

# Accepted Manuscript

Frontiers article

Sulphuric acid-catalysed formation of hemiacetal from glyoxal and ethanol

Farzaneh Sarrami, Li-Juan Yu, Wenchao Wan, Amir Karton

PII: S0009-2614(17)30211-7

DOI: <http://dx.doi.org/10.1016/j.cplett.2017.02.084>

Reference: CPLETT 34597

To appear in: *Chemical Physics Letters*

Received Date: 23 January 2017

Revised Date: 27 February 2017

Accepted Date: 27 February 2017



Please cite this article as: F. Sarrami, L-J. Yu, W. Wan, A. Karton, Sulphuric acid-catalysed formation of hemiacetal from glyoxal and ethanol, *Chemical Physics Letters* (2017), doi: <http://dx.doi.org/10.1016/j.cplett.2017.02.084>

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.

## Sulphuric acid-catalysed formation of hemiacetal from glyoxal and ethanol

Farzaneh Sarrami, Li-Juan Yu, Wenchao Wan, and Amir Karton\*

School of Molecular Sciences, The University of Western Australia, Perth, WA 6009, Australia

### Abstract

We examine the reaction of ethanol with glyoxal to form hemiacetal by means of the high-level G4(MP2) procedure. In this reaction, an intermolecular proton transfer is coupled with the formation of a covalent C–O bond between the two molecules. We find a novel catalytic reaction mechanism in which an H<sub>2</sub>SO<sub>4</sub> catalyst reduces the barrier height from  $\Delta H_{298}^{\ddagger} = 140.2$  to 16.3 kJ mol<sup>-1</sup>. It is well established that H<sub>2</sub>SO<sub>4</sub> can effectively catalyse intramolecular proton transfers. This letter shows that H<sub>2</sub>SO<sub>4</sub> can catalyse an intermolecular proton transfer that is coupled with a covalent bond formation.

Keywords: Sulfuric acid catalyst, Intermolecular proton transfer, Glyoxal, G4(MP2), CCSD(T).

\*Corresponding author: Amir Karton, E-mail: amir.karton@uwa.edu.au

Download English Version:

<https://daneshyari.com/en/article/5377976>

Download Persian Version:

<https://daneshyari.com/article/5377976>

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