Experimental report

26/01/2016

Proposal: **4-01-1409** **Council:** 4/2014

Title: The magnon spectrum in $FePS_3$, a 2DIsing system on a honeycomb lattice

Research area: Physics

This proposal is a new proposal

Main proposer: **Andrew WILDES**

Experimental team: Diane LANCON
Helen WALKER

Local contacts: Andrew WILDES

Samples: $FePS_3$

Instrument	Requested days	Allocated days	From	To
IN8	0	8	12/11/2014	20/11/2014
IN1	8	0		

Abstract:

$FePS_3$ appears to be a very good example of a 2D Ising antiferromagnet on a honeycomb lattice, which makes it rare. We have previously estimated the magnon dispersion based on neutron spectrometry from a powder, but now wish to verify our conclusions by measuring the dispersion in a single crystal. We have begun by measuring using a thermal three-axis with graphite monochromators and analysers, however we soon struck limits when attempting to measure large energy transfers with sufficient resolution at small Q. We now require a three axis with copper monochromators to continue our experiments, and therefore request IN1.

Local contact : A. Wildes
Experimental team : A. Wildes, H. Walker and D. Lançon

Experimental details :
sample : 2 co-aligned $FePS_3$ crystals with (110) and (001) in scattering plane, Al mount, total mass 0.07g.
a=5.947 Å, b=10.30 Å, c=6.722 Å
$\alpha = 90, \beta = 107.16, \gamma = 90$

Background

$FePS_3$ is a quasi 2D antiferromagnet that belongs in the MPS_3 family, where M are the transition metal atoms which forms an honeycomb lattice in the ab plane. Using measurements of the magnetic density of states on a powder sample, the data had been successfully modeled using a Heisenberg Hamiltonian with a single ion anisotropy, calculated for a two-dimensional structure and spin S = 2. A recent experiment was performed on the merlin spectrometer at ISIS on 17 co-aligned crystals in order to measure the magnon dispersion along high symetry directions, and to refine the magnetic exchange parameters.

The aim of this experiment was to use the high flux of IN8 to measure the magnons in the direction normal to the ab plane (i.e. along l) in order to confirm that this direction is dispersionless. We also wished to check whether the sample presented magnetic domains.

Measurements

We used the PG002 analyser and did several tests with vertical collimation, flat analyser, and different monochromator (Si111, PG002, Cu200). The optimal configuration were the following :
- Si111, no collimation, $k_f = 2.662$ Å^{-1} For elastic scans and inelastic for energy transfer 12-28 meV
- Cu200, no collimation, $k_f = 4.1$ Å^{-1} For inelastic scans with energy transfers 28.5-50 meV.

Figure 1 shows a long QL scan at Q=(0.5 0.5 L) at 1.5K, 110K and 130K, showing that we have no twinning with inverted c*. We observe Bragg peaks at L=-2/3 and L=+1/3. We have an increase of diffuse scattering close to L=0 which goes up with temperature, as expected. Above T_n=123K, the Bragg peaks have disappeared.
Figure 2 show energyscans performed at base temperature at various L values. We observe the magnon mode at ΔE=16 meV (left) and ΔE=39 meV, as expected. They appear dispersionless along Ql. The increase in scattering around

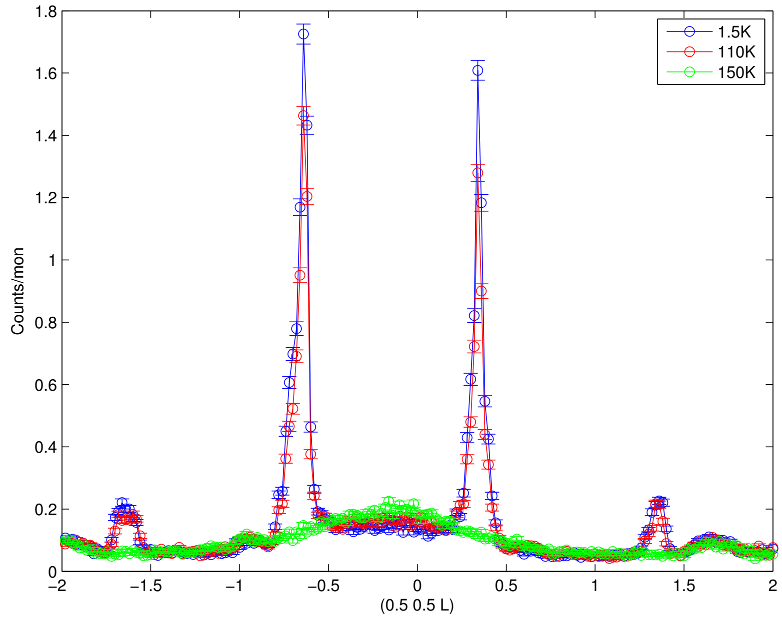

Figure 1: Ql scans at Q=(0.5 0.5 L) at 1.5, 110 and 130K showing magnetic Bragg peaks of $FePS_3$

25 meV was explained as the scattering from the dispersive mode in one of the magnetic domain of $FePS_3$ (rotated by 60 in ab plane).

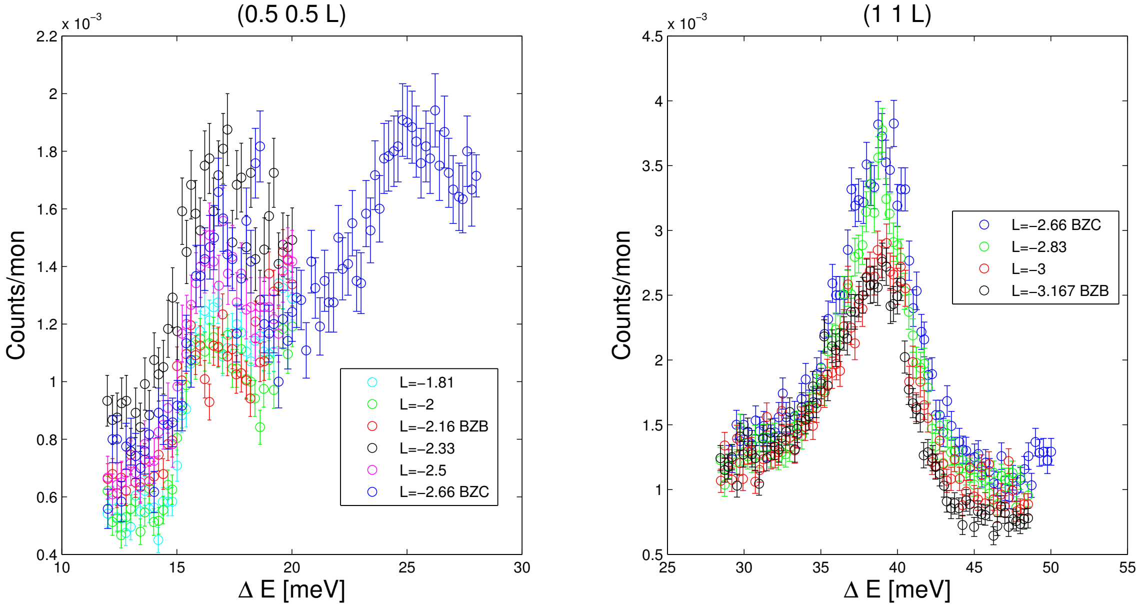

Figure 2: (left) Energy scans at Q=(0.5 0.5 L) for L=-1.81,-2,-2.16,-2.33,-2.5,-2.666 at T=1.5K. (right) Energy scans at Q=(1 1 L) for L=-2.666,-2.83,-3,-3.16 at T=1.5K.