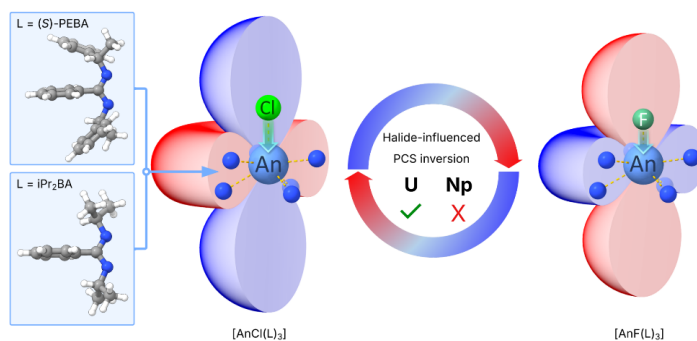


Paramagnetic NMR as a probe into the electronic structure

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Transition-metal and *f*-element complexes often have an intricate electronic structure. This is especially important for actinide compounds as spin-orbit coupling makes the electronic structure even more complex. Most of these complexes have unpaired electrons, and hence interesting NMR spectra. The coupling of the electron spin to the nuclear spin and the external magnetic field can lead to extreme shifts. These shifts can be split into two contributions, the contact shift (also fermi-contact shift or FCS) and the pseudo contact shift (PCS). The latter part propagates through space and can be sizeable for nuclei far from the paramagnetic centre.



We will discuss how the PCS can be calculated and visualized. Two different approaches, namely the point dipole approximation and the Kurov model will be presented and compared. For two sets of amidinate complexes we will demonstrate how small changes in the ligand field can have a major impact on the NMR shifts¹. Furthermore we will show how the pNMR data and the calculated magnetic properties give insight into the electronic structure of the investigated compounds.

Reference

[1] A.Näder, M.Patzschke et al., PCCP *accepted*