Theo KurtÃ©n

List of Publications by Year
in descending order

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172	13,456	28242	26591
papers	citations	55 h-index	107 g-index

178	178	178	5904
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Magnetically induced ring currents in metallocenothiaporphyrins. Physical Chemistry Chemical Physics, 2022, 24, 1666-1674.	1.3	9
2	Pathways to Highly Oxidized Products in the Î”3-Carene + OH System. Environmental Science & Technology, 2022, 56, 2213-2224.	4.6	8
3	Fragmentation inside proton-transfer-reaction-based mass spectrometers limits the detection of ROOR and ROOH peroxides. Atmospheric Measurement Techniques, 2022, 15, 1811-1827.	1.2	14
4	Energy transfer, pre-reactive complex formation and recombination reactions during the collision of peroxy radicals. Physical Chemistry Chemical Physics, 2022, 24, 10033-10043.	1.3	6
5	Odd-Number Cyclo[n]Carbons Sustaining Alternating Aromaticity. Journal of Physical Chemistry A, 2022, 126, 2445-2452.	1.1	7
6	Gas-Phase Peroxyl Radical Recombination Reactions: AÂComputational Study of Formation and Decomposition of Tetroxides. Journal of Physical Chemistry A, 2022, 126, 4046-4056.	1.1	9
7	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
8	Fast estimation of the internal conversion rate constant in photophysical applications. Physical Chemistry Chemical Physics, 2021, 23, 6344-6348.	1.3	16
9	Reaction Mechanisms Underlying Unfunctionalized Alkyl Nitrate Hydrolysis in Aqueous Aerosols. ACS Earth and Space Chemistry, 2021, 5, 210-225.	1.2	9
10	Aqueous-phase behavior of glyoxal and methylglyoxal observed with carbon and oxygen K-edge X-ray absorption spectroscopy. Atmospheric Chemistry and Physics, 2021, 21, 2881-2894.	1.9	5
11	Role of iodine oxoacids in atmospheric aerosol nucleation. Science, 2021, 371, 589-595.	6.0	94
12	Molecular mechanism for rapid autoxidation in Î±-pinene ozonolysis. Nature Communications, 2021, 12, 878.	5.8	47
13	Heterogeneous Nucleation of Butanol on NaCl: A Computational Study of Temperature, Humidity, Seed Charge, and Seed Size Effects. Journal of Physical Chemistry A, 2021, 125, 3025-3036.	1.1	6
14	Gas-to-Particle Partitioning of Cyclohexene- and Î±-Pinene-Derived Highly Oxygenated Dimers Evaluated Using COSMOtherm. Journal of Physical Chemistry A, 2021, 125, 3726-3738.	1.1	16
15	New Particle Formation from the Vapor Phase: From Barrier-Controlled Nucleation to the Collisional Limit. Journal of Physical Chemistry Letters, 2021, 12, 4593-4599.	2.1	8
16	Measurement of iodine species and sulfuric acid using bromide chemical ionization mass spectrometers. Atmospheric Measurement Techniques, 2021, 14, 4187-4202.	1.2	13
17	Atmospheric gaseous hydrochloric and hydrobromic acid in urban Beijing, China: detection, source identification and potential atmospheric impacts. Atmospheric Chemistry and Physics, 2021, 21, 11437-11452.	1.9	12
18	Predicting gasâ€“particle partitioning coefficients of atmospheric molecules with machine learning. Atmospheric Chemistry and Physics, 2021, 21, 13227-13246.	1.9	15

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19	A pH dependent sulfate formation mechanism caused by hypochlorous acid in the marine atmosphere. Science of the Total Environment, 2021, 787, 147551.	3.9	4
20	Franck-Condon factors and vibronic patterns of singlet-triplet transitions of 16O3 molecule falling near the dissociation threshold and above. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 273, 107834.	1.1	8
21	Computational Investigation of the Formation of Peroxide (ROOR) Accretion Products in the OH- and NO₃-Initiated Oxidation of Î±-Pinene. Journal of Physical Chemistry A, 2021, 125, 10632-10639.	1.1	13
22	Solubility and Activity Coefficients of Atmospheric Surfactants in Aqueous Solution Evaluated Using COSMOtherm. Journal of Physical Chemistry A, 2020, 124, 430-443.	1.1	10
23	Atmospheric Sulfuric Acidâ€Dimethylamine Nucleation Enhanced by Trifluoroacetic Acid. Geophysical Research Letters, 2020, 47, e2019GL085627.	1.5	33
24	Highly oxygenated organic molecule cluster decomposition in atmospheric pressure interface time-of-flight mass spectrometers. Atmospheric Measurement Techniques, 2020, 13, 3581-3593.	1.2	4
25	Unprecedented Ambient Sulfur Trioxide (SO₃) Detection: Possible Formation Mechanism and Atmospheric Implications. Environmental Science and Technology Letters, 2020, 7, 809-818.	3.9	34
26	Is either direct photolysis or photocatalysed H-shift of peroxyl radicals a competitive pathway in the troposphere?. Royal Society Open Science, 2020, 7, 200521.	1.1	0
27	Comparing Reaction Routes for ³(ROÂ·Â·Â·ORâ€²) Intermediates Formed in Peroxy Radical Self- and Cross-Reactions. Journal of Physical Chemistry A, 2020, 124, 8305-8320.	1.1	24
28	First-principles calculations of anharmonic and deuteration effects on the photophysical properties of polyacenes and porphyrinoids. Physical Chemistry Chemical Physics, 2020, 22, 22314-22323.	1.3	32
29	Molecular Origin of the Sign Preference of Ion- Induced Heterogeneous Nucleation in a Complex Ionic Liquidâ€“Diethylene Glycol System. Journal of Physical Chemistry C, 2020, 124, 26944-26952.	1.5	8
30	Aromaticity of Even-Number Cyclo[n]carbons (n = 6â€“100). Journal of Physical Chemistry A, 2020, 124, 10849-10855.	1.1	30
31	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
32	Modeling the formation and growth of atmospheric molecular clusters: A review. Journal of Aerosol Science, 2020, 149, 105621.	1.8	98
33	Can Plasmon Change Reaction Path? Decomposition of Unsymmetrical Iodonium Salts as an Organic Probe. Journal of Physical Chemistry Letters, 2020, 11, 5770-5776.	2.1	27
34	Identification of molecular cluster evaporation rates, cluster formation enthalpies and entropies by Monte Carlo method. Atmospheric Chemistry and Physics, 2020, 20, 15867-15906.	1.9	7
35	Seedâ€“Adsorbate Interactions as the Key of Heterogeneous Butanol and Diethylene Glycol Nucleation on Ammonium Bisulfate and Tetramethylammonium Bromide. Journal of Physical Chemistry A, 2020, 124, 10527-10539.	1.1	3
36	Technical note: Estimating aqueous solubilities and activity coefficients of mono- and <i>Î±-</i>,<i>Ï‰</i>-dicarboxylic acids using COSMO<i>therm</i>. Atmospheric Chemistry and Physics, 2020, 20, 13131-13143.	1.9	6

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37	Calculating rate constants for intersystem crossing and internal conversion in the Franckâ€“Condon and Herzbergâ€“Teller approximations. Physical Chemistry Chemical Physics, 2019, 21, 18495-18500.	1.3	38
38	Intersystem Crossings Drive Atmospheric Gas-Phase Dimer Formation. Journal of Physical Chemistry A, 2019, 123, 6596-6604.	1.1	35
39	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
40	Thermalized Epoxide Formation in the Atmosphere. Journal of Physical Chemistry A, 2019, 123, 10620-10630.	1.1	11
41	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
42	Strong Even/Odd Pattern in the Computed Gas-Phase Stability of Dicarboxylic Acid Dimers: Implications for Condensation Thermodynamics. Journal of Physical Chemistry A, 2019, 123, 9594-9599.	1.1	10
43	Computational Study of the Effect of Mineral Dust on Secondary Organic Aerosol Formation by Accretion Reactions of Closed-Shell Organic Compounds. Journal of Physical Chemistry A, 2019, 123, 9008-9018.	1.1	4
44	The role of highly oxygenated organic molecules in the Boreal aerosol-cloud-climate system. Nature Communications, 2019, 10, 4370.	5.8	91
45	Configurational Sampling of Noncovalent (Atmospheric) Molecular Clusters: Sulfuric Acid and Guanidine. Journal of Physical Chemistry A, 2019, 123, 6022-6033.	1.1	54
46	How well can we predict cluster fragmentation inside a mass spectrometer?. Chemical Communications, 2019, 55, 5946-5949.	2.2	43
47	Clustering of H2SO4 with BX3 (Xâ€¯=â€¯H, F, Cl, Br, CN, OH) compounds creates strong acids and superacids. Computational and Theoretical Chemistry, 2019, 1153, 34-43.	1.1	12
48	Reaction between Peroxy and Alkoxy Radicals Can Form Stable Adducts. Journal of Physical Chemistry Letters, 2019, 10, 2051-2057.	2.1	11
49	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
50	Temporal and Spatial Variation in Scots Pine Resin Pressure and Composition. Frontiers in Forests and Global Change, 2019, 2, .	1.0	9
51	Clustering of HClO₄ with BrÃ¸nsted (H₂SO₄, HClO₄,) Tj ETQq1 1 0.784314 rgBT Chemistry, 2019, 43, 16932-16944.	1.4	4
52	Unexpected quenching effect on new particle formation from the atmospheric reaction of methanol with SO ₃. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 24966-24971.	3.3	32
53	Rate enhancement in collisions of sulfuric acid molecules due to long-range intermolecular forces. Atmospheric Chemistry and Physics, 2019, 19, 13355-13366.	1.9	31
54	Modeling on Fragmentation of Clusters inside a Mass Spectrometer. Journal of Physical Chemistry A, 2019, 123, 611-624.	1.1	32

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55	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
56	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
57	Estimating the saturation vapor pressures of isoprene oxidation products C₅H₁₂O₆ and C₅H₁₀O₆ using COSMO-RS. Atmospheric Chemistry and Physics, 2018, 18, 17589-17600.	1.9	19
58	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
59	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
60	Flight Deployment of a Highâ€Resolution Timeâ€ofâ€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
61	Self-Catalytic Reaction of SO₃ and NH₃ To Produce Sulfamic Acid and Its Implication to Atmospheric Particle Formation. Journal of the American Chemical Society, 2018, 140, 11020-11028.	6.6	86
62	Clustering mechanism of oxocarboxylic acids involving hydration reaction: Implications for the atmospheric models. Journal of Chemical Physics, 2018, 148, 214303.	1.2	22
63	Computational Comparison of Acetate and Nitrate Chemical Ionization of Highly Oxidized Cyclohexene Ozonolysis Intermediates and Products. Journal of Physical Chemistry A, 2017, 121, 2172-2179.	1.1	25
64	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
65	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
66	What Is Required for Highly Oxidized Molecules To Form Clusters with Sulfuric Acid?. Journal of Physical Chemistry A, 2017, 121, 4578-4587.	1.1	56
67	Formation of atmospheric molecular clusters consisting of sulfuric acid and C₈H₁₂O₆ tricarboxylic acid. Physical Chemistry Chemical Physics, 2017, 19, 4877-4886.	1.3	47
68	Phosphoric acid â€“ a potentially elusive participant in atmospheric new particle formation. Molecular Physics, 2017, 115, 2168-2179.	0.8	15
69	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
70	Diamines Can Initiate New Particle Formation in the Atmosphere. Journal of Physical Chemistry A, 2017, 121, 6155-6164.	1.1	72
71	Computational and Experimental Investigation of the Detection of HO₂ Radical and the Products of Its Reaction with Cyclohexene Ozonolysis Derived RO₂ Radicals by an Iodide-Based Chemical Ionization Mass Spectrometer. Journal of Physical Chemistry A, 2017, 121, 6778-6789.	1.1	31
72	Can COSMOTherm Predict a Salting in Effect?. Journal of Physical Chemistry A, 2017, 121, 6288-6295.	1.1	17

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73	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
74	Atmospheric Fate of Monoethanolamine: Enhancing New Particle Formation of Sulfuric Acid as an Important Removal Process. Environmental Science & Technology, 2017, 51, 8422-8431.	4.6	95
75	New particle formation from sulfuric acid and amines: Comparison of monomethylamine, dimethylamine, and trimethylamine. Journal of Geophysical Research D: Atmospheres, 2017, 122, 7103-7118.	1.2	97
76	Modeling the role of highly oxidized multifunctional organicÂmolecules for the growth of new particles overÂtheÂborealÂforestÂregion. Atmospheric Chemistry and Physics, 2017, 17, 8887-8901.	1.9	29
77	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. Atmospheric Measurement Techniques, 2016, 9, 1505-1512.	1.2	132
78	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
79	Hydroxyl radical-induced formation of highly oxidized organic compounds. Nature Communications, 2016, 7, 13677.	5.8	178
80	The Effect of Water and Bases on the Clustering of a Cyclohexene Autoxidation Product C₆H₈O₇ with Sulfuric Acid. Journal of Physical Chemistry A, 2016, 120, 2240-2249.	1.1	30
81	Î±-Pinene Autoxidation Products May Not Have Extremely Low Saturation Vapor Pressures Despite High O:C Ratios. Journal of Physical Chemistry A, 2016, 120, 2569-2582.	1.1	95
82	Strong Hydrogen Bonded Molecular Interactions between Atmospheric Diamines and Sulfuric Acid. Journal of Physical Chemistry A, 2016, 120, 3693-3700.	1.1	70
83	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
84	Effect of Conformers on Free Energies of Atmospheric Complexes. Journal of Physical Chemistry A, 2016, 120, 8613-8624.	1.1	36
85	Molecular-scale evidence of aerosol particle formation via sequential addition of HIO3. Nature, 2016, 537, 532-534.	13.7	237
86	Efficient Isoprene Secondary Organic Aerosol Formation from a Non-IEPOX Pathway. Environmental Science & Technology, 2016, 50, 9872-9880.	4.6	100
87	Density functional theory basis set convergence of sulfuric acid-containing molecular clusters. Computational and Theoretical Chemistry, 2016, 1098, 1-12.	1.1	53
88	Pan-Eurasian Experiment (PEEX): towards a holistic understanding of the feedbacks and interactions in the landâ€“atmosphereâ€“oceanâ€“society continuum in the northern Eurasian region. Atmospheric Chemistry and Physics, 2016, 16, 14421-14461.	1.9	57
89	Heterogeneous Nucleation onto Ions and Neutralized Ions: Insights into Sign-Preference. Journal of Physical Chemistry C, 2016, 120, 7444-7450.	1.5	45
90	Coupled Cluster Evaluation of the Stability of Atmospheric Acidâ€“Base Clusters with up to 10 Molecules. Journal of Physical Chemistry A, 2016, 120, 621-630.	1.1	83

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91	Molecular Composition and Volatility of Organic Aerosol in the Southeastern U.S.: Implications for IEPOX Derived SOA. Environmental Science & Technology, 2016, 50, 2200-2209.	4.6	141
92	Modeling the Detection of Organic and Inorganic Compounds Using Iodide-Based Chemical Ionization. Journal of Physical Chemistry A, 2016, 120, 576-587.	1.1	93
93	Highly functionalized organic nitrates in the southeast United States: Contribution to secondary organic aerosol and reactive nitrogen budgets. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1516-1521.	3.3	269
94	Computational Study on the Effect of Hydration on New Particle Formation in the Sulfuric Acid/Ammonia and Sulfuric Acid/Dimethylamine Systems. Journal of Physical Chemistry A, 2016, 120, 1886-1896.	1.1	68
95	Can Highly Oxidized Organics Contribute to Atmospheric New Particle Formation?. Journal of Physical Chemistry A, 2016, 120, 1452-1458.	1.1	32
96	Acidâ€Mediated Formation of Radicals or Baeyerâ€“Villiger Oxidation from Criegee Adducts. Angewandte Chemie - International Edition, 2015, 54, 11848-11851.	7.2	39
97	Introduction: The Pan-Eurasian Experiment (PEEX) â€“ multidisciplinary, multiscale and multicomponent research and capacity-building initiative. Atmospheric Chemistry and Physics, 2015, 15, 13085-13096.	1.9	49
98	Formation of highly oxidized multifunctional compounds: autoxidation of peroxy radicals formed in the ozonolysis of alkenes â€“ deduced from structureâ€“product relationships. Atmospheric Chemistry and Physics, 2015, 15, 6745-6765.	1.9	162
99	The charging of neutral dimethylamine and dimethylamineâ€“sulfuric acid clusters using protonated acetone. Atmospheric Measurement Techniques, 2015, 8, 2577-2588.	1.2	1
100	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
101	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
102	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
103	Computational Study of the Effect of Glyoxalâ€“Sulfate Clustering on the Henryâ€™s Law Coefficient of Glyoxal. Journal of Physical Chemistry A, 2015, 119, 4509-4514.	1.1	35
104	Comment on â€˜Enhancement in the production of nucleating clusters due to dimethylamine and large uncertainties in the thermochemistry of amine-enhanced nucleationâ€™ by Nadykto et al., Chem. Phys. Lett. 609 (2014) 42â€“49. Chemical Physics Letters, 2015, 624, 107-110.	1.2	12
105	Modeling the Charging of Highly Oxidized Cyclohexene Ozonolysis Products Using Nitrate-Based Chemical Ionization. Journal of Physical Chemistry A, 2015, 119, 6339-6345.	1.1	99
106	Computational Study of the Clustering of a Cyclohexene Autoxidation Product C₆H₈O₇ with Itself and Sulfuric Acid. Journal of Physical Chemistry A, 2015, 119, 8414-8421.	1.1	45
107	Glyoxal and Methylglyoxal Setschenow Salting Constants in Sulfate, Nitrate, and Chloride Solutions: Measurements and Gibbs Energies. Environmental Science & Technology, 2015, 49, 11500-11508.	4.6	64
108	Effect of Hydration and Base Contaminants on Sulfuric Acid Diffusion Measurement: A Computational Study. Aerosol Science and Technology, 2014, 48, 593-603.	1.5	9

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109	An Iodide-Adduct High-Resolution Time-of-Flight Chemical-Ionization Mass Spectrometer: Application to Atmospheric Inorganic and Organic Compounds. Environmental Science & Technology, 2014, 48, 6309-6317.	4.6	406
110	Hydration of Atmospherically Relevant Molecular Clusters: Computational Chemistry and Classical Thermodynamics. Journal of Physical Chemistry A, 2014, 118, 2599-2611.	1.1	98
111	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
112	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
113	Molecular Interaction of Pinic Acid with Sulfuric Acid: Exploring the Thermodynamic Landscape of Cluster Growth. Journal of Physical Chemistry A, 2014, 118, 7892-7900.	1.1	64
114	A large source of low-volatility secondary organic aerosol. Nature, 2014, 506, 476-479.	13.7	1,448
115	Reactivity of stabilized Criegee intermediates (sCIs) from isoprene and monoterpene ozonolysis toward SO₂ and organic acids. Atmospheric Chemistry and Physics, 2014, 14, 12143-12153.	1.9	94
116	Electrical charging changes the composition of sulfuric acidâ€“ammonia/dimethylamine clusters. Atmospheric Chemistry and Physics, 2014, 14, 7995-8007.	1.9	59
117	Comparing simulated and experimental molecular cluster distributions. Faraday Discussions, 2013, 165, 75.	1.6	33
118	Criegee Intermediates React with Ozone. Journal of Physical Chemistry Letters, 2013, 4, 2525-2529.	2.1	76
119	Molecular understanding of sulphuric acidâ€“amine particle nucleation in the atmosphere. Nature, 2013, 502, 359-363.	13.7	774
120	Direct Observations of Atmospheric Aerosol Nucleation. Science, 2013, 339, 943-946.	6.0	876
121	Experimental studies of the formation of cluster ions formed by corona discharge in an atmosphere containing SO2, NH3, and H2O. International Journal of Mass Spectrometry, 2013, 341-342, 1-6.	0.7	7
122	Hydration of pure and base-Containing sulfuric acid clusters studied by computational chemistry methods. , 2013, , .		1
123	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
124	The charging properties of protonated acetone and acetone clusters. , 2013, , .		1
125	Linking neutral and charged sulfuric acid-ammonia and sulfuric acid-dimethylamine clusters. , 2013, , .		0
126	Free energy barrier in the growth of sulfuric acidâ€“ammonia and sulfuric acidâ€“dimethylamine clusters. Journal of Chemical Physics, 2013, 139, 084312.	1.2	164

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127	Molecular understanding of atmospheric particle formation from sulfuric acid and large oxidized organic molecules. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 17223-17228.	3.3	300
128	Proton affinities of candidates for positively charged ambient ions in boreal forests. Atmospheric Chemistry and Physics, 2013, 13, 10397-10404.	1.9	11
129	Exploring the atmospheric chemistry of O₂SO₃<sup>â^'</sup& and assessing the maximum turnover number of ion-catalysed H₂SO₄ formation. Atmospheric Chemistry and Physics, 2013, 13, 3695-3703.	1.9	24
130	Rethinking the application of the first nucleation theorem to particle formation. Journal of Chemical Physics, 2012, 136, 094107.	1.2	35
131	On the formation of sulphuric acid â€“ amine clusters in varying atmospheric conditions and its influence on atmospheric new particle formation. Atmospheric Chemistry and Physics, 2012, 12, 9113-9133.	1.9	119
132	From quantum chemical formation free energies to evaporation rates. Atmospheric Chemistry and Physics, 2012, 12, 225-235.	1.9	247
133	Structures and reaction rates of the gaseous oxidation of SO₂ by an O₃^{â^'}(H<sub>2</sub& cluster â€“ a density functional theory investigation. Atmospheric Chemistry and Physics, 2012, 12, 3639-3652.	1.9	24
134	Atmospheric Cluster Dynamics Code: a flexible method for solution of the birth-death equations. Atmospheric Chemistry and Physics, 2012, 12, 2345-2355.	1.9	226
135	Amine substitution into sulfuric acid â€“ ammonia clusters. Atmospheric Chemistry and Physics, 2012, 12, 3591-3599.	1.9	82
136	Structural Rearrangements and Magic Numbers in Reactions between Pyridine-Containing Water Clusters and Ammonia. Journal of Physical Chemistry A, 2012, 116, 4902-4908.	1.1	25
137	A new atmospherically relevant oxidant of sulphur dioxide. Nature, 2012, 488, 193-196.	13.7	465
138	Nitrogenated and aliphatic organic vapors as possible drivers for marine secondary organic aerosol growth. Journal of Geophysical Research, 2012, 117, .	3.3	44
139	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
140	Kinetic (T = 201â€“298 K) and Equilibrium (T = 320â€“420 K) Measurements of the C3H5 + O2 â‡† C3H5O2 Reaction. Journal of Physical Chemistry A, 2012, 116, 3969-3978.	1.1	19
141	MRCISD Studies of the Dissociation of Vinylhydroperoxide, CH₂CHOOH: There Is a Saddle Point. Journal of Physical Chemistry A, 2012, 116, 6823-6830.	1.1	51
142	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
143	Quantum chemical studies on peroxodisulfuric acidâ€“sulfuric acidâ€“water clusters. Computational and Theoretical Chemistry, 2011, 967, 219-225.	1.1	1
144	Ab initio studies of O₂^{â^'}(H<sub>2</sub& and O₃^{â^'}(H<sub>2</sub& anionic molecular clusters, <i>n</i>â‰12. Atmospheric Chemistry and Physics, 2011, 11, 7133-7142.	1.9	43

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145	The effect of H₂SO₄ â€“ amine clustering on chemical ionization mass spectrometry (CIMS) measurements of gas-phase sulfuric acid. Atmospheric Chemistry and Physics, 2011, 11, 3007-3019.	1.9	69
146	Large methane releases lead to strong aerosol forcing and reduced cloudiness. Atmospheric Chemistry and Physics, 2011, 11, 6961-6969.	1.9	14
147	Carbon dioxideâ€“water clusters in the atmosphere of Mars. Computational and Theoretical Chemistry, 2011, 965, 353-358.	1.1	11
148	Density-functional study of the sign preference of the binding of 1-propanol to tungsten oxide seed particles. Computational and Theoretical Chemistry, 2011, 966, 322-327.	1.1	2
149	Experimental Observation of Strongly Bound Dimers of Sulfuric Acid: Application to Nucleation in the Atmosphere. Physical Review Letters, 2011, 106, 228302.	2.9	72
150	A Comment on Nadytko et al., â€œAmines in the Earthâ€™s Atmosphere: A Density Functional Theory Study of the Thermochemistry of Pre-Nucleation Clustersâ€• Entropy 2011, 13, 554â€“569. Entropy, 2011, 13, 915-923.	1.1	19
151	Atmospheric nucleation: highlights of the EUCAARI project and future directions. Atmospheric Chemistry and Physics, 2010, 10, 10829-10848.	1.9	144
152	Factors influencing the contribution of ion-induced nucleation in a boreal forest, Finland. Atmospheric Chemistry and Physics, 2010, 10, 3743-3757.	1.9	48
153	Composition and temporal behavior of ambient ions in the boreal forest. Atmospheric Chemistry and Physics, 2010, 10, 8513-8530.	1.9	170
154	The role of cluster energy nonaccommodation in atmospheric sulfuric acid nucleation. Journal of Chemical Physics, 2010, 132, 024304.	1.2	21
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