Potential of fourier transform near-infrared spectroscopy in studies of the dissociation of fatty acids in the liquid phase.

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Streszczenie

Fourier transform near-infrared (FT-NIR) technique has been employed to determine the degree of dissociation and the thermodynamic parameters of octanoic acid in the liquid phase. FT-NIR absorption spectra of the acid over a temperature range of 15 to 92°C were recorded. From the spectra, intensities of the first overtone of the OH stretching mode due to the monomer form of the acid were extracted and were used to calculate the degree of dissociation and the thermodynamic parameters for the process of dissociation of dimeric octanoic acid into monomer species. In the 7400–6700 cm^{-1} region there appear many bands that are heavily overlapped; the attempts to apply curve-fitting and deconvolution algorithms to separate individual bands have failed. Here, a simple and reliable method of calculation of the intensities of the first overtone of the OH stretching mode due to the monomer is proposed. Also, an excellent procedure of determining the molar absorption coefficients (integrated and at peak position) through a series of measurements in CCl_4 solution at very low concentrations is presented. The bands due to CH vibrations were eliminated in two ways; one way involved taking the concentration as a reference, and the other used the band area of the second overtone of the CH stretching modes as a reference. In the operation the spectrum of neat octanoic acid at 15.1°C was employed. The coefficients obtained by both methods are compared and discussed. The present studies indicate that both band areas and peak heights give results which are found to be in very good agreement.