

INFRARED SPECTROSCOPIC AND QUANTUM CHEMICAL EXPLORATION OF AMMONIUM IODATE CLUSTERS

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New particle formation (NPF) comprises a substantial part of secondary aerosol particle formation in the atmosphere, and these particles play an important role in the radiative forcing balance governing climate change. Significant uncertainties in current global climate models persist in part due to the uncertainty surrounding NPF growth mechanisms. Establishing the surface structure and growth mechanisms of early-stage NPF clusters is necessary to develop accurate descriptions of particle formation and growth rates that can be included in climate models. Clusters containing ammonium, bisulfate, and water have previously been studied via mass spectrometry coupled with infrared spectroscopy as well as via quantum chemical calculations which provided structural and bonding information as well as potential isomer stability. Here we focus on an emerging class of clusters made of ammonium and iodate, which may be important for particle formation in coastal and polar regions. Cationic clusters containing zero, one, or two ammonia, iodic acid, and diiodide pentoxide molecules are the focus of this study. Ammonia appears to stabilize the clusters and promote the formation of larger iodine oxides with presumably lower vapor pressure, which would be expected to lead to higher stability and faster growth. Halogen bonding competes with hydrogen bonding in determining the minimum energy structures of these clusters. These studies are key benchmarks for computational efforts to model these clusters for their inclusion in larger-scale modeling efforts.