INTERMOLECULAR HYDROGEN BOND IN TERTIARY BUTYL ALCOHOL AND ITS SOLUTIONS. RAMAN SCATTERING SPECTRA

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S u m m a r y

It is found that the 750 cm^{-1} band in pure tertiary butyl alcohol shows attributes of a complex structure that can be interpreted as a result of the superposition of several closely located lines belonging to different aggregates of alcohol molecules. As the alcohol is diluted with neutral solvents, the width of this band passes through a maximum that corresponds to the concentration of the mixture with comparable contents of various most stable aggregates in the solution. The performed quantum-chemical calculations confirm the complexity of the 750-cm^{-1} band of pure alcohol caused by the aggregation of molecules by means of hydrogen bonds. The calculated energy gain due to the formation of a hydrogen bond (dimer) amounts to 19.7 kJ/mole, and the length of the hydrogen bridge equals 2.068 Å.