Full Paper _____ *Thematic Section:* Quantum Chemistry.
Registration Code of Publication: 10-21-9-8 *Subsection:* Polymer Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: September 20, 2010.

Quantum-chemical research of geometry and oscillation spectra of hydrogen bonded associates of aromatic urethanes

© **Galina G. Suchkova**,[+] and **Lev I. Maklakov***
Department of physics. Kazan state university of architecture and construction. Zelenaya St., 1. Kazan, 420043. Republic Tatarstan. Russia. Phone: +7 (843) 510-47-38. E-mail: galinasd@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *aromatic urethanes, quantum-chemical calculations, molecular structure, oscillation spectra.*

Abstract

Density functional (DFT) calculations at B3LYP/6-31G(d) level have been employed as an efficient way for calculating "amide" frequencies of several simple aromatic urethanes. Bands attributable to cis and trans conformers in aromatic naphthyl-urethanes have been detected. Structures, harmonic frequencies and their intensities were calculated for hydrogen-bond dimers of these compounds. The calculated dimer spectra are in good agreement with experimental spectra in solution phases.