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Near-infrared spectroscopic study of liquid propanols.

Autorzy

Natalia Michniewicz

Mirosław A. Czarnecki

Jerzy P. Hawranek

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Streszczenie

The effect of temperature on self-association of liquid propan-1-ol and propan-2-ol has been studied by using generalized two-dimensional (2D) Fourier-transform near-infrared (FT-NIR) correlation spectroscopy. Obtained results indicate that the population of the free OH groups increases at the expense of the higher multimers with increasing temperature. However, the molecular mechanism of this process is complex and it proceeds through the intermediate species. The comparison of the present results with those obtained for other alcohols reveals that the extent of self-association decreases on increasing chain length both for the primary and secondary alcohols. As expected, the primary alcohols are more associated as compared with the secondary alcohols. The conclusions derived from 2D correlation analysis are supported by estimated values of the fraction of the free OH groups for several alcohols with different chain length and the molecular structure.

Słowa kluczowe

Propan-1-ol, Propan-2-ol, NIR spectra, 2D correlation analysis, Hydrogen-bonding

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