Full Paper_____*Thematic Section:* Theoretical and Computational Chemistry.
Registration Code of Publication: 9-15-1-65 *Subsection:* Physical Organic Chemistry.
Publication is available for discussion in the framework of on-line conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed to editorial board: March 3, 2009.

Thematic Division: Influence of Media on Reactivity. Part XV.

Calculations of activation energy of cycloaddition reaction in solution

© **Vladimir G. Uryadov**
Department of Organic Chemistry. Kazan State Technological University. K. Marx St., 68. Kazan, 420015. Republic Tatarstan. Russia. Phone: +7 (843) 272-12-53. E-mail: uryadov@kstu.ru

*Supervising author; +Corresponding author

Keywords: *activation energy, theoretical calculation.*

Abstract

With the method, principally different from the quantum ones, there has been performed the calculation of activation energies of 36 cycloaddition reactions in solutions. The objects under examination included: non-catalyzed reactions of diene synthesis, reactions of 1,3-dipolar cycloaddition, reactions of polar [2+2]-cycloaddition and catalyzed reactions of diene synthesis. Calculation results have been compared with the experimental data. The comparison testifies in favor of closeness of calculated values and experimental data.