

Quantitative description of the hydrophobic effect: The enthalpic contribution

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Abstract

A new method of experimental determination of the hydrophobic effect enthalpy is proposed. The method is based on regarding the hydration enthalpy as the sum of the nonspecific 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. 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 by assuming that the specific interaction enthalpies of alcohols in water and in methanol are equal. The hydrophobic effect enthalpy values for the aliphatic alcohols ($-10.0 \pm 0.9 \text{ kJ}\cdot\text{mol}^{-1}$) were found to be close to the alkanes hydrophobic effect enthalpies ($-10.7 \pm 1.5 \text{ kJ}\cdot\text{mol}^{-1}$). © 2006 American Chemical Society.

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