Two-dimensional near-infrared correlation spectroscopy, principal component analysis and water structure

VEGARD H. SEGTNAN[*1], SLOBODAN ŠAŠIČ[1], TOMAS ISAKSSON[1] AND YUKIHIRO OZAKI[2]

Department of Chemistry, School of Science, Kwansei-Gakuin University, Uegahara, Nishinomiya 662-8501, Japan
Department of Food Science, Agricultural University of Norway, N-1432 Ås, Norway

The structure of water molecules in the pure liquid state has been subjected to extensive research for several decades. Questions still remain unanswered, however, and no single model has been found capable of explaining all the anomalies of water. In the present study near-infrared spectra of water in the temperature region 6-80°C have been analysed by use of principal component analysis (PCA) and two-dimensional correlation spectroscopy in order to study the dynamic behaviour of the water band centred at 1440 nm, which is due to the combination of symmetric and antisymmetric O-H stretching modes. It has been found that the wavelengths 1412 and 1491 nm account for more than 99% of the spectral variation, representing two major water species with weaker and stronger hydrogen bonds, respectively. A third species located at 1438 nm, whose concentration was relatively constant as a function of temperature, is also indicated. A somewhat distorted two-state structural model for water is suggested.