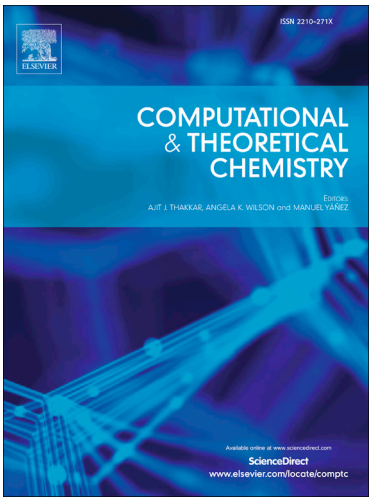

The energetics and kinetics of the $CH_3CHO + (CH_3)_2NH/CH_3NH_2$ reactions catalyzed by a single water molecule in the atmosphere

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The energetics and kinetics of the $CH_3CHO + (CH_3)_2NH/CH_3NH_2$ reactions catalyzed by a single water molecule in the atmosphere

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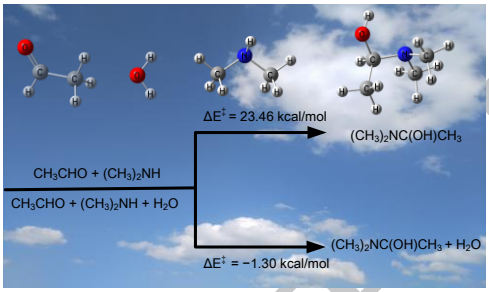
Highlights

- 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 $CH_3CHO + (CH_3)_2NH$ reactions more feasible than the $CH_3CHO + CH_3NH_2$ reaction because the energy barrier of the $CH_3CHO + (CH_3)_2NH$ reaction is about 3 kcal/mol lower than that of the $CH_3CHO + CH_3NH_2$ reaction. In addition, a single water molecule can substantially reduce the energy barriers of the $CH_3CHO + (CH_3)_2NH/CH_3NH_2$ reactions. In particular, the reaction barrier of $CH_3CHO + (CH_3)_2NH$ is decreased from 23.46 to −1.3 kcal/mol with a single

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