Thematic Section: Quantum-Chemical Research. **Full Paper**
Subsection: Physical Inorganic Chemistry. *Reference Object Identifier* – ROI: jbc-02/18-53-1-79
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
The article is published based on the materials of the 2nd stage of the Mini-Symposium "Butlerov Heritage – 17-18" (Kazan)
Submitted on January 21, 2018.

Noncatalytic oxidation of sulfur dioxide

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Keywords: sulfur dioxide, sulfuric acid, sulfur trioxide, oxidation, activation energy, quantum chemical calculations.

Abstract

The theoretical research of process of oxidation dioxide sulfur without catalyst with use of the quantum and chemical Priroda 6 program is conducted. This program is an available software package for scientific and study, she doesn't demand big time expenditure and allows to receive high precision of calculations, and there is also an opportunity to carry out parallel calculations. The ChemCraft program visualizer was used for process modeling. During the sulfur dioxide oxidation process mechanism research for a singletny state it is revealed that this process is difficult and multistage, during reaction formation of several products is possible. At the first stage of the studied process two molecules SO_3 separate, further there is a regrouping to formation of the SO_5 and SO complex. Then the way of process is divided into two in parallel the proceeding stages. One of stages leads to formation, most likely, of the final products of SO_3, SO and O_2. Another in parallel the proceeding stage leads to formation of by-products of SO_4 and SO_2. The most power-intensive stage is the second, E act = 232 kJ/mol. On the obtained data the power chart of a way of reaction of oxidation of dioxide of sulfur is constructed. For all sites of process thermodynamic characteristics are calculated, and for stages values of energy of activation and thermal effects are found. All stages, except the second, go spontaneously with low energy of activation, the third stage is surmountable in temperature conditions of synthesis. The most part of an activation barrier of homogeneous oxidation of dioxide of sulfur is caused by energy expense for a rupture of communication of S-O and transition of one atom of oxygen to the molecule SO_4 with formation of the SO_5 complex. The obtained data, namely the second energy of activation, prove need of carrying out process in the presence of the catalyst. At selection of catalysts of process of oxidation it is necessary to consider probability of a molecule of dioxide of sulfur to react with oxygen atoms, connected with the catalyst less strongly, than with each other in the molecule O_2, for overcoming a power barrier.

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