INTERMOLECULAR H-BONDS IN ACETONITRILE AND ITS SOLUTIONS. RAMAN SPECTRA AND AB INITIO CALCULATIONS

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The band of CN vibrations in pure acetonitrile in Raman spectra is located at 2254 cm^{-1}, and it is asymmetric in low-frequency region. In mixture with acetic acid we observed appearance of a band of aggregations of acetonitrile molecules with those of acetic acid in high-frequency region. Relative intensity of the band increases with decreasing concentration of acetonitrile.
Calculations showed that in monomer molecule of acid one of H atoms of CH_3 group participates in formation of weak intramolecular H-bond with = O atom. Length of this bond is 2,55 A. For monomer molecule interaction of = O atom with H atom of O - H group also takes place. Optimized model of dimer ”acetonitrile - acetic acid” represents closed aggregation with H-bond between N atom and H atom of O-H group. Moreover, there is a possibility of formation of intramolecular H - bond between = O atom of acid and one of H atoms of CH_3 group of acetonitrile. The length of H-bond N...H-O is 2,21 A, and for H_2C - H ... O is 2,61 A. Energy profit in this case is 5,3 kcal/mole. Weak intramolecular H-bond between O atom of C = O group and one of H atoms of CH_3 group of acid is preserved also in dimer ”acetonitrile - acetic acid”.