Thematic Section: Chemical and Technological Research. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 14-39-7-47
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: October 3, 2014.

Reactivity indices of alkenes in amino-methylation reactions

© Rifkat F. Talypov, **Ivan V. Vakulin**,* **Azamat R. Galyakhmetov**,
Elvira R. Latypova,+ and **Guzaliya R. Talypova**
Department of Organic and Bioorganic Chemistry. Bashkir State University.
Zaky Validy St., 32. Ufa, 450074. Republic of Bashkortostan. Russia.
Phone: +7 (347) 229-97-29. E-mail: lelvirar@mail.ru

*Supervising author; +Corresponding author

Keywords: amino-methylation of alkenes, aminomethyl carbocation, Mannich reaction, DFT (Density Functional Theory), NBO-analysis, reactivity indices.

Abstract

The peculiarities of alkenes interaction with aminomethyl carbocations by quantum and chemical methods were considered. The calculations in the approximation B3LYP/6-31G(d,p) and further NBO analysis demonstrate that the correct reactivity index can be obtained on the basis of atomic orbitals contribution values Csp^2 to the multiple bond formation. It accords with the literature data on the alkenes reactivity in the reaction of electrophylic addition of aminomethyl carbocations on multiple bonding.