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The potential role of malonic acid in the atmospheric sulfuric acid - ammonia clusters formation

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Abstract

Malonic acid (**MOA**), one of the major dicarboxylic acids (DCAs) in aerosols, has been identified experimentally and computationally to be a strong acid. However, its potential role in the atmospheric clusters formation is still ambiguous. Hence, the participant mechanism of **MOA** on the formation of atmospheric sulfuric acid (**SA**)- ammonia (**A**) clusters was investigated by combining computational methods with atmospheric cluster dynamics code (ACDC). The most stable molecular structures obtained at the M06-2X/6-311++G(3df,3pd) level of theory shows that the added **MOA** molecule in the **SA**-**A**-based clusters presents a promotion on the interactions between **SA** and **A** molecules. ACDC simulations indicate directly an obvious enhancement strength $R_{\mathbf{MOA}}$ on the clusters formation rates at 218 K and the concentration of **MOA** ([**MOA**]) larger than 10^8 molecules cm^{-3}, up to five orders of magnitude. Meanwhile, enhancement strength of **MOA** is compared with that of glycolic acid, and as

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