Experimental report

16/01/2017

Proposal:	**5-41-874**		**Council:**	4/2016

Title: Magnetic field inducing co-existing antiferromagnetic phases in SrYb2O4 (Continuation)

Research area: Physics

This proposal is a continuation of 5-41-806

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Samples: SrYb2O4

Instrument	Requested days	Allocated days	From	To
D10	8	8	08/11/2016	16/11/2016

Abstract:

SrYb2O4 is an insulating magnet, consisting of two types of zigzag chains running along the c-axis and forming a honeycomb structure in the ab-plane. The similar first and second-neighbor distances suggest high geometrically frustrated magnetic interactions. This frustration sums up to strong single ion anisotropy to produce a highly degenerate ground state manifold reflected by a very complex and anisotropic magnetic phase diagram. Despite of SrYb2O4 having a CurieWeiss temperature of −110K, the compound only orders at 0.9K at zero field, the magnetic structure is found to be noncollinear with a reduction of the ordered magnetic moment from the full ionic moment. Due the competition between frustration and high single ion anisotropy, SrYb2O4 has very rich and complex magnetic phase diagram. The different magnetic phases formed when applying a field along the c-axis have been investigated by neutron diffraction on D10. However, due to technical issues with the dilution refrigerator and an unexpected reactor shut down a completed data set was not possible to be acquired. Here, we propose to continue with this experiment.

Report, 16.01.2016

Magnetic field inducing co-existing antiferromagnetic phases in $SrYb_2O_4$

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$SrYb_2O_4$ is an insulating magnet, consisting of two types of zigzag chains running along the c-axis and forming a honeycomb structure in the ab-plane. The similar first and second-neighbor distances suggest high geometrically frustrated magnetic interactions. This frustration sums up to strong single ion anisotropy to produce a highly degenerate ground state manifold reflected by a very complex and anisotropic magnetic phase diagram (see Fig. 1). Despite of $SrYb_2O_4$ having a CurieWeiss temperature of −110K, the compound only orders at 0.9K at zero field, the magnetic structure is found to be non-collinear with a reduction of the ordered magnetic moment from the full ionic moment [1]. The different magnetic phases formed when applying a field along the c-axis have been investigated by neutron diffraction on D10.

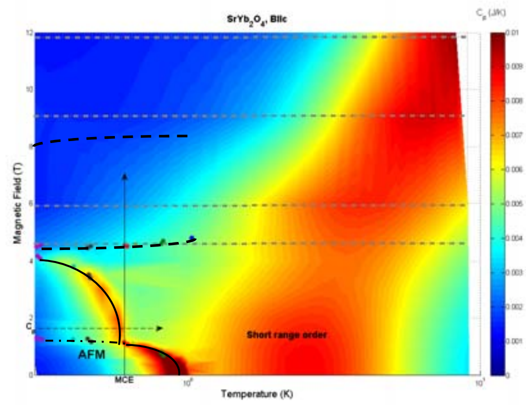

Figure 1. Magnetic phase diagram with magnetic field along the c-axis. The colors indicate the heat capacity in units of J/K. The circles indicate the critical fields extracted from magnetocaloric effect measurements.

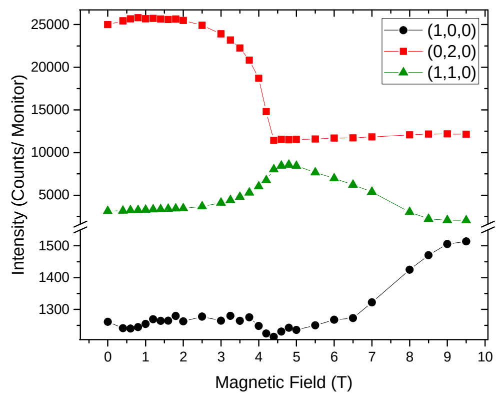

Figure 2. Fitted integrated intensity of the most relevant magnetic plus nuclear Bragg peaks measured on D10. These data have been taken at 40mK.

For the experiment at D10 a neutron wavelength $\lambda = 2.36$ Å was used. A sample of 3.2g was mounted in a cupper holder, aligned to have the c-axis vertical with ab-plane in the horizontal plane and mounted in a dilution stick. A vertical magnet was used to reach fields of up to 9.5T.

In order to determine the magnetic moments of the Yb^{3+} ions we had to determine the overall scale factor and the extinction parameter from crystal structure refinements. Therefore we have used a full data set of 166 *hk*0 reflections (54 unique), which are allowed in the orthorhombic space group *Pnam* (No. 62). Due to the relatively small number of nuclear Bragg reflections we have used the positional parameters *x* and *y* obtained in our earlier study (Ref. 1) and they were not allowed to vary during the refinements. The data were collected in the paramagnetic range at 10 K, well above the magnetic ordering temperature $T_N = 0.9$ K, and in a 2θ-range between 6 and 135°. Further we have measured the intensity of forbidden reflections *h*00 and 0*k*0 with *h* and *k* = odd to check the presence of multiple scattering. This contribution had to be subtracted for the reflections which contribute magnetic intensities. At 40 mK magnetic and nuclear intensities of Bragg reflections were only measured up to 2θ = 92 °, since the magnetic contribution of the high-order reflections is negligible due to the strong decrease of the magnetic form factor of Yb^{3+}. For the refinements of the magnetic structure we finally used 53 reflections (20 unique), where the contribution of nuclear intensity is relatively weak. For the refinements of the magnetic structure only the magnetic moments of the Yb^{3+} ions were allowed to vary. The overall scale factor and the extinction parameter taken from the refinement of the crystal structure from the 10 K data set were fixed during the refinements. In order to follow the change of the magnetic structure as a function of the magnetic field we have collected data sets at $\mu_0 H$ = 0, 2, 6, and 9.5 T. For a reduced set of some prominent magnetic reflections we were able to determine the change of intensity in smaller steps of increasing magnetic fields (see Fig. 2).

The refinements of the crystal and magnetic structure were carried out with the program *FullProf* (Ref. 2) with the nuclear scattering lengths b(O) = 5.805 fm, b(Sr) = 7.02 fm, b(Yb) = 12.40 fm.[3] The magnetic form factors of the Yb^{3+}-ions were taken from Ref. 4.

Table 1: Results of the refinements of the magnetic structure of $SrYb_2O_4$. The magnetic moments were determined at 40 mK, and at magnetic fields at $\mu_0 H$ = 0, 2, 6, and 9.5 T. The spin sequences of the moments along the *x*, *y* and z directions are $A_x(+--+)$, $A_y(+-+-)$, and $F_z(++++)$, respectively.

$SrYb_2O_4$				
	40mK, 0 T	40 mK, 2 T	40 mK, 6 T	40 mK, 9.5 T
μ_x (Yb1)	1.75(3)	1.76(3)	0.02(10)	0.46(5)
μ_y (Yb1)	0.57(4)	0.66(4)	0.23(24)	0.21(8)
μ_z (Yb1)	-	-	2.70(5)	3.09(3)
μ_{exp}(Yb1)	1.83(3)	1.88(3)	2.71(4)	3.16(3)
μ_x (Yb2)	0.57(3)	0.60(3)	0.47(10)	0.16(5)
μ_y (Yb2)	0.62(4)	0.63(4)	0.08(12)	0.07(16)
μ_z (Yb2)	-	-	1.28(5)	2.82(3)
μ_{exp}(Yb2)	0.85(3)	0.87(3)	1.37(4)	2.83(3)

Table 1 shows a summary of the refined magnetic moments in each magnetic phase. The zero field results are in agreement with previously published results [1], however total ordered moment is smaller than previously found. When a magnetic field is applied along the c-axis a ferromagnetic mode is formed along the field direction. The experiment was totally successful.

Additional test measurements were performed with the field along the b-axis. Above 6T the sample was through a spin-flop transition and the crystal orientation was lost. A continuation proposal will be submitted to investigate the phases with the field along the b-axis. Careful sample preparation will be necessary to ensure the crystal orientation at higher fields.

References:

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[3] V. F. Sears, in *International Tables for Crystallography*, edited by A. J. C. Wilson (Kluwer Academic Publishers, Dordrecht/Boston/London, 1995), Vol. C, p. 383.
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