Experimental report

25/01/2024

Proposal: 5-41-1222 **Council:** 4/2023

Title: Determination of magnetic superstructures in HoTe3

Research area: Materials

This proposal is a continuation of 5-41-1146

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Samples: HoTe3

Instrument	Requested days	Allocated days	From	To
D10	6	6	27/11/2023	04/12/2023
ORIENTEXPRESS	1	1	09/11/2023	10/11/2023

Abstract:

Rare-earth layer chalcogenides of type RTe3 (R: Ce, Ne, Gd, Tb, Dy, Ho, Er, Tm) are prominent examples which undergo charge (CDW) and magnetic order and superconductivity under pressure. In our preliminary experiments on IN22 (CRG-2702 and 7-02-188) and on THALES (4-01-1670), we found that charge and magnetic orders in TbTe3 are highly entwined. However, while TbTe3 is remarkable in having three very closely spaced transitions between 5.3 and 5.8 K, all of the compounds in the series exhibit two successive magnetic transitions. The goal of the proposed experiment is to determine for the first time the magnetic superstructures in the parent compound HoTe3 ((Tmag1= 3.25K and Tmag2= 2.87K): modulations vectors incommensurate or commensurate) below TN, temperature dependence and collection of magnetic intensities aiming at a magnetic structure refinement. These measurements are of a great importance with respect to the joint proposal on THALES entitled "Determination of the magnetic excitations in the charge density wave compound HoTe3 by inelastic neutron scattering". To that end we apply for 6 days on the 4-circle diffractometer D10 featuring low background and high resolution.

Experiment 5-41-1222 report

Determination of magnetic superstructures in $HoTe_3$

$HoTe_3$ is a member of the family of rare-earth tri-tellurides, $RETe_3$, that display one or two charge density waves CDW) ordering at fairly high temperatures. In addition, the rare earth ion orders magnetically at low temperatures, below 10K. $HoTe_3$ displays 2 successive antiferromagnetic phase transitions below 4K and the determination of the magnetic moment arrangement was the goal of this experiment.

To that end, we used D10 in a 4-circle configuration with a Displex and PS detector. The sample was grown in our laboratory and checked for quality on D19. Sample quality and the space group of the nominal HoTe3, *Cmcm*, was checked at 20K, as well as the occurrence of the CDW peaks at modulation wavevector (0,0, 0.28).

Figure 1 shows an intensity map of the line (½ , K, 0) as a function of temperature, where the two different transitions clearly appear.

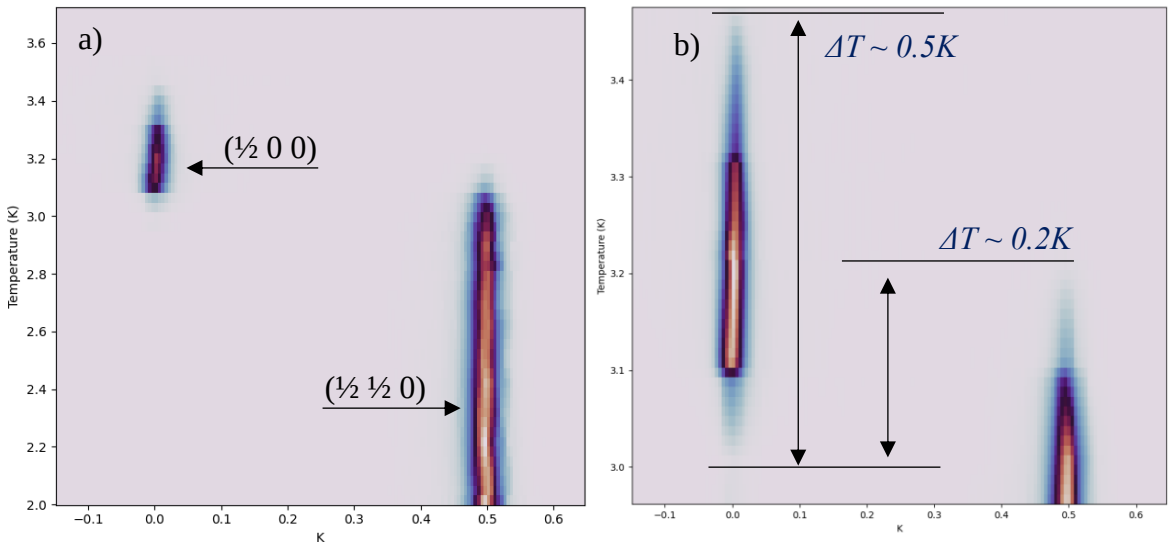

Fig.1: Temperature evolution of magnetic peaks corresponding to wave vectors q_1=(½ 0 0) and q_3=(½ ½ 0).

In the table below, we show a number of parameters characterizing the peak collection at different temperatures.

Name	*Nuclear*	q_1 1.8K	q_3 3.2K
Number of reflections read	430	228	492
Number of valid independent reflections	91	122	230
Number of obs. with equival. reflections	181	183	449
Number of rejected (absences) reflections	215	0	0
R-internal for equivalent reflections (%)	4.14	4.91	9.54
R-weighted for equivalent reflections (%)	4.22	6.32	9.66
Average Intensity of reflections	13636.70	2559.15	781.52
Average sigma for equivalent reflections	192.50	65.81	35.16
1	2	3	4

A first collection of q_1= (½, ½, 0) and q_2=(0, 0, ½) antiferromagnetic peaks was carried out at 1.8K. Reflections of the second type turned out to be very small in intensity, as compared to, for instance, $TbTe_3$. We were not able to refine the structure corresponding to q_2. Next we proceed to carry out a data collection at q_3=(½ , 0, 0) at 3.2K. Results of the refinement and agreement are displayed in the figures below

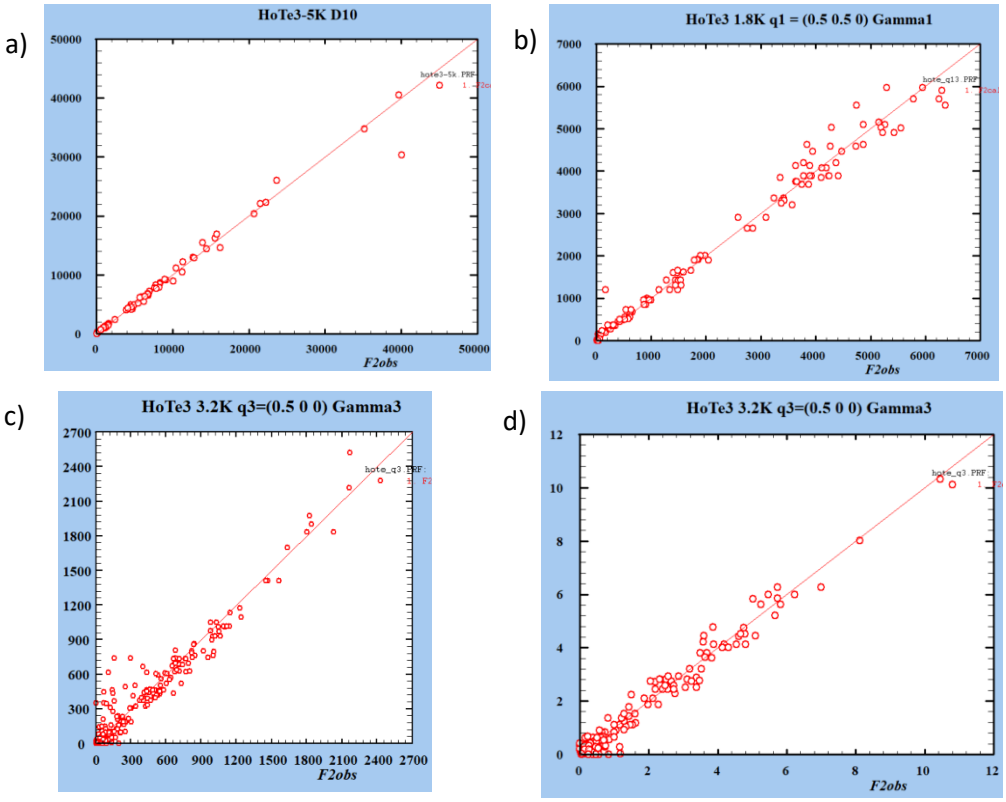

Fig.1: Comparison of model and measured integrated intensities for (a) nuclear, (b) q_1 T=1.8K , (c-d) q_3 T=3.2 K

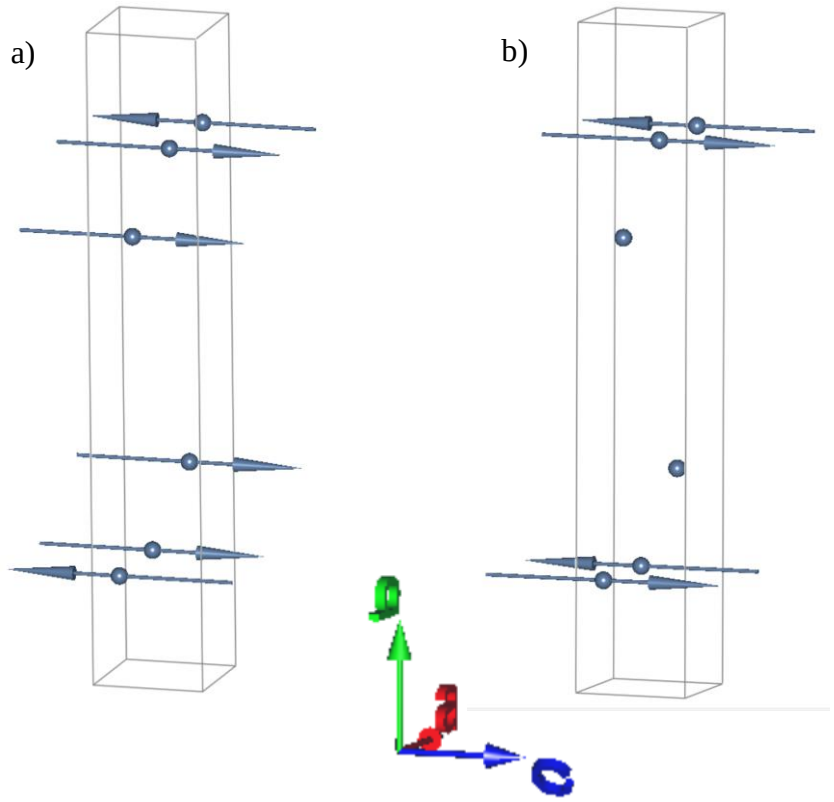

Fig.2: Magnetic structures measured at 1.8K (a) and 3.2K (b).