Thematic Section: Kinetics and Catalysis. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 12-29-1-7
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: December 29, 2011.

Thematic course: Kinetics and mechanism of acyl transfer reactions. Part 2.

Kinetics of heterocyclic amines arensulfonylation in aqueous 1,4-dioxane

© **Natalia R. Sokolova**,[1] **Ekaterina V. Nikitina**,[2] **Ludmila B. Kochetova**,[1]
Natalia V. Kalinina,[2] and **Tatiana P. Kustova**[1]*[+]
[1] *Department of Organic and Biological Chemistry. Ivanovo State University.*
Ermak St., 39. Ivanovo, 153025. Russia. Phone: +7 (84932) 37-37-03. E-mail: kustova_t@mail.ru
[2] *Department of Inorganic and Analytical Chemistry. Ivanovo State University.*
Ermak St., 39. Ivanovo, 153025. Russia. Phone: +7 (84932) 37-37-03.

*Supervising author; [+]Corresponding author

Keywords: *kinetics, arensulfonylation, reaction mechanism, morpholine, piperidine, 4-toluenesulfonyl chloride, benzenesulfonyl chloride, water – 1,4-dioxane, PES.*

Abstract

At the present work results of kinetic investigation of morpholine and piperidine arensulfonylation by 4-toluenesulfonyl chloride and benzenesulfonyl chloride in solvent water (40 % wt.) – 1,4-dioxane in polythermal conditions are presented. Rate constants of all the examined processes are determined, and also activation parameters of the reactions. The kinetic characteristics obtained are compared with data on similar acyl transfer reactions with participation of heterocyclic amines in water-organic media. Potential energy surface is calculated for piperidine reaction with benzenesulfonyl chloride by RHF/6-31G* method. A gas phase reaction occurrence by S_N2-mechanism is established.