Thematic Section: Quantum-Chemical Research. **Full Paper**
Subsection: Organic Chemistry. *Reference Object Identifier* – ROI: jbc-02/16-48-11-7
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Submitted on December 10, 2016.

Theoretical study of the mechanism of model sulfur aquathermolysis asphaltene using of the Priroda program

© **Alexander G. Shamov**,[1]* **Ilia V. Aristov**,[2+] **Guzel G. Garifzianova**,[3]
and **Grigory M. Khrapkovsky**[3]
[1] *IT Department;* [2] *Computational Chemistry Department;* [3] *Department of Catalysis. Kazan National Research Technological University. K. Marx St., 68. Kazan, 420015. Republic of Tatarstan. Russia.*
Phone: [2)] *+7 (843) 231-42-11. E-mail:* [2)] *aristov@kstu.ru*

*Supervising author; +Corresponding author

Keywords: quantum-chemical calculation, aquathermolysis, asphaltene, method QM_N3.

Abstract

The oil fields of Republic of Tatarstan contain various organic sulfur compounds. The removal of organic sulfur compounds is a prerequisite for further refining. One possible way to remove sulfur contaminants is their destruction during aquathermolysis directly into oil wells. Finding the optimal conditions aquathermolysis (temperature, pressure, chemical additives) can be determined on the basis of information on the mechanism of the process. Experimental data on the mechanism of destruction of sulfur-containing impurities during aquathermolysis is absent. The quantum-chemical methods were used to study the mechanism of aquathermolysis in this work.

Since the most difficult problem is the destruction of asphaltenes was to investigate the mechanism of aquathermolysis phenanthro[4,5-bcd]thiophene – the simplest model of the sulfur-containing asphaltenes. Quantum-chemical study was conducted using Priroda 15 program, which includes a semi-empirical method QM_N3 density functional. The *P-AutoExtremum* shell was used to find the extreme points and the construction of reaction paths on the potential energy surface. The program P-Analysis was used for the processing of the elementary acts of studies, which calculates the values of the activation parameters and barriers to the forward and reverse reactions, and thermodynamic functions of the reactants and products. In this paper we consider only beneficial in terms of energy processes for the carbon–carbon of the studied reactions (more than 20 reactions). Elementary stage rupture processes of the thiophene rings are considered by the sulfur–carbon with one and three water molecules. Estimates barriers of aquathermolysis above processes were evaluated. The paper presents the basic geometric parameters of the transition states and products of aquathermolysis reactions.