

**Experiment title:**EXAFS studies of local order in LaBr₃ and LaCl₃ aqueous solutions**Experiment number:**

CH - 791

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3

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Report:

EXAFS experiments on lanthanum bromide and lanthanum chloride aqueous solutions for different concentrations (~ 3 M, 2 M, 1 M and 0.5 M) were done in order to investigate the structure around the La⁺³ ion in both halide solutions.

The EXAFS experiments were performed in the transmission mode at the La K-edge (38924.6 eV) using a Si 311 flat monochromator and ionization cameras filled with krypton as detectors for I and I₀. La₂O₃ was used as reference. The samples were contained in planoparallel cells with collodium or kapton windows.

χ (k) EXAFS modulations of the absorption coefficient were normalized following a standard procedure. EXAFS simulations and Fourier transforms

were carried out using the program EXCURV90 (1). Phase shifts were calculated internally by the program EXCURV90.

For each halide all the spectra have been analysed over the same energy range of about 44 - 1290 eV (corresponding to a wavevector of about 3.3 - 18 \AA^{-1})

The experimental spectra of $k\chi(k)$, the EXAFS simulation on the lanthanum edge and its Fourier transforms for one of the samples (LaBr_3 , 3 M) is shown on the figure. The spectra were found to be almost identical at all concentrations of each halide solution.

In the first coordination shell of lanthanum we found no halide ion, only oxygen atoms at 2.54 \AA from the La^{+3} ion, the number of coordination varying between 7 and 8. The value '8' agrees with a fit of the intensity observed in an X-ray diffraction pattern (not yet published) by a profile calculated from a molecular model where eight water molecules are included in the first hydration shell of the cation.

(1) "SERC Daresbury Laboratory EXCURV90 program", Binsted N, Campbell J W, Gurman S J and Stephenson P C (1990)

