

Effect of temperature and concentration on the structure of *tert*-butyl alcohol/water mixtures: near-infrared spectroscopic study.

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The effect of temperature and concentration on the structure of *tert*-butyl alcohol/water binary mixtures in the alcohol-rich region ($X(\text{H}_2\text{O}) < 0.3$) has been studied by using Fourier transform near-infrared (FT-NIR) spectroscopy. The obtained results demonstrate that the addition of a small amount of water to *tert*-butyl alcohol (2-methyl-2-propanol, abbreviated as TBA) leads to minor changes in the structure of neat TBA and suggest that molecules of TBA in the mixture are in the same environment as those in pure TBA. The bands of water are red-shifted in the mixture relative to bulk water, implying that the molecules of water in TBA are involved in stronger hydrogen bonding. The present experimental data give no evidence for the existence of nonbonded water in the mixture. Even at a very low content of water, the main NIR bands of water ($\nu(2) + \nu(3)$ and $\nu(1) + \nu(3)$) have two components showing markedly different behavior upon an increase in temperature. From the power spectra, it is seen that the extent of intensity changes due to the free OH groups of TBA is smaller in the mixture relative to pure TBA. All of these results support the model of chain-end bonding of water molecules to TBA associates. An increase in $X(\text{H}_2\text{O})$ reduces the population of nonbonded OH groups of TBA, yet both processes do not appear at the same rate. The amount of bonded OH groups of water increases faster than that of the nonbonded ones. It seems that the water-water interaction becomes more important as $X(\text{H}_2\text{O})$ increases. At high alcohol content, the position of the CH alkyl stretching bands is constant, evidencing a negligible role of the hydrophobic hydration in the mixture.

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