

Chemical bonding, core spectroscopy, and magnetic properties of actinide complexes

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Actinide complexes exhibit fascinating magnetic properties and interesting chemical bonding. An on-going research project in our group is devoted to first-principles calculations of magnetic resonance parameters (NMR, EPR), magnetic susceptibilities, magnetic circular dichroism, core excitation spectra, and other types of spectra, of actinide complexes, and how the observed properties relate to the chemical bonding involving the actinide. Of particular interest is the involvement of the 5f shell in metal-ligand bonding. We will present results from recent computational studies of the aforementioned magnetic and spectroscopic properties of f-element complexes utilizing relativistic quantum chemical methods.

References

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