Full Paper Reference Object Identifier - ROI: jbc-02/15-43-8-140 The article is published on materials of the report on "International Scientific Forum Butlerov Heritage – 2015". http://foundation.butlerov.com/bh-2015/ (English Preprint) Submitted on April 21, 2015.

Bond dissociation energy of C-X (X = F, Cl, Br, I) bonds in halogencontaining hydrocarbons: correlation ratios with electronegativity, force constants of bonds and radii of atom X

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Keywords: bond dissociation energy, enthalpy of radical formation, enthalpy of molecule formation, electronegativity, force constant, atom radius, correlation ratio, regression equation.

Abstract

In this paper dissociation energies of C-X-bonds (X=F, Cl, Br, I) in halogen-containing hydrocarbons are calculated or specified using enthalpies of free radical formation derived from the experimental kinetic data. Comparison of the obtained results with the literary data is made. Correlation connection between the dissociation energy of C-X-bond of the replaced hydrocarbons and their electronegativity, force constant and atom radius of X is established. The regression equations for various groups of halogen-containing hydrocarbons $D_{C-X} = \omega_1 \sqrt{D_{X-X} D_{C-C}} + \omega_2 b r_{XX} + \omega_3$ are suggested, where $D_{F-F} = 158.670 \pm 0.096$ kJ/mol, $D_{Cl-Cl} =$ $242.58 \pm 0.004 \text{ kJ/mol}, D_{\text{Br-Br}} = 193.859 \pm 0.120 \text{ kJ/mol}, D_{\text{I-I}} = 152.25 \pm 0.57 \text{ kJ/mol}, D_{\text{C-C}}$ are calculated using enthalpies of free radical formation.

Subsection: Physical Organic Chemistry.