

  ROBL-CRG	Experiment title: Interactions of the halophilic archaeon <i>Halobacterium noricense</i> DSM-15987 with uranium	Experiment number: 20-01-773
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Report:

The interactions of the halophilic archaeon *Halobacterium noricense* DSM-15987 with uranium were investigated in detail by X-ray absorption spectroscopy (XAS). The background of this study is associated to the final storage of radioactive waste in the potential host formation rock salt where this microorganism is indigenously occurring. Previous batch-experiments showed an interesting time and uranium concentration depending bioassociation behavior with hints for biomineralization of uranium. Hence, this project aims to get more insights into this unexpected bioassociation behavior down to a molecular level. The cells were incubated with different uranium concentrations (30 μM , 50 μM , 85 μM) for different exposure times (1 h, 5 h, 48 h, 7d,

14 d). After collecting the cell pellet, it was transferred as wet paste in a 3 mm thick polyethylene, double confined sample holder.

Principal component analysis (PCA) of the acquired XANES data calculates two eigenvectors, indicating that two different oxidation states (U(IV) and U(VI)) are occurring. Especially samples exposed to uranium for only a short time, independent of uranium concentration, exhibit significant high fractions of U(IV), which was unexpected. PCA on the U L_{III}-edge EXAFS spectra lead to three significant eigenvectors, indicating at least three independent uranium species in the samples. Based on these three principal components, target transformation analysis (TFA) for a series of possible reference compounds was tested to identify the most reasonable reference compounds. The analysis results in the following three compounds: Na₆[U^{IV}(CO₃)₅], meta-autunite and uranium (VI)-lactate. Based on these three references the EXAFS data were further analyzed to estimate the fractions of these compounds in all the samples by Iterative Transformation Factor Analysis (ITFA) and TFA.

Differences in species distribution become obvious in dependence on uranium concentration. For the lower uranium concentration (30 μM) meta-autunite is the dominating species over the whole time frame. The fraction of the minor species uranium(VI)-lactate is increasing with increasing exposure time, whereas the fraction of uranium(IV)-carbonate is decreasing. However, the major fraction of the highest uranium concentration (85 μM) is the uranium(VI)-lactate and meta-autunite occurring on a constant low level over the whole time frame.

Analysis results of XANES data (i.e., oxidation states information) and those of the EXAFS data (i.e., speciation information) are complementary to each other, suggesting the reliability of these data analyses as well as the acquired results. The results obtained with XAS also support our previous knowledge and are essential for interpreting the bioassociation process. Based on these experimental outcomes, a manuscript for publication is currently being prepared. The manuscript is planned to be submitted by October 2016.