Accepted Manuscript

Synthesis and characterization of sulfolane-based amino alcohols: A combined experimental and computational study

Vitalii A. Palchykov, Iryna S. Zarovnaya, Serhii V. Tretiakov, Alyona V. Reshetnyak, Iryna V. Omelchenko, Oleg V. Shishkin, Sergiy I. Okovytyy

PII: S0022-2860(17)31676-9

DOI: 10.1016/j.molstruc.2017.12.055

Reference: MOLSTR 24674

To appear in: Journal of Molecular Structure

Received Date: 12 November 2017

Accepted Date: 14 December 2017

Please cite this article as: V.A. Palchykov, I.S. Zarovnaya, S.V. Tretiakov, A.V. Reshetnyak, I.V. Omelchenko, O.V. Shishkin, S.I. Okovytyy, Synthesis and characterization of sulfolane-based amino alcohols: A combined experimental and computational study, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2017.12.055.

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.



Synthesis and characterization of sulfolane-based amino alcohols:

a combined experimental and computational study

Vitalii A. Palchykov¹*, Iryna S. Zarovnaya¹, Serhii V. Tretiakov¹,

Alyona V. Reshetnyak¹, Iryna V. Omelchenko², Oleg V. Shishkin^{2†} and Sergiy I. Okovytyy¹

¹Oles Honchar Dnipro National University, 72 Gagarina Ave., Dnipro 49010, Ukraine

²SSI «Institute for Single Crystals», National Academy of Sciences of Ukraine, 60 Lenina Ave.,

Kharkiv 61001, Ukraine

Corresponding author e-mail: palchikoff82@gmail.com. Tel. +38 066 3007157.

[†]Deceased

Abstract

Aminolysis of 3,4-epoxysulfolane in aqueous media leads to a very complex mixture of products with unresolved stereochemistry. Herein, we report a detailed theoretical and experimental mechanistic investigation of this reaction along with extensive spectroscopic characterization of the resulting amino alcohols, using 1D and 2D NMR techniques (¹H, ¹³C, NOE, NOESY, COSY, HSQC, HMBC) as well as XRD analysis. In addition to simple amines such as ammonia and benzylamine, our study also employed the more sterically hindered *endo*-bicyclo[2.2.1]hept-5-en-2-ylmethanamine. The mechanism of the aminolysis of 3,4-epoxysulfolane by aqueous ammonia was studied in more detail using quantum chemical calculations at the MO6-2X/6-31++G** level of theory. The computational results led us to conclude that the most probable way of initial epoxide transformation is base-catalyzed rearrangement to a corresponding allylic alcohol. Subsequent formation of vicinal amino alcohols and diols proceeds *via* addition of ammonia or hydroxy-anions to activated double C=C bond with some preference of a *cis*-attack. Detailed analytical data obtained in the course of our work will be useful for the stereochemical identification of new sulfolane derivatives.

Keywords amino alcohols, rearrangement, quantum chemical calculations, XRD analysis, 2D NMR investigation

Download English Version:

https://daneshyari.com/en/article/7808190

Download Persian Version:

https://daneshyari.com/article/7808190

Daneshyari.com