Experimental report

25/05/2019

Proposal: **EASY-295** **Council:** 4/2017

Title: Elucidating Magnetic Order in a Quantum Spin Liquid Mother Compound, Cu4(OD)6FBr

Research area: Physics

This proposal is a new proposal

Main proposer: **Lucy CLARK**

Experimental team:

Local contacts: Clemens RITTER

Samples: Cu4(OD)6FBr

Instrument	Requested days	Allocated days	From	To
D20	8	8	04/07/2018	05/07/2018

Abstract:

Quantum spin liquids are intriguing states of matter in which magnetic frustration and strong quantum fluctuations prevent classical long-range magnetic order. To date, one of the best experimental realisations of such a system is herbertsmithite, ZnCu3(OH)6Cl2, but the exact nature of its ground state remains a matter of debate. Recently, we have explored Zn-doping in the related compound barlowite, ZnxCu4-x(OH)6FBr, which like herbertsmithite contains frustrated corner-sharing triangular layers of Cu2+ ions. The x = 0 member of this series undergoes a magnetic ordering transition at 15 K, and we were awarded beamtime on the GEM diffractometer at the ISIS Facility to determine the magnetic structure of the Cu4(OH)6FBr ground state. We do see magnetic Bragg peaks in our GEM data at the expected d-spacings based on our predictions of the magnetic structure, but given the small ordered moment, the flux on GEM was not sufficient to clearly resolve the magnetic Bragg scattering. As such, we request EASY access on D20 to make use of its extremely high flux to complete our experiment and solve the magnetic structure. We require two measurements - 4 hours at 1.7 K and 4 hours at 20 K.

EASY-295 Experimental Report

Elucidating Magnetic Order in a Quantum Spin Liquid Mother Compound, $Cu_4(OD)_6FBr$

May 2019

One day of EASY access was granted on D20 to determine the magnetic structure of the frustrated S = ½ kagome compound, $Cu_4(OD)_6FBr$. From preliminary studies, we knew that this material adopts an orthorhombic *Pnma* crystal structure below 250 K and that it orders magnetically below 15 K. As such we collected data on a 4-g deuterated sample on D20 with λ = 2.4188 Å and a monochromator take-off angle 42 ° at 1.5 K and 20 K. Subtraction of the data below and above the Néel ordering transition revealed 10 magnetic Bragg peaks corresponding to a $\boldsymbol{k}$ = (0, 0, 0) magnetic structure. As such, the high-flux afforded by the D20 instrument was critical in giving us the best possible chance to solve the magnetic structure of this material.

Using the MAXMAGN application on the Bilbao Crystallographic Server we identified the symmetry allowed magnetic structures of $Cu_4(OD)_6FBr$ and uniquely identified that described by the *Pn'm'a* magnetic space group as giving the best fit to our data. The Rietveld fit of this model to our subtracted data and the corresponding magnetic structure are shown in the figure below.

There are a number of important outcomes of this EASY experiment. First, the data will make an important contribution to the PhD thesis of K. Tustain at the University of Liverpool. Second, we were able to publish our data in a rapid communication to Physical Review Materials – see K. Tustain *et al.*, *Phys. Rev. Mater.* **2**, 111405(R) (2018). Finally, we have secured further beamtime on D20 in summer 2019 to explore the magnetic ground states of the related $Cu_4(OD)_6FCl$ and $Cu_4(OD)_6FI$ systems.