

Solvation Structures of Iodide Anion in Various Solvents

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Our previous studies on the solvation structures of Br^- in various solvents indicated that the hydration number in protic solvents correlates with the acceptor number of solvents and that the first shell distances, corresponding to Br-O length, are almost the same in various protic solvents from water to alkylalcoholes, while the distance is longer in aprotic solvents corresponding to that of Br-C(in methyl group). Based on such information we are studying the ion pair structure of alkylammonium- X^- , i.e. whether the ion-pair includes solvent molecules inbetween the ions. Since the solvation of I^- is far more weaker than Br^- . the ion-pair structure for alkylammonium- I^- should be different from that for Br^- . The aim of the present study is thus two folds, one to collect the XAFS data for I^- in various solvents in order to compare with those for Br^- and the other to study the extent of dehydration for iodide in the ion-pair.

The XAFS study for iodine K-edge has been insufficient mostly due to its high energy, 33keV. It requires high beam energy for SR, and the monochromator needs higher precision and stability.

The XAFS experiments were performed at BL01B1 station. During the allotted beamtime several runs were devoted to obtain the same XAFS spectra, I K-edge for 0.1M KI aqueous solution. One of the results is illustrated in the figure. The spectrum was obtained by using the mirror system, thus there should not exist the higher harmonic contamination problem. As is clear from the spectrum, the EXAFS oscillation amplitude is far smaller than

that for bromide case. Thus it is obvious that the EXAFS analyses on the iodide solvation structures is not easy.

The present experiments also indicated that the double crystal monochromator at BL01B1 needs improvement, since the resolution and EXAFS amplitude are not reproducible. At the high energy region, the monochromator must be operated under the continuous adjustment of $\Delta\theta$.

