



# Groundbreaking actinide research: The discovery of unique metal–ligand bonding

May 14, 2020

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Researchers in the Los Alamos Theoretical Division discovered two new types of metal–ligand bonding in actinide metal complexes. How orbitals align within a complex plays into the chemical bonding, and *f*-elements offer particularly exotic opportunities.

The alignments seen in the new bonds include “head-to-side”  $\pi$  in metallacyclopropenes and “side-to-side”  $\pi$  back-bonding in metallacyclocumulenes. These new bonds are the first to defy the typical bond length contraction trend that usually happens in actinide complexes, underscoring the importance of the discovery.

### Research includes uranium and plutonium

Los Alamos is the Plutonium Center of Excellence, and understanding actinides is a primary Lab mission. The chemistry and corresponding behavior of actinides are often quite complex and exotic.

This study, published in [Nature Communications](#), looked at known complexes of thorium and uranium propenes and cumulenes as well as accurately predicted complexes of protactinium, neptunium, and plutonium. Structures of the complexes were optimized via Density Functional Theory with the PBE functional. The chemical bonding was analyzed with the AdNDP method. Although the techniques were simulation based, the models were shown to well represent reality.

The researchers were able to explain in detail the increase in actinide–ligand bond length across the actinide series. In particular, the  $\pi$  and  $\pi$  back-donations are crucial in explaining this non-classical trend.

Understanding this type of bonding and the role it plays in actinide complexes aides in simulation, prediction, and experiment. Actinides are vital to our national security, and better understanding their chemistry firmly supports our mission.

