



ROBL-CRG

Experiment title: Local Structure of Th Complexes on Montmorillonite Clay Mineral Determined by Extended X-ray Absorption Fine Structure (EXAFS) Spectroscopy	Experiment number: ME-49
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Abstract

The research at the Waste Management Laboratory, PSI, concentrates on the understanding of safety relevant mechanisms and processes that govern the release of radionuclides from waste matrices, and their transport through engineered barrier systems and the surrounding geosphere. For this reason, detailed sorption studies of radionuclides in clay and cement systems are conducted. The studies are combined with extended X-ray absorption fine structure (EXAFS) spectroscopy measurements in order to understand the sorption mechanisms on an atomic level.

In this manuscript, a case study of Th(IV) uptake on montmorillonite is presented. EXAFS samples were prepared by incubating a montmorillonite suspension with Th

for 7 days at pH = 5 ($\text{Th}_{\text{initial}}$: 4.3×10^{-5} - 4×10^{-4} M). The resulting Th loadings on the clay varied between 14 and 166 $\mu\text{mol/g}$. L_{III} -Th EXAFS spectra of Th treated montmorillonite were measured at the Rossendorfer Beamline at the European Synchrotron Radiation Facility. Data analysis revealed the presence of two O shells at 2.27 Å and 2.45 Å in all samples. The spectra at low Th uptake suggest the presence of Si/Al and Th backscattering atoms at distances of 3.85 Å and 3.77 Å respectively. The presence of a Th-Si/Al backscattering pair suggests that Th is bound to Si tetrahedra in a double corner-sharing manner. At higher Th uptake, however, the spectrum shows a strong similarity with the spectrum of amorphous $\text{Th}(\text{OH})_4$ and suggests that Th is predominately present as a newly formed $\text{Th}(\text{OH})_4$ -like phase.

Dähn, R., Scheidegger, A. M., Manceau A., Baeyens, B., and Bradbury, M. H., 2001. "Local Structure of Th Complexes on Montmorillonite Clay Mineral Determined by Extended X-ray Absorption Fine Structure (EXAFS) Spectroscopy." *Speciation, Techniques and Facilities for Radioactive Materials at Synchrotron Light Sources*, NEA Publication, in press