ABSTRACT SYMPOSIUM NAME: Lanthanide & Actinide Chemistry (Poster)

ABSTRACT SYMPOSIUM PROGRAM AREA NAME: INOR

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PRESENTATION TYPE: Poster Preferred : Consider for Sci-Mix

TITLE: EPR of lanthanide complexes: exploring the consequences of ligand induced anisotropy

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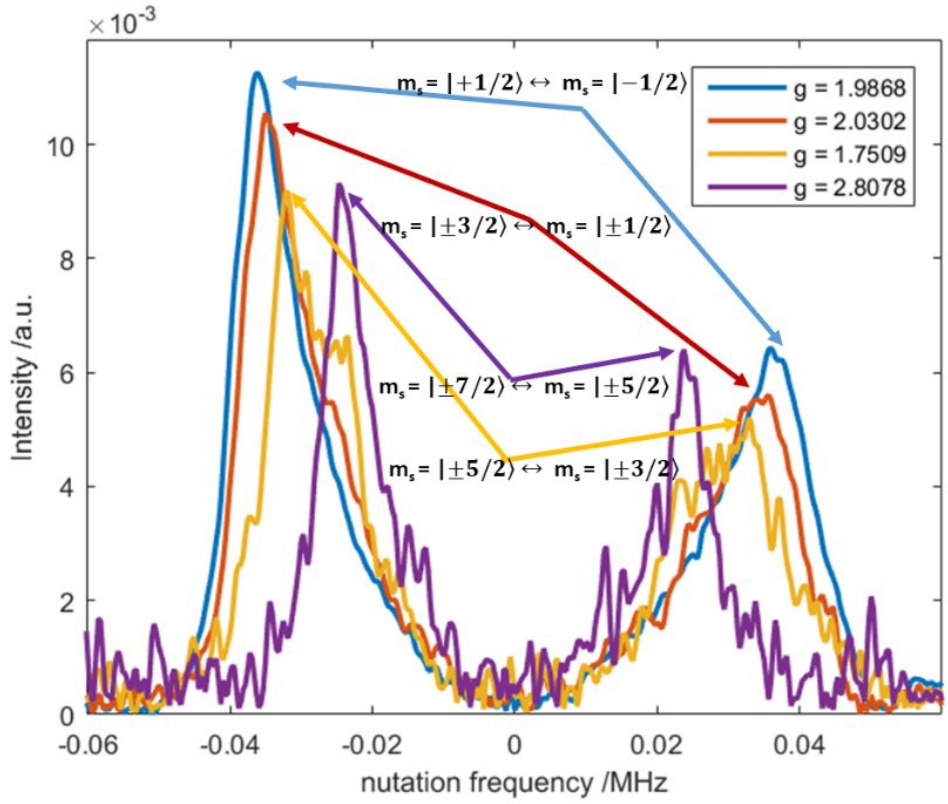
ABSTRACT BODY:

Abstract: Ligand field anisotropy plays a key role in defining the spectroscopic properties of lanthanide complexes. We have recently shown how changes to the local ligand field can have profound consequences for the NMR, luminescence and EPR properties of lanthanide ions with inherent anisotropy, such as europium and ytterbium. In this study, we extend our existing work to the behaviour of gadolinium complexes, where the ground state of the free ion has an isotropic electron distribution. In these systems, changes to the ligand field and the axial donor are shown to have dramatic effects on the form of the EPR spectrum. These can be rationalised through considering the donor set, and the variation in structural isomerism between square antiprismatic and twisted square antiprismatic geometries. A number of EPR techniques have been used to characterise the systems: CW EPR and pulsed PEANUT (phase-inverted echo-amplitude detected nutation) measurements can be correlated with the splitting of the m_s states within the ^8S ground state of Gd(III). These variations, with relatively small changes to the local field, can provide useful information and aid in the development of new contrast media. The figure shows the 4 nutation frequency transitions observed in PEANUT measurements on Gd.DOTAMPh in the presence of benzylamine as an axial ligand.


×10-3
Intensity /a.u.
nutation frequency /MHz
g = 1.9868
g = 2.0302
g = 1.7509
g = 2.8078
ms = |+1/2⟩ ↔ ms = |−1/2⟩
ms = |±3/2⟩ ↔ ms = |±1/2⟩
ms = |±7/2⟩ ↔ ms = |±5/2⟩
ms = |±5/2⟩ ↔ ms = |±3/2⟩