# Comparing Single and Multiple Base Systems in Secondary Aerosol Formation

Fern Morrison, Berhane Temelso, George C. Shields
Department of Chemistry, College of Arts & Sciences, Bucknell University, Lewisburg PA 17837

Atmospheric aerosols have a great impact on our global climate. They cool the planet by directly reflecting light away from the earth, and indirectly by acting as cloud condensation nuclei that brighten and extend the lifespan of clouds. Despite their importance in the earth's radiation balance, the lack of understanding about their formation has led to uncertainties about their effect on the global climate.

Previous experimental works have shown that sulfate systems with ammonia and an amine tend to have higher formation rates than those with ammonia or an amine alone. This study attempts to explain that behavior by exploring the clustering of sulfuric acid [$H_2(SO)_4$, (S)], ammonia [$NH_3$, (A)], and trimethylamine [$(CH_3)_3N$, (TMA)]. Initial configurational sampling was performed using genetic algorithm (GA) interfaced to semi-empirical methods (PM7 and SCC-DFTB) to find a large number of low energy configurations. These structures were then subject to quantum mechanical calculations using PW91, M06-2X and wB97X-D functionals with large basis sets. The thermodynamics of formation for the most stable structures was then reviewed to determine why multiple base systems have higher rates of aerosol formation than single base ones. The combined data showed that the binding energy of the cluster is related to the $pK_b$ value of the base; the more basic the amine group the stronger the binding. This trend was consistent for dimethylamine (DMA) and methylamine (MA) groups as well. Further research is being conducted to assess the evaporation rate of sulfuric acid from single and multiple base systems.

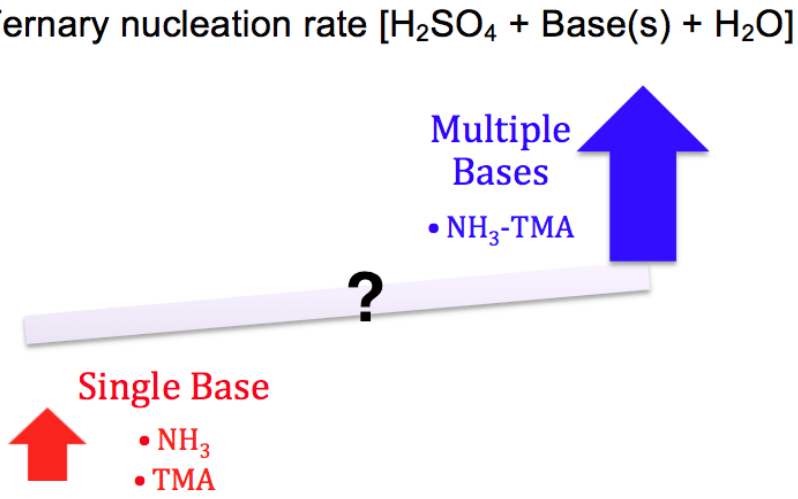


Figure 1: Why is the formation rate of aerosols higher for multiple base systems?