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

Haijie Zhang<sup>a</sup>, Hao Li<sup>a</sup>, Ling Liu<sup>a</sup>, Yunhong Zhang<sup>a</sup>, Xiuhui Zhang<sup>a,\*\*</sup>,  
Zesheng Li<sup>a,\*\*</sup>

<sup>a</sup>Key Laboratory of Cluster Science, Ministry of Education of China, School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing 100081, Peoples Republic of China

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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  $R_{\text{MOA}}$  on the clusters formation rates at 218 K and the concentration of **MOA** ( $[\text{MOA}]$ ) larger than  $10^8$  molecules  $\text{cm}^{-3}$ , up to five orders of magnitude. Meanwhile, enhancement strength of **MOA** is compared with that of glycolic acid, and as

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\*Xiuhui Zhang

\*\*Zesheng Li

Email addresses: zhangxiuhui@bit.edu.cn (Xiuhui Zhang), zeshengli@bit.edu.cn (Zesheng Li)

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