Jonas Elm

List of Publications by Year in descending order

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82 papers	3,088 citations	126708 33 h-index	182168 51 g-index
87 all docs	87 docs citations	87 times ranked	1694 citing authors

#	Article	IF	Citations
1	Assessment of Density Functional Theory in Predicting Structures and Free Energies of Reaction of Atmospheric Prenucleation Clusters. Journal of Chemical Theory and Computation, 2012, 8, 2071-2077.	2.3	168
2	Assessment of binding energies of atmospherically relevant clusters. Physical Chemistry Chemical Physics, 2013, 15, 16442.	1.3	130
3	Methane sulfonic acid-enhanced formation of molecular clusters of sulfuric acid and dimethyl amine. Atmospheric Chemistry and Physics, 2014, 14, 12023-12030.	1.9	110
4	Modeling the formation and growth of atmospheric molecular clusters: A review. Journal of Aerosol Science, 2020, 149, 105621.	1.8	98
5	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
6	The role of highly oxygenated organic molecules in the Boreal aerosol-cloud-climate system. Nature Communications, 2019, 10, 4370.	5.8	91
7	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
8	Basis set convergence of the binding energies of strongly hydrogen-bonded atmospheric clusters. Physical Chemistry Chemical Physics, 2017, 19, 1122-1133.	1.3	82
9	Towards Solar Energy Storage in the Photochromic Dihydroazuleneâ€“Vinylheptafulvene System. Chemistry - A European Journal, 2015, 21, 7454-7461.	1.7	79
10	Computational approaches for efficiently modelling of small atmospheric clusters. Chemical Physics Letters, 2014, 615, 26-29.	1.2	75
11	Diamines Can Initiate New Particle Formation in the Atmosphere. Journal of Physical Chemistry A, 2017, 121, 6155-6164.	1.1	72
12	Strong Hydrogen Bonded Molecular Interactions between Atmospheric Diamines and Sulfuric Acid. Journal of Physical Chemistry A, 2016, 120, 3693-3700.	1.1	70
13	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
14	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
15	Elucidating the Limiting Steps in Sulfuric Acidâ€“Base New Particle Formation. Journal of Physical Chemistry A, 2017, 121, 8288-8295.	1.1	60
16	An Atmospheric Cluster Database Consisting of Sulfuric Acid, Bases, Organics, and Water. ACS Omega, 2019, 4, 10965-10974.	1.6	58
17	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
18	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

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19	Interaction of Glycine with Common Atmospheric Nucleation Precursors. Journal of Physical Chemistry A, 2013, 117, 12990-12997.	1.1	55
20	Aromaticityâ€Controlled Energy Storage Capacity of the Dihydroazuleneâ€Vinylheptafulvene Photochromic System. Chemistry - A European Journal, 2016, 22, 14567-14575.	1.7	55
21	Density functional theory basis set convergence of sulfuric acid-containing molecular clusters. Computational and Theoretical Chemistry, 2016, 1098, 1-12.	1.1	53
22	Hydration of Atmospheric Molecular Clusters: A New Method for Systematic Configurational Sampling. Journal of Physical Chemistry A, 2018, 122, 5026-5036.	1.1	53
23	Influence of Nucleation Precursors on the Reaction Kinetics of Methanol with the OH Radical. Journal of Physical Chemistry A, 2013, 117, 6695-6701.	1.1	51
24	Methanesulfonic Acid-driven New Particle Formation Enhanced by Monoethanolamine: A Computational Study. Environmental Science & Technology, 2019, 53, 14387-14397.	4.6	50
25	Formation of atmospheric molecular clusters consisting of sulfuric acid and C₈H₁₂O₆ tricarboxylic acid. Physical Chemistry Chemical Physics, 2017, 19, 4877-4886.	1.3	47
26	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
27	Atmospheric Oxidation of Piperazine Initiated by Â·Cl: Unexpected High Nitrosamine Yield. Environmental Science & Technology, 2018, 52, 9801-9809.	4.6	45
28	Piperazine Enhancing Sulfuric Acid-Based New Particle Formation: Implications for the Atmospheric Fate of Piperazine. Environmental Science & Technology, 2019, 53, 8785-8795.	4.6	41
29	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
30	Assessment of the DLPNO Binding Energies of Strongly Noncovalent Bonded Atmospheric Molecular Clusters. ACS Omega, 2020, 5, 7601-7612.	1.6	38
31	Computational study of the Rayleigh light scattering properties of atmospheric pre-nucleation clusters. Physical Chemistry Chemical Physics, 2014, 16, 10883-10890.	1.3	37
32	Ambient reaction kinetics of atmospheric oxygenated organics with the OH radical: a computational methodology study. Physical Chemistry Chemical Physics, 2013, 15, 9636.	1.3	36
33	Effect of Conformers on Free Energies of Atmospheric Complexes. Journal of Physical Chemistry A, 2016, 120, 8613-8624.	1.1	36
34	Hydration of Atmospheric Molecular Clusters II: Organic Acidâ€“Water Clusters. Journal of Physical Chemistry A, 2018, 122, 8549-8556.	1.1	36
35	Structural Effects of Amines in Enhancing Methanesulfonic Acid-Driven New Particle Formation. Environmental Science & Technology, 2020, 54, 13498-13508.	4.6	36
36	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

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37	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
38	Guanidine: A Highly Efficient Stabilizer in Atmospheric New-Particle Formation. Journal of Physical Chemistry A, 2018, 122, 4717-4729.	1.1	32
39	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
40	Towards Storage of Solar Energy in Photochromic Molecules: Benzannulation of the Dihydroazulene/Vinylheptafulvene Couple. ChemPhotoChem, 2017, 1, 206-212.	1.5	29
41	Clusteromics II: Methanesulfonic Acidâ€“Base Cluster Formation. ACS Omega, 2021, 6, 17035-17044.	1.6	28
42	Formation of Low-Volatile Products and Unexpected High Formaldehyde Yield from the Atmospheric Oxidation of Methylsiloxanes. Environmental Science & Technology, 2020, 54, 7136-7145.	4.6	27
43	Clusteromics I: Principles, Protocols, and Applications to Sulfuric Acidâ€“Base Cluster Formation. ACS Omega, 2021, 6, 7804-7814.	1.6	27
44	Direct probing of ion pair formation using a symmetric triangulenium dye. Photochemical and Photobiological Sciences, 2011, 10, 1963-1973.	1.6	26
45	Large area, soft crystalline thin films of N,Nâ€²,Nâ€²â€²-trialkyltriazatriangulenium salts with homeotropic alignment of the discotic cores in a lamellar lattice. Journal of Materials Chemistry, 2012, 22, 4797.	6.7	26
46	Thermodynamic properties of isoprene- and monoterpene-derived organosulfates estimated with COSMO<i>therm</i>. Atmospheric Chemistry and Physics, 2020, 20, 5679-5696.	1.9	25
47	Atmospheric chemistry of iodine anions: elementary reactions of I^{â˜}, IO^{â˜}, and IO₂^{â˜} with ozone studied in the gas-phase at 300 K using an ion trap. Physical Chemistry Chemical Physics, 2018, 20, 28606-28615.	1.3	24
48	Secondary aerosol formation from dimethyl sulfide â€“ improved mechanistic understanding based on smog chamber experiments and modelling. Atmospheric Chemistry and Physics, 2021, 21, 9955-9976.	1.9	24
49	Fine-tuning the lifetimes and energy storage capacities of meta-stable vinylheptafulvenes via substitution at the vinyl position. RSC Advances, 2016, 6, 49003-49010.	1.7	23
50	Benchmark Study of the Structural and Thermochemical Properties of a Dihydroazulene/Vinylheptafulvene Photoswitch. Journal of Physical Chemistry A, 2017, 121, 3148-3154.	1.1	23
51	The Aarhus Chamber Campaign on Highly Oxygenated Organic Molecules and Aerosols (ACCHA): particle formation, organic acids, and dimer esters from <i>Î±</i>-pinene ozonolysis at different temperatures. Atmospheric Chemistry and Physics, 2020, 20, 12549-12567.	1.9	21
52	Atmospheric Chemistry of Allylic Radicals from Isoprene: A Successive Cyclization-Driven Autoxidation Mechanism. Environmental Science & Technology, 2021, 55, 4399-4409.	4.6	20
53	Toward a Holistic Understanding of the Formation and Growth of Atmospheric Molecular Clusters: A Quantum Machine Learning Perspective. Journal of Physical Chemistry A, 2021, 125, 895-902.	1.1	20
54	The role of organic acids in new particle formation from methanesulfonic acid and methylamine. Atmospheric Chemistry and Physics, 2022, 22, 2639-2650.	1.9	20

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55	The reaction of hydrated iodide I(H₂O)^{â˜} with ozone: a new route to IO₂^{â˜} products. Physical Chemistry Chemical Physics, 2019, 21, 17546-17554.	1.3	19
56	Clusteromics III: Acid Synergy in Sulfuric Acidâ€“Methanesulfonic Acidâ€“Base Cluster Formation. ACS Omega, 2022, 7, 15206-15214.	1.6	19
57	Racemization Mechanisms and Electronic Circular Dichroism of [4]Heterohelicenium Dyes: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 12025-12033.	1.1	18
58	Atmospheric Autoxidation of Organophosphate Esters. Environmental Science & Technology, 2022, 56, 6944-6955.	4.6	18
59	Quantum Machine Learning Approach for Studying Atmospheric Cluster Formation. Environmental Science and Technology Letters, 2022, 9, 239-244.	3.9	18
60	Can COSMOTherm Predict a Salting in Effect?. Journal of Physical Chemistry A, 2017, 121, 6288-6295.	1.1	17
61	Large Discrepancy in the Formation of Secondary Organic Aerosols from Structurally Similar Monoterpenes. ACS Earth and Space Chemistry, 2021, 5, 632-644.	1.2	17
62	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
63	Hydration of Atmospheric Molecular Clusters III: Procedure for Efficient Free Energy Surface Exploration of Large Hydrated Clusters. Journal of Physical Chemistry A, 2020, 124, 5253-5261.	1.1	16
64	Phosphoric acid â€“ a potentially elusive participant in atmospheric new particle formation. Molecular Physics, 2017, 115, 2168-2179.	0.8	15
65	Unexpected Growth Coordinate in Large Clusters Consisting of Sulfuric Acid and C₈H₁₂O₆ Tricarboxylic Acid. Journal of Physical Chemistry A, 2019, 123, 3170-3175.	1.1	15
66	New Particle Formation and Growth from Dimethyl Sulfide Oxidation by Hydroxyl Radicals. ACS Earth and Space Chemistry, 2021, 5, 801-811.	1.2	15
67	Obtaining Enhanced Circular Dichroism in [4]Heterohelicenium Analogues. Journal of Physical Chemistry A, 2012, 116, 8744-8752.	1.1	14
68	Rayleigh light scattering properties of atmospheric molecular clusters consisting of sulfuric acid and bases. Physical Chemistry Chemical Physics, 2015, 17, 15701-15709.	1.3	14
69	Azulenium chemistry: towards new derivatives of photochromic dihydroazulenes. Organic and Biomolecular Chemistry, 2016, 14, 2403-2412.	1.5	14
70	Amine-Enhanced Methanesulfonic Acid-Driven Nucleation: Predictive Model and Cluster Formation Mechanism. Environmental Science & Technology, 2022, 56, 7751-7760.	4.6	13
71	New Particle Formation and Growth. , 2018, , 315-352.		12
72	Tri-Base Synergy in Sulfuric Acid-Base Clusters. Atmosphere, 2021, 12, 1260.	1.0	12

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73	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
74	Mechanism and predictive model development of reaction rate constants for N-center radicals with O2. Chemosphere, 2019, 237, 124411.	4.2	8
75	Neutral Sulfuric Acidâ€“Water Clustering Rates: Bridging the Gap between Molecular Simulation and Experiment. Journal of Physical Chemistry Letters, 2020, 11, 4239-4244.	2.1	6
76	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
77	Modeling the Binding Free Energy of Large Atmospheric Sulfuric Acidâ€“Ammonia Clusters. ACS Omega, 2022, 7, 8077-8083.	1.6	6
78	Benchmarking sampling methodology for calculations of Rayleigh light scattering properties of atmospheric molecular clusters. Physical Chemistry Chemical Physics, 2019, 21, 17274-17287.	1.3	4
79	Gas-Phase Spectroscopy of a Vinylheptafulvene Chromophore. European Journal of Mass Spectrometry, 2015, 21, 569-577.	0.5	3
80	The reaction of isotope-substituted hydrated iodide I(H182O)^{â^’} with ozone: the reactive influence of the solvent water molecule. Physical Chemistry Chemical Physics, 2020, 22, 19080-19088.	1.3	2
81	Reply to the â€˜Comment on â€œAtmospheric chemistry of iodine anions: elementary reactions of I^{â^’}, IO^{â^’}, and IOâ^’2 with ozone studied in the gas-phase at 300 K using an ion trapâ€â€™ by D. Britz, Phys. Chem. Chem. Phys., 2019, 21, C9CP03851E. Physical Chemistry Chemical Physics, 2019, 21, 22656-22656.	1.3	0
82	Real-time monitoring of aerosol particle formation from sulfuric acid vapor at elevated concentrations and temperatures. Physical Chemistry Chemical Physics, 2022, , .	1.3	0