



Experiment title: Investigations of the structure of ion complexes in aqueous electrolyte solution: an anomalous X-ray scattering study of La³⁺, In³⁺ and Br⁻

Experiment number:
CH-813

Beamline:
ID01

Date of experiment: from: 13th July to: 17th July 2000
and from: 9th December to: 12th December 2000

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54

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Report:

Previous investigations on the structure of lanthanum bromide aqueous solutions by X-ray diffraction, EXAFS and Raman spectroscopy [1] lead to some information on the structure of the lanthanum complexes and on their distribution in the solution. These different experimental methods allowed us to conclude that the first coordination shell of lanthanum cations is only constituted by water molecules (plausibly nine), without any bromine anion in direct contact with the cation. Obviously, from EXAFS results the distances of the hydration water to the cation were also obtained. No study having been made on the hydration of the bromine anion on those solutions, we intended to study it by AXD (Anomalous X-ray Diffraction).

In the case of the indium bromine aqueous solutions the indium complexes contain two bromine and five or six water molecules around each indium cation. Those solutions were investigated by X-ray diffraction [2,3] and by EXAFS [4] at both K edges, the indium and the bromine one. It seemed interesting to us to compare the results obtained by EXAFS and by AXD about the solvation shell of the bromine anion. As a matter of fact, AXD seems to be an accurate technique for this purpose. Moreover, similar experiments by AXD on other aqueous solutions, were done with success by the Bristol group [5].

The first experiments on indium bromide aqueous solutions took place at ID-01 beam line from 13 till 17 July 2000. Due to difficulties with the instrument we did not get any useful data, so the experiment had to be re-done later on from 9 to 12 December 2000. The experiments were repeated with indium bromide this time with success. New ones with lanthanum bromide aqueous solutions were also done.

Diffraction experiments were made at 200 eV and 5 eV below the bromine K-edge (13422 eV). The samples used were 1.23 mol.dm^{-3} LaBr_3 aqueous solution and 1.76 mol.dm^{-3} InBr_3 aqueous solution.

Figures 1 and 2 show the row intensities measured at 200 eV and at 5 eV below the bromine K edge for the lanthanum bromide and for the indium bromide aqueous solutions respectively. A clear difference can be seen between the two energies.

The data will be analysed following the same procedures used by the Bristol group .

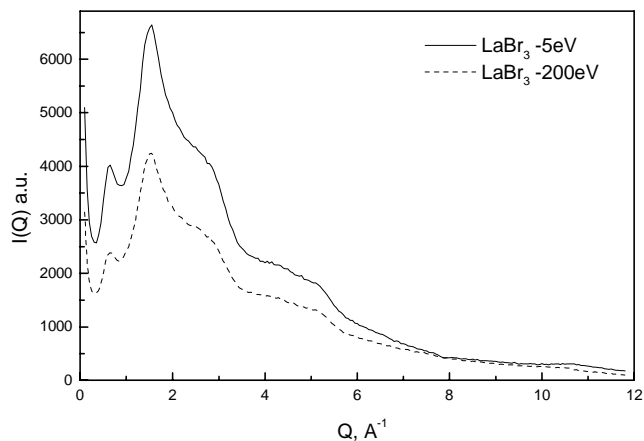


Figure 1. LaBr_3 solutions Br edge.

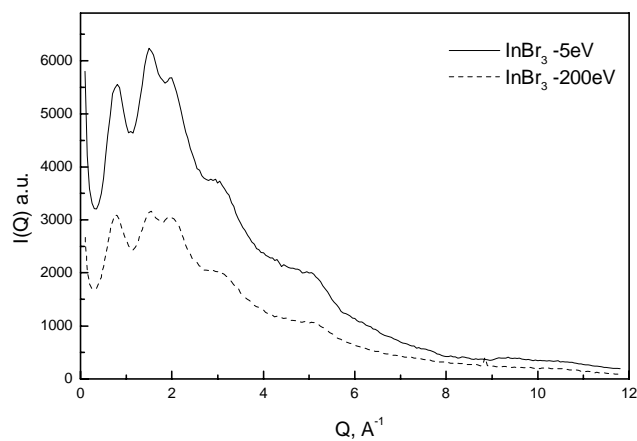


Figure 2. InBr_3 solutions Br edge

References

- [1] Alves Marques M, Cabaço M I, de Barros Marques M I, Gaspar A M, de Morais C M 2001 J. Phys.: Condensed Matter **13** 4367
- [2] de Barros Marques M I, Cabaço M I, Oliveira M A and Alves Marques M 1982 Chem. Phys. Letters 91 222
- [3] Cabaço M I, Gaspar A M, de Morais C M, Alves Marques M 2000 J. Phys.: Condensed Matter **12** 2623
- [4] de Barros Marques M I and Lagarde P 1990 J.Phys.: Condensed Matter 231
- [5] Ramos S, Barnes A C, Neilson G W, Thiaudaire D, Lequien S 1999 J.Phys.: Condensed Matter **11** A203