

# Use of principal components analysis in a near infrared study of the dissociation process of oleyl alcohol in carbon tetrachloride

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## Introduction

Near infrared (NIR) spectroscopy has been employed for studies of self-associated compounds for nearly forty years. Recent rapid progress both in hardware and software brought about innovative changes in the NIR studies of self-associated compounds.<sup>1–3</sup> For example, in our previous paper,<sup>2</sup> we demonstrated the usefulness of principal component analysis (PCA) in the NIR study of the dissociation process of oleyl alcohol in the pure liquid. The present paper deals with a similar study for the alcohol in CCl<sub>4</sub>.

## Experimental

The sample of oleyl alcohol of very high purity was supplied by Nippon Oil and Fats Co. Ltd (Amagasaki, Japan) and was used without further purification.

The instrumentation and experimental conditions for the Fourier transform (FT) NIR measurements and the methods for data analysis were the same as those described in our previous paper.<sup>2</sup>

## Results and discussion

Figure 1 shows FT-NIR spectra in the 9000–6000 cm<sup>-1</sup> region of oleyl alcohol in CCl<sub>4</sub> (0.1 M) measured over a temperature range of 6.5–72°C.<sup>3</sup> Bands at 8555 and 8254 cm<sup>-1</sup> are assigned to the second overtones of CH stretching modes of CH<sub>3</sub> and CH<sub>2</sub> groups, respectively. A sharp

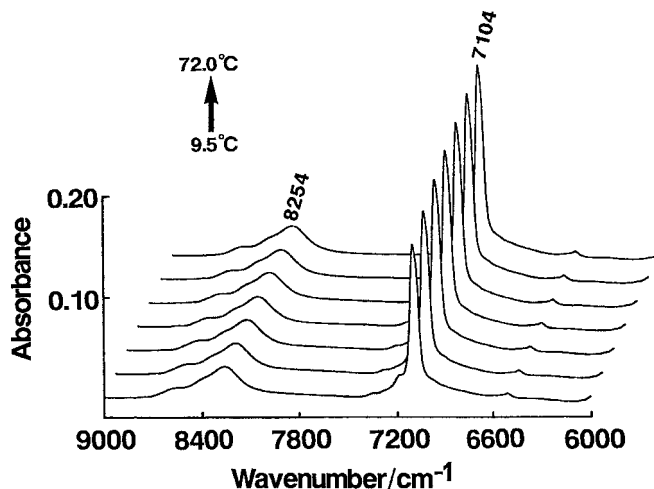


Figure 1. Temperature-dependent FT-NIR spectra of oleyl alcohol in  $\text{CCl}_4$  (0.1 M). [Reproduced from Reference 3 with permission. Copyright (1995) Society for Applied Spectroscopy].

band at  $7090\text{ cm}^{-1}$  is assigned to the first overtone of an OH stretching mode of the monomer. This band heavily overlaps with bands arising from combinations of CH vibrations. A broad feature in the  $6600\text{--}6200\text{ cm}^{-1}$  region is assigned to the first overtones of OH stretching modes of polymeric forms of the alcohol. The intensity changes of the bands due to the first overtones of the OH stretching modes indicate that the hydrogen-bonded species dissociate into the monomeric species with temperature.

We can evaluate the concentration of the monomer at each temperature by Beer's law.<sup>2</sup> Then, the degree of dissociation,  $\alpha$ , can be calculated from the concentrations. The peak intensity of the

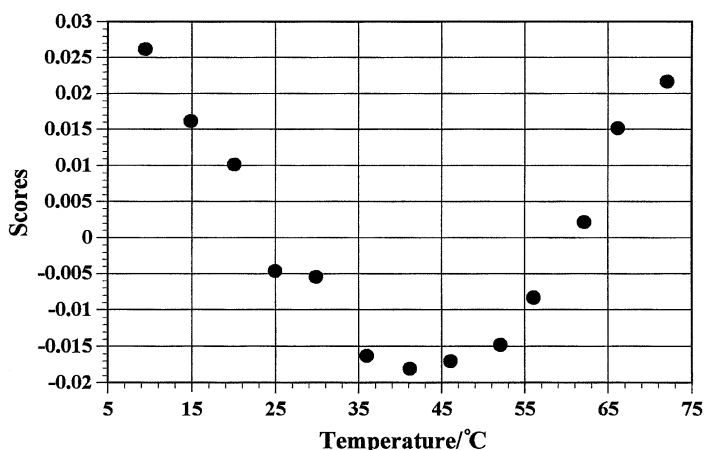


Figure 2. Principal component analyses (PCA) of FT-NIR spectra of the alcohol in  $\text{CCl}_4$  (0.1 M) in the  $9000\text{--}6000\text{ cm}^{-1}$  region.

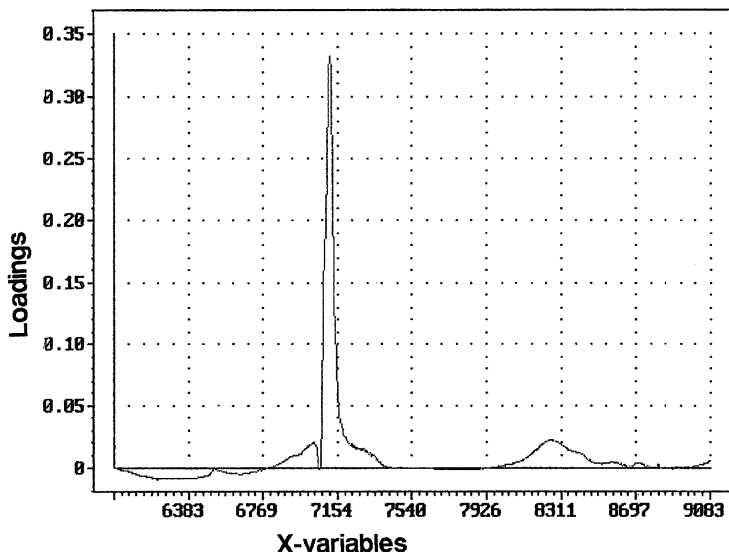


Figure 3. Loading plot of factor 1 for PCA in Figure 2.

first overtone of the OH stretching mode of the monomer was employed to estimate the degree of dissociation. The  $\alpha$  value increases gradually with temperature without a clear turning point.

Figure 2 shows the score plots from the PCA model for the 9000–6000  $\text{cm}^{-1}$  region. Of particular note is that the plots have a turning point at 41°C. This means that the aggregation of oleyl alcohol in  $\text{CCl}_4$  changes greatly near 41°C. The present results are in good agreement with the results obtained by Iwahashi *et al.*<sup>1</sup> for oleyl alcohol in the pure liquid and decane solution. However, it should be noted that PCA gives clearer results.

Figure 3 depicts the loading plot of factor 1 for PCA in Figure 2. A peak dominating the plot corresponds to the first overtone of the OH stretching of the monomer. Of note is that PCA also gives a negative band at *c.* 7070  $\text{cm}^{-1}$  due to the terminal OH groups.<sup>3</sup>

## References

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