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Effect of temperature and concentration on self-association of octan-3-ol studied by vibrational spectroscopy and dielectric measurements.

Autorzy

Mirosław A. Czarnecki

Kazimierz Orzechowski

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Streszczenie

The effects of temperature and concentration on self-association of octan-3-ol both in pure liquid and CCl_4 solution have been studied by two-dimensional (2D) Fourier transform near-infrared (FT-NIR) correlation spectroscopy, conventional FT-IR spectroscopy, and dielectric measurements. The interpretation of 2D correlation spectra was supported by simulation studies. A particular attention has been paid for comparison of the present results with that previously published for octan-1-ol. The obtained results indicate that population of the free OH groups changes faster than that of the associated species with increasing temperature. This results from the fact that in the open-chain multimers the terminal hydrogen bonds break easier than the interior ones. The open-chain dimers are less favorable than the higher associates due to the lack of the cooperativity effect. Hence, these species appear as a result of temperature-induced dissociation of higher multimers in concentrated solutions and in neat alcohols. At low concentration of alcohol in CCl_4 the nonpolar (cyclic) species dominates. An increase in the concentration of the sample increases the number and length of the linear associates, and this effect is more pronounced for primary alcohols. In octan-1-ol, formation of the linear associates is favored, whereas in octan-3-ol the cyclic species dominates. The present results reveal the presence of at least two kinds of associated species and argue against frequently assumed equilibrium between the monomers and one kind of associates at all concentrations.

Słowa kluczowe

Alcohols, Insulators, Monomers, Noncovalent interactions, Oligomers

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