

A near-infrared study of hydrogen bonds in alcohols-comparison of chemometrics and spectroscopic analysis.

Autorzy

H. Maeda

Yuan Wang

Yukihiro Ozaki

M. Suzuki

Mirosław A. Czarnecki

M. Iwahashi

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Streszczenie

Near-infrared (NIR) spectra of *n*-, *sec*-, and *tert*-butanol in CCl₄ were measured over a temperature range of 10–60°C. The spectra obtained were analyzed by both spectroscopic analytical methods such as calculations of the difference spectra and the second derivatives, and chemometrics, namely partial least squares (PLS) regression. The present study aims at comparing the spectroscopic analytical methods with chemometrics in the analysis of NIR spectra of *n*-, *sec*-, and *tert*-butanols in CCl₄. The three kinds of alcohol showed an intense band due to the first overtone of the OH stretching mode in the 7120–7030 cm⁻¹ (1404–1422 nm) region. The calculations of the difference spectra and the second derivatives revealed that the above bands of *n*- and *sec*-butanol consist of three and four component bands, respectively, due to the rotational isomerism of the monomer, the OH group weakly hydrogen-bonded with CCl₄, and the terminal free OH groups of the self-associated species. For *tert*-butanol, which does not have the rotational isomerism, the corresponding band splits into only two components. Temperature of the alcohols was predicted by use of PLS regression. The regression coefficients for the models predicting the temperature of the alcohols were almost identical with the difference spectra of the alcohols between 10 and 60°C. Both the regression coefficients and the difference spectra reflect strongly the changes in the hydrogen bonds of the alcohols.

Słowa kluczowe

Hydrogen bonds, Near-infrared spectroscopy, Butanol, CCl₄, PLS regression, Regression coefficient

Adres publiczny

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