ESRF	Experiment title: EXAFS contribution to evidence rare earth elements / humic acid binding change with the metal loading	Experiment number: EC817
Beamline:	Date of experiment : from: 8-04-2011 at 8 am to: 03-05-2011 at 8 am	Date of report: Sep 12, 2011
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Report:

The objective of this proposal was to investigate the molecular environment of Rare Earth Elements (REE) bound to humic acid at various loadings in order to determine which organic functional sites are involved in REE complexation to humics. The present beamtime was used to complete a set of data previously recorded at the Tokyo photon factory in order to study the binding of Sm and Yb to purified humic acid. The present experiment consisted of collecting EXAFS spectra of both REE-humic complexes and model compounds complexes including Sm and Yb - EDTA, NTA and IDA.

During the 15 shifts beamtime, EXAFS data were recorded at the Sm and Yb L3-edge in fluorescence detection mode using a 13 Ge-elements detector, at room temperature. The monochromator was equipped with Si(111) crystals and we used harmonic rejection mirrors.

Samples consist of solution of 1:1 Sm- or Yb-model organic ligand containing 500ppm of Sm and Yb at pH 5 or 1:1 Sm- or Yb- organic resins containing 1000 ppm of Sm and Yb. The data were of good quality to k values of 11 Å⁻¹ after 20 to 30 EXAFS scans.

Comparisons of spectra obtained for Yb-EDTA, Yb-NTA and Yb-IDA complexes indicated that the first coordination sphere around Yb consists of both O and N and it also revealed an increase of the C contribution in the second coordination sphere of Yb from IDA to NTA and EDTA. This observation is consistent with the molecular structure of these chelating complexes, as determined from crystallographic structures of the crystalline compounds, Yb being surrounded with 4 C atoms with EDTA, 3 C atoms with NTA and 2 C atoms with IDA.

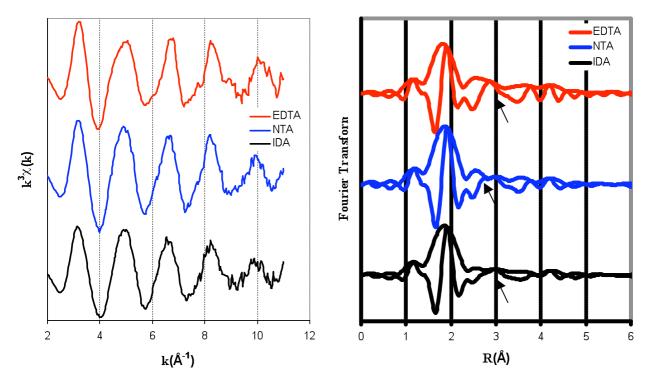


Figure 1: Examples of Yb-L3 edge EXAFS data of some samples studied showing an increase of the C contribution in the second coordination sphere of Yb.

This data will be further compared with dataset of Sm-, Yb- and Pr- model organic ligands and Yb-, Sm- and Pr-HA complexes obtained at the Tokyo Japan photon factory and at Soleil. This work will allow to determine the nature of the REE binding site in HA, as a function of REE loading and pH conditions. These results will provide evidence that REE pattern shape is a fingerprint of the HA sites involved in the binding REE-HA.