Molecular structure and hydrogen bonding of 2-aminoethanol, 1-amino-2-propanol, 3-amino-1-propanol, and binary mixtures with water studied by Fourier transform near-infrared spectroscopy and density functional theory calculations.

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Streszczenie

The effect of temperature and water content on the molecular structure and hydrogen bonding of 2-aminoethanol (2AE), 1-amino-2-propanol (2AP), and 3-amino-1-propanol (3AP) has been examined by Fourier transform near-infrared (FT-NIR) spectroscopy. The experimental spectra were analyzed using the two-dimensional (2D) correlation approach and chemometrics methods. Interpretation of the spectra was guided by density functional theory (DFT) calculations. The novelty of the present work relates to the interpretation of the spectra of aminoalcohols in the liquid phase and their mixtures with water based on dimeric structures. The molecules of 2AE and 2AP form stable cyclic dimers through the intermolecular O-H...N hydrogen bonds (HBs), whereas the intramolecular HBs are absent. In contrast, the molecules of 3AP create two kinds of dimers. The first dimer has two intermolecular O-H...N HBs and two intramolecular N-H...O HBs, while the second dimer has the opposite. In the liquid phase the cyclic dimers interact with each other and form higher associates through the intermolecular N-H...O HBs. The temperature rise weakens these interactions but the structure of the dimers remains intact. The majority of the molecules of water act as double proton donors to oxygens linking different molecules of aminoalcohol. This cooperative hydrogen bonding is stronger than that in bulk water. A small amount of one-bonded water occurs in the mixtures, and the population of this species increases with the temperature rise. At higher water content small clusters of water are formed. On the basis of the present results one can conclude that addition of water does not lead to noticeable variations in the structure of liquid aminoalcohols. More significant changes are induced by the temperature variations.

Adres publiczny

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