Full Paper _____ *Thematic Section:* Preparative Research.
Registration Code of Publication: 14-39-10-58 *Subsection:* Structural Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/ *(English Preprint)*
Contributed: December 12, 2014.

Quantum-chemical study of ozone protonation

© **Quyen Quy Ngo**, **Alexander Ya. Samuilov**,* **Yakov D. Samuilov**,
Fanis F. Valiullin, **Evgeny I. Grigoriev**,[+] and **Alexander A. Petukhov**
Department of Technology of Synthetic Rubber. Kazan National Research Technological University.
K. Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia.
Phone: +7 (843) 231-42-14. E-mail: grigoriev@kstu.ru

*Leading direction; [+]Corresponding author

Keywords: ozone, quantum chemistry, B3LYP, protonation, DFT.

Abstract

The process of protonation of ozone in the singlet and triplet states was studied using B3LYP/6-311++G(df,p) quantum-chemical method. The geometric structure of the products of protonation were studied. The thermodynamic parameters of the reaction of protonation of ozone in the singlet and triplet electronic configurations were described. It was shown that the process of protonation of ozone in all cases is exothermic and proceeds with free energy and entropy decrease.