INTERMOLECULAR H-BOND IN PROPAN-2-OL AND ITS SOLUTIONS WITH ACETONITRILE

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Formation of propan-2-ol-acetonitrile dimers is manifested in Raman spectra as an appearance of the band of aggregates in the high-frequency side of CN vibration of liquid acetonitrile (2 cm^{-1}). Intensity of the band of aggregates changes with changing the concentration of mixture. For iso-propyl alcohol we carried out non-empirical calculations of structure of isolated dimer aggregates. Formation of intramolecular H-bond between H atom of HCOH group and O atom of this group with the bond8217;s length 2.045 A is possible in monomer molecule. 1057;1053;3 groups of alcohol are not equivalent. The indicated peculiarities of monomer molecule are preserved in dimer formation. Intermolecular H-bond with the length 2.045 A and energy 3.6 kcal/mole is formed between H atom of O-H group of one molecule and O atom of other molecule. Calculations of the length and energy of H-bond for propan-2-ol-acetonitrile dimer formations give 2.27 A and 3.1 kcal/mole, respectively. The H-bond is formed by sigma-electrons of nitrogen. Experimental data and results of calculations are in good agreement.