ENTIALPY OF FORMATION AND ENERGY REORGANIZATION OF NAPHTHALENE RADICALS

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Abstract: Based on the method of double-difference, the enthalpy of formation of radicals of naphth-1-yl and naphth-2-yl (405.0 ± 2.0 kJ/mol) has been calculated. As objects of study, data on the enthalpies of formation of naphthalene derivatives were used and as the reference values, the phenyl radical and benzene derivatives have been applied. The obtained data on the enthalpies of formation of radicals of naphth-1-yl and naphth-2-yl were applied to adjust the existing enthalpies of formation of naphthalene derivatives in the gas phase. For 1- and 2-nitronafthalines, the same value was obtained equal to 133 kJ/mol. The literature data were 111.2 ± 5.3 and 145.0 ± 1.9 kJ/mol for 1-nitronaftaline and 129.8 kJ/mol for 2-nitronaftaline (calculation). The data obtained allowed calculating the dissociation of bonds $D(C–NO_2)$ in 1- and 2-nitronaftaline which was 306 ± 2.0 kJ/mol and close to the energy of this bond in benzene (305.4 ± 1.3 kJ/mol). To determine the identity of bonds in naphthalene and benzene, a joint calculation of C–N and C–C bonds in naphthalene and benzene from the enthalpy of atomization of these compounds was performed. The energies of bonds are obtained identical, i. e., the values are the same which means that the energies of the rearrangement of radicals naphth-1-yl and naphth-2-yl are equal to 0 kJ/mol.

Keywords: enthalpy of radical formation; double-difference method; aromatic homologues; formation of derivatives of 1- and 2-naphthalenes; rearrangement energy of radicals; dissociation energy of bonds

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