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Theoretical Study on the Mechanism and Kinetics of Acetaldehyde and Hydroperoxyl Radical: An Important Atmospheric Reaction

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ABSTRACT

A systematic theoretical study was performed on the mechanism and kinetics of the atmospheric reaction of acetaldehyde (CH_3CHO) and hydroperoxyl radical (HO_2) in the gas phase. The DFT-B3LYP/6-311++G(3df,3pd) and CCSD(T)/6-311++G(d,p) methods were employed for calculations. Based on the calculations, this reaction leads to four different products through radical addition and hydrogen abstraction mechanisms which are very important in atmospheric and combustion chemistry. The favorable reaction paths begin with α-hydroxyethylperoxy radical, $CH_3CH(OO)OH$, in a exothermic process and finally leads to the product P1 ($CH_3COOH+OH$). The overall rate constants for favorite reaction paths have been calculated at different temperatures (200-2500 K).

Keywords: Acetaldehyde, Hydroperoxyl radical, Atmospheric reaction, B3LYP, Rate constant

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