

Accepted Manuscript

Modeling of stability and properties of anionic and cationic tautomers of the 3-hydroxypyridin-4-one system

Mehrdad Mohammadpour, Krzysztof K. Zborowski, S. Heidarpoor, Grzegorz Żuchowski, Leonard M. Proniewicz

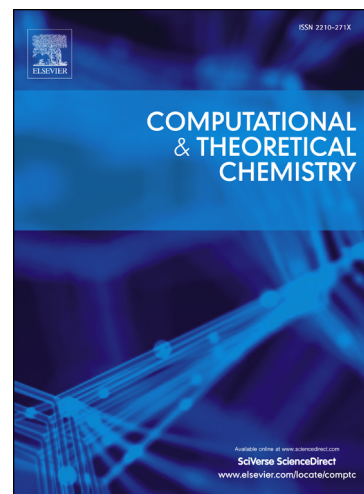
PII: S2210-271X(15)00504-6
DOI: <http://dx.doi.org/10.1016/j.comptc.2015.12.023>
Reference: COMPTC 2027

To appear in: *Computational & Theoretical Chemistry*

Received Date: 1 November 2015
Revised Date: 22 December 2015
Accepted Date: 23 December 2015

Please cite this article as: M. Mohammadpour, K.K. Zborowski, S. Heidarpoor, G. Żuchowski, L.M. Proniewicz, Modeling of stability and properties of anionic and cationic tautomers of the 3-hydroxypyridin-4-one system, *Computational & Theoretical Chemistry* (2015), doi: <http://dx.doi.org/10.1016/j.comptc.2015.12.023>

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.



Modeling of stability and properties of anionic and cationic tautomers of the 3-hydroxypyridin-4-one system.

Mehrdad Mohammadpour^a, Krzysztof K. Zborowski^{b*}, S. Heidarpoor^a,
Grzegorz Żuchowski^c, Leonard M. Proniewicz^b

^a*Department of Medicinal Chemistry, Faculty of Pharmacy, Isfahan University of Medical Sciences, Isfahan 81746-73461, Iran*

^b*Faculty of Chemistry, Jagiellonian University in Krakow, Ingardena 3,
30-060 Kraków, Poland*

^c*Department of Organic Chemistry, Medical College, Jagiellonian University in Kraków,
9 Medyczna St., 30-688 Kraków, Poland*

* Corresponding author:

Phone: +48-12-663-20-64; fax: +48-12-634-05-15;

E-mail address: zborowsk@chemia.uj.edu.pl (K.K. Zborowski).

Download English Version:

<https://daneshyari.com/en/article/5392935>

Download Persian Version:

<https://daneshyari.com/article/5392935>

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