Insights into the Formation of Ammonium Water Clusters

Thomas E. Morrell, George C. Shields, Thomas C. Castonguay

Hamilton College, Department of Chemistry, Clinton, NY 13323

The formation of aerosols and clouds is known to begin with the interaction of a small number of water and other molecules. Ammonium plays an important role in many atmospheric processes, and this study focused on $NH_4^+(H_2O)_n$ clusters, where n = 1-10. Using configurations sampled from molecular dynamics simulations, free energy changes of cluster formation were calculated at the MP2/CBS extrapolated//MP2/6-31G* level of theory. This method produces energies that are consistent with experimental results and allows us to calculate a theoretical concentration of clusters in the atmosphere. We will discuss the abundance of these clusters under different atmospheric conditions and address the implications of these results.