



Experiment title:
X-ray diffraction investigations of the structure of concentrated aqueous solutions of indium and yttrium chloride, bromide and nitrate at low and room temperatures

Experiment number:
SC-1006

Beamline:	Date of experiment: from: 19 th June 2002 to: 24 th June 2002	Date of report: 28-02-2003
Shifts: 15	Local contact(s): Dr Veijo Honkimaki	<i>Received at ESRF:</i>

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Report:

This experiment was proposed in the frame of investigations of the authors on molecular correlations existing in concentrated aqueous solutions of salts constituted by ions of different valences [1-7]. The authors intended to obtain information about the structure of concentrated aqueous solutions of indium and yttrium salts both in the liquid and in the glassy states.

Monochromatized synchrotron radiation of high energy (88.54 keV, 0.140Å) was chosen. The samples were studied by transmission in layers of 2 mm, contained in a plane parallel cell between kapton windows (25 µm). When obtaining the X-ray diffraction pattern of a glassy sample a closed cycle He cryostat was used, allowing sample temperatures between 11K and 300K. The vacuum chamber was built with mylar windows (100 µm) for the incident and scattered x-rays.

The detection system was a MAR online image plate scanner (2300x2300 pixels: pixel size 0.15mm). The one-dimensional diffraction patterns were obtained by integration of the diffraction rings of the 2D patterns (Figure 1). In order to gather information over the Q region of interest the X-ray diffraction patterns were acquired at two different distances from the sample to the detector: 320 mm and 960 mm. A tube filled with helium was used to reduce significantly the contribution from air scattering to the measurements with the longest path between the sample and the detector.

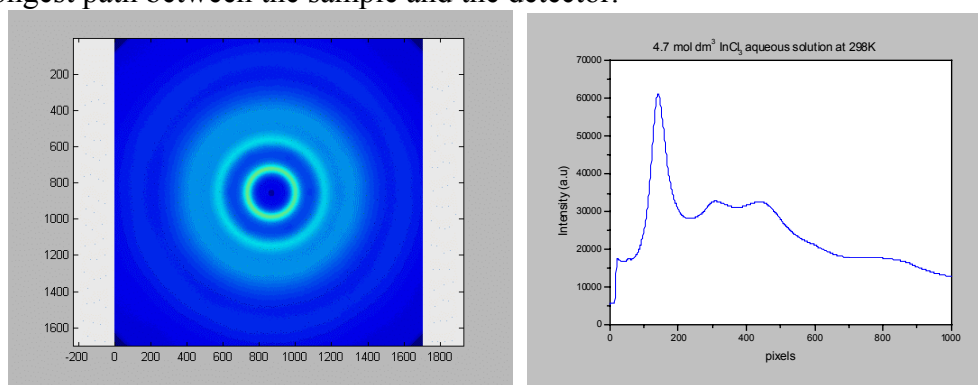


Figure 1 - Diffraction patterns obtained for the 4.7 mol dm³ InCl₃ aqueous solution at 298K. 2D image and corresponding 1D curve.

Corrections were made for background, empty container, air and helium scattering contributions, absorption and geometrical factors and then scaled to electron units using the Krogh-Moe method. A comparison between the experimental results obtained for the indium halide aqueous solutions in the liquid and the glassy states are displayed in Figure 2. Similar results were obtained for the yttrium halides aqueous solutions, as well as for aqueous solutions of lanthanum halides.

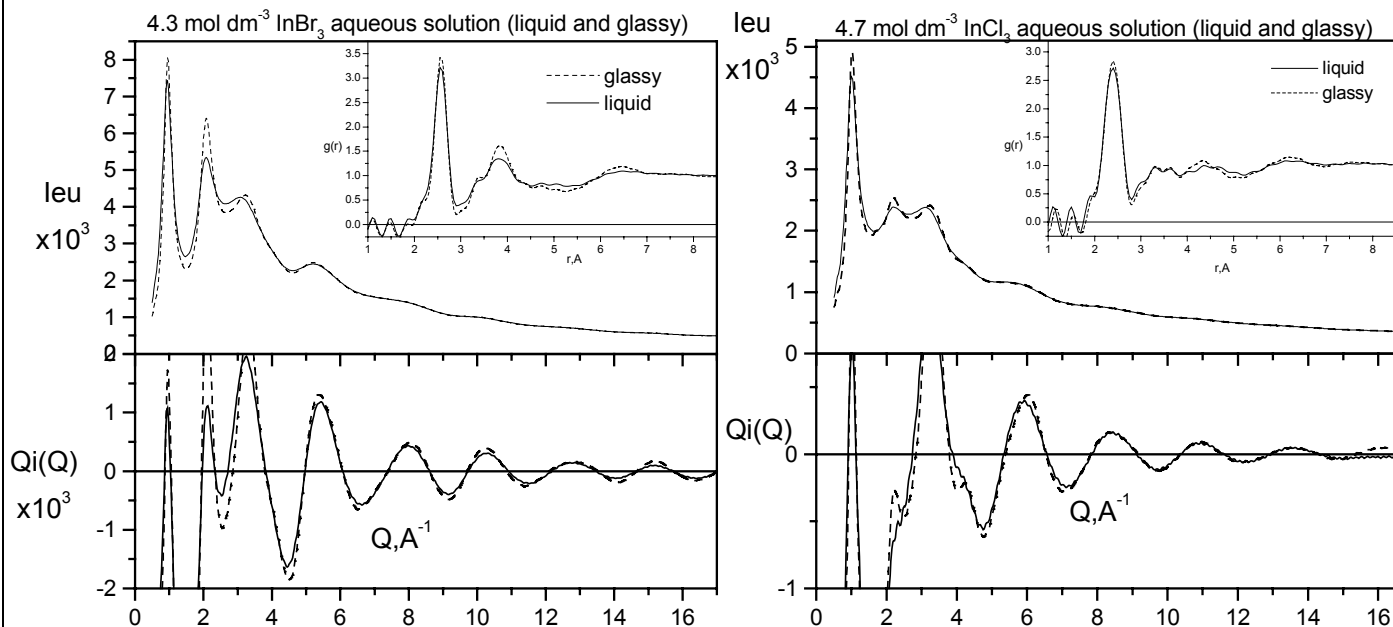


Figure 2 - Experimental X-ray diffraction patterns $I_{eu}(Q)$ and $I_{Qi}(Q)$ and pair correlation function $g(r)$ of concentrated aqueous solutions of InCl_3 and InBr_3 in the glassy state (obtained at 25K) and in the liquid state (obtained at 298K).

Diffraction patterns of indium and yttrium nitrate aqueous solutions were also obtained at room temperature for samples with different concentrations. The interpretation of the results obtained for these and for aqueous solutions of other nitrates*, which is based on building of molecular models, is in progress. Some results were already presented in Rhodes, Greece, during the NATO-ASI conference on the Physical Chemistry of Liquids (September 2002). The results obtained for the $\text{Cu}(\text{NO}_3)_2$ aqueous solutions have already been included in an article recently submitted to Journal of Molecular Liquids.

* see report on experiment sc-916

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