Experimental report

08/02/2021

Proposal: 4-06-14 **Council:** 10/2019

Title: Investigation of Energy States andMagnetic Coupling on a Peroxide bridged Lanthanide dimer

Research area: Chemistry

This proposal is a new proposal

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Samples: DyC19H19N10O9
TbC19H19N10O9
Dy2C38H38N18O14
Tb2C38H38N18O14

Instrument	Requested days	Allocated days	From	To
IN5	4	2	11/02/2020	13/02/2020

Abstract:

In this experiment we intend to study the magnetic excitation spectra of a series of Lanthanide based dimeric Single Molecule Magnets (SMMs). These complexes will be the first ever peroxide-bridged Lanthanide dimers, for which the electronic and magnetic properties is investigated. In addition, studying a series of monomeric, chemically equivalent complexes will allow for the deconvolution of crystal field effects and the super-exchange interaction.

Experiment 4-06-14 Report

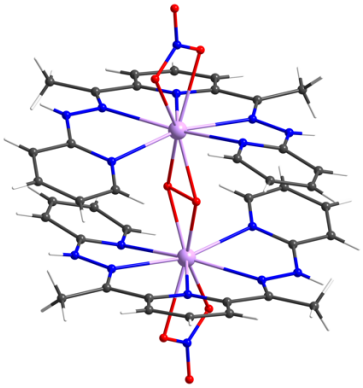

Figure 1: Molecular structure of the investigated compounds. Gray=C, white=H, blue=N, red=O, purple=Dy/Tb/Er

The experiment was performed on an isostructural series of three lanthanide complexes with the molecular structure depicted in figure 1. Each complex consists of two lanthanide ions, which are magnetically coupled through a hitherto unstudied chemical linker, the peroxide ion. Preliminary super conducting quantum interference device measurements have revealed slow relaxation for the dysprosium complex and a comparison with the magnetic data of the fluoride coupled isostructural complexes and the monomeric complexes lead to assume that the magnetic coupling is the key factor for the enhanced single molecular magnetic properties. To investigate the coupling of the two lanthanides, we studied primarily low-energy transfer magnetic excitations, as these are the most perturbed by the magnetic coupling. We were very happy to observe magnetic excitations for the terbium and the erbium sample (figure 2 and figure 3). Now we are engaged in analysing and modelling the data. Our tentative analysis of the Tb analogue is shown together with INS simulation and energy level diagram (figure 4). A preliminary assignment of the signals is given in table 1.

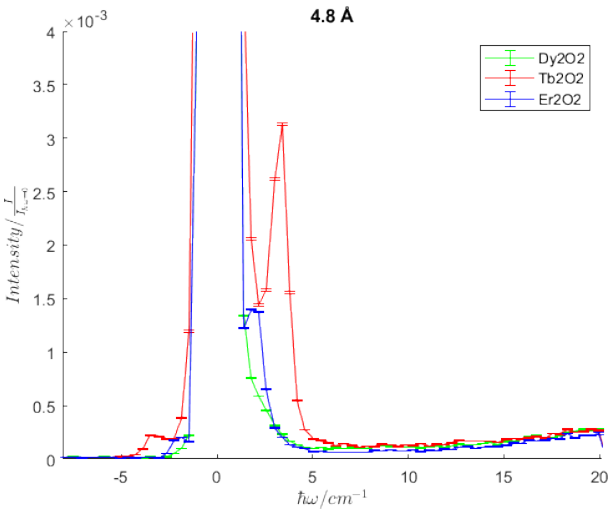

Figure 2: Comparison of the signals for the three investigated compounds in the intensity versus energy plot

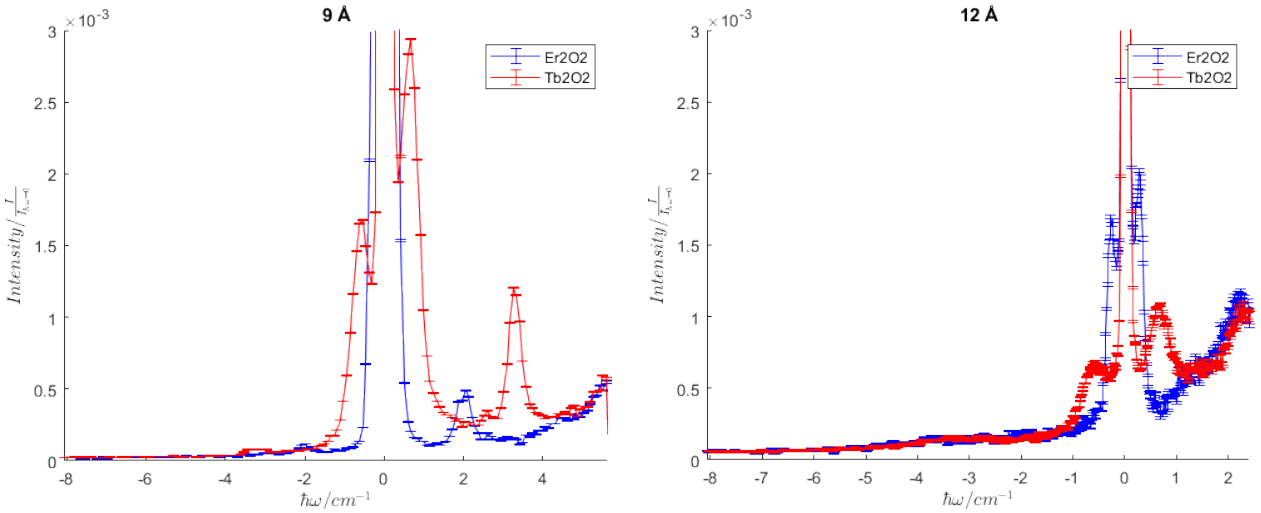

Figure 3: Intensity versus energy plot for the Er and Tb dimers at different Q

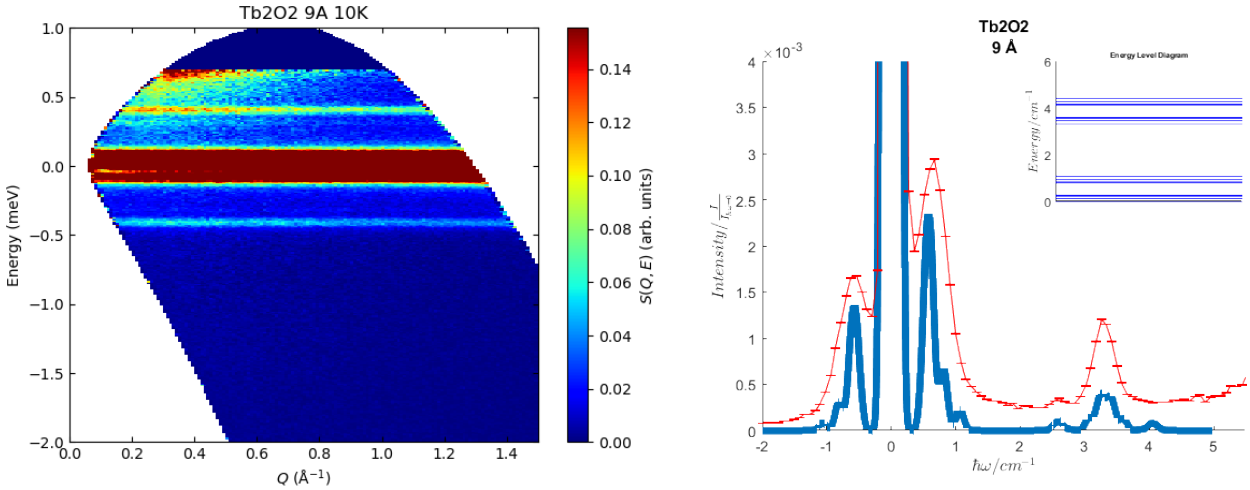

Figure 4: Results of the measurement for the terbium sample (left) and preliminary fitting of the data with extracted energy diagram (right)

Table 1: Preliminary assignment of the signals in the measurements

Sample	Transition Energy
Tb2O2	0.65 cm^{-1} (see Q-dep. & Stokes) 3.31 cm^{-1} (Cold)
Dy2O2	Nothing conclusive
Er2O2	0.28 cm^{-1} (See Q-dep.) 1.4 cm^{-1} (broad) 2.0 cm^{-1} (broad)