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Fundamental Study on the Evaluation of the Water Structure in Salt Solutions by Spectroscopic Method

Daitaro Ishikawa

Faculty of Agricultural Sciences, Fukushima University

Summary

It is known that the addition of salt is directly related to the physical properties and quality of foods and also has an effect on the structure of water. However, in our best knowledge the effect of quality modification by salt addition on the structure of water is not fully understanding physiochemically. Researches have been reported on the evaluation for the structural state of water by ions using vibrational spectroscopy such as infrared spectroscopy and Raman spectroscopy. Especially, the quantum chemical calculation method has strongly contributed to the progress. Nevertheless, it is hard that the effects of ions in salt-added solutions on the water structure have been clarified yet. Therefore, in this study, as the fundamental study for developing quality evaluation method of salt-added foods, infrared / far-infrared spectra in the 4000-100 cm^{-1} region were obtained on salt-added solutions with different concentration. Finally, the purpose of this study was to search for a marker band for evaluating the state of the salt-added solution.

Water activity decreased in all solution as the salt concentration increased. The linearity between water activity and the mole fraction of water decreased. This trend; the non-ideality of the solution changed according to the ionic radius. In infrared region in 4000-900 cm^{-1}, the band due to HOH stretching vibration mode was observed in the 3600-3200 cm^{-1} region. In this study, it is found that the band consisted of three bands; around 3200.3400, and 3600cm^{-1}, A band at 3200 cm^{-1} due to structured water was shifted to higher wavenumber region and the intensity decreased. The band position at 3400 cm^{-1} due to week hydrogen bonding did not change for concentration and the intensity of this band increased. In far infrared region, a broad band was observed in the 900-100cm^{-1} and the peak position of this band changed to lower wavenumber in high concentration sample. The band of NaCl solution has iso-absorbance points so that the solution was defined as two components system. The change in peak position corresponded to the non-ideality of solution described by Raoult's law. Consequently, the results obtained in this study strongly suggested that the spectral behavior in the far infrared (below 900 cm^{-1}) region is effective in evaluating the state of water in salt solutions.