INFRARED SPECTROSCOPIC CHARACTERIZATION OF THE STRUCTURES OF SULFURIC ACID/AMINE/WATER CLUSTERS

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It is estimated that ~50% of climatically relevant atmospheric aerosols arise from new particle formation (NPF), the process by which trace atmospheric gases such as sulfuric acid and ammonia cluster and grow. Amines are expected to enhance NPF, with greater enhancement from larger amines. Using cryogenic ion vibrational predissociation (CIVP) spectroscopy, we studied the structural evolution of clusters with up to 3 sulfuric acids. It is shown that substitution of amines for ammonia can induce structural rearrangement, which is driven by the ability of the alkylamines (MA, DMA, TMA) to form hydrogen bonds, and can lead to direct bisulfate-bisulfate hydrogen bonds. This direct interaction between formal anions indicates that hydrogen bonding can compete with Coulombic force in determining cluster structure. From these observations we have developed a model to predict when these arrangements may arise in ionic and neutral clusters with a variety of compositions. This structural motif is correlated with the fastest growing amines, and could play a role in the mechanism of NPF.