# Usefulness of the second overtone of the OH stretching mode for the study of the dissociation of hydrogen-bonded Z-9-octadecen-1-ol in the pure liquid state.

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Rok wydania

1993

Czasopismo

Applied Spectroscopy

Numer woluminu

47

Strony

2169-2171

DOI

10.1366/0003702934066262

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Recently, Iwahashi et al. demonstrated that near-infrared (NIR) spectroscopy is a powerful technique in investigating the structure and thermodynamic properties of fatty acids and alcohols In order to extract useful information from NIR spectra, they examined temperature behaviors of the first overtone (~7000 cm<sup>−1</sup>) of the OH stretching mode of the monomeric forms of cis-9-octadecenoic acid and octan-1-ol. Since the first overtone bands are heavily overlapped with bands due to combination modes of CH<sub>3</sub> and CH<sub>2</sub> groups, they had to subtract the contributions from CH modes to obtain net spectra for the free and hydrogen-bonded OH groups. They adopted a computational method, which employed as a reference the peak heights of the second overtone of the CH stretching mode of decane to cancel the contributions from the CH modes of octan-1-ol. In a companion paper, we proposed an improved method, which eliminates the bands due to the CH vibrations by subtraction of the spectrum of the same sample measured at a temperature close to the melting point. At the same time, we showed that FT-NIR is more profitable than conventional NIR in the studies of such spectral changes; by using FT-NIR one can calculate more accurate difference spectra with a higher signal-to-noise ratio.