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Enthalpies of fusion and enthalpies of solvation of aromatic hydrocarbons derivatives: Estimation of sublimation enthalpies at 298.15 K

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ABSTRACT

Enthalpy of sublimation of solid compound can be found using the values of solution enthalpy and solvation enthalpy in any solvent. In this work enthalpies of solution at infinite dilution of a number of aromatic hydrocarbons derivatives in benzene were measured at 298.15 K. Comparison between experimental and literature solution enthalpies in benzene at 298.15 K and fusion enthalpies at melting temperature of aromatic hydrocarbon derivatives showed, that these values are approximately equal. Thereby, fusion enthalpies at melting temperature can be used instead of their solution enthalpies in benzene at 298.15 K for calculation of sublimation enthalpies at 298.15 K. Solvation enthalpies in benzene at 298.15 K required for this procedure were calculated using group additivity scheme. The sublimation enthalpies of 80 aromatic hydrocarbons derivatives at 298.15 K were evaluated as a difference between fusion enthalpies at melting temperature and solvation enthalpies in benzene at 298.15 K. Obtained in this work values of sublimation enthalpy at 298.15 K for studied compounds were in a good agreement with available literature data.

1. Introduction

We developed a new approach for determination of vaporization/sublimation enthalpy [1–6]. This approach is based on a well-known relationship between vaporization/sublimation enthalpy of studied compound at 298.15 K and its solution and solvation enthalpies at 298.15 K in the same solvent. Solution enthalpy at 298.15 K is measured experimentally, while solvation enthalpy at 298.15 K is calculated using a number of simple empirical approaches. These approaches include determination of values of solvation enthalpy of solute Ai in solvent S from linear relationship between solvation enthalpy and molar refraction [1,3,4,6] or using group-additivity schemes [2,5]. The latter present solvation enthalpy as a sum of contributions of unsubstituted compound and substituents. Group-additivity scheme was successfully implemented for determination of solvation enthalpies of 78 polycyclic and polysubstituted aromatic hydrocarbons and pyridine derivatives in different solvents.

In work [5] a simple method for calculation of solvation enthalpy at 298.15 K of the polyaromatic hydrocarbons in various solvents was proposed. According to this method, the enthalpy of solvation of any polyaromatic hydrocarbon can be calculated based on the value of solvation enthalpy of benzene in a solvent of interest, the quantity of carbon and hydrogen atoms in studied molecule. Furthermore, in work [5] we demonstrated that solution enthalpies of polyaromatic hydrocarbons in benzene at 298.15 K are approximately equal to their fusion enthalpies at melting temperature. Sublimation enthalpies at 298.15 K of a number of polyaromatic hydrocarbons were successfully calculated using fusion enthalpies at melting temperature instead of solution enthalpies in benzene at 298.15 K.

In present work we continue the testing of our method which is based on usage of fusion enthalpy at melting temperature instead of solution enthalpy in benzene at 298.15 K for determination of sublimation enthalpy at 298.15 K. Various derivatives of aromatic hydrocarbons, which contain nitro-, alkyl-, halogen-, cyano-, alkylcarboxy- and other substituents were taken as objects of our study.

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