

FT-near-IR and FT-IR studies of *cis*-9-octadecen-1-ol: molar absorption coefficient of a band due to the first overtone of the stretching mode of the terminal OH group and comparison of anharmonicity of an OH stretching mode among the monomeric and associa.

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Fourier transform near-infrared (FT-near-IR) and FT-IR spectra have been measured for *cis*-9-octadecen-1-ol in CCl_4 solutions at various concentrations and temperatures partly to investigate its self-association and partly to explore its near-IR spectrum. Both spectra have demonstrated the appearances of bands due to free terminal OH groups of the linear dimer (open-chain dimer) and oligomer of the alcohol. They are observed at 3621 and 7070 cm^{-1} in the IR and near-IR regions, whose frequencies are lower by 16 and 34 cm^{-1} , respectively, than those of the corresponding bands due to a free OH group of the monomer. The spectral changes in both regions suggest that (1) at concentrations below 0.10 M, the alcohol exists mostly as the monomer and dimer, and with increasing temperature the dimer dissociates into the monomer; and (2) as the concentration is increased, it associates to form aggregates (such as tetramer), and with temperature increase the aggregates dissociate into the dimer and monomer. The molar absorption coefficient of the band due to the first overtone of the stretching mode of the terminal OH groups has been determined to be 0.139 $\text{dm}^3 \text{mol}^{-1} \text{cm}^{-1}$. It is approximately 8% of that of the first overtone of the monomeric OH group (1.63 $\text{dm}^3 \text{mol}^{-1} \text{cm}^{-1}$). The anharmonicity of an OH stretching mode of the alcohol has been investigated for various OH groups, free, terminal, and hydrogen-bonded, by comparing the frequencies of the bands due to the OH stretching modes with those of the bands due to the corresponding first overtones. The anharmonicity of the stretching mode of the terminal OH groups of the associated species is very similar to that for the free OH group of the monomer.

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