ESRF	Experiment title: Zn speciation in colloidal precipitates and fungi related to Acid Mine Drainage processes	Experiment number: ES-248
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Shifts:	Local contact(s):	Received at ESRF:
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Report:

The aim of this proposal was to study the Zn local environment and speciation in monophase and multiphase colloidal procipitates formed in several Acid Mine Drainage environments (all located in the Liguria Region, ITALY) and to determine Zn structural environment in fungi grown either on colloidal procipitates or in a ZnSO4 solution.

During the present run we managed to collect both XANES and EXAFS spectra of :

5 different <u>colloidal precipitates</u> differering for both mineralogical composition, transition metal and Rare Earth Elements content.

A <u>synthetic Woodwardite</u> has been analysed also by XANES and EXAFS in order to serve as a model compound to interpret xAS spectra of colloidal precipitates where woodwardite is present and to retrieve structural information of the local environment around Zn for this phase for which no Structural information is available in the litterature.

XANES data of <u>**3 model compounds</u>** (synthetic hardystonite, natural tarbuttite and synthetic $ZnSO_4$:7H₂O) with zinc in [4], [5], and [6] coordination have been collected as well in order to aid determining the Zn coordination geometry from the edge energy position.</u>

<u>2 fungi</u> (Tricoderma and Penicillium) grown on a colloidal precipitate mostly consisting of allophane, and for the same two species of fungi grown in a ZnSO4 acqueous solution.

For the fungi samples, a preliminarly test was tried to collect fast XANES spectra at the Cu K-edge: In this kind of fungi Cu is believed to behave like Zn. However, Cu is present inmuch higher amounts (10000ppm) allowing us to try transmission XANES spectra with much shorter data collection times. We performed a series of short XANES spectra (each lasting ca. 6 minutes) to see if some variation occurred with time possibly related to structural damage induced by the X-ray beam. We did not observe any change even after 1 hour collection time. So, we proceeded in collecting Zn K-edge XAS data on these samples. Both XANES and EXAFS data are of good quality and will allow a reliable determination of Zn-O distances and Zn-O coordination number.

All the samples showed the presence of divalent Zinc, and no metallic zinc has been observed within the detection limit of XAS technique. All EXAFS data are currently being analysed in order to retrieve Zn-O bond distances and coordination numbers. The model compounds analysed here and others from the literature [1] will be also used for theoretical XANES calculations. Once a good agreement will be found between theoreticl and experimental XANES spectra of model compounds, theoretical XANES spectra will be calculated also for the fungi samples in order to get further information on the bonding geometry around zinc .

[1] G. Giuli, A. Trapananti, F. Mueller, D. Bresser, F. d'Acapito, S. Passerini (2014), Inorganic chemistry, in press, DOI: 10.1021/acs.inorgchem.5b00493