Experimental report

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Proposal: **4-01-1427** **Council:** 10/2014

Title: Magnetic excitations in the frustrated Cairo pentagon lattice compound Bi4Fe5O13F.

Research area: Physics

This proposal is a new proposal

Main proposer: **Manh Duc LE**

Experimental team: Manh Duc LE
Elisa WHEELER

Local contacts: Bjorn FAK

Samples: Bi4Fe5O13F

Instrument	Requested days	Allocated days	From	To
IN4	3	3	27/10/2015	30/10/2015

Abstract:

The Cairo lattice is a tiling of irregular pentagons, each with 4 long and 1 short sides, thus producing two competing nearest neighbour interactions. When the short bond interaction dominates, a collinear structure is predicted by theory for low spins, whereas a possible spin nematic phase could be stabilised by a 4-spin exchange term when the two interactions are equal or the long bond interactions is larger. Bi4Fe5O13F is a physical realisation of the Cairo lattice, with pentagonal layers of Fe3+ (S=5/2) spins interleaved by a Fe3+/Bi3+ layer where the Fe3+ forms a square lattice, which is expected to be only weakly coupled to the pentagonal plane by an almost 90 degree Fe-O-Fe superexchange. Within the plane, the short interaction is expected to dominate as it involves superexchange via a 180 degrees Fe-O-Fe bond. As an initial determination of these interactions, we propose to measure the powder magnon spectrum of Bi4Fe5O13F on IN4C. Spin wave calculations show that much information may still be extracted from a powder measurement if guided by ab initio calculations, which have been completed.

Magnetic excitations in the frustrated Cairo pentagon lattice compound $Bi_4Fe_5O_{13}F$.

Magnetic ions which lie at the vertex of a Cairo pentagon lattice (a tiling of irregular pentagons with one side of different length to the other four) may be geometrically frustrated if their nearest neighbour interactions are antiferromagnetic. We have recently investigated the magnetic excitations spectrum of $Bi_2Fe_4O_9$, where the Fe^{3+} (S=5/2) spins lie on a Cairo lattice, using the Eiger and IN20 spectrometers, and found that the deduced exchange interactions, whilst different to DFT predictions [1] agree with a theoretical study [2] of the phase diagram of the Cairo lattice as a function of the ratio of interactions along the four equal sides (J_{43}) to the unequal side of the pentagon (J_{33}).

$Bi_4Fe_5O_{13}F$ has a structure very similar to $Bi_2Fe_4O_9$, and is formed by interleaving the pentagonal layers (formed from corner shared (4-fold) $Fe(1)O_4$ tetrahedra and pairs of edge-sharing (3-fold) $Fe(2)O_6$ octahedra) with a layer consisting of $Fe(3)O_6$ octahedra and Bi_4F tetrahedra as shown in fig 1(e). Unlike $Bi_2Fe_4O_9$, which has a single phase transition from paramagnetic to an "orthogonal" magnetically ordered structure, $Bi_4Fe_5O_{13}F$ was found to have two addition phase transitions before adopting the "orthogonal" structure [3], although the magnetic structure of these intermediate phases have not yet been solved.

In this measurement, on a powder sample on the IN4 spectrometer, we aimed to explore the inelastic neutron spectrum of $Bi_4Fe_5O_{13}F$ as a first step to experimentally determine the magnetic exchange interactions, previously calculated using *ab initio* methods [3]. Two main settings, with the monochromator set to λ=1.22Å and λ=2.22Å, were used and we concentrated mainly in the low temperature "orthogonal" phase at around 2K, although some measurements were also carried out in the intermediate phases near the end of the experiment.

The measured data are shown in fig 1, together with calculations using the exchange parameters from [3]. The low temperature data show three bands of magnon modes, a low energy band below 5meV, an intermediate energy band between 5 and 20meV and a high energy band between 25 and 45 meV, with gaps between them [Fig 1(a) and (c)]. As the temperature rises, the low and intermediate energy bands softens [Fig 1(d) and (g)], and above T_2=71K, the low energy band disappears, and the gap to the intermediate band closes [Fig 1(i)]. The high energy band does not appear to change in energy with increasing temperature [Fig 1(k)]. Simulations with the exchange parameters determined in [3] qualitatively reproduces the measurement at low temperatures [Fig 1 (b)]. In the high temperature case, the low energy band, and the gap to the intermediate energy band can be suppressed by making the spins on the Fe3 sites disordered in the simulation [Fig 1(j)]. This was also what has recently been found from new diffraction measurements on this material in the intermediate phases.

Thus we have confidence that the Hamiltonian used for the modelling is correct, and will be working on refining the exchange parameters to better reproduce the measured spectrum.

References

[1] Pchelkina and Streltsov, *Phys. Rev. B* **88** 054424 (2013).
[2] Rousochatzakis et al., *Phys. Rev. B* **85** 104415 (2012).
[3] Abakumov et al., *Phys. Rev. B.* **87** 024423 (2013).

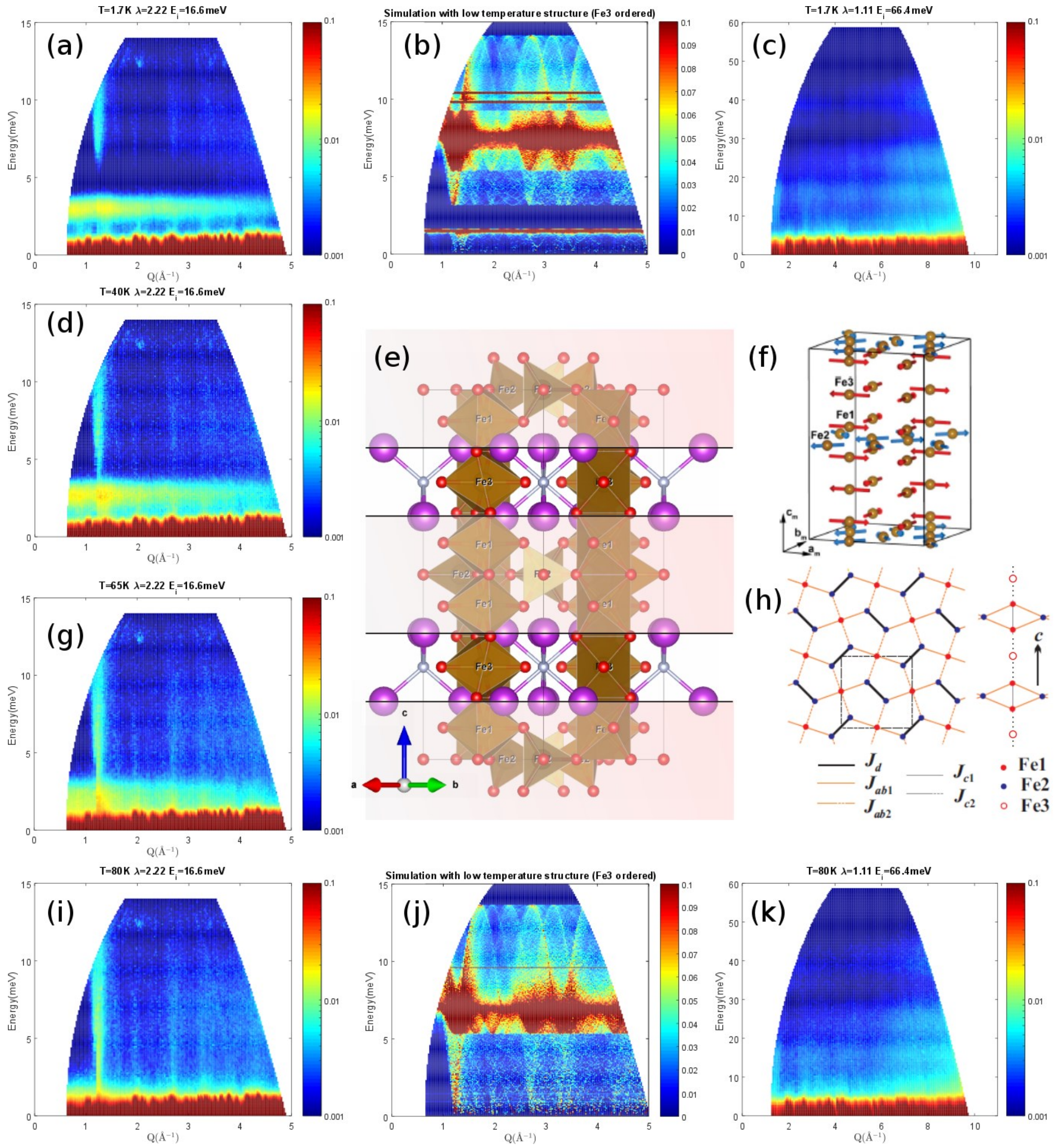

Figure 1. (a-c) The measured (a,c) and simulated (b) neutron spectrum at 1.7K. The simulation was done using exchange parameters in [3] using the spinW program. (d,g) Measured data at 40K and 65K. (e) the crystal structure of $Bi_4Fe_5O_{13}F$, with the pentagonal layers shaded in pink, separated by $Fe(3)O_6$-Bi_4F layers. (f) the magnetic structure at 1.5K, showing the only the Fe^{3+} sites, labeled by the orientation of their spins. (h) the exchange interactions between the Fe^{3+} ions in plan view. (i-k) The measured (i,k) and simulated spectrum at 80K.