Structure of Water-Methanol Mixtures Studied by NIR Spectroscopy

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NIR spectroscopy has been used extensively to investigate the structure of water, alcohol and other self-associate molecules because the frequencies of NIR bands due to OH and NH groups strength of hydrogen bonds. We have studied the structure of water – methanol mixtures by use of NIR spectroscopy. Strong features in the 7200-6300 cm^{-1} region consist of a number of overlapped bands due to the combination of OH antisymmetric and symmetric stretching modes of water and the first overtone of the OH stretching modes of free and hydrogen bonded methanol, while weak features in the 6000-5800 cm^{-1} region are ascribed to the first overtones of CH_3 stretching modes of methanol. We will focus the discussion on the CH_3 stretching bands. They seem to show a significant shift is not clear from the spectra shown in Figure 1(a).

Figure 1(b) depicts the second derivative in the 6000-5700 cm^{-1} region. Now, it is clear from the second derivative that there are two major bands near 5950 and 5900 cm^{-1} and that they do show a shift be about 30 cm^{-1}. Why do the CH_3 bands show the shift with increasing concentration of methanol? Probably, the CH_3 group interacts directly with OH groups of water. The results in Figure 1(b) demonstrate the usefulness of the second derivative in resolution enhancement as well as the potential of NIR spectroscopy in the studies of molecular interactions.

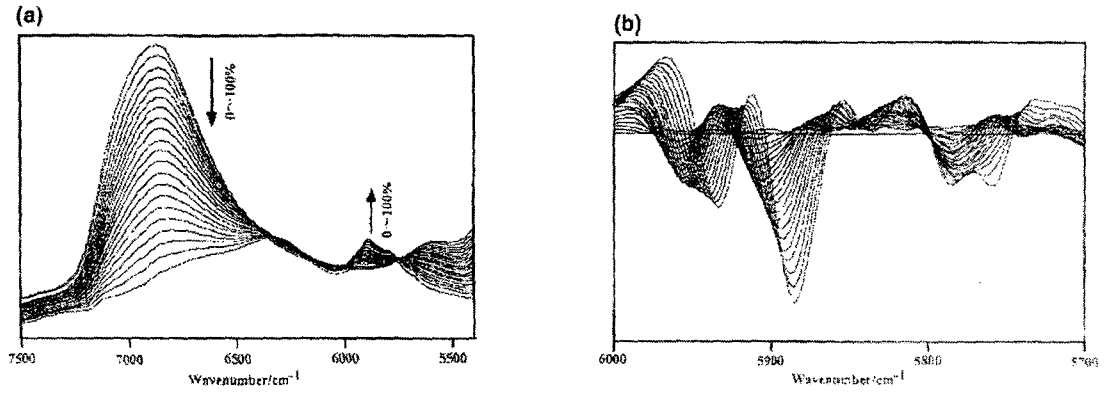

Figure 1. (a) Concentration dependence of NIR spectra of water-methanol mixtures. (b) The second derivative in the 6000-5700 cm^{-1} region of the spectra shown in (a).