

Supplementary Material

Theoretical Study on the Gas-Phase and Aqueous Interface Reaction Mechanism of Criegee Intermediates with 2-Methylglyceric Acid and the Nucleation of Products

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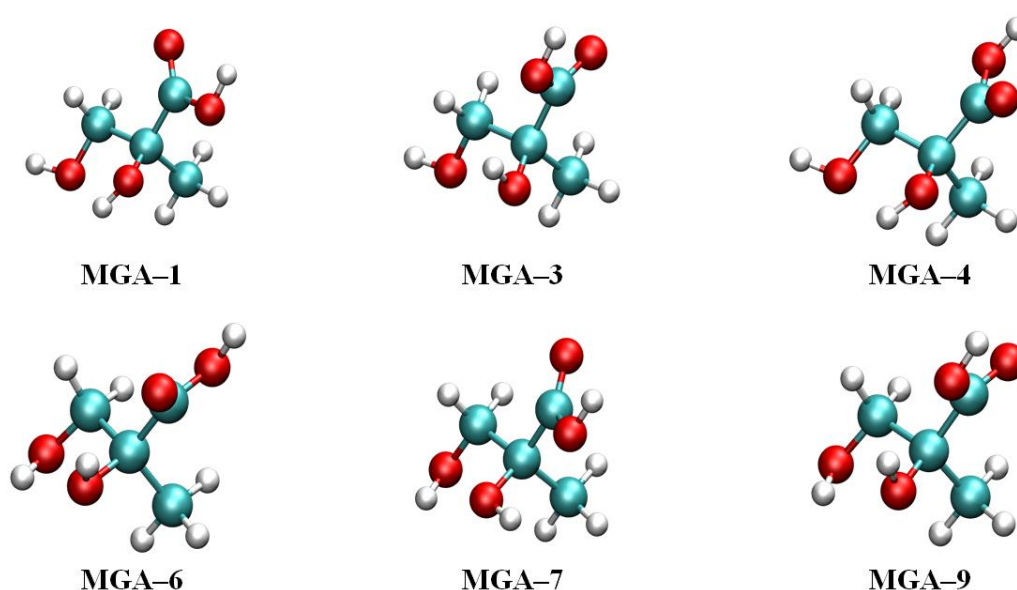


Fig. S1. The six configurations of MGA molecule.

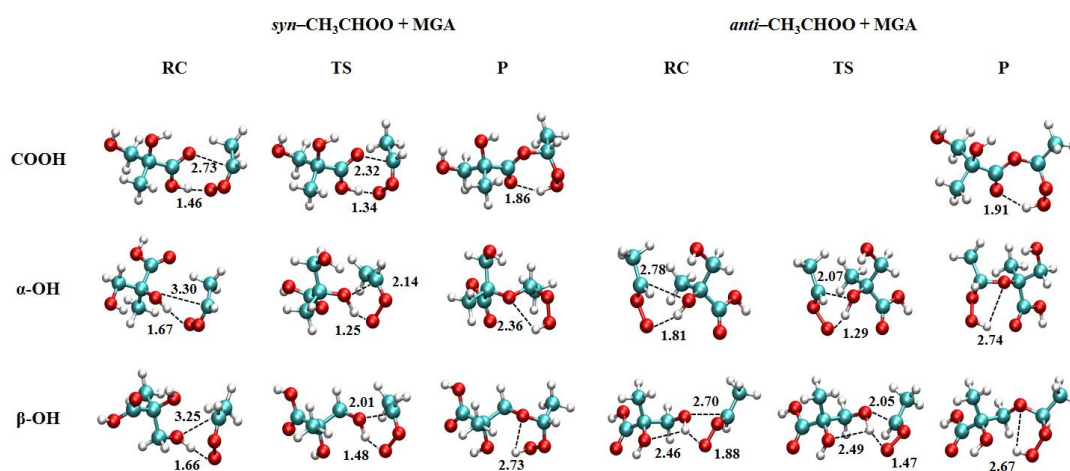


Fig. S2. The structures of bimolecular reaction complexes (RC), transition states (TS) and products (P).

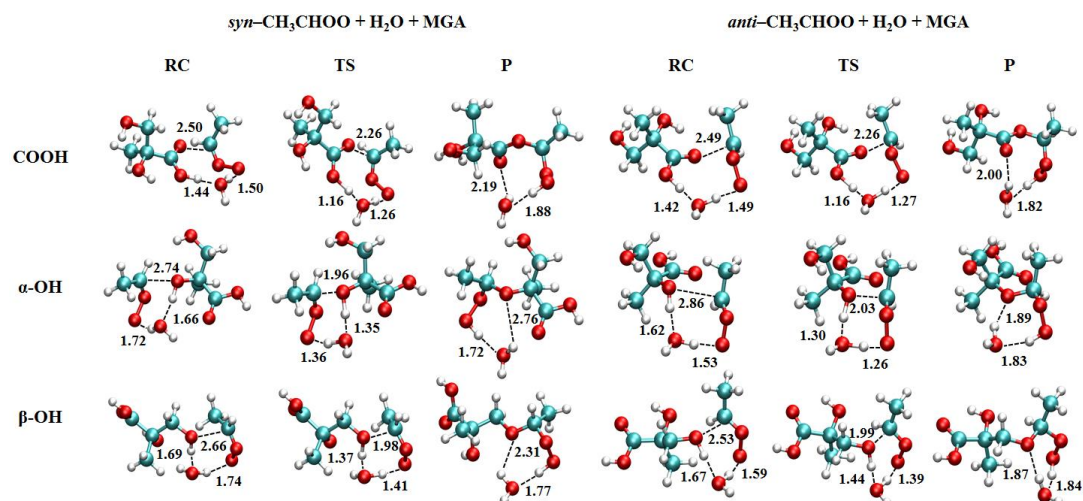


Fig. S3. The structures of water-mediated reaction complexes (RC), transition states (TS) and products (P).

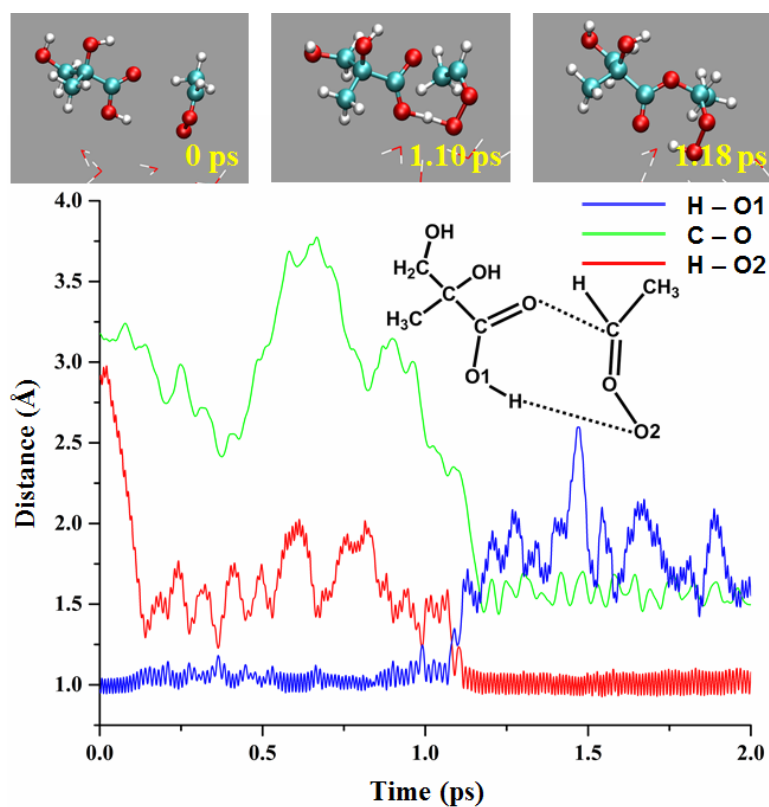


Fig. S4. The key bond length variations and snapshots of the gas-liquid interfacial reaction of *syn*-CH₃CHOO with the MGA COOH group.

System 2

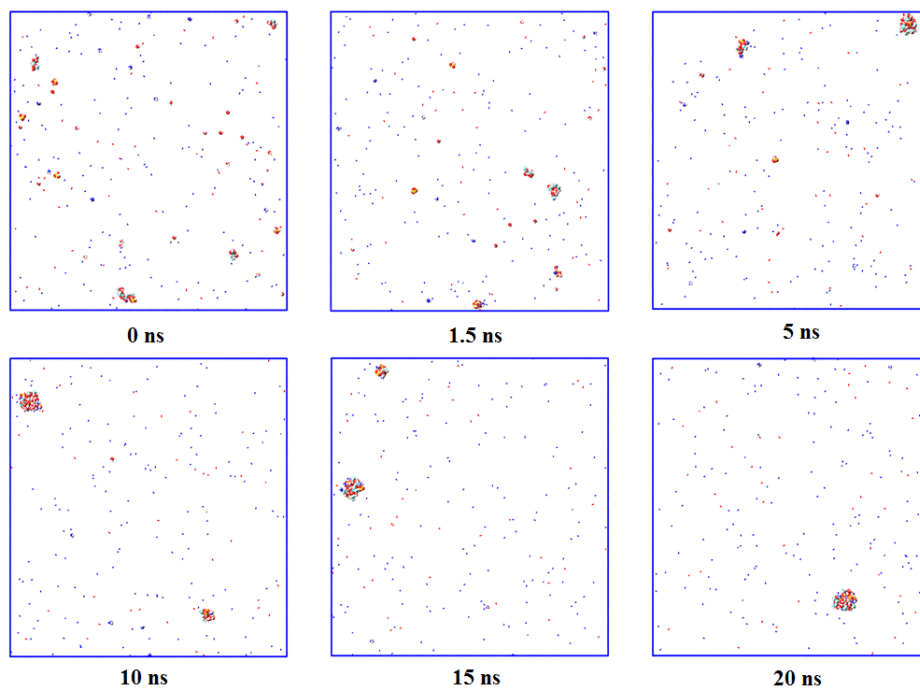


Fig. S5. The snapshots of nucleation simulation for the reaction product of *anti*-CH₃CHOO + MGA-β-OH.

System 3

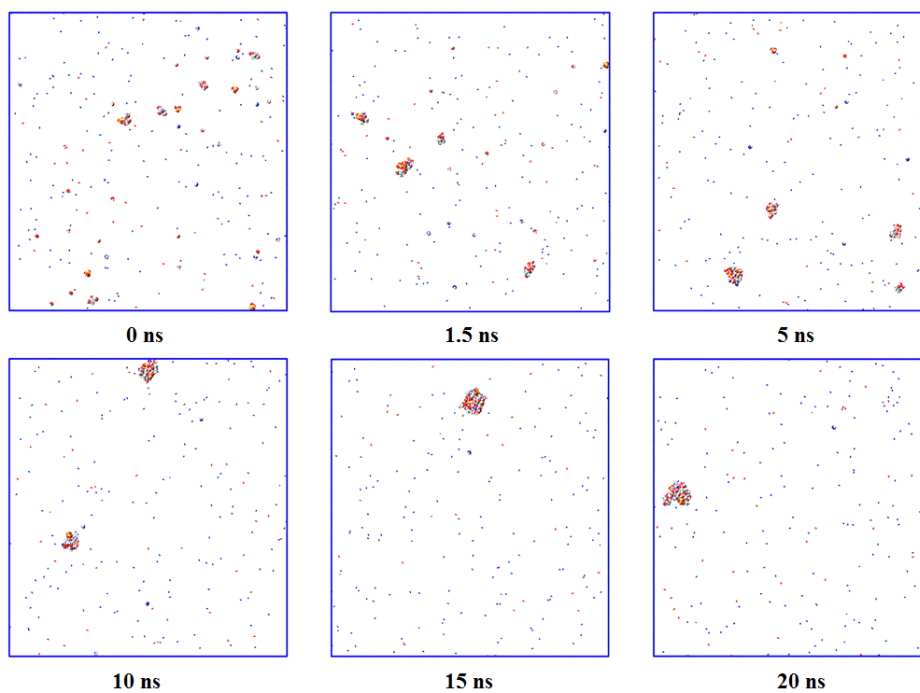


Fig. S6. The snapshots of nucleation simulation for the reaction product of *anti*-CH₃CHOO + MGA-α-OH.

System 4

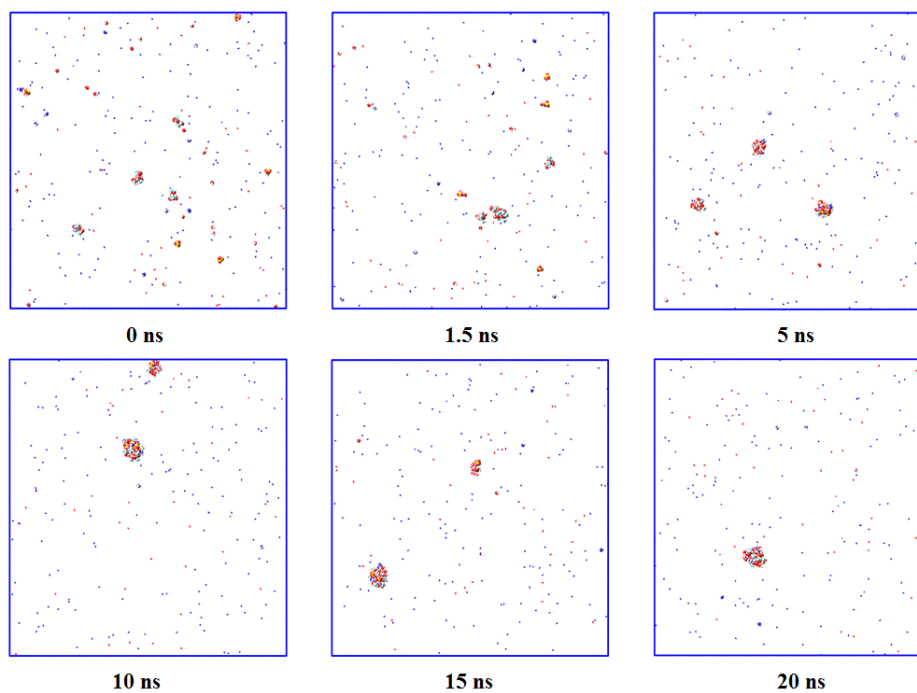


Fig. S7. The snapshots of nucleation simulation for the reaction product of *syn*-CH₃CHOO + MGA-COOH.

System 5

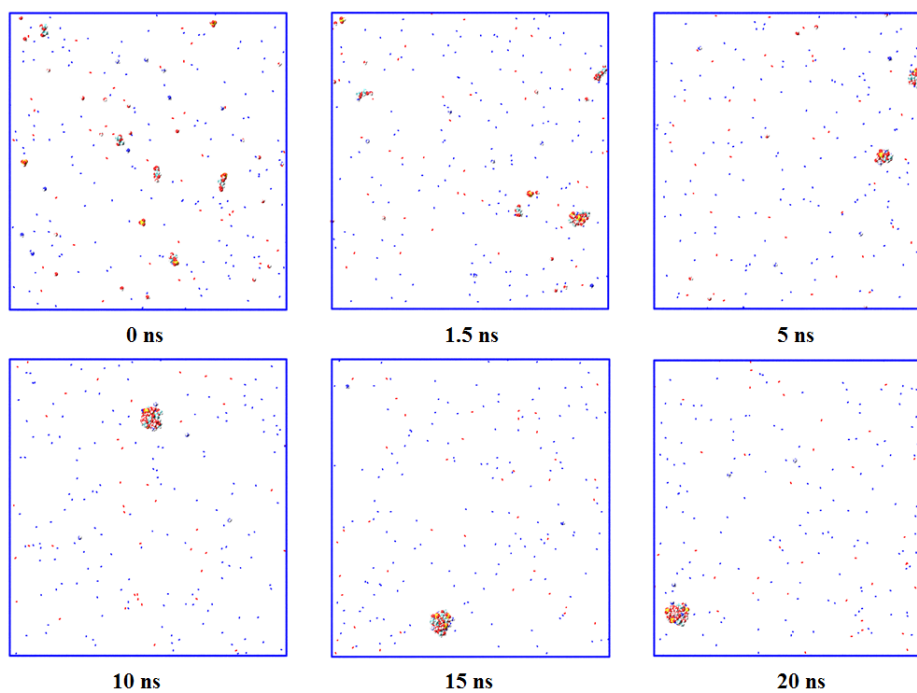


Fig. S8. The snapshots of nucleation simulation for the reaction product of *syn*-CH₃CHOO + MGA-β-OH.

System 6

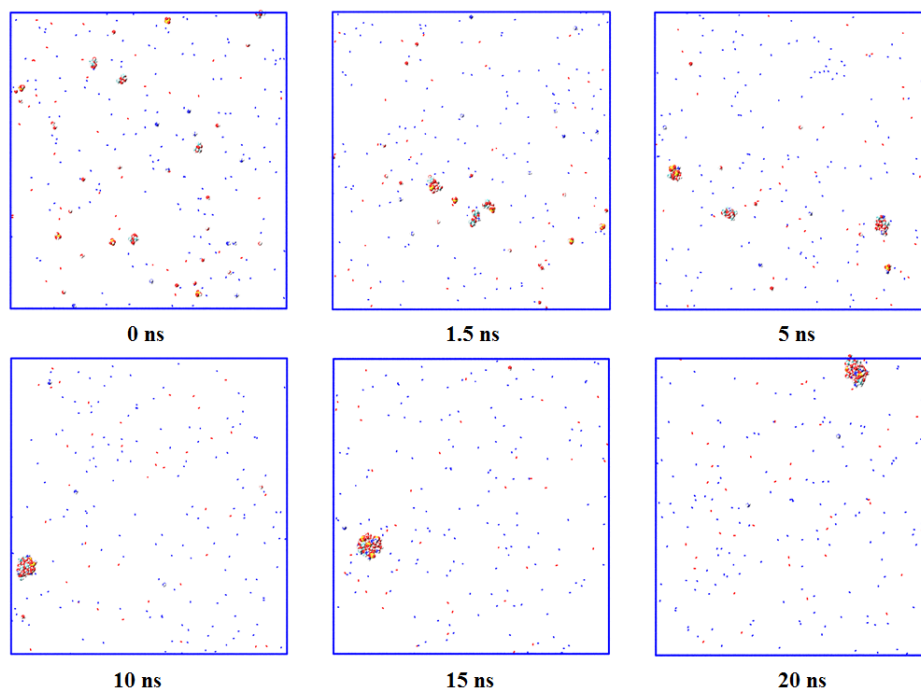


Fig. S9. The snapshots of nucleation simulation for the reaction product of *syn*-
 $\text{CH}_3\text{CHOO} + \text{MGA-}\alpha\text{-OH}$.