

The temperature-induced changes in hydrogen bonding of decan-1-ol in the pure liquid phase studied by two-dimensional Fourier transform near-infrared correlation spectroscopy.

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Streszczenie

Fourier transform near-infrared (FT-NIR) spectra of decan-1-ol in the pure liquid phase were investigated in the regions of the first and second overtones of the OH stretching vibration over the temperature range 15–76°C. The dynamics of temperature-induced changes in the hydrogen bonding were explored by the 2D correlation approach. It was found that the first overtone of the monomer band is split into two peaks (7087 and 7114 cm⁻¹). The peaks originate from the rotational isomerism of the OH group. Although the *trans*-isomer (at 7114 cm⁻¹) is more stable than the *gauche*-isomer (at 7087 cm⁻¹), the intensity of the band due to the former is weaker in the pure liquid phase. In dilute solutions the situation is reversed. This effect can be explained by higher accessibility of the OH proton in the *trans*-position. Therefore, the population of the free protons in the *trans*-position is reduced faster with increase in concentration. The band attributed to the free terminal OH groups in open chain polymers was not observed in the 2D correlation spectra of neat decan-1-ol. As for butanols, studied previously, the populations of the polymers and cyclic dimers vary faster than that of the monomers. When the temperature is raised, the population of the monomers increases faster where that of the polymers decreases more slowly. Hence it is concluded that the growth in the population of the monomeric species comes from dissociation of the intermediate species. These 2D correlation studies on alcohols in the pure liquid state suggest that the degree of association in the saturated straight-chain alcohols decreases with increase in chain length.

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