Formations of Larger Mixed Ammonia-Amine Systems

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Composed of gas phase molecules present in the atmosphere, aerosols have been found to have a net cooling effect on the global climate with its precise process of their formation still not fully understood. Acid-base reactions between the crucial atmospheric nucleation precursor, sulfuric acid, and bases, such as ammonia and amines, promote aerosol formation. For this study, larger configurations containing three sulfuric acid [H_2SO_4, S] molecules and a combination of three bases, either of ammonia [NH_3, A] and/or an amine, such as methylamine [CH_3NH_2, MA], dimethylamine [$(CH_3)_2NH$, DMA], and trimethylamine [C_3H_9N, TMA], were sampled using a genetic algorithm applied on semi-empirical potential energy surfaces (PM7, EFP). Then, the low energy structures were subject to quantum mechanical calculations, such as PW91, M06-2X, wB97X-D with a 6-311++G** basis set. From our data, we have come to the conclusion that binding energies correlate with the basicity of the base, with the exception of TMA, due to possible steric effects. The reasons for these discrepancies are explored.

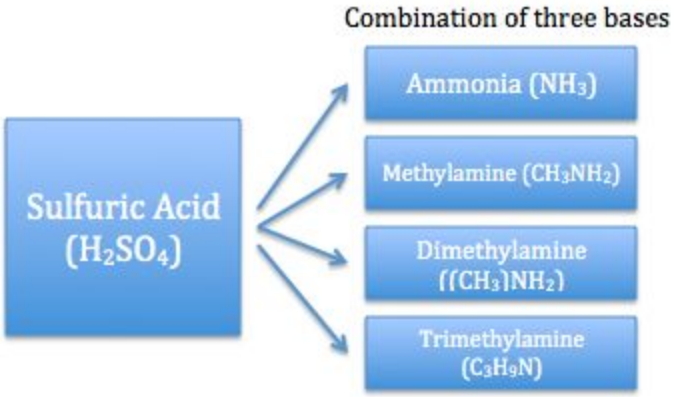

Figure 1: How does the binding energies differ among systems with different combinations of three bases?