Additive Methods for Prediction of Thermochemical Properties. The Laidler Method Revisited. 1. Hydrocarbons

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A new parameterization of the Laidler method for estimation of atomization enthalpies and standard enthalpies of formation at 298.15 K for several families of hydrocarbons (alkanes, alkenes, alkynes, polyenes, poly-ynes, alkyl radicals, cycloalkanes, cycloalkenes, benzene derivatives, and polyaromatics) is presented. A total of 200 compounds (164 for liquid phase) are used for the calculation of the parameters. Comparison between the experimental values and those calculated using the group additive scheme led to an average difference of 1.28 $kJ \cdot mol^{-1}$ for the gas phase enthalpy of formation (excluding the polyaromatic compounds) and of 1.38 $kJ \cdot mol^{-1}$ for the liquid phase enthalpy of formation. The data base used appears to be essentially error free, but for some compounds (e.g., 2,2,4-trimethyl-pentane, with the highest deviation among all compounds except the polyaromatic ones) the experimental values might need a reevaluation. An Excel worksheet is provided to simplify the calculation of enthalpies of formation and atomization enthalpies based on the Laidler terms defined in this paper. © *2006 American Institute of Physics.* [DOI: 10.1063/1.1996609]

Key words: additive methods; atomization enthalpy; bond dissociation enthalpy; bond strength; enthalpy of formation; hydrocarbons; Laidler method.

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