# Water structure studied by difference spectra, PCA, and two- dimensional correlation spectroscopy

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Studies of water by NIR spectroscopy stretch back more than forty years. NIR spectroscopy has been employed to investigate hydrogen bonds of water, hydration, and water content not only in basic science but also in various application fields such as agricultural and food engineering, medical and phamaceutical sciences, and polymer and materials engineering. Since water does not exist as a single species, and water molecules form various cluster structures, It has not been easy to analyze NIR spectra of water.

We investigated water structure by using NIR spectroscopy with the aid of difference spectroscopy, two-dimensional correlation (2DCOS) spectroscopy, and principal component analysis (PCA). An NIR spectrum of water has broad feature centered at 6900 cm$^{-1}$ with a long tail toward a longer wavelength region.

**1) Difference spectra:** We measured temperature-dependent NIR spectra of water over a temperature range of 5 to 85℃. As temperature increase a band at 7050 increases while a band at 6844 cm$^{-1}$ decreases, indicating that a water specie having weaker hydrogen bonds increases while that with stronger hydrogen bonds decreases. We calculated deference spectra by subtracting a spectrum measured at 5℃ from each spectrum. It was found that the difference spectra contain only two species at 7089 and 6718 cm$^{-1}$.

**2) 2DCOS:** Synchronous and asynchronal 2DCOS spectra were calculated by using temperature-dependent NIR spectra of water. The synchronous 2DCOS spectrum develops two autopeaks at 7089 and 6718 cm$^{-1}$ and a pair of cross peaks at (7089, 6718) cm$^{-1}$. Thus 2DCOS results suggested there are two peaks at 7089 and 6718 cm-1 in the spectra of water..

**3) PCA:** PCA was carried out for the same spectra data as those for 2DCOS. It was found that the wavenumbers 7089 and 6718 cm$^{-1}$ account for more than 99% of the spectral variations.

These difference spectra, 2DCOS, and PCA all indicated there are two water species giving bands at 7089 and 6718 cm$^{-1}$. These water species may be those having weaker and stronger hydrogen bonds.