Jonas Elm

List of Publications by Year
in descending order

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	Atmospheric Autoxidation of Organophosphate Esters. Environmental Science & Technology, 2022, 56, 6944-6955.	4.6	18
2	Real-time monitoring of aerosol particle formation from sulfuric acid vapor at elevated concentrations and temperatures. Physical Chemistry Chemical Physics, 2022, , .	1.3	0
3	Quantum Machine Learning Approach for Studying Atmospheric Cluster Formation. Environmental Science and Technology Letters, 2022, 9, 239-244.	3.9	18
4	Modeling the Binding Free Energy of Large Atmospheric Sulfuric Acidâ€“Ammonia Clusters. ACS Omega, 2022, 7, 8077-8083.	1.6	6
5	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
6	Clusteromics III: Acid Synergy in Sulfuric Acidâ€“Methanesulfonic Acidâ€“Base Cluster Formation. ACS Omega, 2022, 7, 15206-15214.	1.6	19
7	Amine-Enhanced Methanesulfonic Acid-Driven Nucleation: Predictive Model and Cluster Formation Mechanism. Environmental Science & Technology, 2022, 56, 7751-7760.	4.6	13
8	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
9	Clusteromics I: Principles, Protocols, and Applications to Sulfuric Acidâ€“Base Cluster Formation. ACS Omega, 2021, 6, 7804-7814.	1.6	27
10	Atmospheric Chemistry of Allylic Radicals from Isoprene: A Successive Cyclization-Driven Autoxidation Mechanism. Environmental Science & Technology, 2021, 55, 4399-4409.	4.6	20
11	New Particle Formation and Growth from Dimethyl Sulfide Oxidation by Hydroxyl Radicals. ACS Earth and Space Chemistry, 2021, 5, 801-811.	1.2	15
12	Clusteromics II: Methanesulfonic Acidâ€“Base Cluster Formation. ACS Omega, 2021, 6, 17035-17044.	1.6	28
13	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
14	Tri-Base Synergy in Sulfuric Acid-Base Clusters. Atmosphere, 2021, 12, 1260.	1.0	12
15	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
16	Structural Effects of Amines in Enhancing Methanesulfonic Acid-Driven New Particle Formation. Environmental Science & Technology, 2020, 54, 13498-13508.	4.6	36
17	The reaction of isotope-substituted hydrated iodide I(H182O)^{âˆ’} with ozone: the reactive influence of the solvent water molecule. Physical Chemistry Chemical Physics, 2020, 22, 19080-19088.	1.3	2
18	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

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19	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
20	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
21	Assessment of the DLPNO Binding Energies of Strongly Noncovalent Bonded Atmospheric Molecular Clusters. ACS Omega, 2020, 5, 7601-7612.	1.6	38
22	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
23	Modeling the formation and growth of atmospheric molecular clusters: A review. Journal of Aerosol Science, 2020, 149, 105621.	1.8	98
24	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
25	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
26	Mechanism and predictive model development of reaction rate constants for N-center radicals with O2. Chemosphere, 2019, 237, 124411.	4.2	8
27	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
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	Methanesulfonic Acid-driven New Particle Formation Enhanced by Monoethanolamine: A Computational Study. Environmental Science & Technology, 2019, 53, 14387-14397.	4.6	50
30	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
31	An Atmospheric Cluster Database Consisting of Sulfuric Acid, Bases, Organics, and Water. ACS Omega, 2019, 4, 10965-10974.	1.6	58
32	The role of highly oxygenated organic molecules in the Boreal aerosol-cloud-climate system. Nature Communications, 2019, 10, 4370.	5.8	91
33	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
34	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
35	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, <i>Phys. Chem. Chem. Phys.</i>, 2019, 21, C9CP03851E. Physical Chemistry Chemical Physics, 2019, 21, 22656-22656.	1.3	0
36	Guanidine: A Highly Efficient Stabilizer in Atmospheric New-Particle Formation. Journal of Physical Chemistry A, 2018, 122, 4717-4729.	1.1	32

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37	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
38	Atmospheric chemistry of iodine anions: elementary reactions of I^{âˆ’}, IO^{âˆ’}, and IO₂^{âˆ’} 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
39	Hydration of Atmospheric Molecular Clusters II: Organic Acidâ€“Water Clusters. Journal of Physical Chemistry A, 2018, 122, 8549-8556.	1.1	36
40	New Particle Formation and Growth. , 2018, , 315-352.		12
41	Atmospheric Oxidation of Piperazine Initiated by Â·Cl: Unexpected High Nitrosamine Yield. Environmental Science & Technology, 2018, 52, 9801-9809.	4.6	45
42	Hydration of Atmospheric Molecular Clusters: A New Method for Systematic Configurational Sampling. Journal of Physical Chemistry A, 2018, 122, 5026-5036.	1.1	53
43	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
44	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
45	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
46	Formation of atmospheric molecular clusters consisting of sulfuric acid and C₈H₁₂O₆ tricarboxylic acid. Physical Chemistry Chemical Physics, 2017, 19, 4877-4886.	1.3	47
47	Phosphoric acid â€“ a potentially elusive participant in atmospheric new particle formation. Molecular Physics, 2017, 115, 2168-2179.	0.8	15
48	Basis set convergence of the binding energies of strongly hydrogen-bonded atmospheric clusters. Physical Chemistry Chemical Physics, 2017, 19, 1122-1133.	1.3	82
49	Towards Storage of Solar Energy in Photochromic Molecules: Benzannulation of the Dihydroazulene/Vinylheptafulvene Couple. ChemPhotoChem, 2017, 1, 206-212.	1.5	29
50	Elucidating the Limiting Steps in Sulfuric Acidâ€“Base New Particle Formation. Journal of Physical Chemistry A, 2017, 121, 8288-8295.	1.1	60
51	Diamines Can Initiate New Particle Formation in the Atmosphere. Journal of Physical Chemistry A, 2017, 121, 6155-6164.	1.1	72
52	Can COSMOTherm Predict a Salting in Effect?. Journal of Physical Chemistry A, 2017, 121, 6288-6295.	1.1	17
53	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
54	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

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55	Strong Hydrogen Bonded Molecular Interactions between Atmospheric Diamines and Sulfuric Acid. Journal of Physical Chemistry A, 2016, 120, 3693-3700.	1.1	70
56	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
57	Effect of Conformers on Free Energies of Atmospheric Complexes. Journal of Physical Chemistry A, 2016, 120, 8613-8624.	1.1	36
58	Aromaticityâ€Controlled Energy Storage Capacity of the Dihydroazuleneâ€Vinylheptafulvene Photochromic System. Chemistry - A European Journal, 2016, 22, 14567-14575.	1.7	55
59	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
60	Density functional theory basis set convergence of sulfuric acid-containing molecular clusters. Computational and Theoretical Chemistry, 2016, 1098, 1-12.	1.1	53
61	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
62	Azulenium chemistry: towards new derivatives of photochromic dihydroazulenes. Organic and Biomolecular Chemistry, 2016, 14, 2403-2412.	1.5	14
63	Gas-Phase Spectroscopy of a Vinylheptafulvene Chromophore. European Journal of Mass Spectrometry, 2015, 21, 569-577.	0.5	3
64	Towards Solar Energy Storage in the Photochromic Dihydroazuleneâ€“Vinylheptafulvene System. Chemistry - A European Journal, 2015, 21, 7454-7461.	1.7	79
65	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
66	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
67	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
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	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
70	Computational approaches for efficiently modelling of small atmospheric clusters. Chemical Physics Letters, 2014, 615, 26-29.	1.2	75
71	Computational study of the Rayleigh light scattering properties of atmospheric pre-nucleation clusters. Physical Chemistry Chemical Physics, 2014, 16, 10883-10890.	1.3	37
72	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

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73	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
74	Assessment of binding energies of atmospherically relevant clusters. Physical Chemistry Chemical Physics, 2013, 15, 16442.	1.3	130
75	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
76	Interaction of Glycine with Common Atmospheric Nucleation Precursors. Journal of Physical Chemistry A, 2013, 117, 12990-12997.	1.1	55
77	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
78	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
79	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
80	Obtaining Enhanced Circular Dichroism in [4]Heterohelicenium Analogues. Journal of Physical Chemistry A, 2012, 116, 8744-8752.	1.1	14
81	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
82	Direct probing of ion pair formation using a symmetric triangulenium dye. Photochemical and Photobiological Sciences, 2011, 10, 1963-1973.	1.6	26