Thematic Section: Theoretical and Computer Chemistry. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 10-23-15-1
Publication is available for discussion in the Internet as a material of "All-Russian Working Chemical Conference "*Butlerov's Heritage-2011*". http://butlerov.com/bh-2011/
Contributed to editorial board: November 9, 2010.

Method for estimating the reactivity of oxidation inhibitors of acrylic acid

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Keywords: *acrylic acid, aromatic amine, hydrogen bond, inhibitor, rate constant, method of intersecting parabolas, multiplicative method, oxidation, semiquinone radical, phenol, activation energy, enthalpy of reaction.*

Abstract

Semi-empirical method has been worked out for calculating activation energies (E) and rate constants (k) of the reactions of peroxyl and alkyl radicals of acrylic acid and oxidation inhibitors. The developed method represents a combination of two methods: the method of intersecting parabolas for calculating E and k of the reaction under investigation in non-polar solvent (hydrocarbon) and multiplicative method for calculating the enthalpy and Gibbs energy of hydrogen bond formation between O-H or N-H-bonds of the inhibitor and solvent (acrylic acid). This method was used to calculate E and k for the reactions of acrylic acid with 29 inhibitors (phenols and aromatic amines) and the reaction of oxygen with 5 semi-quinone radicals.