Thematic section: Quantum Chemistry. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 10-21-8-45
Publication is available for discussion in the framework of on-line conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed to editorial board: September 10, 2010.

Investigation of the potential energy surface of bimolecular reactions of nucleophilic substitution on the base of density functional theory

© **Alexander V. Fateev**, **Anastasiya O. Akulova**, and **Oleg Kh. Poleschuk***[+]
Department of organic chemistry. Tomsk state pedagogical university. Komsomolskiy St., 75. Tomsk, 634041. Russia. Phone: +7 (3822) 59-14-54. E-mail: poleshch@tspu.edu.ru

*Supervising author; [+]Corresponding author

Keywords: *density functional theory; B3LYP/DGDZVP; biomolecular nucleophilic substitution; energy shape of the reaction.*

Abstract

Analysis of the thermodynamic parameters of bimolecular reactions of nucleophilic substitution in the gas phase and in solution using density functional calculations in the program packages GAUSSIAN and ADF using a number of all-electron basis sets has been carried out. The geometry of the transition state, and early- and last transition states for the reaction $CH_3Cl + F^- \rightarrow CH_3F + Cl^-$ have been calculated. Comparative analysis of the energy profiles of reaction in the gas phase, water and carbon tetrachloride was carried out.