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## ACCEPTED MANUSCRIPT

#### Contribution to the special issue in honour of Prof. Kabo's 80th birthday

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# Improving the method of solution calorimetry for evaluation of the enthalpies of phase transitions and condensed state enthalpies of formation

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### Abstract

In the present work, *n*-heptane was tested as a solvent with the zero-thermal effect of solution enthalpy for normal and cyclic alkanes. For alkanes in n-heptane, no obvious dependence of the solution enthalpy on alkyl chain length was found with the absolute values of the solution enthalpy being below the uncertainty of determination.

For aliphatic and aromatic compounds, the linear correlation between solvation enthalpy in *n*-heptane and molar refraction of these solutions was observed. Using evaluated linear fitting and the experimental values of solution enthalpies, the formation enthalpies in the condensed state for some classes of organic compounds were determined. The gas phase enthalpies of formation were computed at DLPNO-CCSD(T)/def2-QZVP level of theory. All experimental and calculated values were in good agreement with the most reliable literature data.

The solution enthalpies for thirty-five compounds were experimentally determined using solution calorimetry.

Keywords: Solvation enthalpy, Aliphatic compounds, Formation enthalpy, Molar refraction

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