

## Combined computational and spectroscopical analysis of tetravalent f-element complexes

Thomas Radoske<sup>1</sup>, Peter Kaden<sup>1</sup>, Roger Kloditz<sup>1</sup>, Juliane März<sup>1</sup> and Michael Patzschke<sup>1</sup>

<sup>1</sup> *Helmholtz-Zentrum Dresden-Rossendorf, Institute of Resource Ecology, Bautzner Landstraße 400, 01328 Dresden, Germany*  
m.patzschke@hzdr.de

The rich chemistry of actinide complexes makes them an interesting object for scientific investigations. This resulting enthusiasm can be curbed by the difficulties that arise in the treatment of actinides, both *in vitro* and *in silico*. It is of course the partially filled f-shell and the similarity of the f and d orbital energies, that make especially the first half of the actinide row so interesting, see e.g. [1]. Computationally as well as experimentally it is interesting and educating to compare lanthanide and actinide complexes.

We present here an analysis of the electron density of several salene and amidinate complexes of tetravalent actinides and lanthanides (See Figure 1) that have been synthesised in our laboratories.

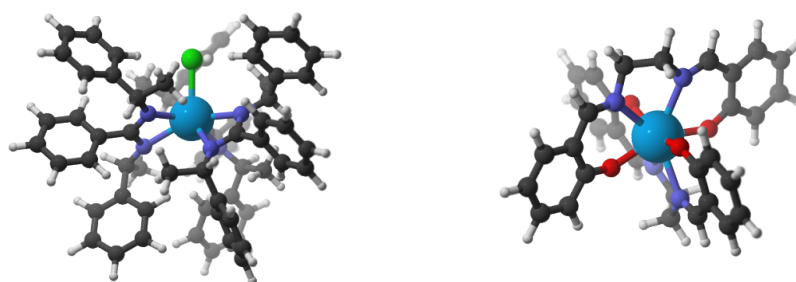


Figure 1: Structure of the amidinate complex  $[ThCl((S)\text{-PEBA})_3]$  (left) and of the Schiff-base complex  $[Th(\text{Salen})_2]$  (right).

The complex structures were optimised at DFT level and subjected to QTAIM analysis, we will also present density difference plots and plots of weak interactions (known as non-covalent interaction plots, NCI). We then proceeded to multi-reference calculations, some preliminary results will be shown.

We then discuss some features of the NMR spectra of these complexes. Finally we will present some features of the UV/VIS and TRFS spectra of selected actinide complexes.

Our results should help to improve the understanding of actinide bonding. This will then allow us to predict the behaviour of actinides in the environment as well as in technical processes. This knowledge is of course important in amongst others, the context of nuclear waste disposal.

### References

1. M. L. Neidig, D. L. Clark and R. L. Martin, *Coord. Chem. Rev.* **257** (2013), 394.