



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

Autorzy

Dagmara Wojtków

Mirosław A. Czarnecki

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The effect of temperature and concentration on the structure of sec-butyl alcohol and isobutyl alcohol/water binary mixtures in the alcohol-rich region (mole fraction of water $X(\text{H}_2\text{O}) < 0.3$) has been studied using Fourier transform (FT) near-infrared (NIR) spectroscopy. The experimental data were analyzed by a two-dimensional (2D) correlation approach and chemometric methods. It was found that molecules of both alcohols in the mixture with water are in the same environment as those in the pure alcohols. Even at very low water content ($X(\text{H}_2\text{O}) = 0.001$) we did not observe water free from any specific interactions. The molecules of water are attached to the end free OH groups in the open chain associates of alcohol. In this way the structure of neat alcohol remains intact by addition of water. The water-alcohol interactions in sec-butyl alcohol and isobutyl alcohol/water mixtures are stronger than those in bulk water. The results obtained at higher water content or elevated temperatures indicate the possibility of water-water interaction. In the alcohol-rich region the hydrophobic effects are of minor importance and the structure and properties of these systems are determined by hydrogen bonding through the hydroxyl groups. Both alcohols behave similarly on the temperature or water content variation; the minor difference results from a different degree of self-association for sec-butyl alcohol and isobutyl alcohol.

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<https://www.acs.org/content/acs/en.html>