



	<b>Experiment title:</b> Molecular scale mechanism of arsenic scavenging by nanocrystalline iron-hydroxysulfate minerals	<b>Experiment number:</b> EC127
<b>Beamline:</b> BM 29	<b>Date of experiment:</b> from: 29-NOV-06 to: 03-DEC-06	<b>Date of report:</b> Sept. 20 2008
<b>Shifts:</b> 12	<b>Local contact(s):</b> <b>Giuliana AQUILANTI</b>	<i>Received at ESRF:</i>

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**Report:**

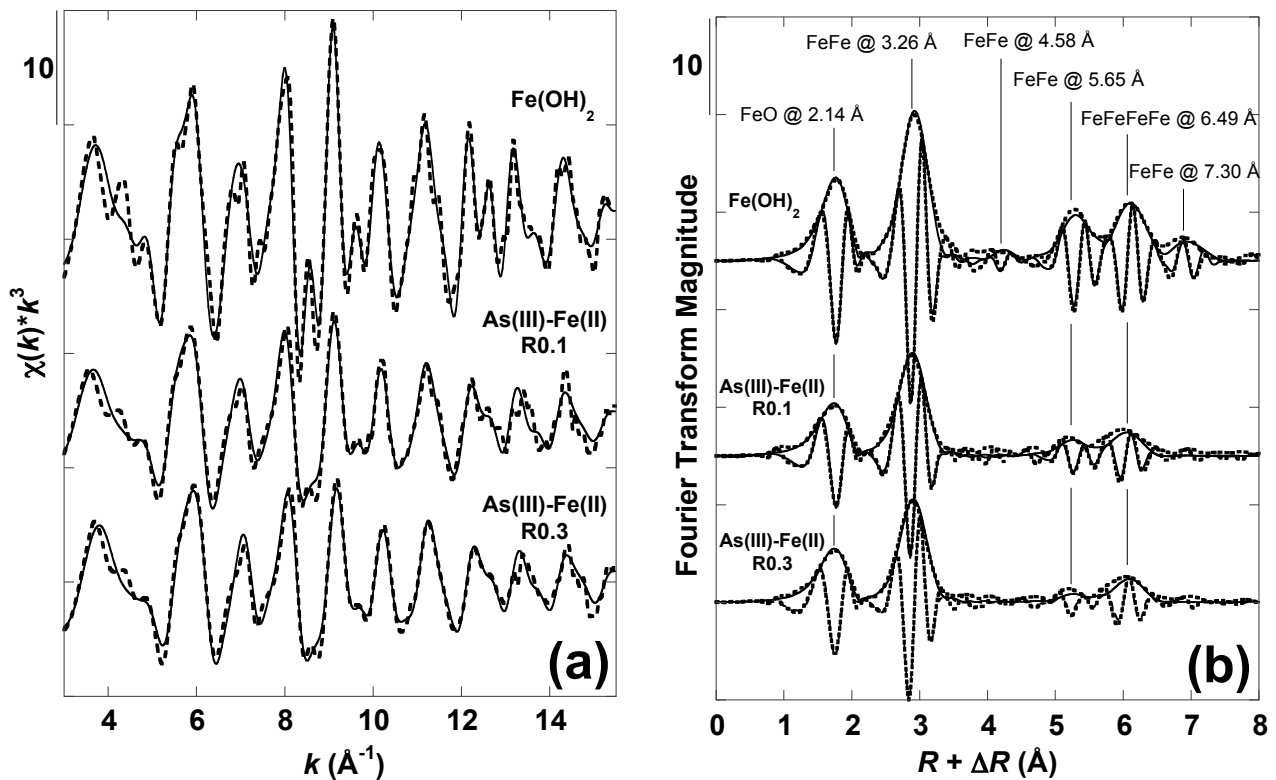
The objective of this proposal was to determine local structural environment of iron in Arsenic rich nanocrystalline phases able to immobilize arsenic in impacted environments, as acid mine drainage, or contaminated sediments. Particular emphasis was put on the understanding of the role of arsenic in the breakdown of Fe-minerals structures, which significantly influences their solubility.

During the 4 days (12 shifts) beamtime, XAS data were recorded at the Fe K-edge in transmission detection mode, in order to complement XAS data previously recorded at ESRF and SSRL at the As K-edge. The monochromator was equipped with Si(111) crystals and the whole experiment.

EXAFS and XANES data were recorded at the Fe K-edge on a set of 25 samples containing 10 – 40 wt% of iron, at a temperature of 10-15 K, using a liquid He cryostat. Samples were previously diluted in appropriate amounts of cellulose to get absorption edge-jump of 1-2, without exceeding total absorption factor of 2.5 above the Fe K-edge.

XANES data were recorded within the same scans as EXAFS data, by defining various regions in the scan.

The data were of excellent quality, combining good energy resolution (Figure 1) to excellent signal to noise ratio after 1 to 3 scans (Figures 1 and 2). Part of these data are about to be published (Ona-Nguema et al. accepted). XANES data on model compounds recorded during this session were also used in Miot et al. (accepted).



Iron K-edge EXAFS data recorded at 10K for three selected model compounds: crystalline  $\text{Fe(OH)}_2$ ,  $\text{Fe(II)-As(III)}$  hydroxides R0.1 and R0.3 (see text). (a)  $k^3$ -weighted  $\chi(k)$  EXAFS, and (b) their corresponding Fourier transforms (FT), including the magnitude and imaginary part of the FT. Experimental and calculated curves are displayed as dashed and solid lines, respectively. (from Ona-Nguema et al. Accepted)

## References

- G. Ona-Nguema, G. Morin, Y. Wang, N. Menguy, F. Juillot, L. Olivi, G. Aquilanti, M. Abdelmoula, C. Ruby, J. R. Bargar, F. Guyot, G. Calas, and G. E. Brown Jr. (2009) Arsenite sequestration at the surface of nano- $\text{Fe(OH)}_2$ , ferrous-carbonate hydroxide, and green-rust after bioreduction of arsenic-sorbed lepidocrocite by *Shewanella putrefaciens*. *Geochimica et cosmochimica Acta* (accepted)
- J. Miot, K. Benzerara, G. Morin, A. Kappler, S. Bernard, M. Obst, C. Férard, F. Skouri-Panet, J-M Guigner, N. Posth, M. Galvez, G.E. Brown Jr, F. Guyot (2009) Iron biomineralization by anaerobic neutrophilic iron-oxidizing bacteria. *Geochimica et cosmochimica Acta* (accepted)