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Gas phase transformation from organic acid to organic sulfuric anhydride: Possibility and atmospheric fate in the initial new particle formation

Haijie Zhang, Wei Wang, Shuangqi Pi, Ling Liu, Hao Li, Yu Chen, Yunhong Zhang, Xiuhui Zhang, Zesheng Li



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1 Gas phase transformation from organic acid to organic  
2 sulfuric anhydride: possibility and atmospheric fate in  
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4 Haijie Zhang<sup>a</sup>, Wei Wang<sup>a</sup>, Shuangqi Pi<sup>a</sup>, Ling Liu<sup>a</sup>, Hao Li<sup>a</sup>, Yu Chen<sup>b</sup>,  
5 Yunhong Zhang<sup>a</sup>, Xiuhui Zhang<sup>a,\*\*</sup>, Zesheng Li<sup>a,\*\*</sup>

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

9 <sup>b</sup>School of Materials Science and Engineering, Beijing Institute of Technology, Beijing  
10 100081, Peoples Republic of China

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11 **Abstract**

12 New particle formation (NPF) process has been observed frequently in various  
13 environments and produces a large fraction of atmospheric aerosols. However,  
14 the chemical species participating in the nucleation as well as the corresponding  
15 nucleation mechanism in the atmosphere still remain ambiguous. Recent re-  
16 search by Leopold et al. shows that cycloaddition reaction of SO<sub>3</sub> to carboxylic  
17 acids could contribute to the formation of organic sulfuric anhydride which  
18 would have lower vapor pressure compared with the corresponding carboxylic  
19 acid and hence kick-start new particle formation in the gas phase. In the present  
20 study, energy profile for the formation of 3-methyl-1,2,3-butanetricarboxylic sul-  
21 furic anhydride (MBTCSA) through the cycloaddition of SO<sub>3</sub> to 3-methyl-1,2,3-  
22 butanetricarboxylic acid (MBTCA) has been investigated using computational  
23 methods. As a result, such a process would be effectively barrierless for one of  
24 the terminal carboxy group and has very low energy barriers for the other two  
25 carboxy groups (0.6 and 2.8 kcal/mol, respectively), indicating the whole process

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

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