

Experimental report

13/09/2024

Proposal: 5-41-1217

Council: 4/2023

Title: Field induced magnetic state of the ζ Faraday-rotator ζ KTb3F10

Research area: Physics

This proposal is a new proposal

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Samples: KTb3F10

Instrument	Requested days	Allocated days	From	To
D23	7	7	28/08/2023	04/09/2023

Abstract:

In recent years, the study of the coupling between the 4f electronic density and lattice degrees of freedom has aroused a lot of attention. Such interactions are suspected to play a key role in a number of issues, ranging from highly frustrated magnetism to the design of smart materials in optics. Preliminary single-crystal neutron diffraction experiments performed on the Faraday rotator KTb3F10 have revealed a decrease of the intensity on several Bragg reflections in a magnetic field up to 2 T, anomaly which can be interpreted as originating from a magneto-elastic coupling. To confirm this hypothesis, we need a more comprehensive study of the evolution of the crystal structure of KTb3F10 in an applied magnetic field. This will also lead to a better description of the Tb³⁺ environment, which will be used for crystal electric field modellings. For this study, we would require the D23 diffractometer, working in the 2-300 K range, up to 6 T.

**Experimental report on
Magneto-elastic coupling in the “Faraday-rotator” $\text{KTb}_3\text{F}_{10}$
@D23**

Scientific context: As is well known for non-Kramers ions, the crystal-electric field (CEF) splits the $(2J+1)$ -fold degenerate J-multiplet into a series of doublets but also singlets. The class of magnetic materials whose CEF ground state is *such a singlet*, like in $\text{KTb}_3\text{F}_{10}$ is quite remarkable. Depending on the precise value of the gap to the excited states, the singlet state could be either well protected, or much more subtle, (so called “induced magnetism”) [1 -8].

In $\text{KTb}_3\text{F}_{10}$, the Tb ions occupy the vertices of a network of corner-sharing octahedra (cubic $Fm-3m$ space group, see Ref [7]). Its CEF scheme encompasses a singlet ground state $|O\rangle = |J=6, J_z=0\rangle$ and an excited doublet $|\pm\rangle = |J=6, J_z=\pm 1\rangle$ at about 2.7 meV. Importantly, the z quantification axis changes from site to site, being one of the cubic axes [2]. Our modelling of the CEF levels leads to the fact that any field induced magnetic moment appears within the plane perpendicular to this local z quantification axis. Depending on the site, this plane is perpendicular to the local a , b or c axis of the cell. This experiment was dedicated to carry out diffraction measurements on $\text{KTb}_3\text{F}_{10}$ to study the induced magnetism. The magnetic field was applied along the [110] direction.

The D23 diffractometer was operated at the wavelength of $\lambda = 1.28 \text{ \AA}$. It was equipped with a 6T cryomagnet. A high-quality single crystal ($5 \times 5 \times 5 \text{ mm}^3$, commercial, Northrop-Grumman) was oriented with [110] vertical, along the magnetic field direction.

We spent 6 days to record data collections at various magnetic fields and temperature, ranging from 0 to 4.5 T at 1.5 K. We also ramped the field on a series of reflections to obtain a continuous evolution of the induced magnetic structure.

Representative results are shown in Figure 1. The direction of the field splits make non-equivalent the terbium sites. Indeed, the terbium sites with their 4-fold axis orthogonal to the field (4-fold axis parallel to [001]) have to be distinguished from other sites. On the figure 1, M_0 represents the magnetic moment component parallel to the 4 fold axis for sites having their 4-fold axis with a non-zero projection on the magnetic field direction. M_1 is the magnetic moments component parallel to the magnetic field and orthogonal to the 4-fold axis of the Tb with their 4-fold axis either parallel to [100] or [010]. Finally, M_2 represents the magnetic moments component parallel to the field of the terbium sites with their 4-fold axis along [001].

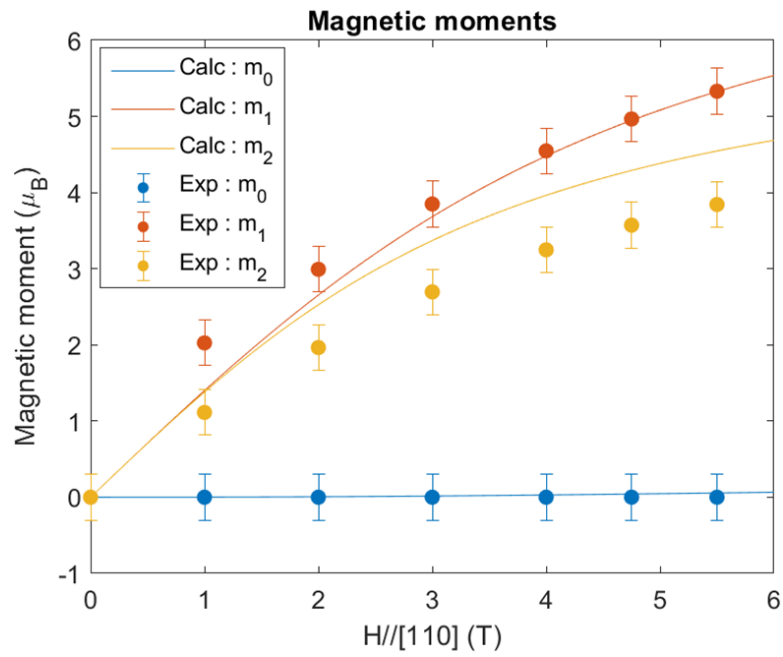


Figure 1 : Evolution of magnetic moments carried by magnetic ions.

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