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Complexation of actinides by ramified N-macrocycle DOTA

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The comprehension of the actinides affinity for interest ligands has been a pivotal issue. The difference in interaction between N-donors ligands and O-donor ligands is a hint on the selectivity difference between trivalent and tetravalent actinides. The study of molecules featuring both N and O-donor functions may be a way to reach a better understanding. Thus, the poly-amino-carboxylate ligands form an interesting family of f-element cations chelating agents. One specific ligand has been selected for this study: the DOTA macrocycle (1,4,7,10-tetraazacyclododecane-tetraacetic acid). EXAFS experiments proved DOTA forms complexes with both AnIII and AnIV. Complexation of AnIII is similar to what has been observed with LnIII, the system slowly evolves towards the final species, as shown on the UV-Vis spectra. In equivalent chemical conditions, Np(IV) and Pu(IV) behaves as the AnIII. Theoretical structures (DFT) were used to fit the experimental data, leading to the conclusion of a final complex is the (1:1) species: the cation gets inside the cavity formed by the N-cycle and the carboxylate arms and one water molecule is completing the coordination sphere. An-O and An-N distances are discussed regarding equivalent lanthanides species.

Primary author: Mr AUDRAS, Matthieu (CEA)

Co-authors: BERTHON, Laurence (CEA); MOISY, Philippe (cea); Dr DUMAS, Thomas (CEA)

Presenter: Dr DUMAS, Thomas (CEA)

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