PROBING THE STRUCTURE AND HYDRATION BEHAVIOR OF NEWLY-FORMED ATMOSPHERIC CLUSTERS

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New particle formation is a process in which particles form from trace vapors in the atmosphere and grow into climatically relevant clusters in a complex and still poorly understood process. Clusters of amines and sulfuric acid are known to yield NPF rates similar to those in the ambient atmosphere and provide a useful window into the surface structural motifs present in these clusters. Identifying the complete structure of clusters of a climatically relevant size is extremely difficult. It is excessively computationally expensive, and validating computed structures is made more difficult by a lack of experimental data containing explicit structural information. A core-shell type of structure has been proposed to explain, among other puzzles, the synergistic effects of ammonia and alkylamines on formation and growth rates, with the bulky amines with lower hydrogen bonding numbers tending to partition to the surface of the cluster and a core with fully hydrogen-bonded ammonium ions. We seek to elucidate the structural motifs of several smaller, experimentally accessible cationic clusters of amines and sulfuric acid that represent surface structural motifs of larger clusters using cryogenic ion vibrational predissociation spectroscopy. By mapping structural features to specific vibrational bands we can create a library of spectral markers through which we can identify surface structural motifs of larger clusters, allowing us to more easily identify the climatically relevant surface groups and better predict the behavior of the clusters. Additionally, work is underway to investigate the role water plays in the growth of these structures and how a variety of structural features influence the likely binding sites for water and the water uptake properties of these clusters.