

FRAME COMPOUNDS. ENERGY REARRANGMENTS OF RADICALS

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Abstract: On the basis of the relations connecting the energy characteristics of compounds (enthalpy of formation, enthalpy of atomization, energy of dissociation of chemical bonds, average thermochemical energy of bonds, and energy of rearrangement of fragments of molecules into radicals — energy of restructuring of radicals), the energies of restructuring of radicals of frame compounds are determined. The application of a simple difference method and a double difference method for the evaluation and control of enthalpy of formation of radicals and substances is demonstrated. In the calculations, patterns previously identified for average thermochemical energies of the bonds of aliphatic compounds and energies of the rearrangement of the radicals have been used.

Keywords: frame compounds; chemical bond energies; bond dissociation energies; enthalpy of radical formation; enthalpy of atomization; energy of radical rearrangement

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