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# Molecular structures of actinide ions in solution from theoretical chemistry combined with experimental data

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## T7. Ressources and sustainability

### Molecular structures of actinide ions in solution from theoretical chemistry combined with experimental data

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Understanding the structure and bonding in actinide compounds provides fundamental information that is essential for developing effective separation for actinide recovery. A thorough characterization of their molecular structures in solution is of particular interest for the development of hydrometallurgical process for waste remediation in advanced nuclear fuel cycles or for the uranium extraction from ores. The chemistry of actinide ions is particularly rich because a large number of oxidation states are accessible to them and their coordination sphere is very flexible. The bonds formed between actinides and ligands are mainly ionic with a partially covalent character. They can therefore be easily broken and reformed. In solution, small changes in concentration, pH, or solvent can alter the coordination sphere of an actinide ion. In addition, mono- and polynuclear species can be present and complex equilibria often exist, complicating experimental characterization. In order to obtain accurate structural and bonding properties, it is essential to combine experimental data with theoretical chemistry. In our studies, actinides ions with oxidation states ranging from III to VI have been characterized in aqueous and organic solution from spectroscopies combined with theoretical chemistry calculations. We will discuss the specific coordination features of actinides for mono- and polynuclear species with oxygen-donor ligands. [1-3]

#### References

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- [3] G. Chupin, C. Tamain, T. Dumas, P. L. Solari, P. Moisy, D. Guillaumont, *Inorg. Chem.* **2022**, 61, 4806.