

Supplementary Material for

**Theoretical Study on the Gas Phase and Gas-Liquid
Interface Reaction Mechanism of Criegee Intermediates
with Glycolic Acid Sulfate**

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Keywords: Criegee intermediates, Glycolic acid sulfate, Gas-phase reaction, Aqueous-surface reaction, Proton transfer

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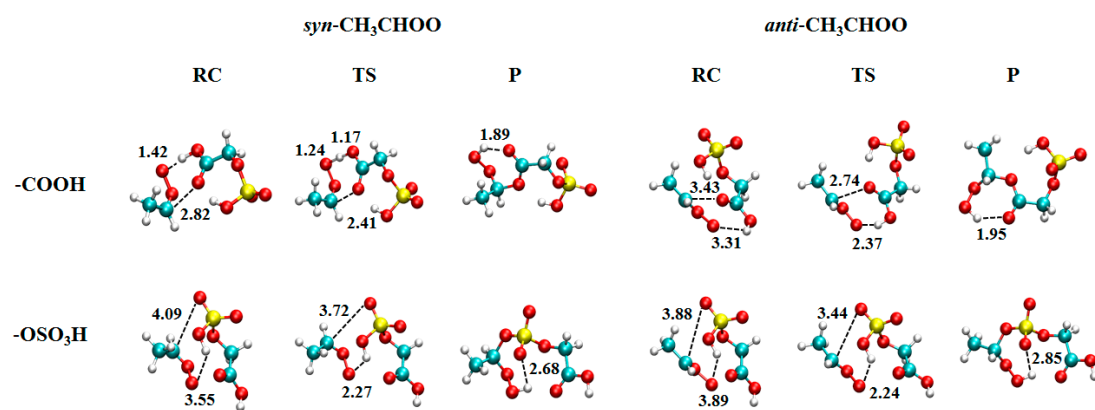


Figure. S1. The configurations of the direct reaction stages (reaction complex, transition state, product).

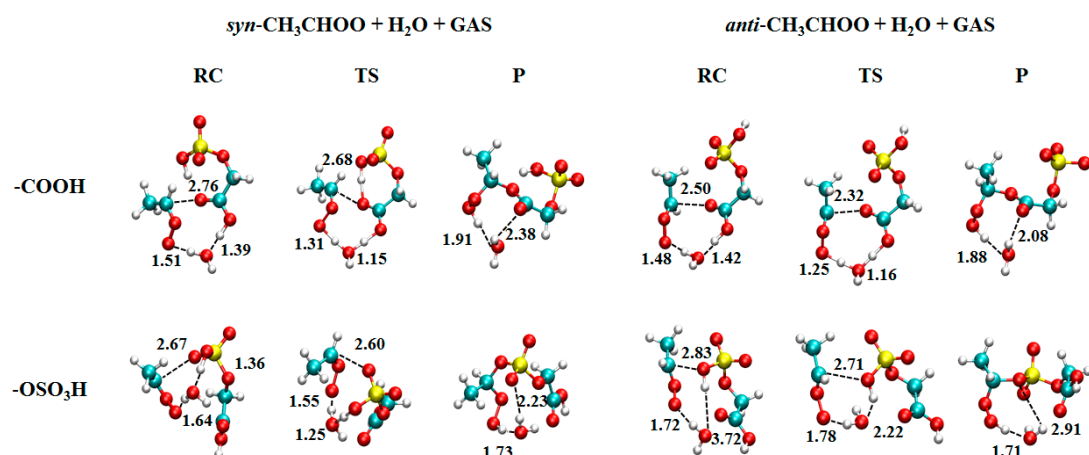


Figure. S2. The configurations of the direct and water-mediated reaction stages (reaction complex, transition state, product).