Hydration of Sulfuric Acid-Methylamine Clusters

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Sulfuric acid (H_2SO_4) drives the formation of secondary aerosol particles in the atmosphere, but the process is significantly enhanced by the presence of bases and organic acids. In this study, I have evaluated the effect of the base methylamine (CH_3NH_2) which is abundant in the atmosphere particularly near animal husbandry sites. The acid−base reactions between sulfuric acid and bases influence aerosol particle formation and growth. The basicity of methylamine (pK_b = 3.35) is stronger than ammonia's (pK_b = 4.75) and slightly weaker than dimethylamine's. However, the methylamine emissions are 83 ± 26 Gg N a^{-1} compared to 33 ± 19 Gg N a^{-1} for dimethylamine and 50 000 ± 30 000 Gg N a^{-1} for ammonia.

For $(H_2SO_4)_2(CH_3NH_2)(H_2O)_n$ where n=0-3, the possible configurations were sampled using genetic algorithm (GA) with the PM7 and SCC-DFTB semi-empirical methods involving an initial pool of 500 structures refined over 10,000-20,000 global optimization steps. After removing duplicates from the final pool of structures, the unique ones were minimized using the MP2/6-31G* *ab initio* method. One of the main observations were the presence of proton transfer between the sulfuric acids and methylamine even in the absence of water. Both the protonated methylamine and water typically serve as a bridging role between the sulfuric acids instead of solvating an intact sulfuric acid dimer. The implication of these findings for aerosol formation will be discussed.

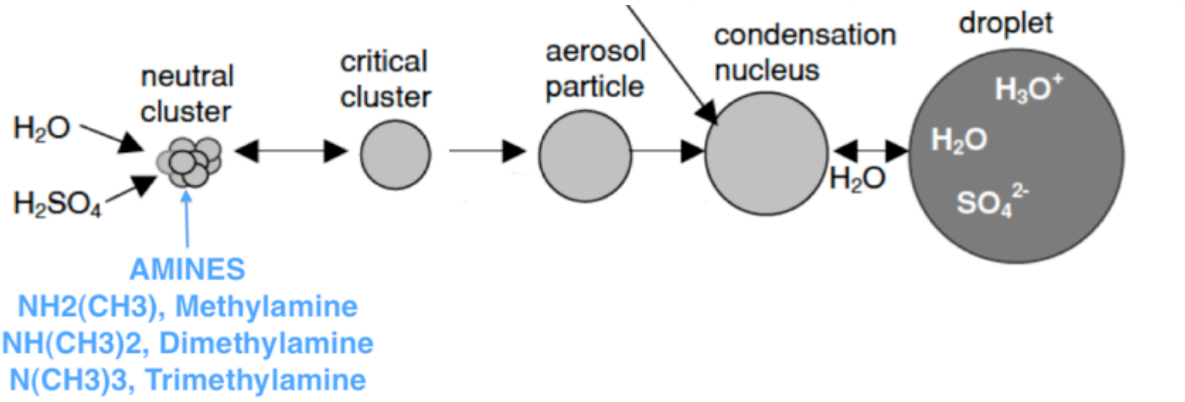

Figure 1. The role of bases in aerosol nucleation. Adapted from Curtius, J. EPJ Web of Conferences 2009, *1*, 199-209