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Calorimetric determination of hydrogen-bonding enthalpy for neat aliphatic alcohols

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Abstract

Hydrogen bonding in pure aliphatic alcohols is investigated using a novel calorimetric approach. Average enthalpies of hydrogen bonding were determined for methanol, ethanol, propan-1-ol, propan-2-ol, butan-1-ol, hexan-1-ol and octan-1-ol. For all the studied alcohols except methanol the average hydrogen-bonding enthalpies fall in the range from -16.9 to -17.7 kJ mol⁻¹. A slightly smaller value of -15.1 kJ mol⁻¹ was observed for methanol. From the enthalpies of the specific interactions of the alcohols and chloroform (as proton donors) formed with the alcohols and diethyl ether (as proton acceptors), the dimerization enthalpies were determined for the investigated alcohols: -8.6 ± 0.7 kJ mol⁻¹. The specific interaction and dimerization enthalpies obtained are concurrent with the Badger-Bauer rule and the hydrogen-bond cooperativity effects. The calorimetric data obtained are supported by literature Fourier transform infrared data on dimer and multimer formation for ethanol and octan-1-ol in tetrachloromethane solution. Copyright © 2005 John Wiley & Sons, Ltd.

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Keywords

Aliphatic alcohols, Calorimetry: Infrared spectroscopy, Cooperativity factors, Enthalpy of solution, Hydrogen bond