

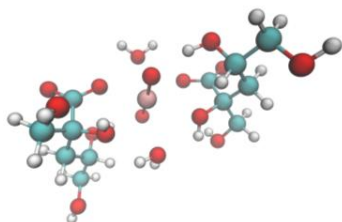
Structural elucidation of U(VI)-isosaccharinic acid complexes under acidic conditions: spectroscopic and theoretical investigations

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The alkaline degradation of cellulosic material present in low and intermediate level waste leads to the formation of water soluble organic compounds. α -Isosaccharinic acid (ISA) as main degradation product can act as complexing agent for radionuclides [1]. This may affect the mobility as well as the sorption behavior adversely. Studies regarding to the interaction of ISA with U(VI) are scarce. Hence, the aim of this study is to describe the U(VI)-ISA complexes formed under acidic conditions on a molecular level. Since U(VI) can coordinate to different binding sites of the polyhydroxy carboxylic acid, the number of possible complexes is large. To elucidate the number and structure of those U(VI)-ISA species, different spectroscopic methods were applied to obtain information from the metal and from the ligand.

UV-vis measurements lead to the conclusion that three complexes are formed and that both, the carboxylic as well as hydroxylic groups, are involved. Attenuated total reflection-Fourier-transformation-infrared spectroscopy (ATR-FTIR) and extended X-ray absorption fine structure-spectroscopy (EXAFS) offer structural information of the formed complexes. DFT-calculations provide data of optimized structures (e.g. figure below: $[\text{UO}_2(\text{ISA})_2(\text{H}_2\text{O})_2]$), which were used to underpin experimental results in order to identify the formed U(VI)-ISA species.



These results are the basis for further investigations under neutral and alkaline conditions. Moreover, this study helps to elucidate the U(VI) speciation in long term tissue degradation experiments in the presence of microorganisms.

[1] Glaus, M. A. *et al.*, *Analytica Chimica Acta* (1999), 398,111-122.