THE ANALYSIS OF THE FT-NIR SPECTRA OF WATER ON THE BASIS OF TWO-STATE MODEL

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Robinson with coworkers[1] have introduced two-state outer-neighbor bonding model to explain the anomalies of water. The studies on the properties of water as a function of temperature and pressure revealed that, unlike other ideas, all H_2O molecules in liquid are tetrabonded. On the average they are forming two different bonding types. One type is the regular tetrahedral water-water bonding similar to that found in the ordinary ice Ih, whereas the other is a more dense nonregular tetrahedral bonding similar to that appearing in the ice II. The transformation between these two bonding forms is evidenced by FT-NIR experiment.

The FT-NIR measurements were done for liquid water in the temperature range from 20℃ up to 80℃ in a wide extent of frequencies: 12 000 - 4000 cm^{-1}. Temperature dependent variations in the volume fraction of these two structures are directly related to the spectral changes. The absorbance variations are explored by means of the two-dimensional correlation spectroscopy (2DCOS), principal component analysis (PCA), curve fitting and second derivatives.

The presence of the isosbestic points in a range of the combination and overtone transitions indicates that the experimental spectra are a superposition of two temperature independent components. One component of diminishing intensity with temperature increase, is assigned to a stronger hydrogen bonds occurred in the Ih type, whereas the second component showing an opposite behavior, one can attribute to a weaker H-bonds characteristic for the II type.

The understanding of the hydrogen bonding network in the liquid water is very important in interpretation of the interaction between water and protein chain. The two-state model of water surrounding the protein surface could advance an understanding of the hydration process.

[1] M.-P. Bassez, J. Lee, G.W. Robinson, *J. Phys. Chem.* 91, 5818 (1987)