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The energetics and kinetics of the $\text{CH}_3\text{CHO} + (\text{CH}_3)_2\text{NH}/\text{CH}_3\text{NH}_2$ reactions catalyzed by a single water molecule in the atmosphere

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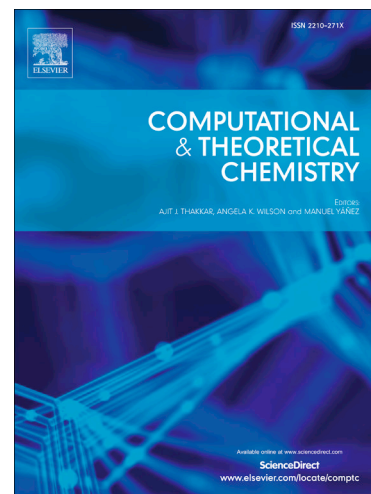
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The energetics and kinetics of the $\text{CH}_3\text{CHO} + (\text{CH}_3)_2\text{NH}/\text{CH}_3\text{NH}_2$ reactions catalyzed by a single water molecule in the atmosphere

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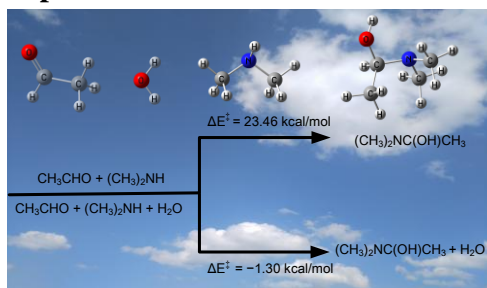
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Highlights

- Dimethylamine is more easily reacted with acetaldehyde than methylamine.
- A single water molecule can significantly reduce the energy barrier of the dimethylamine reaction with acetaldehyde.
- The reaction of dimethylamine with acetaldehyde in the presence of water should contribute to the formation of secondary aerosols in the atmosphere.

Graphical abstract



We report that a single water molecule plays a catalytic role in the reaction of dimethylamine with acetaldehyde.

Abstract: We have used quantum chemical methods and transition state theory with Eckart tunneling to study the water-catalyzed addition reaction of dimethylamine ((CH_3)₂NH) and methylamine (CH_3NH_2) to acetaldehyde (CH_3CHO) responsible for the formation of organic amines acted as the important precursors in the atmospheric nucleation processes. The calculated results show that the $\text{CH}_3\text{CHO} + (\text{CH}_3)_2\text{NH}$ reactions more feasible than the $\text{CH}_3\text{CHO} + \text{CH}_3\text{NH}_2$ reaction because the energy barrier of the $\text{CH}_3\text{CHO} + (\text{CH}_3)_2\text{NH}$ reaction is about 3 kcal/mol lower than that of the $\text{CH}_3\text{CHO} + \text{CH}_3\text{NH}_2$ reaction. In addition, a single water molecule can substantially reduce the energy barriers of the $\text{CH}_3\text{CHO} + (\text{CH}_3)_2\text{NH}/\text{CH}_3\text{NH}_2$ reactions. In particular, the reaction barrier of $\text{CH}_3\text{CHO} + (\text{CH}_3)_2\text{NH}$ is decreased from 23.46 to -1.3 kcal/mol with a single

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