Studying the Formation of HSO_4^- Water Clusters

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Particles in our atmosphere are thought to play an active role in the formation of aerosols. We looked at the clusters $HSO_4^-(H_3O)^+(H_2O)_n$ and $HSO_4^-(H_2O)_n$ where n=1-5. Studying the thermodynamics of these clusters will help increase our understanding of how and why aerosols form in our atmosphere.

The clusters were initially built using Spartan software and their geometries were minimized. Each system was run through molecular dynamics simulations at varying temperatures. After this, we pulled out 100 structures and converted the output files to Gaussian command files. We ran these using MP2/6-31G* geometry optimization, then calculated the single point energy using the aug-cc- pVDZ basis set. The energies of the structures that minimized were obtained and the structures that were within 2.0 Kcal of the low energy structure were then run using the MP2/aug-cc-pVTZ//MP2/6-31G* method.

This method produced 6 low energy structures for the $HSO_4^-(H_3O)^+(H_2O)_5$ system and 2 low energy structures for the $HSO_4^-(H_2O)_5$ system. Since the thermodynamics of ionic clusters with more than 4 waters are relatively unknown, our goal for the future direction of this project is to keep adding more waters to the systems. We hope to study the effect that many waters surrounding a system has on the formation of aerosols and how these aerosols lead to climate changes.

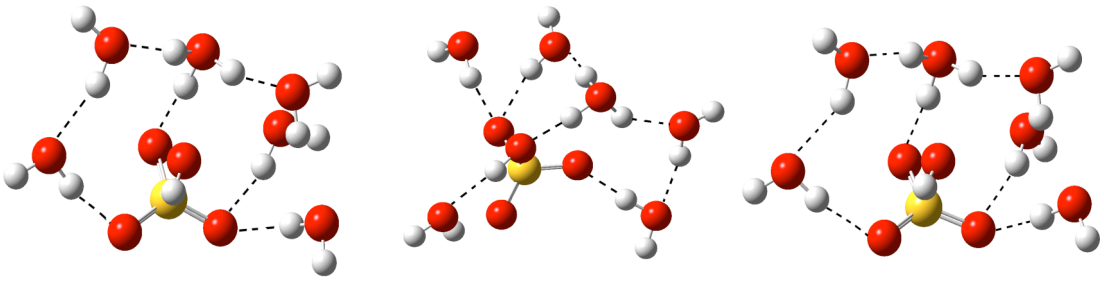

Figure 1. Three low energy structures for $HSO_4^-(H_3O)^+(H_2O)_5$ at the MP2/aug-cc-pVDZ//MP2/6-31G* level of theory