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

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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 $D_{C-X} = \omega_1\sqrt{D_{X-X}D_{C-C}} + \omega_2 br_{XX} + \omega_3$ are suggested, where $D_{\text{F-F}}$ = 158.670 ± 0.096 kJ/mol, $D_{\text{Cl-Cl}}$ = 242.58 ± 0.004 kJ/mol, $D_{\text{Br-Br}}$ = 193.859 ± 0.120 kJ/mol, $D_{\text{I-I}}$ = 152.25 ± 0.57 kJ/mol, $D_{\text{C-C}}$ are calculated using enthalpies of free radical formation.