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Theoretical study of the Thorium structural in solution by EXAFS techniques

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Abstract

Thorium with symbol Th is radioactive metal which emits the alpha rays. This metal can be founded in different forms and can cause the negatives impacts on human health and environment. This is the reason which explains the importance to know the structure of this metal in different forms including the structure of hydrated Thorium. Structural information helps to understand and assess peculiarities this ion in different natural and technological processes taking place in aqueous solutions. The most and efficacy technique to know about distances between atoms and coordination numbers is EXAFS (extended X Ray Absorption Fine Structure) technique because it permits to know these above informations. My project research is was to determine the structure of hydrated, solvated Thorium ion in metal ions. For my research, I preferred to use the EXAFS method to study the structure of the hydrated Th ion and to determine the Th-O bond distance, and from that estimate the coordination number. Th-O distance in the case of hydrated Thorium appeared to be 2.44 Å which corresponds to 9-coordination, as also found in the solids.
The Th-O bond distance in solvated plutonium is ca. 2.41 Å, which corresponds to eightcoordination. These informations have shown me that for Thorium ligand size and coordination number are correlated. In case of Thorium hydrated studies, I saw that shown don't precipitate at the law concentration.
As conclusion, when pH is in range, centrifugation is possible and thorium is in monomeric form, but for pH above 4 Thorium is restrained and centrifuging shown that Thorium is in non-ionic form.

Key notes: EXAFS (extended X-ray Absorption Fine Structure), hydrated thorium, Solvated thorium, monomeric form, non-ionic form

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