Full Paper _____ *Thematic Section:* Quantum-Chemical Research.
Reference Object Identifier – ROI: jbc-02/16-45-3-128 *Subsection:* Physical Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Submitted on April 01, 2016.

Computation of vibrational spectra of 5-methyl-4-nitrobenzofuroxan and 7-methyl-4-nitrobenzofuroxan molecules in coordinates X_δ^0 with an estimation of a force fields in DFT

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Keywords: 5-methyl-4-nitrobenzofuroxan, 7-methyl-4-nitrobenzofuroxan, the generalized force constants, coordinates Xδ0, calculations DFT, vibration frequencies.

Abstract

Within the framework of approach B3LYP/6-311++G(3df,3pd) the force field of 5-methyl-4-nitrobenzofuroxan and 7-methyl-4-nitrobenzofuroxan molecules in coordinates X_δ^0 for the first time is received. Frequencies of normal vibrations were calculated. Comparison of the received generalized force constants with those of molecule was carried out. It is received that for pair compounds, such as 5-metil-4-nitrobenzofuroksan and 7-metil-4-nitrobenzofuroksan, Boulton-Katritzky rearrangement leads to compound with the greatest value of the generalised force constants of bond C-N_3. The Same picture is observed for the generalised force constants of bonds N_1-O_2 and O_2-N_3. Thus value of the generalised force constants of bond N→O decreases.

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