

# Henrik G Kjaergaard

## List of Publications by Citations

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223  
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54  
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239  
ext. papers

14,616  
ext. citations

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6.46  
L-index

#	Paper	IF	Citations
223	Definition of the hydrogen bond (IUPAC Recommendations 2011). <i>Pure and Applied Chemistry</i> , <b>2011</b> , 83, 1637-1641	2.1	1111
222	A large source of low-volatility secondary organic aerosol. <i>Nature</i> , <b>2014</b> , 506, 476-9	50.4	1078
221	Defining the hydrogen bond: An account (IUPAC Technical Report). <i>Pure and Applied Chemistry</i> , <b>2011</b> , 83, 1619-1636	2.1	738
220	Unexpected epoxide formation in the gas-phase photooxidation of isoprene. <i>Science</i> , <b>2009</b> , 325, 730-3	33.3	726
219	Isoprene photooxidation: new insights into the production of acids and organic nitrates. <i>Atmospheric Chemistry and Physics</i> , <b>2009</b> , 9, 1479-1501	6.8	391
218	Are Bond Critical Points Really Critical for Hydrogen Bonding?. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 3263-6	6.4	348
217	Autoxidation of Organic Compounds in the Atmosphere. <i>Journal of Physical Chemistry Letters</i> , <b>2013</b> , 4, 3513-3520	6.4	347
216	Peroxy radical isomerization in the oxidation of isoprene. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 13607-13	3.6	267
215	Highly Oxygenated Organic Molecules (HOM) from Gas-Phase Autoxidation Involving Peroxy Radicals: A Key Contributor to Atmospheric Aerosol. <i>Chemical Reviews</i> , <b>2019</b> , 119, 3472-3509	68.1	262
214	The formation of highly oxidized multifunctional products in the ozonolysis of cyclohexene. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 15596-606	16.4	187
213	Calculation of OH-stretching band intensities of the water dimer and trimer. <i>Journal of Chemical Physics</i> , <b>1999</b> , 110, 9104-9115	3.9	168
212	Design aspects of bright red emissive silver nanoclusters/DNA probes for microRNA detection. <i>ACS Nano</i> , <b>2012</b> , 6, 8803-14	16.7	163
211	Calculation of vibrational transition frequencies and intensities in water dimer: comparison of different vibrational approaches. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 4324-35	2.8	149
210	Photolysis of sulfuric acid vapor by visible solar radiation. <i>Science</i> , <b>2003</b> , 299, 1566-8	33.3	147
209	Atmospheric fate of methacrolein. 1. Peroxy radical isomerization following addition of OH and O <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 5756-62	2.8	145
208	Hydrated Complexes: Relevance to Atmospheric Chemistry and Climate. <i>International Reviews in Physical Chemistry</i> , <b>2003</b> , 22, 203-219	7	128
207	Weak intramolecular interactions in ethylene glycol identified by vapor phase OH-stretching overtone spectroscopy. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 17096-103	16.4	125

206	Calculated OH-stretching and HOH-bending vibrational transitions in the water dimer. <i>Physical Chemistry Chemical Physics</i> , <b>2003</b> , 5, 3100	3.6	124
205	Hydroxyl radical-induced formation of highly oxidized organic compounds. <i>Nature Communications</i> , <b>2016</b> , 7, 13677	17.4	124
204	Intensities in local mode overtone spectra: Propane. <i>Journal of Chemical Physics</i> , <b>1990</b> , 93, 6239-6248	3.9	122
203	Vibrational and Electronic Spectroscopy of Sulfuric Acid Vapor. <i>Journal of Physical Chemistry A</i> , <b>2003</b> , 107, 1112-1118	2.8	102
202	Atmospheric autoxidation is increasingly important in urban and suburban North America. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2018</b> , 115, 64-69	11.5	101
201	Complexes of Importance to the Absorption of Solar Radiation. <i>Journal of Physical Chemistry A</i> , <b>2003</b> , 107, 10680-10686	2.8	100
200	Calculation of vibrational fundamental and overtone band intensities of H <sub>2</sub> O. <i>Journal of Chemical Physics</i> , <b>1994</b> , 100, 6228-6239	3.9	100
199	Accumulation of lipophilic dications by mitochondria and cells. <i>Biochemical Journal</i> , <b>2006</b> , 400, 199-208	3.8	94
198	The relative intensity contributions of axial and equatorial CH bonds in the local mode overtone spectra of cyclohexane. <i>Journal of Chemical Physics</i> , <b>1992</b> , 96, 4841-4851	3.9	94
197	Local modes. <i>Canadian Journal of Chemistry</i> , <b>2002</b> , 80, 1635-1642	0.9	91
196	Infrared measurements and calculations on H <sub>2</sub> O.HO. <i>Journal of the American Chemical Society</i> , <b>2003</b> , 125, 6048-9	16.4	89
195	Mechanism of the hydroxyl radical oxidation of methacryloyl peroxyxynitrate (MPAN) and its pathway toward secondary organic aerosol formation in the atmosphere. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 17914-26	3.6	88
194	Explicitly correlated intermolecular distances and interaction energies of hydrogen bonded complexes. <i>Journal of Chemical Physics</i> , <b>2009</b> , 131, 034307	3.9	87
193	Kinetics and Products of the Reaction of the First-Generation Isoprene Hydroxy Hydroperoxide (ISOPOOH) with OH. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 1441-51	2.8	84
192	Hydrogen bonding to divalent sulfur. <i>Physical Chemistry Chemical Physics</i> , <b>2008</b> , 10, 4113-8	3.6	84
191	Hydrogen bonded OH-stretching vibration in the water dimer. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 567-72	2.8	84
190	Effects of chemical complexity on the autoxidation mechanisms of endocyclic alkene ozonolysis products: from methylcyclohexenes toward understanding $\alpha$ -pinene. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 4633-50	2.8	83
189	Positively Charged Phosphorus as a Hydrogen Bond Acceptor. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 4225-31	6.4	82

188	Influence of intramolecular hydrogen bond strength on OH-stretching overtones. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 10245-50	2.8	80
187	Intensities of CH- and CD-stretching overtones in 1,3-butadiene and 1,3-butadiene-d6. <i>Journal of Chemical Physics</i> , <b>1993</b> , 99, 9438-9452	3.9	79
186	A computational study of the oxidation of SO <sub>2</sub> to SO <sub>3</sub> by gas-phase organic oxidants. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 8669-81	2.8	77
185	Calculated OH-Stretching Vibrational Transitions in the Water-Nitrogen and Water-Oxygen Complexes. <i>Journal of Physical Chemistry A</i> , <b>2002</b> , 106, 8955-8962	2.8	69
184	OH- and CH-Stretching Overtone Spectra of Catechol. <i>Journal of Physical Chemistry A</i> , <b>2002</b> , 106, 258-266	6.8	69
183	Ultrathin reduced graphene oxide films as transparent top-contacts for light switchable solid-state molecular junctions. <i>Advanced Materials</i> , <b>2013</b> , 25, 4164-70	24	68
182	Criegee Intermediates React with Ozone. <i>Journal of Physical Chemistry Letters</i> , <b>2013</b> , 4, 2525-2529	6.4	67
181	Computational Study of Hydrogen Shifts and Ring-Opening Mechanisms in $\alpha$ -Pinene Ozonolysis Products. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 11366-75	2.8	66
180	Fundamental and overtone vibrational spectroscopy, enthalpy of hydrogen bond formation and equilibrium constant determination of the methanol-dimethylamine complex. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 10194-206	3.6	65
179	Towards solar energy storage in the photochromic dihydroazulene-vinylheptafulvene system. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 7454-61	4.8	64
178	Intensities in local mode overtone spectra of dimethyl ether and acetone. <i>Journal of Chemical Physics</i> , <b>1991</b> , 94, 5844-5854	3.9	64
177	Comparison of the Morse and Deng-Fan potentials for X-H bonds in small molecules. <i>Molecular Physics</i> , <b>2003</b> , 101, 2285-2294	1.7	63
176	Global airborne sampling reveals a previously unobserved dimethyl sulfide oxidation mechanism in the marine atmosphere. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2020</b> , 117, 4505-4510	11.5	61
175	Atmospheric fate of methyl vinyl ketone: peroxy radical reactions with NO and HO <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 4562-72	2.8	60
174	The effect of fluorine substitution in alcohol-amine complexes. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 22882-91	3.6	57
173	Fourier transform infrared spectroscopy and theoretical study of dimethylamine dimer in the gas phase. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 12097-104	2.8	57
172	Peroxy radical chemistry and OH radical production during the NO <sub>3</sub> -initiated oxidation of isoprene. <i>Atmospheric Chemistry and Physics</i> , <b>2012</b> , 12, 7499-7515	6.8	57
171	Calculation of the O-H stretching vibrational overtone spectrum of the water dimer. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 6305-12	2.8	57

170	Cost-Effective Implementation of Multiconformer Transition State Theory for Peroxy Radical Hydrogen Shift Reactions. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 10072-10087	2.8	55
169	Identification of the dimethylamine-trimethylamine complex in the gas phase. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 184305	3.9	54
168	Vapor phase near infrared spectroscopy of the hydrogen bonded methanol-trimethylamine complex. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 9597-601	2.8	53
167	Calculation of vibrational (J=0) excitation energies and band intensities of formaldehyde using the recursive residue generation method. <i>Journal of Chemical Physics</i> , <b>1996</b> , 104, 7807-7820	3.9	52
166	Atmospheric fate of methacrolein. 2. Formation of lactone and implications for organic aerosol production. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 5763-8	2.8	51
165	Effect of hydration on the hydrogen abstraction reaction by HO in DMS and its oxidation products. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 4857-63	2.8	51
164	Calculated OH-Stretching Vibrational Transitions of the Water-Nitric Acid Complex. <i>Journal of Physical Chemistry A</i> , <b>2002</b> , 106, 2979-2987	2.8	51
163	Ab initio calculation of dipole moment functions: application to vibrational band intensities of H <sub>2</sub> O. <i>Molecular Physics</i> , <b>1994</b> , 83, 1099-1116	1.7	50
162	Rapid Hydrogen Shift Scrambling in Hydroperoxy-Substituted Organic Peroxy Radicals. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 266-75	2.8	49
161	Benchmarking ab initio binding energies of hydrogen-bonded molecular clusters based on FTIR spectroscopy. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 5316-22	2.8	48
160	Gas Phase Detection of the NH-P Hydrogen Bond and Importance of Secondary Interactions. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 10988-98	2.8	47
159	Identification and characterization of the HCl-DMS gas phase molecular complex via infrared spectroscopy and electronic structure calculations. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 1384-9	2.8	47
158	Similar strength of the NH...O and NH...S hydrogen bonds in binary complexes. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 11074-82	2.8	47
157	Computational methodology study of the optical and thermochemical properties of a molecular photoswitch. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 896-904	2.8	45
156	Identification of OSSO as a near-UV absorber in the Venusian atmosphere. <i>Geophysical Research Letters</i> , <b>2016</b> , 43, 11,146	4.9	45
155	The role of electron correlation on calculated XH-stretching vibrational band intensities. <i>Molecular Physics</i> , <b>1997</b> , 90, 201-213	1.7	45
154	Unimolecular Reactions of Peroxy Radicals Formed in the Oxidation of $\alpha$ -Pinene and $\beta$ -Pinene by Hydroxyl Radicals. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 1661-1674	2.8	43
153	Intramolecular OH... interactions in alkenols and alkynols. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 14183-93	3.6	43

152	The effect of large amplitude motions on the transition frequency redshift in hydrogen bonded complexes: a physical picture. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 184309	3.9	41
151	Absolute intensities of NH-stretching transitions in dimethylamine and pyrrole. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 290-6	2.8	41
150	Ultraviolet absorption cross sections of carbonyl sulfide isotopologues $^{32}\text{S}$ , $^{33}\text{S}$ , $^{34}\text{S}$ and $^{13}\text{C}$ : isotopic fractionation in photolysis and atmospheric implications. <i>Atmospheric Chemistry and Physics</i> , <b>2011</b> , 11, 10293-10303	6.8	41
149	High-level ab initio studies of the electronic excited states of the hydroxyl radical and water-hydroxyl complex. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 6930-4	3.9	41
148	Internal Methyl Rotation in the CH Stretching Overtone Spectra of ortho-, meta-, and para-Xylene. <i>Journal of Physical Chemistry A</i> , <b>2002</b> , 106, 6242-6253	2.8	41
147	The Importance of Peroxy Radical Hydrogen-Shift Reactions in Atmospheric Isoprene Oxidation. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 920-932	2.8	41
146	Intensity of CH- and NH-stretching transitions in the overtone spectra of cyclopropylamine. <i>Journal of Chemical Physics</i> , <b>1993</b> , 99, 5682-5700	3.9	40
145	Isomerization of Second-Generation Isoprene Peroxy Radicals: Epoxide Formation and Implications for Secondary Organic Aerosol Yields. <i>Environmental Science &amp; Technology</i> , <b>2017</b> , 51, 4978-4987	10.3	39
144	Methyl versus Aryl CH and CD Stretching Overtone Intensities in the Vapor Phase Spectra of Toluenes. <i>Journal of Physical Chemistry A</i> , <b>1997</b> , 101, 2589-2596	2.8	39
143	Hydrogen-bonded rotamers of 2,4,6-trihydroxy-3-formylidihydrochalcone, an intermediate in the synthesis of a dihydrochalcone from <i>Leptospermum recurvum</i> . <i>Tetrahedron</i> , <b>2003</b> , 59, 6113-6120	2.4	39
142	Photolysis of sulfuric acid vapor by visible light as a source of the polar stratospheric CN layer. <i>Journal of Geophysical Research</i> , <b>2005</b> , 110,		38
141	CH Stretching Overtone Spectra and Intensities of Vapor Phase Naphthalene. <i>The Journal of Physical Chemistry</i> , <b>1995</b> , 99, 899-904		38
140	XH-stretching overtone transitions calculated using explicitly correlated coupled cluster methods. <i>Journal of Chemical Physics</i> , <b>2010</b> , 132, 174304	3.9	37
139	Calculated intensity in the local mode overtone spectra of hydrogen peroxide. <i>Journal of Chemical Physics</i> , <b>1991</b> , 95, 5556-5564	3.9	37
138	Calculated Hydrogen Shift Rate Constants in Substituted Alkyl Peroxy Radicals. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 8665-8673	2.8	37
137	Spectroscopy and dynamics of double proton transfer in formic acid dimer. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 24654-62	3.6	36
136	CH-stretching overtone spectra and internal methyl rotation in 2,6-difluorotoluene. <i>Journal of Chemical Physics</i> , <b>1997</b> , 107, 691-701	3.9	36
135	Vibrational overtone spectroscopy of phenol and its deuterated isotopomers. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 7345-54	2.8	36

134	Calculation of conformationally weighted dipole moments useful in ion-molecule collision rate estimates. <i>Chemical Physics Letters</i> , <b>2009</b> , 474, 45-50	2.5	35
133	Calculation of overtone O-H stretching bands and intensities of the water trimer. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 9124-32	2.8	35
132	The effect of large amplitude motions on the vibrational intensities in hydrogen bonded complexes. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 094304	3.9	34
131	Intramolecular Hydrogen Bonding in Substituted Aminoalcohols. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 6371-8	2.8	34
130	Overtone spectroscopy of sulfonic acid derivatives. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 5434-40	2.8	34
129	Counterpoise corrected geometries of hydrated complexes. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 14433-7	3.7	34
128	Intramolecular interactions in 2-aminoethanol and 3-aminopropanol. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 10260-73	2.8	33
127	Infrared and Near-Infrared Spectroscopy of Acetylacetone and Hexafluoroacetylacetone. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 7980-90	2.8	32
126	Computational Comparison of Different Reagent Ions in the Chemical Ionization of Oxidized Multifunctional Compounds. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 269-279	2.8	31
125	Photoabsorption cross-section measurements of 32S, 33S, 34S, and 36S sulfur dioxide from 190 to 220 nm. <i>Journal of Geophysical Research D: Atmospheres</i> , <b>2015</b> , 120, 2546-2557	4.4	31
124	SH-stretching vibrational spectra of ethanethiol and tert-butylthiol. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 7576-83	2.8	31
123	Calculated band profiles of the OH-stretching transitions in water dimer. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 7439-47	2.8	31
122	Absolute intensities of CH stretching overtones in alkenes. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 1033-41	2.8	31
121	Calculation of dipole moment functions with density functional theory: application to vibrational band intensities. <i>Molecular Physics</i> , <b>1999</b> , 96, 1125-1138	1.7	31
120	Production and Fate of C4 Dihydroxycarbonyl Compounds from Isoprene Oxidation. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 106-17	2.8	30
119	Solar Thermal Energy Storage in a Photochromic Macrocycle. <i>Chemistry - A European Journal</i> , <b>2016</b> , 22, 10796-800	4.8	30
118	Calculated electronic transitions in sulfuric acid and implications for its photodissociation in the atmosphere. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 4958-64	2.8	29
117	Atmospheric water vapor complexes and the continuum. <i>Geophysical Research Letters</i> , <b>2004</b> , 31, n/a-n/a	4.9	29

116	High level ab initio studies of the excited states of sulfuric acid and sulfur trioxide. <i>Journal of Chemical Physics</i> , <b>2003</b> , 118, 7226	3.9	29
115	Calculated CH-Stretching Overtone Spectra of Naphthalene, Anthracene and Their Cations. <i>Journal of Physical Chemistry A</i> , <b>2000</b> , 104, 11297-11303	2.8	29
114	Subtle differences in the hydrogen bonding of alcohol to divalent oxygen and sulfur. <i>Chemical Physics Letters</i> , <b>2017</b> , 667, 146-153	2.5	28
113	Intramolecular Hydrogen Bonding in Methyl Lactate. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 9692-7028	2.8	28
112	Theoretical Investigation of Substituent Effects on the Dihydroazulene/Vinylheptafulvene Photoswitch: Increasing the Energy Storage Capacity. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 9782-9793	2.8	28
111	Controlling two-step multimode switching of dihydroazulene photoswitches. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 3968-77	4.8	28
110	On the possible catalysis by single water molecules of gas-phase hydrogen abstraction reactions by OH radicals. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 12992-9	3.6	28
109	The lowest 2A <sub>1</sub> excited state of the water-hydroxyl complex. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 204302	3.0	28
108	Resonance coupling in the fourth OH-stretching overtone spectrum of formic acid. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 136-40	3.9	28
107	Vibrational Overtone Spectroscopy of Jet-Cooled Aminophenols as a Probe for Rotational Isomers. <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 4420-4427	2.8	28
106	Intensities of CH-stretching overtones in 2-butenes. <i>Chemical Physics</i> , <b>1995</b> , 195, 129-141	2.3	28
105	Alkoxy Radical Bond Scissions Explain the Anomalously Low Secondary Organic Aerosol and Organonitrate Yields From $\alpha$ -Pinene + NO. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 2826-2834	6.4	26
104	OH-stretch vibrational spectroscopy of hydroxymethyl hydroperoxide. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 7072-9	2.8	26
103	Chemical properties of HULIS from three different environments. <i>Journal of Atmospheric Chemistry</i> , <b>2015</b> , 72, 65-80	3.2	25
102	CH Stretching Overtone Investigation of Relative CH Bond Lengths in Pyridine. <i>The Journal of Physical Chemistry</i> , <b>1996</b> , 100, 19273-19279		24
101	Photoswitchable Dihydroazulene Macrocycles for Solar Energy Storage: The Effects of Ring Strain. <i>Journal of Organic Chemistry</i> , <b>2017</b> , 82, 10398-10407	4.2	23
100	Internal Methyl Rotation in the CH Stretching Overtone Spectra of Toluene- $d_2$ , - $d_1$ , and - $d_0$ . <i>Journal of Physical Chemistry A</i> , <b>2000</b> , 104, 6398-6405	2.8	23
99	Atmospheric Hydroxyl Radical Source: Reaction of Triplet SO and Water. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 4465-4469	2.8	22



98	The gas-phase reaction of methane sulfonic acid with the hydroxyl radical without and with water vapor. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 5140-50	3.6	22
97	Calculated electronic transitions of the water ammonia complex. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 034302	3.9	22
96	Effect of the Methyl Internal Rotation Barrier Height on CH <sub>3</sub> Stretching Overtone Spectra. <i>Journal of Physical Chemistry A</i> , <b>2003</b> , 107, 4607-4611	2.8	22
95	Dependence of an Acoustically Nonresonant Intracavity Photoacoustic Signal on Sample and Buffer Gas Pressure. <i>The Journal of Physical Chemistry</i> , <b>1995</b> , 99, 6327-6332		22
94	Intramolecular Hydrogen Shift Chemistry of Hydroperoxy-Substituted Peroxy Radicals. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 590-600	2.8	22
93	Measurement of ultraweak transitions in the visible region of molecular oxygen. <i>Journal of Molecular Spectroscopy</i> , <b>2004</b> , 228, 83-91	1.3	21
92	Kinetic Energy Density as a Predictor of Hydrogen-Bonded OH-Stretching Frequencies. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 3452-3460	2.8	20
91	Side-by-Side Comparison of Hydroperoxide and Corresponding Alcohol as Hydrogen-Bond Donors. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 2951-2959	2.8	20
90	The most stable conformer of benzyl alcohol. <i>Chemical Physics Letters</i> , <b>2008</b> , 466, 21-26	2.5	20
89	The effect of NH <sub>2</sub> -inversion tunneling splitting on the NH-stretching overtone spectra of aniline vapour. <i>Physical Chemistry Chemical Physics</i> , <b>2004</b> , 6, 719	3.6	20
88	Towards Storage of Solar Energy in Photochromic Molecules: Benzannulation of the Dihydroazulene/Vinylheptafulvene Couple. <i>ChemPhotoChem</i> , <b>2017</b> , 1, 206-212	3.3	19
87	Kinetics and Product Yields of the OH Initiated Oxidation of Hydroxymethyl Hydroperoxide. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 6292-6302	2.8	19
86	Identification of the water amidogen radical complex. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 1358-9	16.4	19
85	Vibrational transitions in hydrogen bonded bimolecular complexes I: A local mode perturbation theory approach to transition frequencies and intensities. <i>Journal of Molecular Spectroscopy</i> , <b>2017</b> , 334, 1-9	1.3	18
84	Double Bonds Are Key to Fast Unimolecular Reactivity in First-Generation Monoterpene Hydroxy Peroxy Radicals. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 2885-2896	2.8	18
83	Infrared identification of matrix isolated H <sub>2</sub> O.O <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 4274-9	2.8	18
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