Experimental report

16/04/2016

Proposal:	**4-01-1428**	**Council:**	10/2014

Title: Determination of the exchange parameters in the frustrated Cairo pentagon lattice compound Bi2Fe4O9.

Research area: Physics

This proposal is a new proposal

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Samples: Bi2Fe4O9

Instrument	Requested days	Allocated days	From	To
IN20	10	7	04/05/2015	11/05/2015

Abstract:

The Cairo lattice is a tiling of irregular pentagons, each with 4 long and 1 short sides, with magnetic ions at the vertices, thus producing two competing nearest neighbour interactions. When the short bond interaction dominates, a collinear structure is predicted by theory for low spins. For classicals spins, a different structure with the spins forming an orthogonal arrangement that are rotated slightly between the two sublattices is expected. This is the structure found in Bi2Fe4O9 where Fe3+ (S=5/2) spins form a Cairo lattice in the a-b plane. Ab initio calculations and previous inelastic neutron scattering measurements confirmed that the short interaction is strongest. However, the measurements were made in the (hhl) plane and so could not clearly determine the in plane exchange interactions in full. In addition they found a large interlayer coupling and large spin anisotropy gap which warrants further investigation. We thus propose to measure the magnon spectrum in the (hk0) plane on IN20 to elucidate where in the theoretical phase diagram Bi2Fe4O9 falls.

Determination of the exchange parameters in the frustrated Cairo pentagon lattice compound $Bi_2Fe_4O_9$.

The Cairo pentagonal lattice is an tiling of irregular pentagons (with one side of different length to the other four). The Fe^{3+} ions (S=5/2 spins) in the compound $Bi_2Fe_4O_9$ lie on the vertices of a Cairo lattice, and are connected by frustrated antiferromagnetic superexchange interactions. In this case, the pentagons have one short and four long sides, so it is expected that the interaction along the short side, denoted J_{33} linking two three-fold sites, should be stronger than the J_{43} interactions along the long sides linking a four-fold coordinated and a three-fold coordinated site. In $Bi_2Fe_4O_9$, however, there is an additional complication in that actually two physical Fe^{3+} ions lie one of the vertex of the Cairo lattice, as a parallel pair of spins displaced above and below the pentagonal plane in the *c*-direction coupled by J_{44} (see figure 1). In addition, there are interactions along the *c*-directions which link the *ab*- pentagonal plane. Finally the oxygen ligands of the long edges are slightly different between two pairs of Fe^{3+} ions leading to two different J_{43} interactions (J_{43} and J'_{43}).

A theoretical study [1] has determined the phase diagram of the Cairo lattice as a function of the ratio J_{43}/J_{33} which is a measure of the degree of frustration in this system. When J_{33} dominates, a long ranged order structure is stabilised, whilst if J_{43} dominates, a ferromagnetic structure, or possibly a spin nematic phase is more favourable. Neutron diffraction has shown [2] that the predicted orthogonal magnetic structure for the case $J_{43}/J_{33}<\sqrt{2}$ is that adopted by $Bi_2Fe_4O_9$. Finally, the exchange constants have also been predicted by DFT [3] which agrees with the criteria $J_{43}/J_{33}<\sqrt{2}$.

The aim of this experiment is to determine these exchange parameters by measuring the magnon spectrum in the ordered phase of $Bi_2Fe_4O_9$. We had completed initial measurements using the Eiger spectrometer at PSI. However, the small sample size forced us to measure at high temperatures (≈200K) near T_N=245K, so the excitations are significantly broadened and may also have softened leading to underestimations of the exchange parameters. In addition measurements were made in the [HH0]-[00L] scattering plane which does not allow the J_{43} and J'_{43} interactions to be easily distinguished. The higher flux on IN20, however, allowed us to measure at base temperature (2K) and we chose to measure the sample in the [H00]-[0K0] plane.

The fixed k_f=2.66Å^{-1} W-configuration with PG(002) monochromator and analysers and open collimation was used, and we observed one clear dispersive mode from 5meV to 30meV (fig. 2). Measurements were made up to 50meV but unfortunately a strong spurious signal from both Bragg scattering from the sample and the Aluminium sample holder and sample environment which is subsequently thermally diffuse scattered from the analyser was observed around 40meV where another magnon mode was expected. From the data, a set of exchange parameters were fitted which is significantly different from that predicted by DFT [3] or from the Eiger measurements (see table). The parameters deduced here have a very large J_{33} compared to J_{43} and J'_{43} thus yielding a very small ration J_{43}/J_{33}. In addition, the interactions J_{44} between the ferromagnetically coupled spins on the four-fold sites is almost as strong as the in-plane interactions, which is another source of frustration not in the Cairo model. The very strong J_{33} interaction between the three-fold dimers in the pentagon plane should also result in strong classical fluctuations as predicted in [1].

The measurements have thus found significant difference to the predicted exchange interactions which indicates that $Bi_2Fe_4O_9$ may harbour other frustrated interactions not considered by theory.

	J_{33}	J_{43}	J'_{43}	J_{44}	J_c
DFT [3]	-6.3 meV	-3.1 meV	-2.0 meV	-0.9 meV	-1.0 meV
Eiger	-3.8 meV	-1.0 meV	-2.8 meV	-0.5 meV	-3.4 meV
IN20	-13.5 meV	-3.6 meV	-5.1 meV	-2.3 meV	-2.0 meV

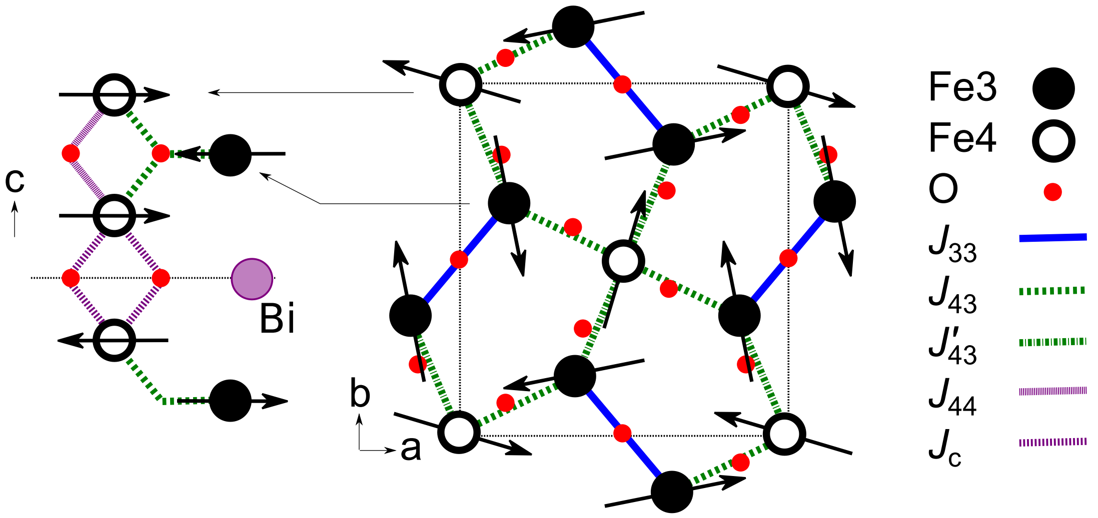

Figure 1. The crystal structure of $Bi_2Fe_4O_9$ showing only the Fe^{3+} ions in the Cairo pentagonal lattice, including the three-fold sites (solid cirlces) and four-fold sites (open circles) and the exchange interactions.

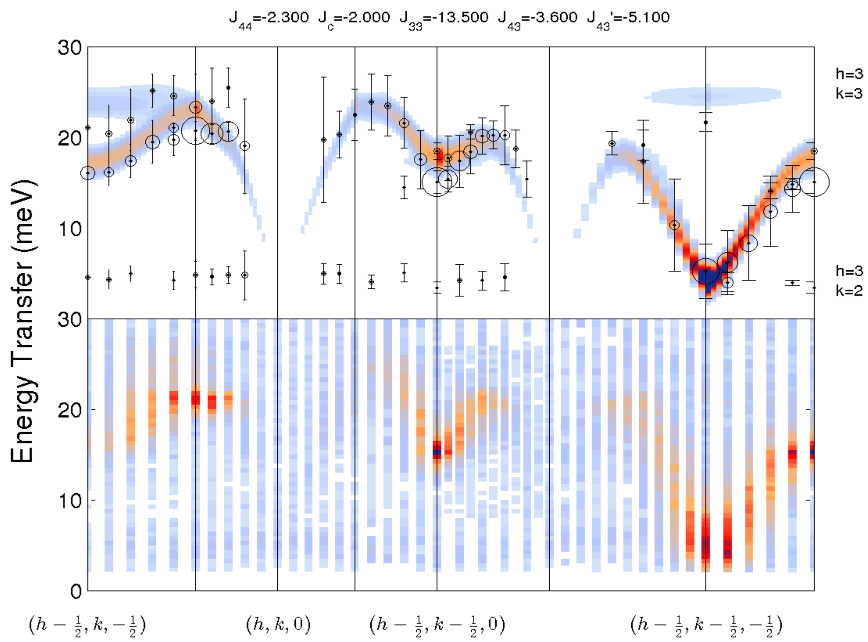

Figure 2. (Top) Simulated magnon dispersion with fitted peak positions and widths as errorbars. (Bottom) Measured constant *q* scans with intensity on a colour scale. One dispersive magnon branch is clearly seen, with a flat optic phonon mode around 5meV.

References

[1] Rousochatzakis et al., *Phys. Rev. B* **85** 104415 (2012).
[2] Ressouche et al., *Phys. Rev. Lett.* **103** 267204 (2009).
[3] Pchelkina and Streltsov, *Phys. Rev. B* **88** 054424 (2013).