Thematic Section: Quantum-Chemical Studies. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 12-32-13-123
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: December 15, 2012.

Quantum chemical research of 1,3-dioxanes formation from formaldehyde dimer and alkenes

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Keywords: *ab initio calculation, transition state, Prins reaction, 1.3-dioxanes, formaldehyde oligomers, alkenes.*

Abstract

Some features of adding formaldehyde dimer to alkenes with formation of alkyl-substituted 1,3-dioxanes by the Prins reaction in the gas phase are studied at the MP2(fc)/6-31G(d,p) computational level. The structure of the transition states and key intermediates are revealed and thermochemical reaction parameters are determined. It is shown that 1,3-dioxanes are mostly formed from the π-complex obtained as a result of formaldehyde dimer interaction with alkenes without intermediate formation of a σ-complex. Here the transformation of π-cation can be considered as a pseudo synchronous process.