

Theo KurtÃ©n

List of Publications by Year in descending order

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172
papers

13,456
citations

28242

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h-index

26591

107
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178
all docs

178
docs citations

178
times ranked

5904
citing authors

#	ARTICLE	IF	CITATIONS
1	A large source of low-volatility secondary organic aerosol. <i>Nature</i> , 2014, 506, 476-479.	13.7	1,448
2	Direct Observations of Atmospheric Aerosol Nucleation. <i>Science</i> , 2013, 339, 943-946.	6.0	876
3	Molecular understanding of sulphuric acid–amine particle nucleation in the atmosphere. <i>Nature</i> , 2013, 502, 359-363.	13.7	774
4	A new atmospherically relevant oxidant of sulphur dioxide. <i>Nature</i> , 2012, 488, 193-196.	13.7	465
5	Highly Oxygenated Organic Molecules (HOM) from Gas-Phase Autoxidation Involving Peroxy Radicals: A Key Contributor to Atmospheric Aerosol. <i>Chemical Reviews</i> , 2019, 119, 3472-3509.	23.0	460
6	Amines are likely to enhance neutral and ion-induced sulfuric acid-water nucleation in the atmosphere more effectively than ammonia. <i>Atmospheric Chemistry and Physics</i> , 2008, 8, 4095-4103.	1.9	424
7	An Iodide-Adduct High-Resolution Time-of-Flight Chemical-Ionization Mass Spectrometer: Application to Atmospheric Inorganic and Organic Compounds. <i>Environmental Science & Technology</i> , 2014, 48, 6309-6317.	4.6	406
8	Molecular understanding of atmospheric particle formation from sulfuric acid and large oxidized organic molecules. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 17223-17228.	3.3	300
9	Highly functionalized organic nitrates in the southeast United States: Contribution to secondary organic aerosol and reactive nitrogen budgets. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 1516-1521.	3.3	269
10	From quantum chemical formation free energies to evaporation rates. <i>Atmospheric Chemistry and Physics</i> , 2012, 12, 225-235.	1.9	247
11	Enhancing effect of dimethylamine in sulfuric acid nucleation in the presence of water – a computational study. <i>Atmospheric Chemistry and Physics</i> , 2010, 10, 4961-4974.	1.9	245
12	Molecular-scale evidence of aerosol particle formation via sequential addition of HIO ₃ . <i>Nature</i> , 2016, 537, 532-534.	13.7	237
13	The Formation of Highly Oxidized Multifunctional Products in the Ozonolysis of Cyclohexene. <i>Journal of the American Chemical Society</i> , 2014, 136, 15596-15606.	6.6	236
14	Atmospheric Cluster Dynamics Code: a flexible method for solution of the birth-death equations. <i>Atmospheric Chemistry and Physics</i> , 2012, 12, 2345-2355.	1.9	226
15	Hydroxyl radical-induced formation of highly oxidized organic compounds. <i>Nature Communications</i> , 2016, 7, 13677.	5.8	178
16	Composition and temporal behavior of ambient ions in the boreal forest. <i>Atmospheric Chemistry and Physics</i> , 2010, 10, 8513-8530.	1.9	170
17	Free energy barrier in the growth of sulfuric acid–ammonia and sulfuric acid–dimethylamine clusters. <i>Journal of Chemical Physics</i> , 2013, 139, 084312.	1.2	164
18	Formation of highly oxidized multifunctional compounds: autoxidation of peroxy radicals formed in the ozonolysis of alkenes – deduced from structure–product relationships. <i>Atmospheric Chemistry and Physics</i> , 2015, 15, 6745-6765.	1.9	162

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19	Atmospheric nucleation: highlights of the EUCAARI project and future directions. <i>Atmospheric Chemistry and Physics</i> , 2010, 10, 10829-10848.	1.9	144
20	Molecular Composition and Volatility of Organic Aerosol in the Southeastern U.S.: Implications for IEPOX Derived SOA. <i>Environmental Science & Technology</i> , 2016, 50, 2200-2209.	4.6	141
21	Constraining the sensitivity of iodide adduct chemical ionization mass spectrometry to multifunctional organic molecules using the collision limit and thermodynamic stability of iodide ion adducts. <i>Atmospheric Measurement Techniques</i> , 2016, 9, 1505-1512.	1.2	132
22	Aerosol size distribution measurements at four Nordic field stations: identification, analysis and trajectory analysis of new particle formation bursts. <i>Tellus, Series B: Chemical and Physical Meteorology</i> , 2007, 59, 350-361.	0.8	131
23	On the formation of sulphuric acid amine clusters in varying atmospheric conditions and its influence on atmospheric new particle formation. <i>Atmospheric Chemistry and Physics</i> , 2012, 12, 9113-9133.	1.9	119
24	A density functional study on water-sulfuric acid-ammonia clusters and implications for atmospheric cluster formation. <i>Journal of Geophysical Research</i> , 2007, 112, .	3.3	111
25	Effects of Chemical Complexity on the Autoxidation Mechanisms of Endocyclic Alkene Ozonolysis Products: From Methylcyclohexenes toward Understanding α -Pinene. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4633-4650.	1.1	101
26	Efficient Isoprene Secondary Organic Aerosol Formation from a Non-IEPOX Pathway. <i>Environmental Science & Technology</i> , 2016, 50, 9872-9880.	4.6	100
27	Modeling the Charging of Highly Oxidized Cyclohexene Ozonolysis Products Using Nitrate-Based Chemical Ionization. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6339-6345.	1.1	99
28	Hydration of Atmospherically Relevant Molecular Clusters: Computational Chemistry and Classical Thermodynamics. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2599-2611.	1.1	98
29	Modeling the formation and growth of atmospheric molecular clusters: A review. <i>Journal of Aerosol Science</i> , 2020, 149, 105621.	1.8	98
30	New particle formation from sulfuric acid and amines: Comparison of monomethylamine, dimethylamine, and trimethylamine. <i>Journal of Geophysical Research D: Atmospheres</i> , 2017, 122, 7103-7118.	1.2	97
31	α -Pinene Autoxidation Products May Not Have Extremely Low Saturation Vapor Pressures Despite High O:C Ratios. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2569-2582.	1.1	95
32	Atmospheric Fate of Monoethanolamine: Enhancing New Particle Formation of Sulfuric Acid as an Important Removal Process. <i>Environmental Science & Technology</i> , 2017, 51, 8422-8431.	4.6	95
33	Reactivity of stabilized Criegee intermediates (sCIs) from isoprene and monoterpene ozonolysis toward SO ₂ and organic acids. <i>Atmospheric Chemistry and Physics</i> , 2014, 14, 12143-12153.	1.9	94
34	Role of iodine oxoacids in atmospheric aerosol nucleation. <i>Science</i> , 2021, 371, 589-595.	6.0	94
35	A Computational Study of the Oxidation of SO ₂ to SO ₃ by Gas-Phase Organic Oxidants. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8669-8681.	1.1	93
36	Modeling the Detection of Organic and Inorganic Compounds Using Iodide-Based Chemical Ionization. <i>Journal of Physical Chemistry A</i> , 2016, 120, 576-587.	1.1	93

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37	Ab Initio and Density Functional Theory Reinvestigation of Gas-Phase Sulfuric Acid Monohydrate and Ammonium Hydrogen Sulfate. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7178-7188.	1.1	92
38	Cost-Effective Implementation of Multiconformer Transition State Theory for Peroxy Radical Hydrogen Shift Reactions. <i>Journal of Physical Chemistry A</i> , 2016, 120, 10072-10087.	1.1	91
39	The role of highly oxygenated organic molecules in the Boreal aerosol-cloud-climate system. <i>Nature Communications</i> , 2019, 10, 4370.	5.8	91
40	The role of ammonia in sulfuric acid ion induced nucleation. <i>Atmospheric Chemistry and Physics</i> , 2008, 8, 2859-2867.	1.9	90
41	Computational Study of Hydrogen Shifts and Ring-Opening Mechanisms in α -Pinene Ozonolysis Products. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11366-11375.	1.1	89
42	Atmospheric Fate of Methyl Vinyl Ketone: Peroxy Radical Reactions with NO and HO ₂ . <i>Journal of Physical Chemistry A</i> , 2015, 119, 4562-4572.	1.1	87
43	Self-Catalytic Reaction of SO ₃ and NH ₃ To Produce Sulfamic Acid and Its Implication to Atmospheric Particle Formation. <i>Journal of the American Chemical Society</i> , 2018, 140, 11020-11028.	6.6	86
44	Coupled Cluster Evaluation of the Stability of Atmospheric Acid-Base Clusters with up to 10 Molecules. <i>Journal of Physical Chemistry A</i> , 2016, 120, 621-630.	1.1	83
45	Amine substitution into sulfuric acid-ammonia clusters. <i>Atmospheric Chemistry and Physics</i> , 2012, 12, 3591-3599.	1.9	82
46	Criegee Intermediates React with Ozone. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2525-2529.	2.1	76
47	Experimental Observation of Strongly Bound Dimers of Sulfuric Acid: Application to Nucleation in the Atmosphere. <i>Physical Review Letters</i> , 2011, 106, 228302.	2.9	72
48	Diamines Can Initiate New Particle Formation in the Atmosphere. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6155-6164.	1.1	72
49	Strong Hydrogen Bonded Molecular Interactions between Atmospheric Diamines and Sulfuric Acid. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3693-3700.	1.1	70
50	The effect of H ₂ SO ₄ -amine clustering on chemical ionization mass spectrometry (CIMS) measurements of gas-phase sulfuric acid. <i>Atmospheric Chemistry and Physics</i> , 2011, 11, 3007-3019.	1.9	69
51	Computational Study on the Effect of Hydration on New Particle Formation in the Sulfuric Acid/Ammonia and Sulfuric Acid/Dimethylamine Systems. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1886-1896.	1.1	68
52	Significance of Ammonia in Growth of Atmospheric Nanoclusters. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10671-10674.	1.1	66
53	Molecular Interaction of Pinic Acid with Sulfuric Acid: Exploring the Thermodynamic Landscape of Cluster Growth. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7892-7900.	1.1	64
54	Glyoxal and Methylglyoxal Setschenow Salting Constants in Sulfate, Nitrate, and Chloride Solutions: Measurements and Gibbs Energies. <i>Environmental Science & Technology</i> , 2015, 49, 11500-11508.	4.6	64

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55	Estimating the ratio of nucleating clusters in atmospheric conditions using quantum chemical methods. <i>Atmospheric Chemistry and Physics</i> , 2007, 7, 2765-2773.	1.9	62
56	Electrical charging changes the composition of sulfuric acid-ammonia/dimethylamine clusters. <i>Atmospheric Chemistry and Physics</i> , 2014, 14, 7995-8007.	1.9	59
57	Benchmarking Ab Initio Binding Energies of Hydrogen-Bonded Molecular Clusters Based on FTIR Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5316-5322.	1.1	58
58	Pan-Eurasian Experiment (PEEX): towards a holistic understanding of the feedbacks and interactions in the land-atmosphere-ocean-society continuum in the northern Eurasian region. <i>Atmospheric Chemistry and Physics</i> , 2016, 16, 14421-14461.	1.9	57
59	What Is Required for Highly Oxidized Molecules To Form Clusters with Sulfuric Acid?. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4578-4587.	1.1	56
60	Configurational Sampling of Noncovalent (Atmospheric) Molecular Clusters: Sulfuric Acid and Guanidine. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6022-6033.	1.1	54
61	Density functional theory basis set convergence of sulfuric acid-containing molecular clusters. <i>Computational and Theoretical Chemistry</i> , 2016, 1098, 1-12.	1.1	53
62	MRCISD Studies of the Dissociation of Vinylhydroperoxide, CH ₂ CHOOH: There Is a Saddle Point. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6823-6830.	1.1	51
63	Alkoxy Radical Bond Scissions Explain the Anomalously Low Secondary Organic Aerosol and Organonitrate Yields From α -Pinene + NO ₃ . <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2826-2834.	2.1	50
64	Introduction: The Pan-Eurasian Experiment (PEEX) – multidisciplinary, multiscale and multicomponent research and capacity-building initiative. <i>Atmospheric Chemistry and Physics</i> , 2015, 15, 13085-13096.	1.9	49
65	Factors influencing the contribution of ion-induced nucleation in a boreal forest, Finland. <i>Atmospheric Chemistry and Physics</i> , 2010, 10, 3743-3757.	1.9	48
66	Formation of atmospheric molecular clusters consisting of sulfuric acid and C ₈ H ₁₂ O ₆ tricarboxylic acid. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 4877-4886.	1.3	47
67	Molecular mechanism for rapid autoxidation in α -pinene ozonolysis. <i>Nature Communications</i> , 2021, 12, 878.	5.8	47
68	Computational Study of the Clustering of a Cyclohexene Autoxidation Product C ₆ H ₈ O ₇ with Itself and Sulfuric Acid. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8414-8421.	1.1	45
69	Heterogeneous Nucleation onto Ions and Neutralized Ions: Insights into Sign-Preference. <i>Journal of Physical Chemistry C</i> , 2016, 120, 7444-7450.	1.5	45
70	Nitrogenated and aliphatic organic vapors as possible drivers for marine secondary organic aerosol growth. <i>Journal of Geophysical Research</i> , 2012, 117, .	3.3	44
71	Ab initio studies of O ₂ and O ₃ anionic molecular clusters. <i>Atmospheric Chemistry and Physics</i> , 2011, 11, 7133-7142.	1.9	43
72	Computational Comparison of Different Reagent Ions in the Chemical Ionization of Oxidized Multifunctional Compounds. <i>Journal of Physical Chemistry A</i> , 2018, 122, 269-279.	1.1	43

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73	How well can we predict cluster fragmentation inside a mass spectrometer?. Chemical Communications, 2019, 55, 5946-5949.	2.2	43
74	A reference data set for validating vapor pressure measurement techniques: homologous series of polyethylene glycols. Atmospheric Measurement Techniques, 2018, 11, 49-63.	1.2	41
75	Acid-Mediated Formation of Radicals or Baeyer-Villiger Oxidation from Criegee Adducts. Angewandte Chemie - International Edition, 2015, 54, 11848-11851.	7.2	39
76	Unimolecular Decay of the Dimethyl-Substituted Criegee Intermediate in Alkene Ozonolysis: Decay Time Scales and the Importance of Tunneling. Journal of Physical Chemistry A, 2017, 121, 6036-6045.	1.1	39
77	Flight Deployment of a High-Resolution Time-of-Flight Chemical Ionization Mass Spectrometer: Observations of Reactive Halogen and Nitrogen Oxide Species. Journal of Geophysical Research D: Atmospheres, 2018, 123, 7670-7686.	1.2	39
78	Calculating rate constants for intersystem crossing and internal conversion in the Franck-Condon and Herzberg-Teller approximations. Physical Chemistry Chemical Physics, 2019, 21, 18495-18500.	1.3	38
79	Chamber-based insights into the factors controlling epoxydiol (IEPOX) secondary organic aerosol (SOA) yield, composition, and volatility. Atmospheric Chemistry and Physics, 2019, 19, 11253-11265.	1.9	38
80	Direct Probing of Criegee Intermediates from Gas-Phase Ozonolysis Using Chemical Ionization Mass Spectrometry. Journal of the American Chemical Society, 2017, 139, 13387-13392.	6.6	37
81	Effect of Conformers on Free Energies of Atmospheric Complexes. Journal of Physical Chemistry A, 2016, 120, 8613-8624.	1.1	36
82	Rethinking the application of the first nucleation theorem to particle formation. Journal of Chemical Physics, 2012, 136, 094107.	1.2	35
83	Computational Study of the Effect of Glyoxal-Sulfate Clustering on the Henry's Law Coefficient of Glyoxal. Journal of Physical Chemistry A, 2015, 119, 4509-4514.	1.1	35
84	Effect of Bisulfate, Ammonia, and Ammonium on the Clustering of Organic Acids and Sulfuric Acid. Journal of Physical Chemistry A, 2017, 121, 4812-4824.	1.1	35
85	Intersystem Crossings Drive Atmospheric Gas-Phase Dimer Formation. Journal of Physical Chemistry A, 2019, 123, 6596-6604.	1.1	35
86	Unprecedented Ambient Sulfur Trioxide (SO ₃) Detection: Possible Formation Mechanism and Atmospheric Implications. Environmental Science and Technology Letters, 2020, 7, 809-818.	3.9	34
87	Impact of Quantum Chemistry Parameter Choices and Cluster Distribution Model Settings on Modeled Atmospheric Particle Formation Rates. Journal of Physical Chemistry A, 2020, 124, 5931-5943.	1.1	34
88	Computational Study of the Reaction between Biogenic Stabilized Criegee Intermediates and Sulfuric Acid. Journal of Physical Chemistry A, 2007, 111, 3394-3401.	1.1	33
89	Comparing simulated and experimental molecular cluster distributions. Faraday Discussions, 2013, 165, 75.	1.6	33
90	CIMS Sulfuric Acid Detection Efficiency Enhanced by Amines Due to Higher Dipole Moments: A Computational Study. Journal of Physical Chemistry A, 2013, 117, 14109-14119.	1.1	33

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91	Atmospheric Sulfuric Acid–Dimethylamine Nucleation Enhanced by Trifluoroacetic Acid. <i>Geophysical Research Letters</i> , 2020, 47, e2019GL085627.	1.5	33
92	On the possible catalysis by single water molecules of gas-phase hydrogen abstraction reactions by OH radicals. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12992.	1.3	32
93	Can Highly Oxidized Organics Contribute to Atmospheric New Particle Formation?. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1452-1458.	1.1	32
94	Unexpected quenching effect on new particle formation from the atmospheric reaction of methanol with SO ₃ . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 24966-24971.	3.3	32
95	Modeling on Fragmentation of Clusters inside a Mass Spectrometer. <i>Journal of Physical Chemistry A</i> , 2019, 123, 611-624.	1.1	32
96	First-principles calculations of anharmonic and deuteration effects on the photophysical properties of polyacenes and porphyrinoids. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22314-22323.	1.3	32
97	Computational and Experimental Investigation of the Detection of HO ₂ Radical and the Products of Its Reaction with Cyclohexene Ozonolysis Derived RO ₂ Radicals by an Iodide-Based Chemical Ionization Mass Spectrometer. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6778-6789.	1.1	31
98	Rate enhancement in collisions of sulfuric acid molecules due to long-range intermolecular forces. <i>Atmospheric Chemistry and Physics</i> , 2019, 19, 13355-13366.	1.9	31
99	The Effect of Water and Bases on the Clustering of a Cyclohexene Autoxidation Product C ₆ H ₈ O ₇ with Sulfuric Acid. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2240-2249.	1.1	30
100	Aromaticity of Even-Number Cyclo[<i>n</i>]carbons (<i>n</i> = 6–100). <i>Journal of Physical Chemistry A</i> , 2020, 124, 10849-10855.	1.1	30
101	Modeling the role of highly oxidized multifunctional organic molecules for the growth of new particles over the boreal forest region. <i>Atmospheric Chemistry and Physics</i> , 2017, 17, 8887-8901.	1.9	29
102	The sign preference in sulfuric acid nucleation. <i>Computational and Theoretical Chemistry</i> , 2009, 901, 169-173.	1.5	28
103	Formation of Highly Oxidized Molecules from NO ₃ Radical Initiated Oxidation of β -3-Carene: A Mechanistic Study. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 1460-1470.	1.2	28
104	Ambient sesquiterpene concentration and its link to air ion measurements. <i>Atmospheric Chemistry and Physics</i> , 2007, 7, 2893-2916.	1.9	27
105	Can Plasmon Change Reaction Path? Decomposition of Unsymmetrical Iodonium Salts as an Organic Probe. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 5770-5776.	2.1	27
106	Structural Rearrangements and Magic Numbers in Reactions between Pyridine-Containing Water Clusters and Ammonia. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4902-4908.	1.1	25
107	Computational Comparison of Acetate and Nitrate Chemical Ionization of Highly Oxidized Cyclohexene Ozonolysis Intermediates and Products. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2172-2179.	1.1	25
108	Stability and Structure of Protonated Clusters of Ammonia and Water, H ⁺ (NH ₃) _{<i>m</i>} (H ₂ O) _{<i>n</i>} . <i>Journal of Physical Chemistry A</i> , 2010, 114, 7301-7310.	1.1	24

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109	Structures and reaction rates of the gaseous oxidation of SO ₂ by an O ₃ cluster " a density functional theory investigation. Atmospheric Chemistry and Physics, 2012, 12,		
110	Exploring the atmospheric chemistry of O ₂ and assessing the maximum turnover number of ion-catalysed H ₂ SO ₄ formation. Atmospheric Chemistry and Physics, 2013, 13, 3695-3703.	1.9	24
111	Comparing Reaction Routes for ³ (RO [•]) ₂ Intermediates Formed in Peroxy Radical Self- and Cross-Reactions. Journal of Physical Chemistry A, 2020, 124, 8305-8320.	1.1	24
112	Computational Study of the Adsorption Energetics and Vibrational Wavenumbers of NH ₃ Adsorbed on the Ni(111) Surface. Journal of Physical Chemistry B, 2005, 109, 8954-8960.	1.2	22
113	Clustering mechanism of oxocarboxylic acids involving hydration reaction: Implications for the atmospheric models. Journal of Chemical Physics, 2018, 148, 214303.	1.2	22
114	Investigating Atmospheric Sulfuric Acid "Water" Ammonia Particle Formation Using Quantum Chemistry. Advances in Quantum Chemistry, 2008, 55, 407-427.	0.4	21
115	The role of cluster energy nonaccommodation in atmospheric sulfuric acid nucleation. Journal of Chemical Physics, 2010, 132, 024304.	1.2	21
116	Unimolecular HO ₂ Loss from Peroxy Radicals Formed in Autoxidation Is Unlikely under Atmospheric Conditions. Journal of Physical Chemistry A, 2016, 120, 3588-3595.	1.1	21
117	Hydration increases the lifetime of HSO ₅ and enhances its ability to act as a nucleation precursor " a computational study. Atmospheric Chemistry and Physics, 2009, 9, 3357-3369.	1.9	19
118	A Comment on Nadytko et al., "Amines in the Earth's Atmosphere: A Density Functional Theory Study of the Thermochemistry of Pre-Nucleation Clusters". Entropy 2011, 13, 554-569. Entropy, 2011, 13, 915-923.	1.1	19
119	Kinetic (T = 201-298 K) and Equilibrium (T = 320-420 K) Measurements of the C ₃ H ₅ + O ₂ † C ₃ H ₅ O ₂ Reaction. Journal of Physical Chemistry A, 2012, 116, 3969-3978.	1.1	19
120	Estimating the saturation vapor pressures of isoprene oxidation products C ₅ H ₁₂ O ₆ and C ₅ H ₁₀ O ₆ using COSMO-RS. Atmospheric Chemistry and Physics, 2018, 18, 17589-17600.	1.9	19
121	Computational Investigation of RO ₂ + HO ₂ and RO ₂ + RO ₂ Reactions of Monoterpene Derived First-Generation Peroxy Radicals Leading to Radical Recycling. Journal of Physical Chemistry A, 2018, 122, 9542-9552.	1.1	19
122	Determination of the collision rate coefficient between charged iodic acid clusters and iodic acid using the appearance time method. Aerosol Science and Technology, 2021, 55, 231-242.	1.5	18
123	Can COSMOTerm Predict a Salting in Effect?. Journal of Physical Chemistry A, 2017, 121, 6288-6295.	1.1	17
124	Closed-Shell Organic Compounds Might Form Dimers at the Surface of Molecular Clusters. Journal of Physical Chemistry A, 2018, 122, 1771-1780.	1.1	16
125	Fast estimation of the internal conversion rate constant in photophysical applications. Physical Chemistry Chemical Physics, 2021, 23, 6344-6348.	1.3	16
126	Gas-to-Particle Partitioning of Cyclohexene- and β -Pinene-Derived Highly Oxygenated Dimers Evaluated Using COSMO-therm. Journal of Physical Chemistry A, 2021, 125, 3726-3738.	1.1	16

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127	Phosphoric acid – a potentially elusive participant in atmospheric new particle formation. <i>Molecular Physics</i> , 2017, 115, 2168-2179.	0.8	15
128	Predicting gas–particle partitioning coefficients of atmospheric molecules with machine learning. <i>Atmospheric Chemistry and Physics</i> , 2021, 21, 13227-13246.	1.9	15
129	Large methane releases lead to strong aerosol forcing and reduced cloudiness. <i>Atmospheric Chemistry and Physics</i> , 2011, 11, 6961-6969.	1.9	14
130	Fragmentation inside proton-transfer-reaction-based mass spectrometers limits the detection of ROOR and ROOH peroxides. <i>Atmospheric Measurement Techniques</i> , 2022, 15, 1811-1827.	1.2	14
131	Measurement of iodine species and sulfuric acid using bromide chemical ionization mass spectrometers. <i>Atmospheric Measurement Techniques</i> , 2021, 14, 4187-4202.	1.2	13
132	Computational Investigation of the Formation of Peroxide (ROOR) Accretion Products in the OH- and NO ₃ -Initiated Oxidation of α -Pinene. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10632-10639.	1.1	13
133	Computational investigation of the possible role of some intermediate products of SO ₂ oxidation in sulfuric acid–water nucleation. <i>Atmospheric Research</i> , 2009, 91, 47-52.	1.8	12
134	Comment on –Enhancement in the production of nucleating clusters due to dimethylamine and large uncertainties in the thermochemistry of amine-enhanced nucleation™ by Nadykto et al., <i>Chem. Phys. Lett.</i> 609 (2014) 42–49. <i>Chemical Physics Letters</i> , 2015, 624, 107-110.	1.2	12
135	Clustering of H ₂ SO ₄ with BX ₃ (X=H, F, Cl, Br, CN, OH) compounds creates strong acids and superacids. <i>Computational and Theoretical Chemistry</i> , 2019, 1153, 34-43.	1.1	12
136	Atmospheric gaseous hydrochloric and hydrobromic acid in urban Beijing, China: detection, source identification and potential atmospheric impacts. <i>Atmospheric Chemistry and Physics</i> , 2021, 21, 11437-11452.	1.9	12
137	Carbon dioxide–water clusters in the atmosphere of Mars. <i>Computational and Theoretical Chemistry</i> , 2011, 965, 353-358.	1.1	11
138	Proton affinities of candidates for positively charged ambient ions in boreal forests. <i>Atmospheric Chemistry and Physics</i> , 2013, 13, 10397-10404.	1.9	11
139	Thermalized Epoxide Formation in the Atmosphere. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10620-10630.	1.1	11
140	Reaction between Peroxy and Alkoxy Radicals Can Form Stable Adducts. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2051-2057.	2.1	11
141	Strong Even/Odd Pattern in the Computed Gas-Phase Stability of Dicarboxylic Acid Dimers: Implications for Condensation Thermodynamics. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9594-9599.	1.1	10
142	Solubility and Activity Coefficients of Atmospheric Surfactants in Aqueous Solution Evaluated Using COSMO <i>therm</i> . <i>Journal of Physical Chemistry A</i> , 2020, 124, 430-443.	1.1	10
143	Effect of Hydration and Base Contaminants on Sulfuric Acid Diffusion Measurement: A Computational Study. <i>Aerosol Science and Technology</i> , 2014, 48, 593-603.	1.5	9
144	Temporal and Spatial Variation in Scots Pine Resin Pressure and Composition. <i>Frontiers in Forests and Global Change</i> , 2019, 2, .	1.0	9

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