

STRUCTURE ANALYSIS OF SODIUM CATION IN AQUEOUS SOLUTION BY SOFT X-RAY ABSORPTION SPECTRA AND THEIR MOLECULAR ORBITAL CALCULATION

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We prepared a new soft X-ray absorption spectrometer system for measuring soft X-ray absorption spectra(50-1500 eV) of wet samples such as bio and environmental materials, and solution samples at the beam line 12 of Kyushu Synchrotron Light Research Center. We measured the concentration dependency of absorption spectra of sodium, magnesium, and calcium cations in aqueous solutions for the biological and environmental purposes, and analyzed the spectra by a DV-Xa molecular method. In case of sodium cation in aqueous solution, there exists clear concentration dependency on the spectra and the calculation results give the hydration difference between higher concentrated solution(5-3 molar solutions) and lower solution(1-0.5 molar solutions).

We will talk about the first, our spectrometer system and the second, the detail of the analysis results of sodium samples.