Exploring the Formation of Sulfuric Acid/ Water Aerosols: $(H_2SO_4)_2(H_2O)_n$

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Sulfuric acid acts as a condensation nuclei for water vapor in the atmosphere, thus forming sulfuric acid/water aerosols. This study concentrated on sulfuric acid/water aerosols in which 2 sulfur molecules and 4-30 water molecules were clustered together. The purpose of this study was to predict the structures and energies of $(H_2SO_4)_2(H_2O)_n$ clusters that are most likely to form. First, molecular dynamics simulations were performed using AMBER 9 for each cluster, with a varying number of water molecules (n). These simulations contribute to our knowledge of the solvation of sulfur in water. We performed these simulations at various temperatures to determine the highest temperature at which the cluster would give us the most sampling of structures. From these results we selected close to 100 structures from each cluster's simulation for MP2 quantum mechanical calculations. We then performed an MP2/6-31G* geometry optimization and frequency calculation on each of these structures using Gaussian 03, followed by a single point calculation at the MP2/aug-cc-pVDZ level. We will use the free energies of the lowest energy structures to predict the concentration of each cluster formed in the atmosphere. Future research will include increasing the amount of sulfur and water molecules in the clusters, and combining other research involving $(H_2SO_4)(H_2O)_n$ to enhance our understanding of the role of sulfuric acid/water aerosols in the atmosphere.

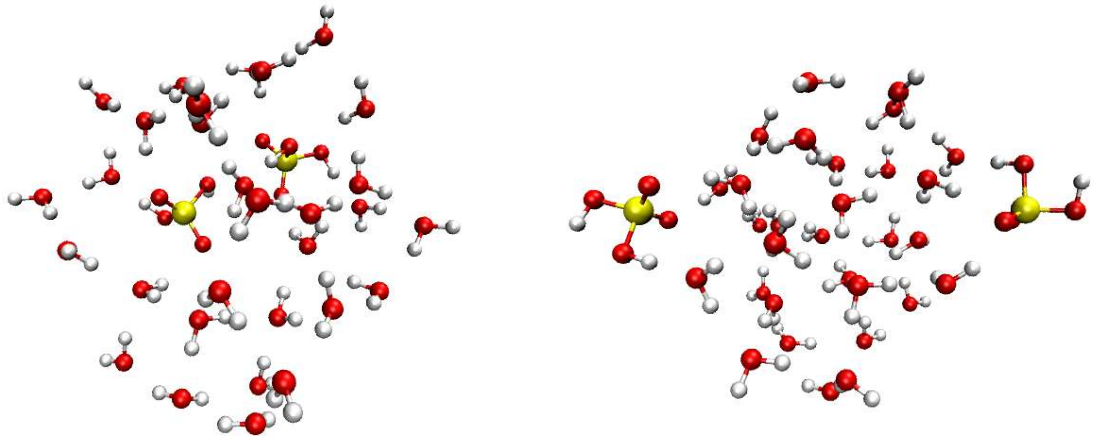

Figure 1. Two configurations of the $(H_2SO_4)_2(H_2O)_{30}$ aerosol, one with the sulfurs on the inside of the cluster, and one with the sulfurs on the outside of the cluster.