

A New Method to Estimate the Hydrophobic Effect Enthalpy

B.N. Solomonov^{C, S} and I.A. Sedov

Department of Chemistry, Kazan State University, Kazan, Russia

Boris.Solomonov@ksu.ru

The hydrophobicity is a well-known and extensively studied phenomenon but it still is not thoroughly explained. To describe the hydrophobic effect quantitatively, thermodynamic parameters (enthalpy, heat capacity, entropy and Gibbs energy) are often used. However, there is no universal scale of the hydrophobicity. In different studies different parameters of the hydrophobicity are used. They can be directly measured magnitudes – the thermodynamic functions of solute transfer from hexane to water, octanol-water and polymethylsiloxane-water partition coefficients as well as various parameters calculated according to some model of solvation from the experimental data such as water-organic solvent mixtures solution enthalpies, noble gases hydration enthalpies etc.

We propose a new method of determination of the hydrophobic effect enthalpy. The method is based on regarding the hydration enthalpy as the sum of the non-specific hydration enthalpy, specific hydration enthalpy and the hydrophobic effect enthalpy. The hydrophobic effect enthalpies of noble and simple substance gases, alkanes, arenes and normal aliphatic alcohols are determined. We used the equation suggested in [1] to calculate the non-specific hydration enthalpy. For the noble gases and alkanes the hydrophobic effect enthalpy is found to be negative and independent of the size of molecule. For aromatic hydrocarbons, it is positive and grows up with the size of the hydrocarbon. The hydrophobic effect enthalpies of normal aliphatic alcohols are determined assuming that the specific interaction enthalpies of alcohols in water and in methanol are equal. The hydrophobic effect enthalpy values for the aliphatic alcohols (-10.0 ± 0.9 kJ·mol⁻¹) were found to be close to the alkanes hydrophobic effect enthalpies (-10.7 ± 1.5 kJ·mol⁻¹). The method will allow us to study the influence of the solute molecule structure to the hydrophobic effect enthalpy for a large number of non-electrolyte solutes.

[1] B.N. Solomonov; V.B. Novikov; M.A Varfolomeev, and N.M. Milesenko. *J. Phys. Org. Chem.* **18**, 49 (2005).