HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF ROBL-CRG	**Experiment title:** EXAFS investigations on uranium complexes formed by fungi and reference samples	**Experiment number**: 20 - 01 - 702
Beamline: BM 20	**Date of experiment**: 23/06/10 – 24/06/10 02/12/10 – 05/12/10	**Date of report**: 31/01/11
Shifts: 12	**Local contact(s)**: André Roßberg	*Received at ROBL:*

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Report:

Experimental

The aim of this study was to determine the structural parameters of the formed uranyl complex species in fungal cells of the *Schizophyllum commune*. The fungal cells were cultivated in an organic liquid full medium. The biomass was harvested and washed with mineral medium. For sorption experiments, the fungal biomass was resuspended (300 mg dry weight / L) in uranium containing mineral medium in a concentration range from $2 \cdot 10^{-6}$ M to $4 \cdot 10^{-4}$ M at pH 4 and 6 at room temperature. After 24 hours the cells were separated from the medium by filtration and washed with 0.1 M $NaClO_4$. Then, the fresh fungal biomass was put into polyethylene sample holders surrounded with Capton tape and shock frozen in liquid nitrogen. The U L_{III}-edge spectra were measured in fluorescence mode at 15 K using a closed-cycle He-cryostat. The EXAFS spectra were analyzed using the program suite EXAFSPAK /1/. The theoretical scattering phases and amplitudes were calculated by using X-ray structural data of meta-autunite and uranyl-triacetate with the scattering code FEFF8.2 /2/.

Results

Figure 1 shows the raw U L_{III}-edge k^3-weighted EXAFS spectra and their corresponding Fourier transforms (FT) of uranium containing fungal cells incubated with $8 \cdot 10^{-5}$ M uranium containing mineral medium at pH 4 and 6 and measured at 15 K after shock freezing of the samples. In all spectra the contribution of two axial oxygen atoms U-O_{ax}

at a distance of 1.77-1.78 Å and one oxygen shell with very short distances between uranium and equatorial oxygen atoms of 2.28-2.30 Å were obtained.

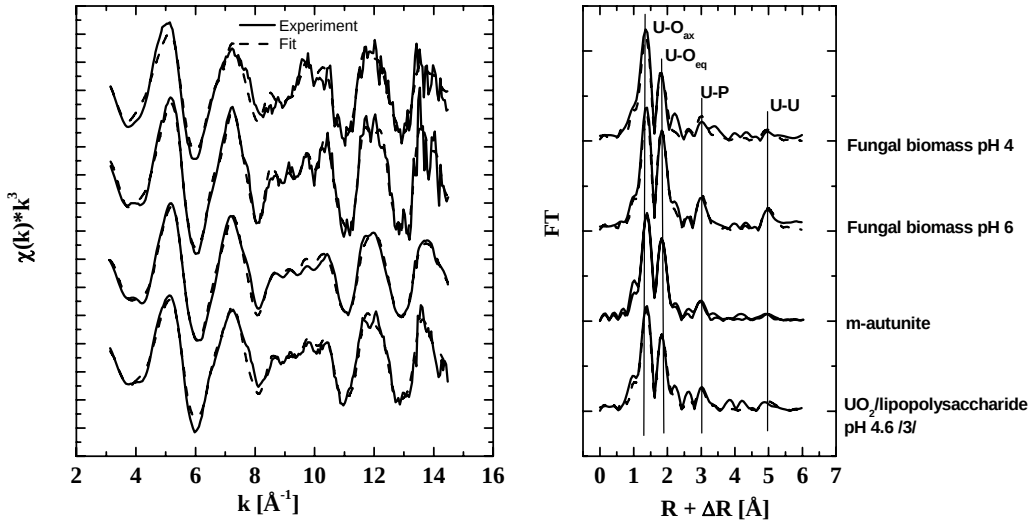

Fig. 1. Raw U L_{III}-edge k^3-weighted EXAFS spectra (left) and corresponding Fourier transforms (right) of uranium containing fungal cells and selected reference samples

Additionally, uranium-phosphorus interactions with a radial distance of 3.59 Å were found and support the TRLFS results, that uranium is mainly bound to phosphate groups on/in the fungal cells. U-U interactions are visible with a radial distance of 5.23-5.24 Å. The number of the coordinated oxygen atoms ($N_{U\text{-}Oeq}$) and phosphorus atoms ($N_{U\text{-}P}$) are different. They are higher in uranyl fungal species formed at pH 6 ($N_{U\text{-}Oeq}$=$N_{U\text{-}P}$=3.8) than those observed at pH 4 ($N_{U\text{-}Oeq}$=$N_{U\text{-}P}$ =2.7). All the spectra including the determined structural parameters could be described with the spectra of the m-autunit first of all, particulary the spectra of uranyl fungal species formed at pH 6. Also the EXAFS spectra of uranyl coordinated by lipopolysaccharide /3/, an organic uranyl phosphate, is very similar to the spectra of uranyl fungal species formed at pH 6 but differs from the spectrum in case of pH 4. So we assume, that at pH 4 and low uranium initial concentration a part of uranium is coordinated in a different way than observed for the other samples. This would support the TRLFS results again.

References

/1/ George, G. N., Pickering, I. J.: EXAFSPAK A Suite of Computer Programs for Analysis of X-Ray Absorption Spectra. Stanford Synchrotron Radiation Laboratory, Stanford, CA. USA. (1995)

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