Thematic Section: Quantum-Chemical Research. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-35-9-1
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: June 5, 2013.

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

Quantum chemical simulation of the mechanism of benzoyl chloride and benzenesulphonyl chloride interactions with amino compounds of different classes

© **Ludmila B. Kochetova**,[1] **Maria G. Paikova**,[1]
Natalia V. Kalinina,[2] and **Tatiana P. Kustova**[1]*[+]
[1] *Department of Organic and Physical Chemistry. Ivanovo State University.*
Ermak St., 39. Ivanovo, 153025. Russia. Phone: +7 (4932) 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 (4932) 37-37-03.

*Supervising author; [+]Corresponding author

Keywords: *acylation, amino compounds,benzoyl chloride, benzenesulfonyl chloride, quantum chemical calculations, reaction mechanism, potential energy surface.*

Abstract

Potential energy surfaces are calculated for reactions of ammonia and a number of amino compounds with benzoyl chloride and benzenesulfonyl chloride in gas phase, as well as for ammonia interaction with benzoyl chloride in water by using the polarized continuum model. It is shown that all the reactions proceed by the concerted mechanism, and benzoylation occurs by the pathway with frontal nucleophilic attack, when whereas arensulfonylation – by the pathway with varying attack angle. Non-specific solvation by water decreases activation energy of ammonia acylation as compared to gas phase reaction**.**