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Atmospheric Oxidation of Carbonyls: Insight to Mechanism, Kinetic and Thermodynamic Parameters

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Abstract : Carbonyls are the first-generation products from tropospheric degradation reactions of volatile organic compounds (VOCs). This computational study examined the mechanism of removal of carbonyls from the atmosphere via hydroxyl radical. The kinetics of the reactions were computed from the activation energy (using enthalpy (ΔH**) and Gibbs free energy (ΔG**). The minimum energy path (MEP) analysis reveals that in all the molecules, the products have more stable energy than the reactants, which implies that the forward reaction is more thermodynamically favorable. The hydrogen abstraction of the aromatic aldehyde, especially without methyl substituents, is more kinetically favorable compared with the other aldehydes in the order of aromatic (without methyl or meta methyl) > alkene (short chain) > diene > long-chain aldehydes. The activation energy is much lower for the forward reaction than the backward, indicating that the forward reactions are more kinetically stable than their backward reaction. In terms of thermodynamic stability, the aromatic compounds are found to be less favorable in comparison to the aliphatic. The study concludes that the chemistry of the carbonyl bond of the aldehyde changed significantly from the reactants to the products.

Keywords : atmospheric carbonyls, oxidation, mechanism, kinetic, thermodynamic
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