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A new method for the extraction of specific interaction enthalpy from the enthalpy of solvation

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Abstract

A new, simple method for the extraction of specific interaction enthalpy from the enthalpy of solvation is proposed. It is based on empirical but very general relationships describing the non-specific solvation enthalpy. The specific interaction enthalpy is calculated from the solution enthalpies in the solvent under consideration, cyclohexane and tetrachloromethane. The solution enthalpy of at least one linear alkane in the solvent must also be available. The solution enthalpies of a 'model compound' or homomorph are not required. This method is applicable not only for proton-donor solutes but also for acceptor solutes such as iodine. It can be used also for solvents associated by hydrogen bonding (e.g. alcohols). The enthalpies of specific interaction for 280 solute-solvent systems were calculated. Solution enthalpy data were mainly obtained from the literature and partially measured by the authors. The results were compared with literature data on complexation enthalpy. Copyright © 2004 John Wiley & Sons, Ltd.

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Keywords

Enthalpy of solution, Hydrogen bonds, Solvent scales, Specific interactions