Selected recent publications with group members as authors

2019:

- Siddharth Iyer, Matti P. Rissanen and Theo Kurtén. Reaction between Peroxy and Alkoxy Radicals Can Form Stable Adducts. J. Phys. Chem. Letters (2019), 10, 2051-2057.
- Federico Bianchi, Theo Kurtén et al. Highly-oxygenated organic molecules (HOM) from gas-phase autoxidation involving organic peroxy radicals: A key contributor to atmospheric aerosol. Chem. Rev. (2019), 119, 3472-3509.
- Evgeni Zapadinski et al. Modelling on Fragmentation of Clusters Inside a Mass Spectrometer. J. Phys. Chem. A (2019), 123, 611-624.
- Younes Valadbeigi and Theo Kurtén. Clustering of H2SO4 with BX3 (X=H, F, Cl, Br, CN, OH) compounds creates strong acids and superacids. Comput. There. Chem. (2019), 1153, 34-43.

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- Siddharth Iyer et al. Computational Investigation of RO2 + HO2 and RO2 + RO2 Reactions of Monoterpene Derived First-Generation Peroxy Radicals Leading to Radical Recycling. J. Phys. Chem. A (2018), 122, 9542-9552.
- Theo Kurtén et al. Estimating the saturation vapor pressures of isoprene oxidation products C5H12O6 and C5H10O6 using COSMO-RS. Atmos. Chem. Phys. (2018), 18, 17589-17600.
- Noora Hyttinen et al. Computational Comparison of Different Reagent Ions in the Chemical Ionization of Oxidized Multifunctional Compounds. J. Phys. Chem. A (2018), 122, 269-279.
- Viivi Hirvonen et al. Closed-Shell Organic Compounds Might Form Dimers at the Surface of Molecular Clusters. J. Phys. Chem. A (2018), 122, 1771-1780.
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- Torsten Berndt et al. Direct probing of Criegee intermediates from gas-phase ozonolysis using chemical ionization mass spectrometry. J. Am. Chem. Soc. (2017), 139, 13387–13392.
- Siddharth Iyer et al. 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. J. Phys. Chem. A (2017), 121, 6778-6789.
- Greg Drozd et al. Unimolecular Decay of the Dimethyl Substituted Criegee Intermediate in Alkene Ozonolysis: Decay Timescales and the Importance of Tunneling. J. Phys. Chem. A (2017), 121, 6306–6045.
- Martta Toivola et al. Can COSMOTherm Predict a Salting in Effect? J. Phys. Chem. A (2017), 121, 6288–6295.
- Theo Kurtén et al. Alkoxy Radical Bond Scissions Explain the Anomalously Low Secondary Organic Aerosol and Organonitrate Yields from alpha-Pinene + NO3. J. Phys. Chem. Lett (2017), 8, 2826–2834.
- Jonas Elm et al. What Is Required for Highly Oxidized Molecules To Form Clusters with Sulfuric Acid? J. Phys. Chem. A (2017), 121, 4578-4587.
- Jonas Elm et al. Formation of atmospheric molecular clusters consisting of sulfuric acid and C8H12O6 tricarboxylic acid. Phys. Chem. Chem. Phys. (2017), 19, 4877-4886.
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- Torsten Berndt et al. Hydroxyl radical-induced formation of highly oxidized organic compounds. Nature Communications (2016), 7, 13677
- Kristian Holten Möller et al. Cost-Effective Implementation of Multiconformer Transition State Theory for Peroxy Radical Hydrogen Shift Reactions. J. Phys. Chem. A (2016), 120, 10072-10087.
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- Siddharth Iyer et al. Modeling the Detection of Organic and Inorganic Compounds Using Iodide-Based Chemical Ionization. J. Phys. Chem. A (2016), 120, 576-587.
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- Theo Kurtén et al. Computational Study of Hydrogen Shifts and Ring-Opening Mechanisms in -Pinene Ozonolysis Products. J. Phys. Chem. A (2015), 119, 11366-11375
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- Theo Kurtén et al. Computational Study of the Effect of Glyoxal–Sulfate Clustering on the Henry's Law Coefficient of Glyoxal. J. Phys. Chem. A (2015), 119, 4509-4514.
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For a full list of publications, see Theo Kurtén's Reseacher ID page: http://www.researcherid.com/rid/G-2120-2012