ESRF	**Experiment title:** X-ray diffraction experiments on concentrated aqueous solutions of salts of yttrium and lanthanum	**Experiment number**: SC-916
Beamline: ID15b	**Date of experiment**: 15th November – 20th November 2001	**Date of report**: 30-08-2002
Shifts: 15	**Local contact(s)**: Dr. Veijo HONKIMAKI	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Professor Manuel Alves Marques
*Dr. Maria Isabel de Barros Marques
*Dr. Maria Isabel Cabaço
*Ms Ana Gaspar

Centro de Física da Matéria Condensada da Universidade de Lisboa, Avenida Professor Gama Pinto, 2, 1649-003 Lisboa, PORTUGAL

Report:

This experiment, performed on the ID15b ESRF beam line, was proposed in the frame of our investigations on positional correlations existing in concentrated aqueous solutions of salts constituted by ions of different valence [1-8]. We asked for beam time in order to obtain X-ray diffraction patterns of aqueous solutions of lanthanum and yttrium nitrates as well as on yttrium halides. During the experiment we also had the opportunity to obtain X-ray diffraction patterns of aqueous solutions of other nitrates, namely cadmium and strontium nitrate aqueous solutions whose results are also presented in this report.

Monochromatized synchrotron radiation of high energy (88.539keV, 0.140Å) was chosen. The samples were studied by transmission in layers of 2mm, contained in a plane parallel cell between kapton windows. 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. In order to gather information over the momentum transfer region of interest ($Q=(4\pi/\lambda)\sin(\theta/2)$) the acquisition of the X-ray diffraction patterns was performed at two different distances from the sample to the detector: 321mm and 951mm. A tube filled with helium was used to significantly reduce the contribution from air scattering to the measurements with the longest path between the sample and the detector. Typical raw data are shown in Figures 1a and 1b, where measured intensities normalised to the intensity of the incident beam are displayed.

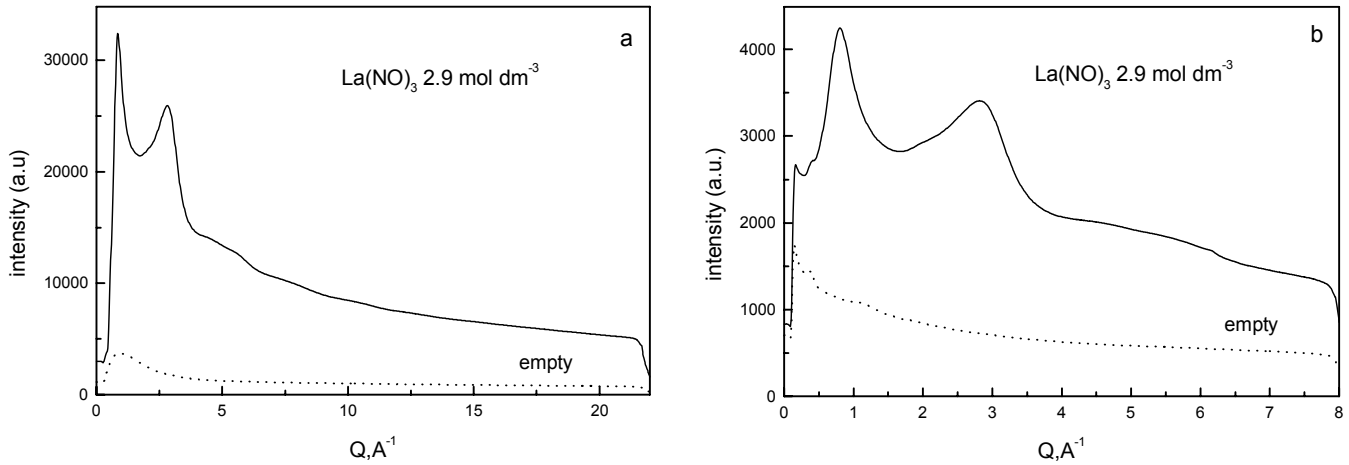

Figure 1: X-ray diffraction patterns obtained at different distances : a) 321 mm, b) 951 mm

Corrections were made for background, empty container, air and helium scattering contributions, absorption and geometrical factors. The intensities, scaled to electron units, are displayed in Figures 2a and 2b. Fourier inversion of the coherent dependent intensities allowed obtaining the corresponding total pair correlation functions g(r), presented in Figures 3a and 3b.

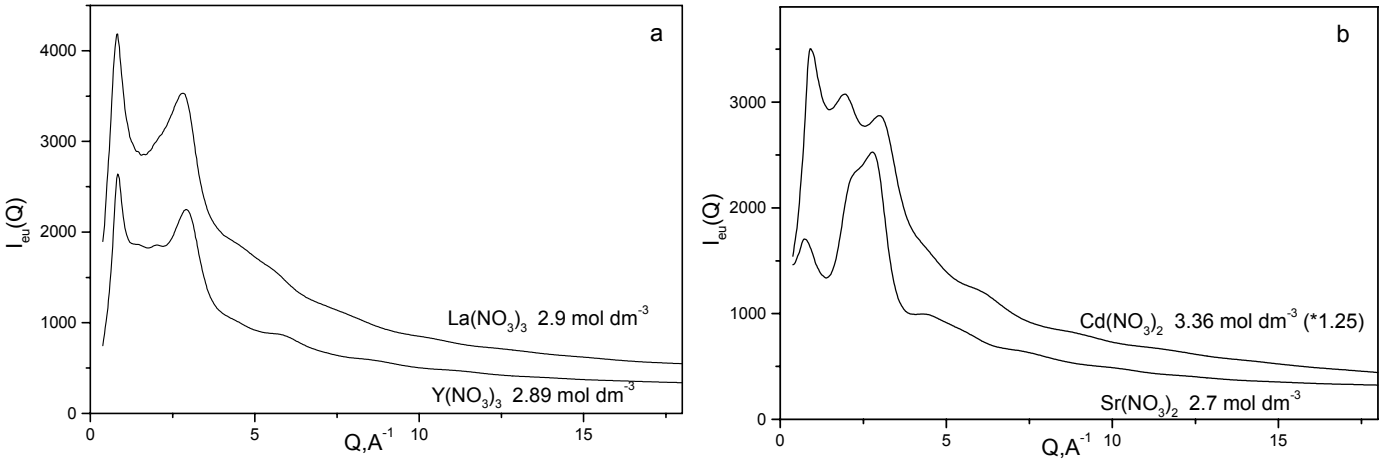

Figure 2: X-ray diffraction patterns: a) $La(NO_3)_3$ and $Y(NO_3)_3$, b) $Sr(NO_3)_2$ and $Cd(NO_3)_2$

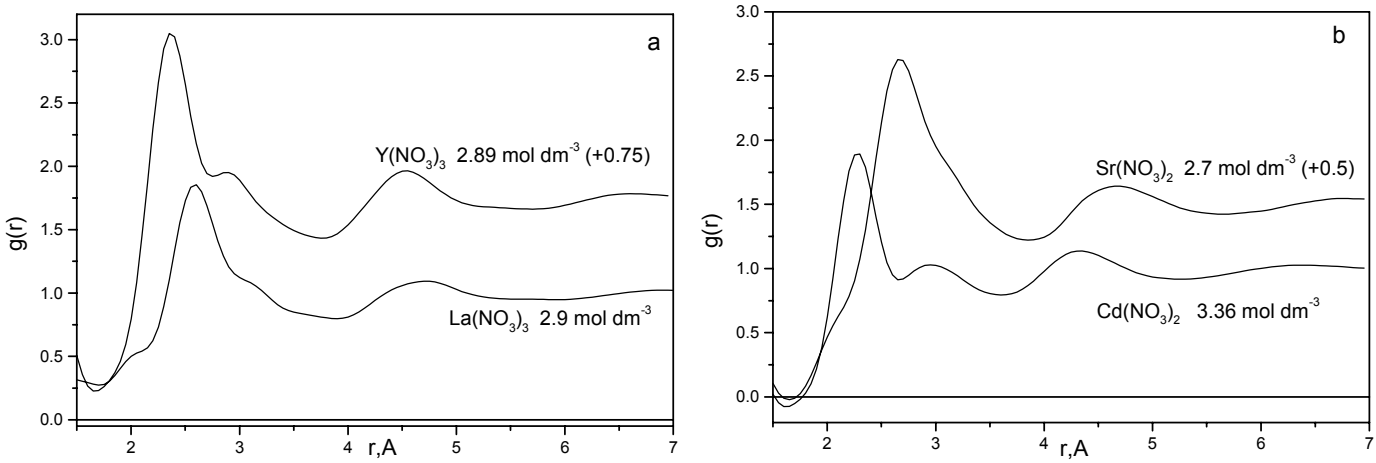

Figure 3: Pair correlation functions g(r): a) $La(NO_3)_3$ and $Y(NO_3)_3$, b) $Sr(NO_3)_2$ and $Cd(NO_3)_2$

The interpretation of these results and of those obtained with the other solutions, which is based on the building of molecular models, is in progress. Preliminar results were already presented in Plymouth NH, United States, during the Gordon Conference on Water and aqueous solutions (Aug 2002) and will be presented in Rhodes, Greece during the NATO-ASI Conference on the Physical Chemistry of Liquids (Sept 2002).

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