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Fundamental Study on the Evaluation of Hydration Structure in Salt Solution by Using Spectroscopy

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Summary

Water is the main component in food and plays an important role for food quality. It has been known that the ions affect the hydrogen bonding of water molecules and is also involved in the structuring of water, but there is still insufficient knowledge on the structuring of water. Since the 2020 grant, the spectroscopic analysis by infrared/far-infrared region of salt solutions were conducted to establish an essential quality evaluation method for salt-added foods. In 2021, marker bands in infrared region were investigated to suggest new spectroscopic regions that can be used in the food industry as well as the effects of changes in the hydration structure of water on the spectra.

Solutions with different cations such as NaCl, KCl, CsCl, $BaCl_2$, etc., and salts with different anions relative to sodium were prepared. Infrared/far infrared spectra in the region of 4000-10 cm^{-1} were measured using the ATR method, and near infrared spectra in the region of 1000-2500 nm were also measured. Water activity of each solution was quantified after spectral measurement t to investigate the relationship with the spectral behavior. The position of the collective band around 3200 cm^{-1} for the chloride solution with different cation shifted to higher wavenumbers as the water activity decreased. This may be attributed that the decrease in water activity due to the addition of salt leads to the cleavage of hydrogen bonds, which increases molecular mobility. The wavenumber shift occurred even when the anion was changed, with almost no change in intensity in the test samples except for Na_2CO_3. To evaluate the ion dependence of the hydrogen bonding state, the ion hydration area was estimated from Raoult's law, and in addition to the amount of shift, the intensity ratio of the two peaks corresponding to water activity (3400/3200) and the band width at half maximum were investigated. The intensity ratios of the spectra of ions other than Li and Ca tended to decrease linearly with water activity. It was shown that the band ratios could be explained by a single straight line even for different ion species. In other words, the ratio of the total state of structured water and weak hydrogen bonds was considered to be independent of the type of these ions. Although the non-ideality of water causes deviations from Raoult's law, the electrostatic potentials of the ions become overlapped, suggesting that the state of hydrogen bonding in the solution may change. The band ratios proposed in this study also essentially correspond to the non-ideality of water, namely, the band ratios suggest that they can be applied to the evaluation of the influence of ions on the structure of water in foods.