

Journal of Solution Chemistry 1995 vol.24 N6, pages 579-586

Evaluation of the contribution to hydration of nonelectrolytes from the hydrophobic effect

Borisover M., Baitalov F., Solomonov B.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

A new method was suggested for estimating the hydrophobic effect of contributions to the Gibbs energies and enthalpies of hydration of hydrocarbons, inorganic gases and rare gases. In accordance with this method the hydrophobic effect contribution to the Gibbs energy was evaluated from the difference between the hydration Gibbs energy of a solute and the non hydrophobic contribution. To estimate the latter value, the known dependence connecting the Gibbs energies of solvation of a solute in a number of aprotic solvents to the Hildebrand solubility parameter for these solvents was used. The non hydrophobic contribution to the Gibbs energy of hydration was calculated for various solutes from such dependences extended to water as solvent. The Hildebrand solubility parameter for water used in the calculation was corrected for the effect of association through hydrogen bonding. This correction was made by subtraction of the water self-association enthalpy from the enthalpy of vaporization of water. The evaluated Gibbs energies of the hydrophobic effect are positive for saturated hydrocarbons, inorganic gases and rare gases and linearly depend on the solute molecular refraction. The hydrophobic contribution to the hydration enthalpies of the solutes was calculated in the same manner as was made to calculate the hydrophobic contribution to Gibbs energies of hydration. Enthalpies of the hydrophobic effect for the solutes under study are negative. © 1995 Plenum Publishing Corporation.

<http://dx.doi.org/10.1007/BF00973208>

Keywords

enthalpy, Gibbs energy, Hydration of nonelectrolytes, hydrophobic effect