Thermodynamics of the $NH_3 \bullet H_2O$ Dimer

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It has been proposed that the presence of ammonia in the atmosphere increases the rate of nucleation among atmospheric particles. Studying $NH_3 \bullet H_2O$ clusters will increase our understanding of how aerosols form in the atmosphere.

The $NH_3 \bullet H_2O$ cluster was initially built two different ways, one in which H_2O acts as a hydrogen bond acceptor, the other where H_2O acts as a hydrogen donor, using Spartan software. The clusters were optimized, and frequencies were obtained using the MP2/aug-cc-pVnZ, n=D, T, Q and B3LYP/aug-cc-pVnZ, n=D, T, Q, B3LYP/6-31G*, G3, and G3B3 levels of theory. The ΔG°_{298K}, ΔE°_{0K}, and ΔH°_{298K} for formation values were calculated at each of these levels of theory. It was found that the $NH_3 \bullet H_2O$ cluster in which H_2O acts as a hydrogen bond accceptor, changes conformation to the cluster in which the H_2O donates a proton, at both levels of theory. At the MP2/aug-cc-pVDZ level of theory, the energy ranged from 2.742217 $kcal \bullet mol^{-1}$ to 3.179967 $kcal \bullet mol^{-1}$. At the B3LYP/aug–cc-pVDZ level of theory the range of energies was -0.024034 $kcal \bullet mol^{-1}$ to 0.245042 $kcal \bullet mol^{-1}$.

We will add more waters around the ammonia and run these clusters using the Amber8 program to obtain different hydrogen bonding configurations. We can then group similar structures and

find the ones with the lowest energy. Understanding how clusters affect nucleation in the atmosphere will lead to a better knowledge of why aerosols affect our environment the way they do.