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Determining the Gibbs energies of hydrogen-bonding interactions of proton-accepting solutes in aqueous solutions from thermodynamic data at 298 K with regard to the hydrophobic effect

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Abstract

Reaction rate and equilibrium constants in aqueous solutions are affected by the strength of hydrogen bonds formed between dissolved species and water molecules. Thermodynamic functions of hydrogen bonding with bulk water cannot be measured directly using spectroscopic methods, but the contribution of hydrogen-bonding processes to the thermodynamic functions of hydration may be determined using some model of aqueous solutions. We determined the Gibbs energies of hydrogen-bonding interactions in water for various simple proton-accepting organic molecules on the basis of two different models that allow the contributions of nonspecific van der Waals interactions and the hydrophobic effect to be quantified. It is shown that hydrogen bonding with bulk water may be stronger than with a single water molecule. The influence of solute structure on the Gibbs energy of hydrogen-bonding interactions is discussed.

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