

Accepted Manuscript

Catalytic effect of water, water dimer, or formic acid on the tautomerization of nitroguanidine

Benni Du, Weichao Zhang

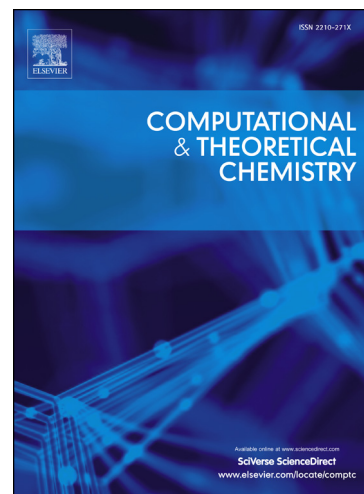
PII: S2210-271X(14)00431-9
DOI: <http://dx.doi.org/10.1016/j.comptc.2014.09.025>
Reference: COMPTC 1616

To appear in: *Computational & Theoretical Chemistry*

Received Date: 10 August 2014
Revised Date: 21 September 2014
Accepted Date: 22 September 2014

Please cite this article as: B. Du, W. Zhang, Catalytic effect of water, water dimer, or formic acid on the tautomerization of nitroguanidine, *Computational & Theoretical Chemistry* (2014), doi: <http://dx.doi.org/10.1016/j.comptc.2014.09.025>

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.



**Catalytic effect of water, water dimer, or formic acid on the
tautomerization of nitroguanidine**

Benni Du, Weichao Zhang*

College of Chemistry and Chemical Engineering, Jiangsu Key Laboratory of Green Synthetic Chemistry for Functional Materials, Jiangsu Normal University, Xuzhou, Jiangsu 221116, People's Republic of China

Abstract

We have investigated the reaction mechanisms and kinetics of water, water dimer, or formic acid catalyzed gas-phase isomerization of α -nitroguanidine to β -nitroguanidine by means of high level theoretical methods and transition state theory. The potential energy surface profile has been characterized at the CCSD(T)/6-311++G(2df,2pd)//M06-2X-D3/6-311++G(3df,3pd) level with zero-point energy correction. The calculations indicate that incorporation of water, water dimer, or formic acid molecule into the reactant α -nitroguanidine can noticeably reduce the energy barrier. The reductions are found to be small for water and most significant for formic acid. Most importantly, the kinetics calculations show that the rate constants for the water, water dimer or formic acid assisted reactions are about 14, 14 or 19 orders of magnitude larger than those for the uncatalyzed reaction, respectively. These results suggest that formic acid should play a larger role than both water and water dimer on isomerization of α -nitroguanidine to β -nitroguanidine

* Corresponding author. Tel.: +86 516 83403165; fax: +86 516 83403164.
E-mail address: zwc@jsnu.edu.cn

Download English Version:

<https://daneshyari.com/en/article/5393520>

Download Persian Version:

<https://daneshyari.com/article/5393520>

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