Experimental report

16/08/2021

Proposal: 4-06-17 **Council:** 4/2020

Title: Correlation between phononic structure and magnetic properties in a new family of Ln(DOTA) complexes

Research area: Chemistry

This proposal is a new proposal

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Samples: K4W2OCl10
DyC28H75Cl2N6O4
ErC28H75Cl2N6O4
HoC28H75Cl2N6O4
YbC28H75Cl2N6O4

Instrument	Requested days	Allocated days	From	To
IN5	3	3	09/09/2020	12/09/2020

Abstract:

In this experiment we aim to study the magnetic and phononic excitations of a series of isostructural mononuclear lanthanide complexes of formula NMe4[LnDOTA] (Ln=Dy, Er, Ho and Yb; DOTA=1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetate, Me=methyl). The compounds are strongly related to the previously reported Na[LnDOTA(H2O)] compounds, but they are devoid of a coordinated water. Since the water molecule has been shown to be a key detrimental component for the relaxation of the compound, we propose the study of these complexes using inelastic neutron scattering to experimentally obtain the crystal fields and phonon spectra to unravel their interplay in magnetic relaxation.

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Our aim of this experiment was to investigate the influence of the famous DOTA-ligand (DOTA=1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetate) on the electronic and magnetic properties of lanthanides, for which this ligand has been used in a multitude of applications. To fully characterize the magnetic INS spectrum of lanthanide single-molecule magnets, a series of isostructural complexes of different Lanthanides must be measured with a wide range of wavelengths and temperatures. The experiment was conducted accordingly, and the most prominent results are shown here. The results exceeded all our expectations, as we were able to extract crystal field excitations for all the measured lanthanides. That provides a phenomenal basis of analysis to unravel the magnetic properties of these compounds. Furthermore, we observed very complex magnetic excitations (see 6Å data for Ho and Tb), that could be indications of systematic hyper-fine interactions, which is a key research interest with applications in molecular spintronics.

The high symmetry of these compounds allows us to fully correlate the magnetic INS excitations to a complete crystal field model, and we are presently engaged in modelling the information gained from INS with previous analyses.