



Two-dimensional attenuated total reflection infrared and near-infrared correlation study of the structure of butyl alcohol/water mixtures.

Autorzy

Dagmara Wojtków

Mirosław A. Czarnecki

Rok wydania

2007

Czasopismo

Applied Spectroscopy

Numer woluminu

61

Strony

928-934

DOI

10.1366/000370207781745900

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The effect of temperature on attenuated total reflection infrared (ATR-IR) and near-infrared (NIR) transmission spectra of pure butan-1-ol, butan-2-ol, 2-methyl-propan-1-ol, 2-methyl-propan-2-ol, and mixtures with a small water content ($X(\text{H}_2\text{O}) \leq 0.1$) have been examined. The spectra were analyzed using a two-dimensional (2D) correlation approach. Two kinds of correlation analysis were performed: IR-IR and NIR-NIR homo-correlation and IR-NIR hetero-correlation. Our results reveal that the addition of small to moderate amounts of water does not destroy the structure of alcohol. The presence of water stabilizes the structure of alcohols and this effect is more evident for sec-butanol and tert-butanol. The ATR-IR spectra provide information on the most associated species, whereas absorption of the smaller associates and the free OH group is hardly seen. On the contrary, in the NIR spectra the absorption of the free OH groups dominates. The ability of resolution enhancement in the hetero-correlation asynchronous spectra is reduced as compared to that in the homo-correlation spectra. On the other hand, peaks may appear in the hetero-correlation synchronous spectra that are not observed in the homo-correlation contour plots. The positions of the synchronous peaks were used for evaluation of anharmonicity constants. These values for the free OH group do not depend on the experimental conditions. In contrast, the anharmonicity constants for the bonded OH groups determined from the spectra of pure alcohols may significantly differ from those obtained from diluted solutions.

Adres publiczny

[https://doi.org/ 10.1366/000370207781745900](https://doi.org/10.1366/000370207781745900)