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Report:

The structural parameters of the uranium complexes formed at the surfaces of three *A. ferrooxidans* eco-types were studied, using extended X-ray absorption fine structure (EXAFS) spectroscopy. The EXAFS spectra demonstrated that the phosphorus or sulphur-containing residues of A. ferrooxidans cells are involved in interaction with uranium.

Sequence analysis of the 16S rRNA genes of several reference strains and uranium-mining waste-pile isolates of *A. ferrooxidans* revealed specific signatures which distinguish three types within the species /1/. These types differ in their capability to accumulate and tolerate uranium /2/.

In this study applying EXAFS spectroscopy, we analysed the nature of the uranium complexes formed at the cell surfaces of the three *A. ferrooxidans* types.

The samples were measured at the Rossendorf Beamline (ROBL) at the European Synchrotron Facility (ESRF), Grenoble, France. The samples studied were: Dry biomass samples of *A. ferrooxidans* W1, 33020 and D2, (a), (c) and (e), and wet paste samples of A. ferrooxidans W1, 33020 and D2, (b), (d) and (f), respectively. In all samples uranium is coordinated by two axial oxygen atoms (Oax) at a distance of 1.77-1.78 Å. The average distance between uranium and the equatorial oxygen atoms (Oeq) is 2.35 Å. The coordination number of Oeq is 5-6.

Using U-C and U-P phase and amplitude functions, the third and fourth peaks in the FT of A. ferrooxidans indicate a distance of 2.91 and 3.58 $\pm$ 0.02Å, respectively. The latter is the same U-P bond distance as for the organic uranyl phosphate (U(VI)-ATP complex). But we do not exclude the possibility of implication of sulphur because these 2 elements (P and S) are close to each other in the periodic system of elements and EXAFS cannot distinguish between them. In addition, P (or S) is bonded in a monodentate mode to the uranyl ion. Bidentate bonding would result in an atomic distance of approximately 3.2 Å. No structural differences were observed between the uranium complexes formed by the 3 types of *A. ferrooxidans*. However, the EXAFS spectra indicate a formation of uranium complexes different from those formed by Bacilli.

References

/1/ Selenska-Pobell, S., et al., Antonie van Leeuwen-huek (in press).
/2/ Merroun, M. and Selenska-Pobell, S. Biometals (in press).

Tab. 1: Structural parameters of the *A. ferrooxidans*

uranium complexes

SAMPLE	SHELL	N	R [Å]	σ^2 [Å^2]
a	**U-O$_{ax}$**	2[a]	1.78	0.0014
	U-O$_{eq}$	4.7(5)	2.35	0.0071
	U-C	1.6(4)	2.92	0.0037[a]
	U-P	0.9(3)	3.58	0.0070
b	**U-O$_{ax}$**	2[a]	1.77	0.00126
	U-O$_{eq}$	5.4(5)	2.35	0.0089
	U-C	1.6(3)	2.92	0.002[a]
	U-P	1.3(3)	3.56	0.007[a]
c	**U-O$_{ax}$**	2[a]	1.77	0.0015
	U-O$_{eq}$	4.5(4)	2.35	0.0076
	U-C	1.0(3)	2.92	0.004[a]
	U-P	0.8(3)	3.59	0.008[a]
d	**U-O$_{ax}$**	2[a]	1.78	0.00127
	U-O$_{eq}$	5.1(5)	2.35	0.0082
	U-C	1.6(4)	2.90	0.0033[a]
	U-P	0.9(4)	3.58	0.008[a]
e	**U-O$_{ax}$**	2[a]	1.77	0.00155
	U-O$_{eq}$	5.7(5)	2.35	0.0093
	U-C	1.2(4)	2.90	0.004[a]
	U-P	1.4(3)	3.59	0.007[a]
f	**U-O$_{ax}$**	2[a]	1.77	0.00146
	U-O$_{eq}$	5.2(3)	2.35	0.0087
	U-C	1.4(2)	2.91	0.003[a]
	U-P	1.0(1)	3.59	0.004[a]

Fig.1: Uranium L_{III}-edge k^3–weighted EXAFS spectra (left) and corresponding FT (right) of the *A. ferrooxidans* uranium complexes