Thematic Section: Quantum Chemistry. **Full Paper**
Subsection: Inorganic Chemistry. *Registration Code of Publication:* 10-20-5-1
Publication is available for discussion in the framework of on-line conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed to editorial board: July 10, 2010.

Quantum-mechanical research of electroreduction of bismuth(III) complexes from aqueous solutions, containing thiocyanate-ions

© **Andrey M. Kuznetsov**,*+ and **Alexandr M. Shapnik**
Department of inorganic chemistry. Kazan state technological university. K. Marx St., 68. Kazan, 420015. Republic of Tatarstan. Russia. Phone: +7 (843) 231-41-22. E-mail: am_kuznetsov@kstu.ru

*Supervising author; +Corresponding author

Keywords: *thiocyanate-ion, complexing, Bi(III), electroreduction, dissociative electronic electron transport, activation energy, quantum-chemical calculations, method of density functional, B3LYP, model PCM.*

Abstract

On the basis of quantum-chemical calculations with functional density method and quantum-mechanical theory of charge transport in polar media there have been carried out the model estimations of the activetion energy of the elementary act of the first stage of electroreduction of aquacomplex $[Bi(Hvation_2O)_6]^{3+}$, monoisothiocyanate complex $[Bi(H_2O)_4NCS]^{2+}$, as well as hexaisothiocyanate complex $[Bi(NCS)_6]^{3-}$. The conclusion was made about the accelerating effect of thiocyanate-ion on electroreduction owing to its complexing with the ion of Bi(III), which allowed to explain the observed regularities.