

# Experimental report

02/02/2022

**Proposal:** 5-32-910

**Council:** 4/2020

**Title:** Probing Short-Range Magnetic Order in Magnetocaloric HoF<sub>3</sub>

**Research area:** Materials

**This proposal is a resubmission of 5-32-896**

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**Experimental team:** Andrew WILDES  
Paul SAINES

**Local contacts:** Andrew WILDES

**Samples:** HoF<sub>3</sub>

Instrument	Requested days	Allocated days	From	To
D7	3	3	08/03/2021	11/03/2021

## Abstract:

The development of magnetocaloric materials optimised for cooling between 4 and 20 K is a promising route to replace increasing scarce and expensive liquid He. The requires the development of new optimised magnetocalorics that work efficiently for small applied field changes that can be achieved using permanent magnets; such properties appear to be strongly associated with ferromagnetic chains coupled with magnetic frustration. HoF<sub>3</sub> appears to be a particularly promising material in this regard with a structure incorporating face-sharing chains of Ho cations giving magnetocaloric performance that only modestly declines with increasing temperature above 4 K. This experiment will measure the magnetic diffuse scattering of this material from a polycrystalline sample using XYZ polarisation. This data will be analysed using reverse Monte Carlo refinements to determine the nature of the magnetic anisotropy and interactions within this material and how these change with temperature. Understanding gained from this will enable the development of precise design rules for developing improved magnetocaloric materials capable of reducing dependence on liquid He in the longer term.

## Probing Short-Range Magnetic Order in Magnetocaloric HoF<sub>3</sub>

### Overview:

This is a report describing the result of experiment 5-32-910 carried out in March 2021 on D7 lasting for 3 days, by Paul Saines, Richard Dixey and Andrew Wildes. Diffraction measurements were conducted using 3.1 Å polarised neutrons on a 7.977g polycrystalline sample of HoF<sub>3</sub>, loaded in a vanadium can. This experiment was performed in order to probe the magnetic correlations as a function of temperature, and was expected to have 1D Ising ferromagnetic correlations contributing to the high efficiency magnetocaloric effect observed below 20 K.

### Report:

Initial diffraction measurements were performed on cooling down to 1.5 K and showed no long or short range order. However, a change in the paramagnetic form factor was detected. At high temperature the scattering function approached 0 at  $Q = 0$ , but lowering the temperature resulted in a scattering function that increased in intensity at low  $Q$ , which was initially interpreted as indicating a change in the magnetic correlation from antiferromagnetic to ferromagnetic (Figure 1.).

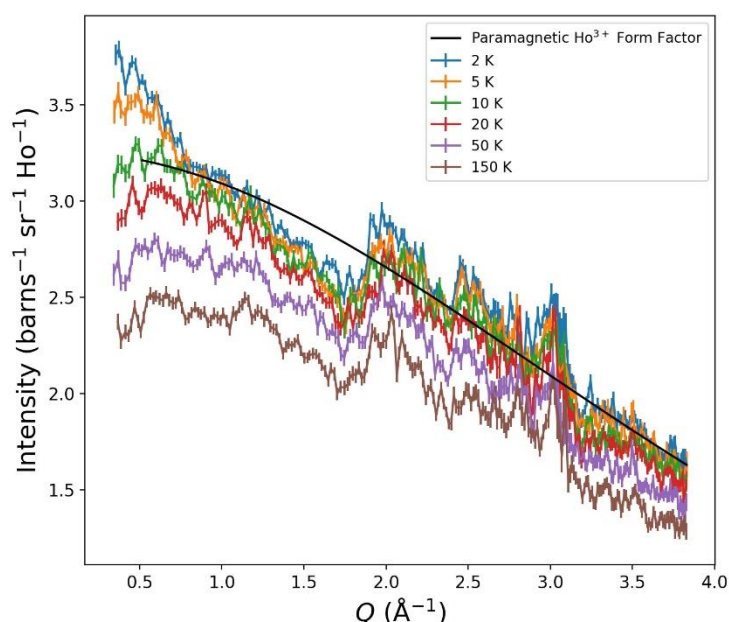


Figure 1. Magnetic scattering function of HoF<sub>3</sub> as a function of temperature.

Anomalous scattering between 2-3 Å<sup>-1</sup> was observed but was not due to magnetic order as no change was observed between the high and low temperature measurements nor was there any signal in our previous magnetometry measurements.

The chopper was subsequently put in the incident beam and the scattering from the sample was measure in time-of-flight mode at an incident energy of  $E_i = 8.5$  meV, in order to examine the scattering between 2-3 Å<sup>-1</sup> and determine whether this was the result of low lying magnetic excitations.

The inelastic measurements revealed a magnetic excitation at 4.8 meV, separated by a spin gap from a more low lying feature at about 0.5 meV. This signal indicates presence of spins with significant anisotropy and behaving as an Ising type spin. Only limited scattering is observed at the elastic line

suggesting magnetic excitations rather than diffraction dominates the patterns observed in diffraction mode limiting the ability to interpret meaningful data from these patterns.

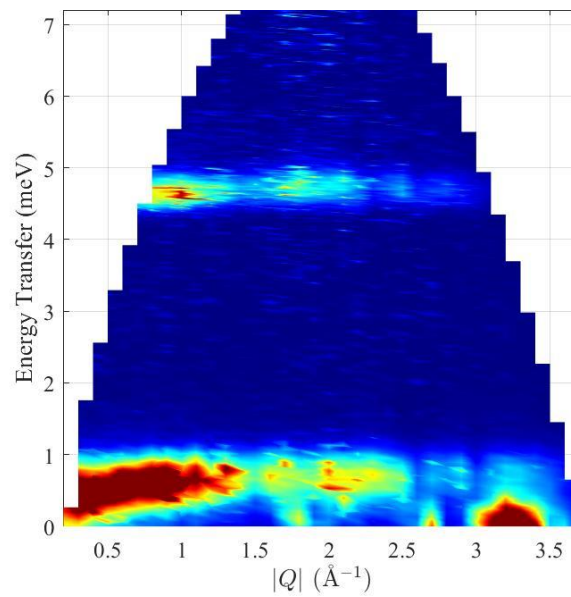


Figure 2. The inelastic magnetic excitations of HoF<sub>3</sub> at 1.5 K.

Likely outcome from experiment:

The results from this experiment are currently being written into a journal publication which is expected to be published in the coming months, which will focus on the magnetocaloric properties of HoF<sub>3</sub> along with a report on the measured spectra.