Temperature-dependent water structural transitions examined by near-IR and mid-IR spectra analyzed by multivariate curve resolution and two-dimensional correlation spectroscopy.

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Streszczenie

This work reports application of the multivariate curve resolution (MCR) and the two-dimensional correlation spectroscopy (2DCOS) to the study of temperature induced changes of conformational multiequilibria in water. The phenomena were simultaneously monitored by the mid-infrared (MIR) and the near-infrared (NIR) spectra. Ordinary methods of band shape analysis are not sufficient to distinguish sub-bands that can be unambiguously assigned to specifically hydrogen-bonded assembles. To achieve the best possible resolution of the multicomponent water system, the MCR analysis has been performed on an augmented data matrix. The 2DCOS calculations were carried out in hetero-spectral mode. The simultaneous analysis of the intensity changes for bands assigned to the fundamental stretching vibration and vibration that combines the fundamental stretching and bending vibrations of the OH groups pointed out on a two-component structure in terms of OH coordination manifested by three spectral components that are in a different way involved in hydrogen bond. The use of MCR and 2DCOS for exploring the NIR and MIR spectra of water enabled to postulate one common picture of the temperature-induced structural changes of water that should be very useful in monitoring the conformational transitions of proteins embedded in aqueous environment.

Słowa kluczowe

Water, Infrared spectroscopy, Multivariate curve resolution, Two-dimensional correlation spectroscopy