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| HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF<br>ROBL-CRG | **Experiment title:**<br>EXAFS studies of the structure and bonding in solution of dioxouranium(VI)-nucleotide complexes | **Experiment number**:<br>20 - 01 - 695 |
| **Beamline**:<br>BM 20 | **Date of experiment**:<br>from: to:<br>01/11 03/11/09<br>29/01 31/01/09 | **Date of report**:<br>01/04/11 |
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## Experimental

The aim of this investigation was to prove the existence of the hexameric U(VI)-adenosine-monophosphate (AMP) complex proposed by NMR studies [1]. Eight aqueous samples were prepared in the pH range pH 9.63 to pH 11.36. According NMR at pH 9.63 49% and at pH 11.36 only 10% of the hexameric species is present. The other acting complex is a trimeric species which has nearly 90% at pH 11.36. Fig. 1 shows the proposed structure of the hexamer and the structure of the trimer [1]. The structure of the trimer was determined by XRD and NMR [1]. The $UL_{III}$ EXAFS spectra of the pure complexes were isolated from the spectral mixtures by factor analysis [2].

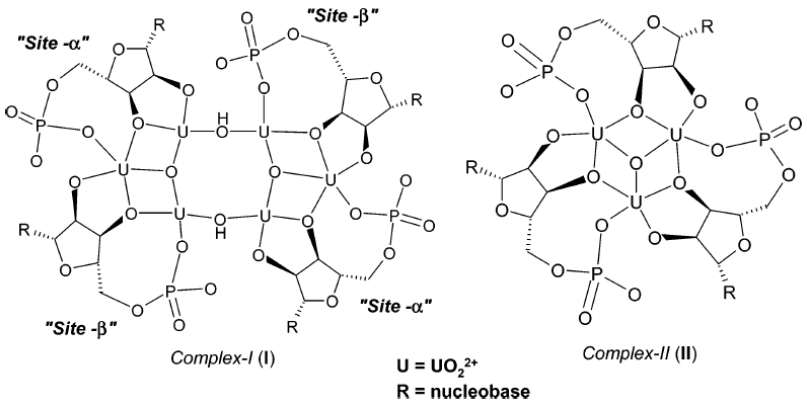


Fig. 1: Proposed hexameric (left) and trimeric U-AMP complex [1].

## Results

Figure 2 contains the best shell fit for the hexamer and the trimer. The fit includes the axial oxygen atoms with the corresponding multiple scattering path, the equatorial(eq) oxygen atoms and the U-U interaction. In case of the hexamer the $O_{eq}$ shell is splitting in two shells (2.30 Å, 2.49 Å) while the trimer shows only one major $O_{eq}$ shell at 2.35 Å. Also the U-U distances are different. In case of the hexamer the U-U distance is 3.83 Å while for the trimer the U-U distance is 0.04 Å longer.

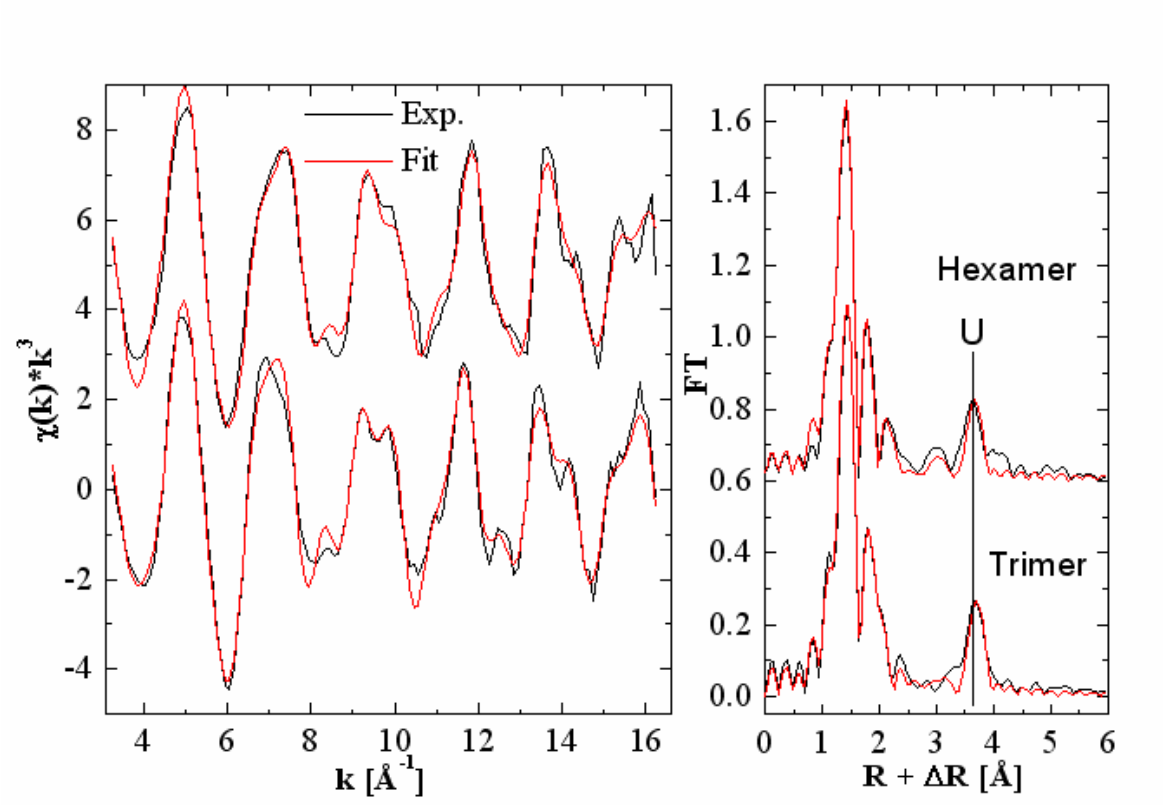


Fig. 2: EXAFS spectra of the hexamer and the trimer (left) with corresponding Fourier transform (FT) (right).

According the proposed hexameric structure (Fig. 1) at least three different U-U distances should be present, hence we expect a highly distorted or several U shell/s. At the moment we investigate this system also by UV-VIS and IR spectroscopy in order to understand the structural features of the hexamer represented by the EXAFS spectrum.

## REFERENCES


[1] Z. Szabo, I. Furo, and I. Csoregh, *Journal of the American Chemical Society* 127 (43), 15236 (2005).

[2] A. Rossberg, T. Reich, and G. Bernhard, *Analytical and Bioanalytical Chemistry* 376 (5), 631 (2003).