Henrik G Kjaergaard

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5877454/publications.pdf

Version: 2024-02-01

226 papers	15,931 citations	25014 57 h-index	20943 115 g-index
240 all docs	240 docs citations	240 times ranked	11014 citing authors

#	Article	IF	Citations
1	Definition of the hydrogen bond (IUPAC Recommendations 2011). Pure and Applied Chemistry, 2011, 83, 1637-1641.	0.9	1,449
2	A large source of low-volatility secondary organic aerosol. Nature, 2014, 506, 476-479.	13.7	1,448
3	Defining the hydrogen bond: An account (IUPAC Technical Report). Pure and Applied Chemistry, 2011, 83, 1619-1636.	0.9	856
4	Unexpected Epoxide Formation in the Gas-Phase Photooxidation of Isoprene. Science, 2009, 325, 730-733.	6.0	837
5	Highly Oxygenated Organic Molecules (HOM) from Gas-Phase Autoxidation Involving Peroxy Radicals: A Key Contributor to Atmospheric Aerosol. Chemical Reviews, 2019, 119, 3472-3509.	23.0	460
6	Isoprene photooxidation: new insights into the production of acids and organic nitrates. Atmospheric Chemistry and Physics, 2009, 9, 1479-1501.	1.9	450
7	Autoxidation of Organic Compounds in the Atmosphere. Journal of Physical Chemistry Letters, 2013, 4, 3513-3520.	2.1	444
8	Are Bond Critical Points Really Critical for Hydrogen Bonding?. Journal of Chemical Theory and Computation, 2013, 9, 3263-3266.	2.3	414
9	Peroxy radical isomerization in the oxidation of isoprene. Physical Chemistry Chemical Physics, 2011, 13, 13607.	1.3	302
10	The Formation of Highly Oxidized Multifunctional Products in the Ozonolysis of Cyclohexene. Journal of the American Chemical Society, 2014, 136, 15596-15606.	6.6	236
11	Hydroxyl radical-induced formation of highly oxidized organic compounds. Nature Communications, 2016, 7, 13677.	5.8	178
12	Design Aspects of Bright Red Emissive Silver Nanoclusters/DNA Probes for MicroRNA Detection. ACS Nano, 2012, 6, 8803-8814.	7.3	177
13	Calculation of OH-stretching band intensities of the water dimer and trimer. Journal of Chemical Physics, 1999, 110, 9104-9115.	1.2	171
14	Atmospheric Fate of Methacrolein. 1. Peroxy Radical Isomerization Following Addition of OH and O₂. Journal of Physical Chemistry A, 2012, 116, 5756-5762.	1.1	166
15	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
16	Photolysis of Sulfuric Acid Vapor by Visible Solar Radiation. Science, 2003, 299, 1566-1568.	6.0	155
17	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.	3.3	149
18	Hydrated Complexes: Relevance to Atmospheric Chemistry and Climate. International Reviews in Physical Chemistry, 2003, 22, 203-219.	0.9	140

#	Article	IF	Citations
19	Calculated OH-stretching and HOH-bending vibrational transitions in the water dimer. Physical Chemistry Chemical Physics, 2003, 5, 3100.	1.3	139
20	Weak Intramolecular Interactions in Ethylene Glycol Identified by Vapor Phase OHâ"Stretching Overtone Spectroscopy. Journal of the American Chemical Society, 2005, 127, 17096-17103.	6.6	135
21	Intensities in local mode overtone spectra: Propane. Journal of Chemical Physics, 1990, 93, 6239-6248.	1.2	128
22	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.	3.3	118
23	Calculation of vibrational fundamental and overtone band intensities of H2O. Journal of Chemical Physics, 1994, 100, 6228-6239.	1.2	112
24	Kinetics and Products of the Reaction of the First-Generation Isoprene Hydroxy Hydroperoxide (ISOPOOH) with OH. Journal of Physical Chemistry A, 2016, 120, 1441-1451.	1.1	111
25	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, 17914-17926.	1.3	108
26	Vibrational and Electronic Spectroscopy of Sulfuric Acid Vapor. Journal of Physical Chemistry A, 2003, 107, 1112-1118.	1.1	107
27	Complexes of Importance to the Absorption of Solar Radiationâ€. Journal of Physical Chemistry A, 2003, 107, 10680-10686.	1.1	105
28	Accumulation of lipophilic dications by mitochondria and cells. Biochemical Journal, 2006, 400, 199-208.	1.7	105
29	Effects of Chemical Complexity on the Autoxidation Mechanisms of Endocyclic Alkene Ozonolysis Products: From Methylcyclohexenes toward Understanding Î±-Pinene. Journal of Physical Chemistry A, 2015, 119, 4633-4650.	1.1	101
30	The relative intensity contributions of axial and equatorial CH bonds in the local mode overtone spectra of cyclohexane. Journal of Chemical Physics, 1992, 96, 4841-4851.	1.2	98
31	Hydrogen bonding to divalent sulfur. Physical Chemistry Chemical Physics, 2008, 10, 4113.	1.3	97
32	Local modes. Canadian Journal of Chemistry, 2002, 80, 1635-1642.	0.6	94
33	A Computational Study of the Oxidation of SO₂ to SO₃ by Gas-Phase Organic Oxidants. Journal of Physical Chemistry A, 2011, 115, 8669-8681.	1.1	93
34	Infrared Measurements and Calculations on H2OÂ·HO. Journal of the American Chemical Society, 2003, 125, 6048-6049.	6.6	92
35	Positively Charged Phosphorus as a Hydrogen Bond Acceptor. Journal of Physical Chemistry Letters, 2014, 5, 4225-4231.	2.1	91
36	Cost-Effective Implementation of Multiconformer Transition State Theory for Peroxy Radical Hydrogen Shift Reactions. Journal of Physical Chemistry A, 2016, 120, 10072-10087.	1.1	91

#	Article	IF	Citations
37	Explicitly correlated intermolecular distances and interaction energies of hydrogen bonded complexes. Journal of Chemical Physics, 2009, 131, 034307.	1.2	89
38	Computational Study of Hydrogen Shifts and Ring-Opening Mechanisms in Î±-Pinene Ozonolysis Products. Journal of Physical Chemistry A, 2015, 119, 11366-11375.	1.1	89
39	Atmospheric Fate of Methyl Vinyl Ketone: Peroxy Radical Reactions with NO and HO₂. Journal of Physical Chemistry A, 2015, 119, 4562-4572.	1.1	87
40	Hydrogen Bonded OH-Stretching Vibration in the Water Dimer. Journal of Physical Chemistry A, 2007, 111, 567-572.	1.1	85
41	Influence of Intramolecular Hydrogen Bond Strength on OH-Stretching Overtones. Journal of Physical Chemistry A, 2006, 110, 10245-10250.	1.1	84
42	Intensities of CHâ€•and CDâ€stretching overtones in 1,3â€butadiene and 1,3â€butadieneâ€d6. Journal of Chemical Physics, 1993, 99, 9438-9452.	1.2	83
43	Towards Solar Energy Storage in the Photochromic Dihydroazuleneâ€“Vinylheptafulvene System. Chemistry - A European Journal, 2015, 21, 7454-7461.	1.7	79
44	Criegee Intermediates React with Ozone. Journal of Physical Chemistry Letters, 2013, 4, 2525-2529.	2.1	76
45	Ultrathin Reduced Graphene Oxide Films as Transparent Topâ€Contacts for Light Switchable Solidâ€State Molecular Junctions. Advanced Materials, 2013, 25, 4164-4170.	11.1	75
46	Unimolecular Reactions of Peroxy Radicals Formed in the Oxidation of Î±-Pinene and Î²-Pinene by Hydroxyl Radicals. Journal of Physical Chemistry A, 2019, 123, 1661-1674.	1.1	75
47	Comparison of the Morse and Deng-Fan potentials for X-H bonds in small molecules. Molecular Physics, 2003, 101, 2285-2294.	0.8	74
48	Calculated OH-Stretching Vibrational Transitions in the Waterâ‹Nitrogen and Waterâ‹Oxygen Complexes. Journal of Physical Chemistry A, 2002, 106, 8955-8962.	1.1	73
49	Fundamental and overtone vibrational spectroscopy, enthalpy of hydrogen bond formation and equilibrium constant determination of the methanolâ€“dimethylamine complex. Physical Chemistry Chemical Physics, 2013, 15, 10194-10206.	1.3	73
50	OH- and CH-Stretching Overtone Spectra of Catechol. Journal of Physical Chemistry A, 2002, 106, 258-266.	1.1	72
51	Peroxy radical chemistry and OH radical production during the NO₃-initiated oxidation of isoprene. Atmospheric Chemistry and Physics, 2012, 12, 7499-7515.	1.9	72
52	Intensities in local mode overtone spectra of dimethyl ether and acetone. Journal of Chemical Physics, 1991, 94, 5844-5854.	1.2	68
53	The Importance of Peroxy Radical Hydrogen-Shift Reactions in Atmospheric Isoprene Oxidation. Journal of Physical Chemistry A, 2019, 123, 920-932.	1.1	66
54	Rapid Hydrogen Shift Scrambling in Hydroperoxy-Substituted Organic Peroxy Radicals. Journal of Physical Chemistry A, 2016, 120, 266-275.	1.1	62

#	Article	IF	Citations
55	Fourier Transform Infrared Spectroscopy and Theoretical Study of Dimethylamine Dimer in the Gas Phase. Journal of Physical Chemistry A, 2011, 115, 12097-12104.	1.1	61
56	The effect of fluorine substitution in alcoholâ€“amine complexes. Physical Chemistry Chemical Physics, 2014, 16, 22882-22891.	1.3	61
57	Calculation of the Oâˆ’H Stretching Vibrational Overtone Spectrum of the Water Dimer. Journal of Physical Chemistry A, 2008, 112, 6305-6312.	1.1	60
58	Identification of OSSO as a nearâ€UV absorber in the Venusian atmosphere. Geophysical Research Letters, 2016, 43, 11,146.	1.5	60
59	Atmospheric Fate of Methacrolein. 2. Formation of Lactone and Implications for Organic Aerosol Production. Journal of Physical Chemistry A, 2012, 116, 5763-5768.	1.1	58
60	Benchmarking Ab Initio Binding Energies of Hydrogen-Bonded Molecular Clusters Based on FTIR Spectroscopy. Journal of Physical Chemistry A, 2014, 118, 5316-5322.	1.1	58
61	Identification of the dimethylamine-trimethylamine complex in the gas phase. Journal of Chemical Physics, 2012, 136, 184305.	1.2	57
62	Similar Strength of the NHÂ·Â·Â·O and NHÂ·Â·Â·S Hydrogen Bonds in Binary Complexes. Journal of Physical Chemistry A, 2014, 118, 11074-11082.	1.1	57
63	Computational Methodology Study of the Optical and Thermochemical Properties of a Molecular Photoswitch. Journal of Physical Chemistry A, 2015, 119, 896-904.	1.1	57
64	Effect of Hydration on the Hydrogen Abstraction Reaction by HO in DMS and its Oxidation Products. Journal of Physical Chemistry A, 2010, 114, 4857-4863.	1.1	56
65	Calculated Hydrogen Shift Rate Constants in Substituted Alkyl Peroxy Radicals. Journal of Physical Chemistry A, 2018, 122, 8665-8673.	1.1	55
66	Calculation of vibrational (J=0) excitation energies and band intensities of formaldehyde using the recursive residue generation method. Journal of Chemical Physics, 1996, 104, 7807-7820.	1.2	54
67	Vapor Phase near Infrared Spectroscopy of the Hydrogen Bonded Methanolâˆ’Trimethylamine Complex. Journal of Physical Chemistry A, 2006, 110, 9597-9601.	1.1	53
68	Gas Phase Detection of the NHâ€“P Hydrogen Bond and Importance of Secondary Interactions. Journal of Physical Chemistry A, 2015, 119, 10988-10998.	1.1	53
69	Isomerization of Second-Generation Isoprene Peroxy Radicals: Epoxide Formation and Implications for Secondary Organic Aerosol Yields. Environmental Science & Technology, 2017, 51, 4978-4987.	4.6	53
70	Ab initiocalculation of dipole moment functions: application to vibrational band intensities of H2O. Molecular Physics, 1994, 83, 1099-1116.	0.8	52
71	Calculated OH-Stretching Vibrational Transitions of the Waterâˆ’Nitric Acid Complex. Journal of Physical Chemistry A, 2002, 106, 2979-2987.	1.1	51
72	Identification and Characterization of the HClâ€“DMS Gas Phase Molecular Complex via Infrared Spectroscopy and Electronic Structure Calculations. Journal of Physical Chemistry A, 2014, 118, 1384-1389.	1.1	51

#	Article	IF	Citations
73	Alkoxy Radical Bond Scissions Explain the Anomalously Low Secondary Organic Aerosol and Organonitrate Yields From Î±-Pinene + NO₃. Journal of Physical Chemistry Letters, 2017, 8, 2826-2834.	2.1	50
74	The role of electron correlation on calculated XH-stretching vibrational band intensities. Molecular Physics, 1997, 90, 201-213.	0.8	49
75	Hydrogen-bonded rotamers of 2â€²,4â€²,6â€²-trihydroxy-3â€²-formyldihydrochalcone, an intermediate in the synthesis of a dihydrochalcone from Leptospermum recurvum. Tetrahedron, 2003, 59, 6113-6120.	1.0	47
76	Intramolecular OHâ‹¯Ï€ interactions in alkenols and alkynols. Physical Chemistry Chemical Physics, 2011, 13, 14183.	1.3	47
77	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.	1.2	47
78	Internal Methyl Rotation in the CH Stretching Overtone Spectra of ortho-, meta-, and para-Xylene. Journal of Physical Chemistry A, 2002, 106, 6242-6253.	1.1	45
79	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.	1.9	45
80	Absolute Intensities of NH-Stretching Transitions in Dimethylamine and Pyrrole. Journal of Physical Chemistry A, 2012, 116, 290-296.	1.1	44
81	Spectroscopy and dynamics of double proton transfer in formic acid dimer. Physical Chemistry Chemical Physics, 2016, 18, 24654-24662.	1.3	44
82	Intensity of CHâ€•and NHâ€stretching transitions in the overtone spectra of cyclopropylamine. Journal of Chemical Physics, 1993, 99, 5682-5700.	1.2	43
83	Calculation of conformationally weighted dipole moments useful in ionâ€“molecule collision rate estimates. Chemical Physics Letters, 2009, 474, 45-50.	1.2	43
84	Infrared and Near-Infrared Spectroscopy of Acetylacetone and Hexafluoroacetylacetone. Journal of Physical Chemistry A, 2015, 119, 7980-7990.	1.1	43
85	Computational Comparison of Different Reagent Ions in the Chemical Ionization of Oxidized Multifunctional Compounds. Journal of Physical Chemistry A, 2018, 122, 269-279.	1.1	43
86	High-levelab initiostudies of the electronic excited states of the hydroxyl radical and waterâ€“hydroxyl complex. Journal of Chemical Physics, 2004, 120, 6930-6934.	1.2	42
87	Photolysis of sulfuric acid vapor by visible light as a source of the polar stratospheric CN layer. Journal of Geophysical Research, 2005, 110, .	3.3	42
88	CH Stretching Overtone Spectra and Intensities of Vapor Phase Naphthalene. The Journal of Physical Chemistry, 1995, 99, 899-904.	2.9	40
89	Methyl versus Aryl CH and CD Stretching Overtone Intensities in the Vapor Phase Spectra of Toluenes. Journal of Physical Chemistry A, 1997, 101, 2589-2596.	1.1	40
90	Intramolecular Interactions in 2-Aminoethanol and 3-Aminopropanol. Journal of Physical Chemistry A, 2013, 117, 10260-10273.	1.1	40

#	Article	IF	Citations
91	Intramolecular Hydrogen Bonding in Substituted Aminoalcohols. Journal of Physical Chemistry A, 2016, 120, 6371-6378.	1.1	40
92	Subtle differences in the hydrogen bonding of alcohol to divalent oxygen and sulfur. Chemical Physics Letters, 2017, 667, 146-153.	1.2	40
93	CH-stretching overtone spectra and internal methyl rotation in 2,6-difluorotoluene. Journal of Chemical Physics, 1997, 107, 691-701.	1.2	39
94	The effect of large amplitude motions on the vibrational intensities in hydrogen bonded complexes. Journal of Chemical Physics, 2015, 142, 094304.	1.2	39
95	Theoretical Investigation of Substituent Effects on the Dihydroazulene/Vinylheptafulvene Photoswitch: Increasing the Energy Storage Capacity. Journal of Physical Chemistry A, 2016, 120, 9782-9793.	1.1	39
96	Calculated intensity in the local mode overtone spectra of hydrogen peroxide. Journal of Chemical Physics, 1991, 95, 5556-5564.	1.2	38
97	Vibrational Overtone Spectroscopy of Phenol and Its Deuterated Isotopomers. Journal of Physical Chemistry A, 2006, 110, 7345-7354.	1.1	38
98	XH-stretching overtone transitions calculated using explicitly correlated coupled cluster methods. Journal of Chemical Physics, 2010, 132, 174304.	1.2	38
99	Production and Fate of C₄ Dihydroxycarbonyl Compounds from Isoprene Oxidation. Journal of Physical Chemistry A, 2016, 120, 106-117.	1.1	38
100	Double Bonds Are Key to Fast Unimolecular Reactivity in First-Generation Monoterpene Hydroxy Peroxy Radicals. Journal of Physical Chemistry A, 2020, 124, 2885-2896.	1.1	37
101	Calculation of dipole moment functions with density functional theory: application to vibrational band intensities. Molecular Physics, 1999, 96, 1125-1138.	0.8	36
102	Counterpoise corrected geometries of hydrated complexes. Journal of Chemical Physics, 2006, 125, 144317.	1.2	36
103	Controlling Twoâ€Step Multimode Switching of Dihydroazulene Photoswitches. Chemistry - A European Journal, 2015, 21, 3968-3977.	1.7	36
104	Solar Thermal Energy Storage in a Photochromic Macrocycle. Chemistry - A European Journal, 2016, 22, 10796-10800.	1.7	36
105	Overtone Spectroscopy of Sulfonic Acid Derivatives. Journal of Physical Chemistry A, 2007, 111, 5434-5440.	1.1	35
106	Calculation of Overtone Oâ€H Stretching Bands and Intensities of the Water Trimer. Journal of Physical Chemistry A, 2009, 113, 9124-9132.	1.1	35
107	Photoabsorption crossâ€section measurements of ³²S, ³³S, ³⁴S, and ³⁶S sulfur dioxide from 190 to 220â€‰nm. Journal of Geophysical Research D: Atmospheres, 2015, 120, 2546-2557.	1.2	35
108	Atmospheric water vapor complexes and the continuum. Geophysical Research Letters, 2004, 31, n/a-n/a.	1.5	34

#	Article	IF	Citations
109	Calculated Band Profiles of the OH-Stretching Transitions in Water Dimer. Journal of Physical Chemistry A, 2008, 112, 7439-7447.	1.1	34
110	Absolute Intensities of CH Stretching Overtones in Alkenes. Journal of Physical Chemistry A, 2005, 109, 1033-1041.	1.1	33
111	SH-Stretching Vibrational Spectra of Ethanethiol and tert-Butylthiol. Journal of Physical Chemistry A, 2009, 113, 7576-7583.	1.1	33
112	Photoswitchable Dihydroazulene Macrocycles for Solar Energy Storage: The Effects of Ring Strain. Journal of Organic Chemistry, 2017, 82, 10398-10407.	1.7	33
113	Atmospheric Hydroxyl Radical Source: Reaction of Triplet SO₂ and Water. Journal of Physical Chemistry A, 2018, 122, 4465-4469.	1.1	33
114	Kinetics and Product Yields of the OH Initiated Oxidation of Hydroxymethyl Hydroperoxide. Journal of Physical Chemistry A, 2018, 122, 6292-6302.	1.1	33
115	Atmospheric Autoxidation of Amines. Environmental Science & Technology, 2020, 54, 11087-11099.	4.6	33
116	On the possible catalysis by single water molecules of gas-phase hydrogen abstraction reactions by OH radicals. Physical Chemistry Chemical Physics, 2012, 14, 12992.	1.3	32
117	New Insights into the Radical Chemistry and Product Distribution in the OH-Initiated Oxidation of Benzene. Environmental Science & Technology, 2020, 54, 13467-13477.	4.6	32
118	Intramolecular Hydrogen Shift Chemistry of Hydroperoxy-Substituted Peroxy Radicals. Journal of Physical Chemistry A, 2019, 123, 590-600.	1.1	31
119	Calculated CH-Stretching Overtone Spectra of Naphthalene, Anthracene and Their Cations. Journal of Physical Chemistry A, 2000, 104, 11297-11303.	1.1	30
120	Calculated Electronic Transitions in Sulfuric Acid and Implications for Its Photodissociation in the Atmosphere. Journal of Physical Chemistry A, 2008, 112, 4958-4964.	1.1	30
121	Chemical properties of HULIS from three different environments. Journal of Atmospheric Chemistry, 2015, 72, 65-80.	1.4	30
122	Intensities of CH-stretching overtones in 2-butenes. Chemical Physics, 1995, 195, 129-141.	0.9	29
123	High level ab initio studies of the excited states of sulfuric acid and sulfur trioxide. Journal of Chemical Physics, 2003, 118, 7226.	1.2	29
124	Resonance coupling in the fourth OH-stretching overtone spectrum of formic acid. Journal of Chemical Physics, 2004, 121, 136.	1.2	29
125	The lowest Aâ€²2 excited state of the water-hydroxyl complex. Journal of Chemical Physics, 2006, 125, 204302.	1.2	29
126	Intramolecular Hydrogen Bonding in Methyl Lactate. Journal of Physical Chemistry A, 2015, 119, 9692-9702.	1.1	29

#	Article	IF	Citations
127	Side-by-Side Comparison of Hydroperoxide and Corresponding Alcohol as Hydrogen-Bond Donors. Journal of Physical Chemistry A, 2017, 121, 2951-2959.	1.1	29
128	Towards Storage of Solar Energy in Photochromic Molecules: Benzannulation of the Dihydroazulene/Vinylheptafulvene Couple. ChemPhotoChem, 2017, 1, 206-212.	1.5	29
129	Vibrational Overtone Spectroscopy of Jet-Cooled Aminophenols as a Probe for Rotational Isomers. Journal of Physical Chemistry A, 2004, 108, 4420-4427.	1.1	28
130	Formation of Highly Oxidized Molecules from NO₃ Radical Initiated Oxidation of Î"-3-Carene: A Mechanistic Study. ACS Earth and Space Chemistry, 2019, 3, 1460-1470.	1.2	28
131	CH Stretching Overtone Investigation of Relative CH Bond Lengths in Pyridine. The Journal of Physical Chemistry, 1996, 100, 19273-19279.	2.9	26
132	OH-Stretch Vibrational Spectroscopy of Hydroxymethyl Hydroperoxide. Journal of Physical Chemistry A, 2006, 110, 7072-7079.	1.1	26
133	Identification of the Water Amidogen Radical Complex. Journal of the American Chemical Society, 2009, 131, 1358-1359.	6.6	26
134	The gas-phase reaction of methane sulfonic acid with the hydroxyl radical without and with water vapor. Physical Chemistry Chemical Physics, 2013, 15, 5140.	1.3	26
135	Unimolecular Reactions Following Indoor and Outdoor Limonene Ozonolysis. Journal of Physical Chemistry A, 2021, 125, 669-680.	1.1	26
136	Calculated electronic transitions of the water ammonia complex. Journal of Chemical Physics, 2008, 128, 034302.	1.2	25
137	Kinetic Energy Density as a Predictor of Hydrogen-Bonded OH-Stretching Frequencies. Journal of Physical Chemistry A, 2017, 121, 3452-3460.	1.1	25
138	Internal Methyl Rotation in the CH Stretching Overtone Spectra of Toluene-Î±-d2, -Î±-d1, and -d0. Journal of Physical Chemistry A, 2000, 104, 6398-6405.	1.1	24
139	Effect of the Methyl Internal Rotation Barrier Height on CHâ^'Stretching Overtone Spectra. Journal of Physical Chemistry A, 2003, 107, 4607-4611.	1.1	23
140	Measurement of ultraweak transitions in the visible region of molecular oxygen. Journal of Molecular Spectroscopy, 2004, 228, 83-91.	0.4	23
141	Competition between chloride and sulphate during the reformation of calcined hydrotalcite. Applied Clay Science, 2016, 132-133, 650-659.	2.6	23
142	Dependence of an Acoustically Nonresonant Intracavity Photoacoustic Signal on Sample and Buffer Gas Pressure. The Journal of Physical Chemistry, 1995, 99, 6327-6332.	2.9	22
143	The most stable conformer of benzyl alcohol. Chemical Physics Letters, 2008, 466, 21-26.	1.2	22
144	Gibbs energy of complex formation â€“ combining infrared spectroscopy and vibrational theory. International Reviews in Physical Chemistry, 2019, 38, 115-148.	0.9	22

#	Article	IF	Citations
145	The effect of NH2-inversion tunneling splitting on the NH-stretching overtone spectra of aniline vapour. Physical Chemistry Chemical Physics, 2004, 6, 719.	1.3	21
146	Theoretical study, and infrared and Raman spectra of copper(II) chelated complex with dibenzoylmethane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 272-279.	2.0	21
147	Unimolecular HO₂ Loss from Peroxy Radicals Formed in Autoxidation Is Unlikely under Atmospheric Conditions. Journal of Physical Chemistry A, 2016, 120, 3588-3595.	1.1	21
148	Vibrational transitions in hydrogen bonded bimolecular complexes â€“ A local mode perturbation theory approach to transition frequencies and intensities. Journal of Molecular Spectroscopy, 2017, 334, 1-9.	0.4	21
149	Conformer-Specific Photolysis of Pyruvic Acid and the Effect of Water. Journal of Physical Chemistry A, 2020, 124, 1240-1252.	1.1	21
150	The OH-stretching and OOH-bending overtone spectrum of HOONO. Journal of Chemical Physics, 2005, 123, 134318.	1.2	20
151	Infrared Identification of Matrix Isolated H2OÂ·O2. Journal of Physical Chemistry A, 2005, 109, 4274-4279.	1.1	20
152	Infrared spectroscopic probing of dimethylamine clusters in an Ar matrix. Journal of Environmental Sciences, 2016, 40, 51-59.	3.2	20
153	Accurate thermodynamic properties of gas phase hydrogen bonded complexes. Physical Chemistry Chemical Physics, 2016, 18, 23831-23839.	1.3	20
154	Deuterium Isotope Effects on the CH Stretching Overtone Spectrum of Toluene-Î±-d1. Journal of Physical Chemistry A, 1998, 102, 6095-6100.	1.1	19
155	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.	1.2	19
156	Ultraviolet Spectroscopy of the Gas Phase Hydration of Methylglyoxal. ACS Earth and Space Chemistry, 2017, 1, 345-352.	1.2	19
157	Computational Investigation of RO₂ + HO₂ and RO₂ + RO₂ Reactions of Monoterpene Derived First-Generation Peroxy Radicals Leading to Radical Recycling. Journal of Physical Chemistry A, 2018, 122, 9542-9552.	1.1	19
158	Stereoselectivity in Atmospheric Autoxidation. Journal of Physical Chemistry Letters, 2019, 10, 6260-6266.	2.1	19
159	SO₂ formation and peroxy radical isomerization in the atmospheric reaction of OH radicals with dimethyl disulfide. Chemical Communications, 2020, 56, 13634-13637.	2.2	18
160	High levelab initiostudies of the low-lying excited states in the H2Oâ‹…O2 complex. Journal of Chemical Physics, 2003, 119, 3717-3720.	1.2	16
161	Fluorosulfonic Acid and Chlorosulfonic Acid:â€‰ Possible Candidates for OH-Stretching Overtone-Induced Photodissociation. Journal of Physical Chemistry A, 2007, 111, 9707-9713.	1.1	16
162	Redox chemistry of an ethenyl complex with isolobal CbCo and CpFe fragments. Inorganica Chimica Acta, 2008, 361, 1616-1623.	1.2	16

#	Article	IF	Citations
163	Methyl chavicol reactions with ozone, OH and NO3 radicals: Rate constants and gas-phase products. Atmospheric Environment, 2013, 77, 696-702.	1.9	16
164	Spectroscopy of OSSO and Other Sulfur Compounds Thought to be Present in the Venus Atmosphere. Journal of Physical Chemistry A, 2020, 124, 7047-7059.	1.1	16
165	Hydrotrioxide (ROOOH) formation in the atmosphere. Science, 2022, 376, 979-982.	6.0	16
166	Modelling and calculation of dipole moment functions for XH bonds. Canadian Journal of Chemistry, 1999, 77, 1775-1781.	0.6	15
167	Atmospheric Photolysis of Sulfuric Acid. Advances in Quantum Chemistry, 2008, 55, 137-158.	0.4	15
168	Oxidation kinetics of n-pentanol: A theoretical study of the reactivity of the 1â€‘hydroxyâ€‘1-peroxypentyl radical. Combustion and Flame, 2020, 219, 20-32.	2.8	15
169	Atmospheric Fate of the CH₃SOO Radical from the CH₃S + O₂ Equilibrium. Journal of Physical Chemistry A, 2021, 125, 8933-8941.	1.1	15
170	Vibrational OH-Stretching Overtone Spectroscopy of Jet-Cooled Resorcinol and Hydroquinone Rotamers. Journal of Physical Chemistry A, 2007, 111, 6028-6033.	1.1	14
171	Overtone Spectra of 2-Mercaptoethanol and 1,2-Ethanedithiol. Journal of Physical Chemistry A, 2010, 114, 12692-12700.	1.1	14
172	Room Temperature Gas-Phase Detection and Gibbs Energies of Water Amine Bimolecular Complex Formation. Journal of Physical Chemistry A, 2020, 124, 7113-7122.	1.1	14
173	Computational Vibrational and Electronic Spectroscopy of the Water Nitric Oxide Complex. Journal of Physical Chemistry A, 2010, 114, 4835-4842.	1.1	13
174	Weak intramolecular OHâ‹Ï€ hydrogen bonding in methallyl- and allyl-carbinol. Chemical Physics Letters, 2013, 582, 31-37.	1.2	13
175	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.	2.1	13
176	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.	1.1	13
177	A new setup for low-temperature gas-phase ion fluorescence spectroscopy. Review of Scientific Instruments, 2021, 92, 033105.	0.6	13
178	Vibrational Spectroscopy of the Water Dimer at Jet-Cooled and Atmospheric Temperatures. Annual Review of Physical Chemistry, 2022, 73, 209-231.	4.8	13
179	Effect of OH Internal Torsion on the OH-Stretching Spectrum of cis,cis-HOONO. Journal of Physical Chemistry A, 2005, 109, 1810-1814.	1.1	12
180	Calculated Spectroscopy and Atmospheric Photodissociation of Phosphoric Acid. Journal of Physical Chemistry A, 2010, 114, 7544-7552.	1.1	12

#	Article	IF	Citations
181	Widening of the hydrogen bonded OH-streching bands due to the wagging and OO-stretching modes in H2OÂ·H2O. Chemical Physics Letters, 2011, 513, 167-172.	1.2	12
182	Spectroscopic Investigation of Subtle CH-Bond Changes between Solid and Vapor Phase Naphthalene. The Journal of Physical Chemistry, 1996, 100, 4749-4754.	2.9	11
183	CH-Stretching Overtone Spectra of 3-Hexyne and Butaneâ€. Journal of Physical Chemistry A, 2003, 107, 3236-3243.	1.1	11
184	CH-Stretching Overtone Spectroscopy of 1,1,1,2-Tetrafluoroethane. Journal of Physical Chemistry A, 2005, 109, 5323-5331.	1.1	11
185	Unusual Low-Energy Near-Infrared Bands for Ferrocenylâ€“Naphthalimide Donorâ€“Acceptor Dyads with Aromatic Spacer Groups: Prediction by Time-Dependent DFT and Observation by OTTLE Spectroscopy. Organometallics, 2015, 34, 2662-2666.	1.1	11
186	Thermalized Epoxide Formation in the Atmosphere. Journal of Physical Chemistry A, 2019, 123, 10620-10630.	1.1	11
187	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.	1.2	11
188	Trimethylamine Outruns Terpenes and Aromatics in Atmospheric Autoxidation. Journal of Physical Chemistry A, 2021, 125, 4454-4466.	1.1	11
189	Effect of Freezing out Vibrational Modes on Gas-Phase Fluorescence Spectra of Small Ionic Dyes. Journal of Physical Chemistry Letters, 2021, 12, 11346-11352.	2.1	11
190	The quantum mechanical Hamiltonian in curvilinear coordinates: A simple derivation. American Journal of Physics, 1990, 58, 344-347.	0.3	10
191	Interactions between tetrathiafulvalene units in dimeric structures â€“ the influence of cyclic cores. Beilstein Journal of Organic Chemistry, 2015, 11, 930-948.	1.3	10
192	Absolute fundamental and overtone OH and OD stretching intensities of alcohols. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 208, 315-324.	2.0	10
193	Computational and Experimental Evidence of Two Competing Thermal Electrocyclization Pathways for Vinylheptafulvene. Chemistry - an Asian Journal, 2019, 14, 1111-1116.	1.7	10
194	Attenuated Deuterium Stabilization of Hydrogen-Bound Complexes at Room Temperature. Journal of Physical Chemistry A, 2020, 124, 1763-1774.	1.1	10
195	Resolving the anomalous infrared spectrum of the MeCNâ€“HCl molecular cluster using ab Initio molecular dynamics. Physical Chemistry Chemical Physics, 2014, 16, 24685-24690.	1.3	9
196	Simulated Electronic Absorption Spectra of Sulfur-Containing Molecules Present in Earthâ€™s Atmosphere. Journal of Physical Chemistry A, 2019, 123, 6605-6617.	1.1	9
197	Room Temperature Gibbs Energies of Hydrogen-Bonded Alcohol Dimethylselenide Complexes. Journal of Physical Chemistry A, 2019, 123, 8427-8434.	1.1	9
198	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.	1.2	9

#	Article	IF	Citations
199	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.	1.0	8
200	Nitrate radical additionâ€“elimination reactions of atmospherically relevant sulfur-containing molecules. Physical Chemistry Chemical Physics, 2010, 12, 12833.	1.3	8
201	Molecular dynamic simulations of OH-stretching overtone induced photodissociation of fluorosulfonic and chlorosulfonic acid. Physical Chemistry Chemical Physics, 2010, 12, 8277.	1.3	8
202	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.	1.1	8
203	Pathways to Highly Oxidized Products in the Î”3-Carene + OH System. Environmental Science & Technology, 2022, 56, 2213-2224.	4.6	8
204	The nature of molecular vibrations selected by various excitation processes. Chemical Physics, 1989, 138, 237-244.	0.9	7
205	On the association of neutral and cationic tris(tetrathiafulvaleno)dodecadehydro[18]annulenes. Organic and Biomolecular Chemistry, 2016, 14, 425-429.	1.5	7
206	The weak fundamental NH-stretching transition in amines. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 173, 201-206.	2.0	7
207	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.	1.1	7
208	CH-Stretching Overtone Spectra ofcis- andtrans-1,3-Pentadiene. Journal of Physical Chemistry A, 2006, 110, 913-920.	1.1	6
209	Vibrational Overtone Spectroscopy of Three-Membered Rings. Journal of Physical Chemistry A, 2007, 111, 5415-5421.	1.1	6
210	Dimethyl Sulfoxide Complexes Detected at Ambient Conditions. Journal of Physical Chemistry A, 2017, 121, 6046-6053.	1.1	6
211	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.	1.3	6
212	Accuracy of XH-stretching intensities with the Dengâ€“Fan potential. Molecular Physics, 2019, 117, 1629-1639.	0.8	6
213	Modelling and calculation of dipole moment functions for XH bonds. Canadian Journal of Chemistry, 1999, 77, 1775-1781.	0.6	6
214	Reduced-dimensional vibrational models of the water dimer. Journal of Chemical Physics, 2022, 156, 164304.	1.2	6
215	Internal Methyl Rotation in the CH Stretching Overtone Spectra of 2-, 3-, and 4-Methylpyridine. Journal of Physical Chemistry A, 2002, 106, 4368-4376.	1.1	5
216	CH stretching overtone spectra of trimethyl amine and dimethyl sulfide. Journal of Molecular Structure, 2004, 687, 87-99.	1.8	4

#	Article	IF	Citations
217	Reactivity of Electronically Excited SO₂ with Alkanes. Journal of Physical Chemistry A, 2018, 122, 7782-7789.	1.1	4
218	Characterisation of dihydroazulene and vinylheptafulvene derivatives using Raman spectroscopy: The CN-stretching region. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 161, 70-76.	2.0	3
219	Fundamental FH-stretching transition frequencies and oscillator strengths in hydrogen bonded FH complexes. Chemical Physics Letters, 2018, 692, 291-297.	1.2	3
220	Atmospheric Chemistry of CH₃OCF₂CHF₂. Journal of Physical Chemistry A, 2021, 125, 10640-10648.	1.1	3
221	Vibrational Overtone Spectroscopy and Overtone Intensities of Cyclohexadiene Iron Tricarbonyl and 1,3-Cyclohexadiene. Journal of Physical Chemistry A, 2001, 105, 3458-3465.	1.1	2
222	Relative Intensities of Nonequivalent CH Bonds in the Local Mode Overtone Spectra of 1,3- and 1,4-Cyclohexadiene. Journal of Physical Chemistry A, 1998, 102, 10230-10237.	1.1	1
223	Calculated two-photon electronic transitions in sulfuric acid and its atmospheric relevance. Chemical Physics Letters, 2010, 498, 18-21.	1.2	1
224	Response to Comment on â€œUnexpected Epoxide Formation in the Gas-Phase Photooxidation of Isopreneâ€• Science, 2010, 327, 644-644.	6.0	1
225	2,6-Diazaanthracene-9,10-dione and its Radical Anionâ€” A Structural and Spectroscopic Investigation. Australian Journal of Chemistry, 2003, 56, 607.	0.5	1
226	Infrared Identification of Matrix Isolated H2OÃ—O2.. ChemInform, 2005, 36, no.	0.1	0