A SPECTROSCOPIC AND COMPUTATIONAL PEEK INTO THE STRUCTURE OF ATMOSPHERICALLY RELEVANT DRY AND HYDRATED AMMONIUM BISULFATE CLUSTERS

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New particle formation (NPF) plays a crucial role in the formation of secondary aerosol particles, which in turn actively influence the climate radiative forcing balance. The magnitude of this impact is currently unclear, which limits the accuracy of climate models and their predictions. In order to minimize this radiative forcing uncertainty due to aerosol particles, information regarding surface structure and growth mechanisms of these precursor NPF clusters is necessary. Using a combination of mass spectrometry and infrared spectroscopy, these clusters containing sulfuric acid, ammonia, and water can be mass selected and irradiated with infrared light as a means to gain insight into bonding and structure of the smallest atmospherically relevant clusters. Quantum chemical calculations also provide important supplementary information regarding potential isomer stability at varying cluster sizes. However, even at the smallest cluster sizes there are several isomers that contribute to the experimental spectrum and there are even more potential isomer arrangements to explore computationally. As cluster size increases, computational expense increases exponentially, and water further complicates the computational process. Combining these experimental and computational efforts allows key structural features impacting cluster growth and stability to be identified for a subset of simple clusters. Cationic clusters containing two ammonium and one bisulfate as well as cationic clusters containing four ammonium and three bisulfate molecules are the focus of the study, as well as their singly hydrated counterparts. By understanding these small cluster binding motifs, growth models can be developed and applied to larger atmospherically relevant clusters, and ultimately help improve the accuracy of climate models.