The surface complexes of the oxoanions of Se(VI) and Tc(VII) at mineral-water interfaces

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^{79}Se and ^{99}Tc are fission products of the nuclear fuel cycle and, thus, are of concern during the safety assessment of a nuclear waste disposal site. For a comprehensive description of their mobility in the near and far field of a deep geological repository, the interactions of respective dissolved species with mineral surfaces are of special interest. In particular, the oxoanions $Se(VI)O_4^{2-}$ and $Tc(VII)O_4^{-}$ are considered as mobile species in aquifer due to their high solubility and negative charge.

In this study, the surface reactions of these anions were studied by *in situ* vibrational spectroscopy which is a dedicated technique for the real time monitoring of the surface processes at the water-mineral interface [1] [2]. For the selenate anion, the formation of two different types of outer-sphere complexes was observed depending on the mineral's surface. Although both types of sorption complexes behave like typical outer-sphere complexes in terms of macroscopic properties, the different spectral signatures clearly reflect two different molecule symmetries. From the spectra, a slightly distorted tetrahedral geometry, which is close to the aqueous species, and a bidendately coordinated species showing a C_{2v} symmetry were derived. These surface species are denoted as "extended" and "classical" outer sphere complexes, respectively [3] [4].

In homology, spectroscopic sorption experiments with Tc(VII) were performed. The aqueous species should share the same symmetry as for Se(VI), that is a tetrahedral TcO_4^{-} ion. From preliminary results of the vibrational spectroscopic sorption experiments, mainly outer-sphere complexes were found which are obviously less specific as it was found for Se(VI).

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