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## Coordination of actinyl ions to N-heterocyclic ligands: A joint theoretical and experimental study

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Nuclear energy represents a critical tool available to meet the demand of increasing energy supply while limiting green house gas emissions. To reduce the need for long-term nuclear waste storage, it is important to develop efficient strategies for selective separations. A better molecular-level understanding of the coordination modes and affinities of ligands with multiple binding sites to actinyl ions can pave the way to designing new ligands with improved extraction efficiency and selectivity. We will discuss the coordination chemistry of actinyl ions with ligands composed of multiple competitive binding sites, including sulfur, nitrogen and oxygen chelating groups. We will present the interactions between actinide centers and selected nitrogenous heterocyclic ligands using first-principle methods that include relativistic effects and electron correlation. The theoretical results will be further validated by gas phase and solution spectroscopic characterizations.

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