Evaluation of enthalpies of free radicals formation by the kinetic data

© **Vladimir E. Tumanov,**[+] and **Evgeny T. Denisov***
Institute of Problems of Chemical Physics RAS. Chernogolovka, 142432.
Moscow Region. Russia. Fax: +7 (496) 522-35-07. E-mail: tve@icp.ac.ru

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*Supervising author; [+]Corresponding author

Abstract

We have proposed a method for calculating the enthalpies of formation of free radicals (R • i) based on the model of intersecting parabolas through the enthalpy of formation of a molecule (RiH), bond dissociation energies (DR-H) and the ratio of the rate constants of the reactions of radical detachment ($X^\bullet + R_iH$, $X^\bullet + R_1H$). With the proposed method the enthalpies of formation of 111 free radicals containing the atoms of C, H, O, S were calculated using the kinetic data. A brief description of the database on the enthalpies of free radicals, published on the Internet site of the Institute of Problems of Chemical Physics is presented.