Thematic Section: Quantum Chemistry. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 11-28-17-11
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: October 13, 2011.

Quantum-chemical modeling of the reaction route of butene-2 with ozone

© **Boris E. Krisyuk**,[2]* **Alexey V. Mayorov**,[1] **Vasily A. Ovchinnikov**,[1+] and **Anatoly A. Popov**[1]
[1] *Laboratory of Physical Chemistry of Synthetical and Natural Polymers. Emmanuel Institute of Biochemical Physics of Russian Academy of Sciences. Kosyigina St., 4. Moscow, 119334. Russia. Phone: +7 (495) 939-71-93. E-mail: fizhim@rambler.ru*
[2] *Laboratory of Kinetics of Processes in Gase Phase. Institute of Chemical Problems of Russian Academy of Sciences, ICP RAS. Academic Semyonov St., 1. Chernogolovka, 142432. Moscow District. Russia. Phone: +7 (495) 993-57-07 E-mail: bkris@mail.ru*

*Supervising author; [+]Corresponding author

Keywords: *ozone, butene-2, double bond, multi-reference approach, concerted and non-concerted addition.*

Abstract

Calculations of potential energy surface profile of reaction of *cis*- and *trans*-butene-2 with ozone were performed with quantum chemistry methods. MP2, B3LYP, MRMP2 methods were used in conjunction of 6-31+G**, 6-311+G**, aug-cc-pVDZ basis sets. Dimensions of active space are (10.9) and (14.11). Two paths of reaction were investigated – concerted (five-membered cyclic transition state (TS1)) and non-concerted (through biradical transition state (TS2)). It has been shown that these methods described reaction well, activation energy and rate constants are in agreement with experimental dates. Reaction through TS1 for butene-2 is much faster then through TS2, so concerted mechanism predominates in this case.