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Program with elements of artificial intelligence to evaluate the enthalpy of formation of radicals on the kinetic data

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Abstract

We have developed the intellectual software agent, which implements the evaluation algorithm of the enthalpy of formation of free radical on kinetics data which is based on hybrid knowledge base. Logical structure of knowledge base and the algorithm of intellectual software agent have been described. The results of numerical experiments on predicting the values of enthalpies of the formation of free radicals derived from acetals have been presented. We conducted the comparison of the calculated values of enthalpy of the radicals formation, derivatived from acetals, nitriles and nitro compounds with literary data. The comparison shows good agreement with the published data. Linear correlations have been constructed between the formation enthalpy of free radicals derived from a series of substituted acetals. The radical stabilization energy of substituted phenyl radicals has been calculated. It is shown that the conjugated system of π-electrons near the radical center destabilizes the radical, both for electron-donor substituents, and for electron-acceptor substituents.