EXPLORING ATMOSPHERICALLY RELEVANT CLUSTERS OF GLYCINE, AMMONIA AND SULFURIC ACID VIA INFRARED SPECTROSCOPY AND MASS SPECTROMETRY

ANNAPOORANI HARIHARAN, *Department of Chemistry, Stony Brook University, Stony Brook, NY, USA*; CONOR J. BREADY, *Department of Chemistry, Furman University, Greenville, SC, USA*; JACK G AJELLO, *Department of Chemistry, Stony Brook University, Stony Brook, NY, USA*; SAMANTHA H. BLACK, *Chemistry, Washington University in St. Louis, St. Louis, MO, USA*; GEORGE C. SHIELDS, *Department of Chemistry, Furman University, Greenville, SC, USA*; CHRISTOPHER J. JOHNSON, *Chemistry, Stony Brook University, Stony Brook, NY, USA*.

The impact of atmospheric aerosols on climate is one of the largest uncertainties in global climate models so far. New particle formation (NPF) is an all-important initial step that brings together trace gases in the atmosphere to form aerosols. Identifying the structural motifs and intermolecular interactions stabilizing newly-formed clusters is key to establishing their growth mechanisms and developing quantitative models for their growth. Sulfuric acid and bases such as ammonia have been heavily studied as prototypical new particles, but recent evidence suggests that organic vapors (such as dicarboxylic acids, amino acids, etc.) are likely to play a significant role in NPF. In this work we explore the structural motifs in cationic clusters composed of glycine, ammonia, and sulfuric acid. We find that glycine stabilizes these clusters, with collision induced dissociation (CID) mass spectra showing that ammonia is preferentially lost from these clusters. Gas phase vibrational spectra and quantum chemical calculations show that the largest of these clusters have strong hydrogen bonds between bisulfate groups, hinting at potential phase separation in pre-nucleation clusters containing both organic and inorganic compounds. Lastly, variable temperature mass spectrometry (VTMS) experiments show that the glycine-containing clusters uptake water at atmospherically relevant temperatures. Combined, these results imply that in the atmosphere, glycine will likely replace ammonia in ammonium bisulfate clusters, forming stable clusters that can potentially increase NPF efficiency.