopy and atmospheric photodissociation of phosphoric acid. *Journal of Physical Chemistry A*, **2010**, 114, 7544-52	2.8	12
95	Computational vibrational and electronic spectroscopy of the water nitric oxide complex. *Journal of Physical Chemistry A*, **2010**, 114, 4835-42	2.8	11
94	Nitrate radical addition-elimination reactions of atmospherically relevant sulfur-containing molecules. *Physical Chemistry Chemical Physics*, **2010**, 12, 12833-9	3.6	8
93	Effect of hydration on the hydrogen abstraction reaction by HO in DMS and its oxidation products. *Journal of Physical Chemistry A*, **2010**, 114, 4857-63	2.8	51
92	Overtone spectra of 2-mercaptoethanol and 1,2-ethanedithiol. *Journal of Physical Chemistry A*, **2010**, 114, 12692-700	2.8	13
91	Molecular dynamic simulations of OH-stretching overtone induced photodissociation of fluorosulfonic and chlorosulfonic acid. *Physical Chemistry Chemical Physics*, **2010**, 12, 8277-84	3.6	7
90	Calculated two-photon electronic transitions in sulfuric acid and its atmospheric relevance. *Chemical Physics Letters*, **2010**, 498, 18-21	2.5	1
89	Explicitly correlated intermolecular distances and interaction energies of hydrogen bonded complexes. *Journal of Chemical Physics*, **2009**, 131, 034307	3.9	87
88	Unexpected epoxide formation in the gas-phase photooxidation of isoprene. *Science*, **2009**, 325, 730-3	33.3	726
87	Co(III) complexes of the type [(L)Co(O2CO)]+ (L = tripodal tetraamine ligand): Synthesis, structure, DFT calculations and 59Co NMR. *Polyhedron*, **2009**, 28, 1459-1468	2.7	7
86	Calculation of conformationally weighted dipole moments useful in ion□olecule collision rate estimates. *Chemical Physics Letters*, **2009**, 474, 45-50	2.5	35
85	Identification of the water amidogen radical complex. *Journal of the American Chemical Society*, **2009**, 131, 1358-9	16.4	19
84	Calculation of overtone O-H stretching bands and intensities of the water trimer. *Journal of Physical Chemistry A*, **2009**, 113, 9124-32	2.8	35
83	SH-stretching vibrational spectra of ethanethiol and tert-butylthiol. *Journal of Physical Chemistry A*, **2009**, 113, 7576-83	2.8	31
82	Isoprene photooxidation: new insights into the production of acids and organic nitrates. *Atmospheric Chemistry and Physics*, **2009**, 9, 1479-1501	6.8	391
81	Atmospheric Photolysis of Sulfuric Acid. *Advances in Quantum Chemistry*, **2008**, 55, 137-158	1.4	15

80	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
79	Hydrogen bonding to divalent sulfur. *Physical Chemistry Chemical Physics*, **2008**, 10, 4113-8	3.6	84
78	Calculated electronic transitions in sulfuric acid and implications for its photodissociation in the atmosphere. *Journal of Physical Chemistry A*, **2008**, 112, 4958-64	2.8	29
77	Calculation of the O-H stretching vibrational overtone spectrum of the water dimer. *Journal of Physical Chemistry A*, **2008**, 112, 6305-12	2.8	57
76	Calculated band profiles of the OH-stretching transitions in water dimer. *Journal of Physical Chemistry A*, **2008**, 112, 7439-47	2.8	31
75	Calculated electronic transitions of the water ammonia complex. *Journal of Chemical Physics*, **2008**, 128, 034302	3.9	22
74	The most stable conformer of benzyl alcohol. *Chemical Physics Letters*, **2008**, 466, 21-26	2.5	20
73	Redox chemistry of an ethenyl complex with isolobal CbCo and CpFe fragments. *Inorganica Chimica Acta*, **2008**, 361, 1616-1623	2.7	15
72	Hydrogen bonded OH-stretching vibration in the water dimer. *Journal of Physical Chemistry A*, **2007**, 111, 567-72	2.8	84
71	Fluorosulfonic acid and chlorosulfonic acid: possible candidates for OH-stretching overtone-induced photodissociation. *Journal of Physical Chemistry A*, **2007**, 111, 9707-13	2.8	15
70	Vibrational overtone spectroscopy of three-membered rings. *Journal of Physical Chemistry A*, **2007**, 111, 5415-21	2.8	6
69	Overtone spectroscopy of sulfonic acid derivatives. *Journal of Physical Chemistry A*, **2007**, 111, 5434-40	2.8	34
68	Vibrational OH-stretching overtone spectroscopy of jet-cooled resorcinol and hydroquinone rotamers. *Journal of Physical Chemistry A*, **2007**, 111, 6028-33	2.8	13
67	Accumulation of lipophilic dications by mitochondria and cells. *Biochemical Journal*, **2006**, 400, 199-208	3.8	94
66	Counterpoise corrected geometries of hydrated complexes. *Journal of Chemical Physics*, **2006**, 125, 144317	3.9	34
65	The lowest $^2A''$ excited state of the water-hydroxyl complex. *Journal of Chemical Physics*, **2006**, 125, 204302	3.9	28
64	CH-stretching overtone spectra of cis- and trans-1,3-pentadiene. *Journal of Physical Chemistry A*, **2006**, 110, 913-20	2.8	6
63	OH-stretch vibrational spectroscopy of hydroxymethyl hydroperoxide. *Journal of Physical Chemistry A*, **2006**, 110, 7072-9	2.8	26

62	Vibrational overtone spectroscopy of phenol and its deuterated isotopomers. *Journal of Physical Chemistry A*, **2006**, 110, 7345-54	2.8	36
61	Vapor phase near infrared spectroscopy of the hydrogen bonded methanol-trimethylamine complex. *Journal of Physical Chemistry A*, **2006**, 110, 9597-601	2.8	53
60	Influence of intramolecular hydrogen bond strength on OH-stretching overtones. *Journal of Physical Chemistry A*, **2006**, 110, 10245-50	2.8	80
59	Infrared identification of matrix isolated H2O.O2. *Journal of Physical Chemistry A*, **2005**, 109, 4274-9	2.8	18
58	Absolute intensities of CH stretching overtones in alkenes. *Journal of Physical Chemistry A*, **2005**, 109, 1033-41	2.8	31
57	CH-stretching overtone spectroscopy of 1,1,1,2-tetrafluoroethane. *Journal of Physical Chemistry A*, **2005**, 109, 5323-31	2.8	11
56	Effect of OH internal torsion on the OH-stretching spectrum of cis,cis-HOONO. *Journal of Physical Chemistry A*, **2005**, 109, 1810-4	2.8	11
55	Photolysis of sulfuric acid vapor by visible light as a source of the polar stratospheric CN layer. *Journal of Geophysical Research*, **2005**, 110,		38
54	Weak intramolecular interactions in ethylene glycol identified by vapor phase OH-stretching overtone spectroscopy. *Journal of the American Chemical Society*, **2005**, 127, 17096-103	16.4	125
53	The OH-stretching and OOH-bending overtone spectrum of HOONO. *Journal of Chemical Physics*, **2005**, 123, 134318	3.9	18
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