

# Determination of Solvation Structure of Chloride and Iodide Ions in Methanol and Ethanol by EXAFS Using BL-4

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## Abstract

The solvation structure of  $\text{Cl}^-$  and  $\text{I}^-$  ions was investigated in water, methanol and ethanol under an atmospheric pressure by using an EXAFS (extended X-ray absorption fine structure) beamline (BL-4), which covers the K-edge absorption energy of elements with relatively low atomic numbers from silicon (atomic number 14) through zinc (30). This is the first case to study the solvation structure of chloride ions by EXAFS.

The chloride ion is solvated with 3.4 methanol and 3.8 ethanol molecules through the alcoholic hydroxyl group and methyl group in methanol and methyl or methylene group in ethanol. On the other hand, the iodide ion interacts with  $3 \pm 1$  molecules in both methanol and ethanol. A possibility of monodentate interactions of some alcohol molecules with the chloride and iodide ions in the solvation shell could not be fully excluded. The  $\text{Cl}^-$ -O and  $\text{Cl}^- \cdots \text{C}$  distances were determined to be  $(317 \pm 1)$  and  $(389 \pm 1)$  pm, respectively, for methanol and  $(320 \pm 1)$  and  $(391 \pm 1)$  pm, respectively, for ethanol. The  $\text{I}^-$ -O and  $\text{I}^- \cdots \text{C}$  distances, on the other hand, were found to be  $(361 \pm 1)$  and  $(405 \pm 1)$  pm, respectively, for methanol and  $(358 \pm 1)$  and  $(404 \pm 1)$  pm, respectively, for ethanol.

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