

Accepted Manuscript

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

Solaleh Farnia, Morteza Vahedpour, Mostafa Abedi, Hossein Farrokhpour

PII: S0009-2614(13)00956-1

DOI: <http://dx.doi.org/10.1016/j.cplett.2013.07.065>

Reference: CPLETT 31435

To appear in: *Chemical Physics Letters*



Please cite this article as: S. Farnia, M. Vahedpour, M. Abedi, H. Farrokhpour, Theoretical Study on the Mechanism and Kinetics of Acetaldehyde and Hydroperoxyl Radical: An Important Atmospheric Reaction, *Chemical Physics Letters* (2013), doi: <http://dx.doi.org/10.1016/j.cplett.2013.07.065>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

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

Solaleh Farnia^a, Morteza Vahedpour^a, Mostafa Abedi^b and Hossein Farrokhpour^{b,*}

^aDepartment of Chemistry, University of Zanjan, Zanjan 38791-45371, Iran

^bDepartment of Chemistry, Isfahan University of Technology, Isfahan 84156-83111, Iran

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, $\text{CH}_3\text{CH}(\text{OO})\text{OH}$, in an exothermic process and finally leads to the product P1 ($\text{CH}_3\text{COOH}+\text{OH}$). 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

Corresponding Author: Hossein Farrokhpour

E-mail: farrokhpoussein@gmail.com

Download English Version:

<https://daneshyari.com/en/article/5381493>

Download Persian Version:

<https://daneshyari.com/article/5381493>

[Daneshyari.com](https://daneshyari.com)