# Solvation Structures of Iodide Anions in Various Solvents

**Iwao Watanabe*[1] 3296, Shuichi Emura[2] 1239, Masao Takahashi[2] 1285, Makoto Harada[1] 1286, Yasuhiko Mizoguchi[1] 3497, Kennichi Kato[1] 3496, Takafumi Miyanaga[3] 3319, Hideto Sakane[4] 3298, Tomoya Uruga[5] 182, Hajime Tanida[6] 1275.**
[1]Graduate School of Science, Osaka University. [2]The Institute of Scientific and Industrial Research, Osaka University. [3]Faculty of Science and Technology, Hirosaki University. [4]Faculty of Engineering, Yamanashi University. [5]SPring-8. [6]The Institute of Physical and Chemical Research(RIKEN).

Several combinations of solute-solvent have been studied at the beamline BL01-B1. The solvents used were water, methyl alcohol, ethyl alcohol, formamide, acetonitrile, and dimetylformamide. The counter ions used were tetrabutylammonium and potassium or lithium ions. The mirror system was used to remove higher harmonics components. From the previous experiences we understand that it is essential for obtaining high quality XAFS spectra at the I K-edge (33 keV) to keep the double crystal monochromator in best tune during the energy scan, therefore the absorbance data have been collected after tuning the $\Delta\theta$ at each energy point during the energy scan.

Though the XAFS data contain only weak EXAFS signals, as was the previous experience (1997B0038-NX np), it is clear that the signal intensity reflects the magnitude of solute-solvent interaction from the plot of the main peak height in the Fourier transform spectrum for iodide ion in solution against the acceptor number AN of the solvent as shown in Figure 1. The peak intensity depends not only upon the coordination number but the Debye-Waller-like parameter. Since both are intimately related with the solute-solvent interaction, then the peak intensity must be in good correlation with AN, the empirical parameter indicating the anion-solvent interaction strength.

The information on solvation number can be obtained from the EXAFS analysis as the coordination number N. However, since the standard sample for this system is difficult to obtain here, the relative coordination numbers were determined as SN as shown in Figure 2. There is almost linear correlation between AN and N for protic solvents, the larger the solvent molecule, the smaller the solvation number. It is interesting to see that in dimethylsulfoxide the solvation number is large although the molecular size is far larger than the other solvents. This seems to be indicating that iodide ion contacts with two methyl groups from a single solvent molecules.

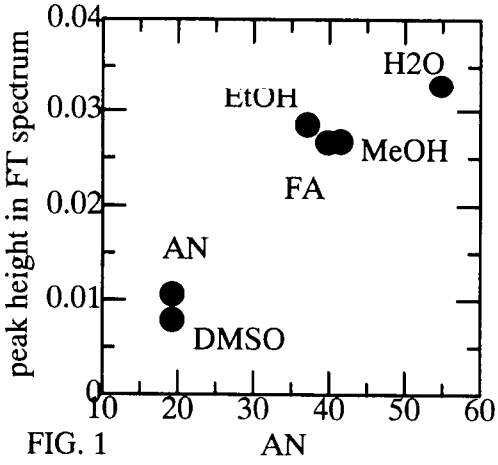

FIG. 1

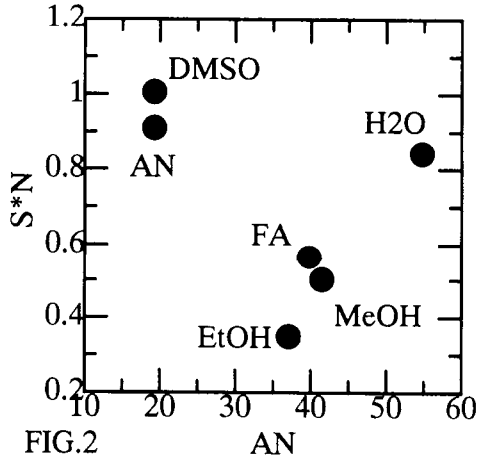

FIG.2