ESRF	<b>Experiment title:</b> Differential anomalous x-ray scattering on a saturated aqueous MnBr2 solution	Experiment number: SC-416
Beamline:	Date of experiment:	Date of report:
ID1	from: 28.04.98 to: 03.05.98	24.08.98
Shifts:	Local contact(s): Stéphane Lequien	Received at ESRF:

Names and affiliations of applicants (\* indicates experimentalists):

Prof. Dr. Helmut Bertagnolli Stefan Batschkowitsch \* Ulrich Eberhardinger Gerhard Heusel

## **Report:**

The knowledge of the coordination and configuration of  $Mn^{2+}$  ions in concentrated aqueous solutions is very limited. In dilute aqueous solutions the bulk water structure remains relatively undistributed except in the near vicinity of the ion. At high concentrations the dielectric strength of the solution has been significantly lowered decreasing the ability of an ion to orient coordinated water molecules. Entropy considerations may favor a degree of association of oppositely charged ions. Water molecules in solvation layers of unassociated ions cannot be considered to be independent of the influence of neighbouring ions. This leads to the conclusion that ion-ion, ion-solvent and solvent-solvent interactions in concentrated solutions are relatively complicated.

The characterization of the structure of aqueous solutions is not an easy task using conventional x-ray scattering method. In binary metal-bromide aqueous solutions, the total structure factor comprises ten partial structure factors (PSF). Therefore the separation of individual contributions of such components is very difficult. The Differential Anomalous Scattering (DAS) technique exploits on the strong variation of the atomic scattering factor close to the absorption edges. Diffraction experiments at different energies give rise to total differential scattering cross sections which differ with respect to the contributions of the anomalous scatterer. This leads to the differential structure factor (DSF), which only includes contributions of the anomalous scatterer itself and other atoms. So the DSF comprises only four Differential Atom Pair Correlation Functions (DAPCF).

The complete technical arrangement for this experiment worked well.

A problem appeared, when we looked at the received spectra. They showed crystalline peaks. The color of the solution turned to brown in the area hit by the x-rays. Further experiments with solutions of the same substances brought the same result. We assume, that this behaviour comes from a photochemical reaction.

Because there where no additional possibilities to finish the planned experiment, we decided to cut our beam time and provided it for other groups.