Experimental Report

13/01/2014

Proposal: **5-32-782** **Council:** 10/2012

Title: The Frustrated Magnetic Order of $Ba_3YIr_2O_9$.

This proposal is a new proposal

Researh Area: Physics

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Samples: $Ba_3YIr_2O_9$

Instrument	Req. Days	All. Days	From	To
D7	7	7	25/03/2013	01/04/2013

Abstract:
Studies of iridium-based compounds are at the forefront of solid state physics research. In these materials the electronic configurations are driven by strong spin-orbit coupling. Adding geometric spin frustration may provide a route to realization of the spin-orbit driven quantum spin liquid state. Here we plan to study the frustrated magnetic order $Ba_3YIr_2O_9$, combining this data with inelastic neutron scattering to understand the magnetic interactions of this material, and possible routes to a magnetic disordered ground state in a high pressure phase cubic phase of $Ba_3YIr_2O_9$.

The Frustrated Magnetic Order of Ba 3YIr2O9.

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Recent interest has been sparked into the magnetic properties of 5*d*-transition metals due to the large degree of spin-orbit coupling in these materials, which for instance can drive these materials towards a Mott insulating state in spite of large covalency, and a small on-site Coulomb repulsion energy *U*[1]. More interestingly in the field of frustrated magnetism enhanced spin-orbit coupling can lead to new magnetic states, such as the quantum compass phase[2]. In this proposal we proposed to investigate the role of spin-orbit interaction in a novel frustrated spin system $Ba_3YIr_2O_9$.

The system we have been studying is $Ba_3BIr_2O_9$ B = Y, Zn or Sc, crystallizes in a hexagonal ($P6_3mmc$) structure with Ir-Ir structural dimers forming an edge-shared triangular network, with the dimers aligned along the crystal c-axis. Ir occupies a unique crystallographic site and has a fractional (+4.5) oxidation state in a purely ionic picture thereby suggesting metallicity. However the materials are likely spin-orbit driven Mott insulators. Reports of reduced moments in these materials have led to the postulation of antiferromagnetic (AFM) Ir dimers[3]. While our structures are similar to $Ba_3BRu_2O_9$ B´ = La, Y[4], a recent diffraction study has determined ferromagnetic (FM) Ru-dimers interacting antiferromagnetically on a hexagonal lattice, with dramatic differences in size of the ordered moment with B´ [5] . In this proposal we tried to determine the magnetic order of the $Ba_3YIr_2O_9$ system using polarized neutron diffraction on D7, whether we have FM or AFM dimers with frustrated spin interactions on a hexagonal lattice. The polarization analysis of D7 would prove vital due to the reduce moment of the reduced Ir moment indicated in our susceptibility data.

For performing a neutron diffraction on D7 with an Ir based sample neutron absorption must be taken into account. The effects of absorption are stronger the longer the wavelength of neutrons used, selecting the shortest available wavelength available on D7 of 3.12 Å. To further reduce the effects of neutron absorption we used a toroidal sample, employing the chewing gum mounting technique. A further advantage of using a toroidal sample is the maximizing of area of the incident neutron beam on D7.

Initially we found that there was no strong magnetic Bragg reflections from the ordered Ir moments at 2 K. The experiment suffered from an unexpected difficulty of a large incoherent scattering rate. This large incoherent scattering could only be accounted for by the absorption of water into the sample, of the order of 2-3 mg per gram. We have since determined that this water can successfully be removed by baking, without any damage to the crystal structure of this and related materials. The large incoherent scattering and lack of a large ordered Ir moment necessitated in long counting times at 2 K, and at 20 K far above the 4.5 K spin ordering temperature, aswell as careful treatment of all background and calibration effects. In figure one we show the magnetic Bragg reflection we observed only at base temperature. The intensity of the magnetic Bragg reflection we observed corresponds to a moment of the order of 0.03-0.04 μ_B, a moment that is on the detection limit of D7.

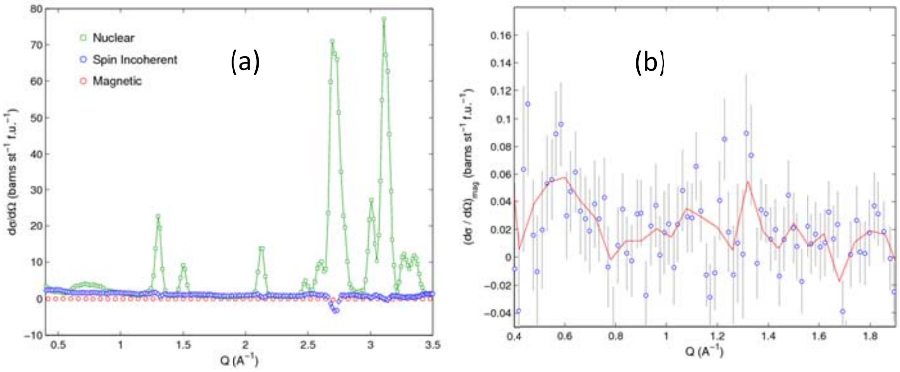

Figure 1: (a) The different scattering components of $Ba_3YIr_2O_9$ measured in 48 hours by polarized neutron diffraction on D7 at the ILL. (b) A zoom of the magnetic scattering, showing a weak magnetic Bragg reflection at Q = 0.6 Å^{-1}. The peak at 1.3 Å^{-1} is due to imperfect correction of a structural Bragg reflection. The red line is the result of re-binning the data.

We have successfully observed magnetic order in $Ba_3YIr_2O_9$, but the size of the ordered moment precludes an extensive study of this material by neutron diffraction. It is unclear whether the peak observed on D7 corresponds to two peaks observed for $Ba_3BRu_2O_9$ B´ = La, Y, or a single diffuse peak. Further investigations by other experimental techniques are required to resolve the magnetic ordering in $Ba_3YIr_2O_9$.

References:

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[4] Y, Hinatsu and Y. Doi, Bull. Chem. Soc. Jpn. **76**, 1093 (2003)

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