

# Gibbs energy of cooperative hydrogen-bonding interactions in aqueous solutions of amines and pyridines

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## Abstract

A method to determine the Gibbs energy of specific (hydrogen bonding) interactions of a solute with water is proposed. The energies of hydrogen bonding in bulk water are very difficult to determine by any method. The Gibbs energy of hydration of substances forming hydrogen bonds with water is considered as the sum of contributions due to non-specific interactions, the hydrophobic effect, and specific interactions. The first two terms were found to be rather accurately described by empirical equations. The Gibbs energies of hydrogen bonding of aliphatic amines and pyridines in bulk water are determined, and the results are compared with the energies of their complexes with one molecule of water. The cooperativity of hydrogen bonding is proved in aqueous solutions of amines and pyridines. To use our equations, experimental values of the Gibbs energies of solvation in 'standard' solvents need to be known. The Gibbs energies of solvation of ten amines and pyridines in dimethyl sulfoxide are determined experimentally using chromatographic head space analysis. The tendencies observed for the series of amines and pyridines are in agreement with other studies. Copyright © 2009 John Wiley & Sons, Ltd.

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## Keywords

Cooperativity, Hydrogen bonding, Hydrophobic effect, Solvation