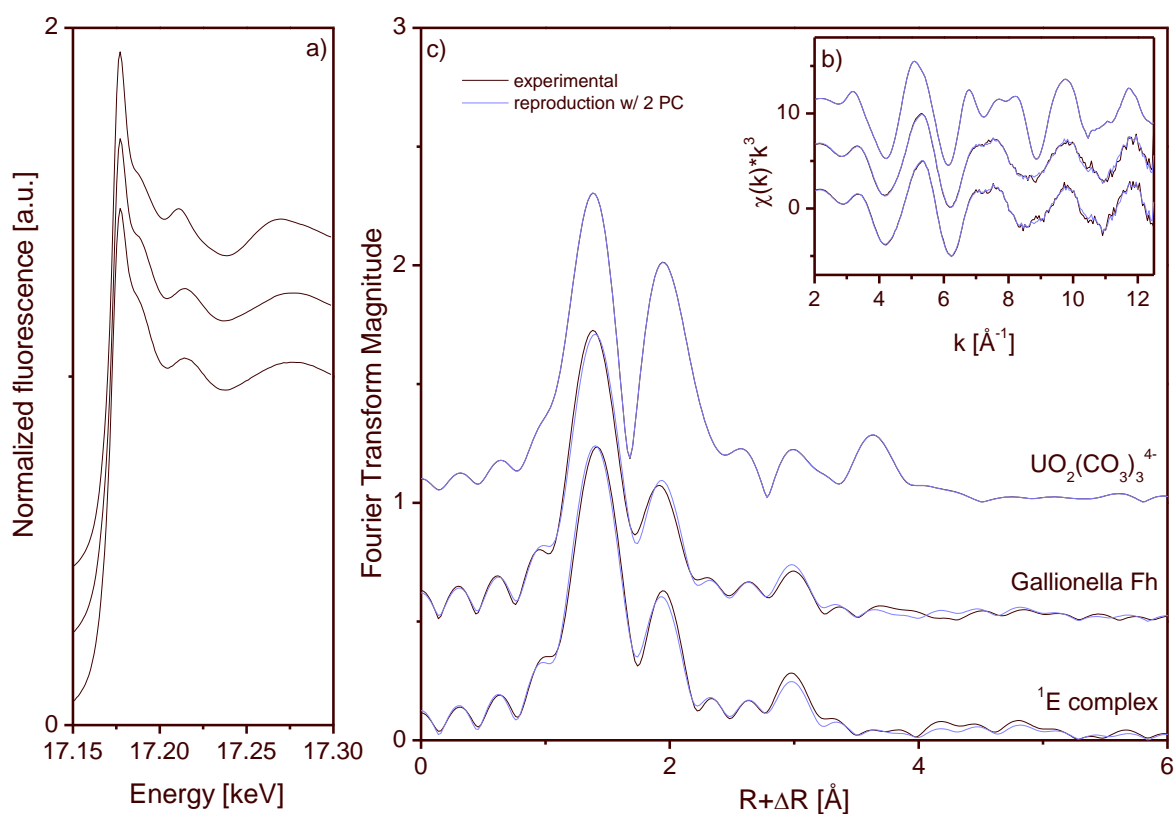
 ROBL-CRG	<b>Experiment title:</b> U and Np sorption on bacteria and biogenically formed ferrihydrite	<b>Experiment number:</b> 20-01-763
<b>Beamline:</b> BM 20	<b>Date of experiment:</b> from: 05.09.15                      to:08.09.15	<b>Date of report:</b> 11.1.2016
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## Report:

XANES (Fig. 1a) and EXAFS spectra (Fig. 1b and c) of the U sorped biogenic ferrihydrite sample are shown along with selected references. The XANES position and especially its fine structure are indicative of the hexavalent uranyl moiety. The “yl-shoulder” at about 17.175 keV is fully expressed, hence gives no indication for a significant amount of U<sup>IV</sup>. The k<sup>3</sup>-weighted chi-spectrum and its Fourier transform magnitude bears close resemblance to the bidentate edge-sharing innersphere sorption complex (<sup>1</sup>E), which is the main sorption species on ferrihydrite. <sup>1</sup> Due to the CO<sub>2</sub>-feeding of the *Gallionella* culture, the biogenic ferrihydrite precipitated in this system may have a relatively high carbonate loading of its surface, potentially causing the formation of a smaller portion of the type-B ternary uranyl –carbonato sorption complex determined for high pH

and high  $p_{\text{CO}_2}$ .<sup>1</sup> To elucidate this potential second sorption species, we performed iterative target test factor analysis (ITFA) using the spectra of the two endmember species<sup>2</sup>. The good reproduction of the *Gallionella* spectrum along with those of the two endmember spectra by 2 principal components (compare the black and blue lines in Fig. 1b and c) proves that the *Gallionella* samples contain no third sorption species. Using the iterative target test modul of the ITFA software package, we determined that the <sup>1</sup>E complex is in fact predominant with 95%, while the ternary uranyl-carbonato complex is present only to 5%.



**Figure 1.** U-L<sub>III</sub> XAS spectra of uranium sorption sample on *Gallionella*-produced ferrihydrite, together with the limiting species observed for ferrihydrite sorption samples, i.e. a bidentate edge-sharing uranyl sorption complex (<sup>1</sup>E) and the aqueous tris-carbonato complex (UO<sub>2</sub>(CO<sub>3</sub>)<sub>3</sub><sup>4-</sup>) representative for a type-B ternary uranyl carbonato sorption complex taken from Rossberg et al. (2009)<sup>1</sup>

- (1) Rossberg, A. et al. *Environ. Sci. Technol.* **2009**, 43 (5), 1400–1406.
- (2) Rossberg, A. et al. *Anal. Bioanal. Chem.* **2003**, 376 (5), 631-638.