

# Experimental report

08/05/2017

**Proposal:** 5-31-2467

**Council:** 4/2016

**Title:** Tuning magnetism in a chiral quantum magnet

**Research area:** Physics

**This proposal is a new proposal**

**Main proposer:** Peter BABKEVICH

**Experimental team:** Peter BABKEVICH

**Local contacts:** Vivian NASSIF

**Samples:** K(NbO)Cu<sub>4</sub>(PO<sub>4</sub>)<sub>4</sub>  
Sr(TiO)Cu<sub>4</sub>(PO<sub>4</sub>)<sub>4</sub>  
Ba(VO)Cu<sub>4</sub>(PO<sub>4</sub>)<sub>4</sub>

Instrument	Requested days	Allocated days	From	To
D20	0	4	01/07/2016	05/07/2016
D1B	4	0		

## Abstract:

In this proposal we aim to examine A(BO)Cu<sub>4</sub>(PO<sub>4</sub>)<sub>4</sub> family of compounds which are possible candidates for a S=1/2 square-lattice antiferromagnets. The prototypical Ba(TiO)Cu<sub>4</sub>(PO<sub>4</sub>)<sub>4</sub> system has been shown to order in a non-collinear antiferromagnetic structure below 9.5 K. At the same time, the crystal structure is non-centrosymmetric giving rise to a chiral nuclear structure. Heat capacity together with XRD measurements on related compounds have found that the change in chirality is closely linked to a change in the magnetic interactions. The aim of this proposal is to systematically study this effect of chirality on the magnetic structure. To do so, we propose to employ the D1B diffractometer. In addition, we have proposed to systematically study the magnetic fluctuations of this family using IN5 spectrometer (proposal #75643).

## Proposal 5-31-2467: Tuning magnetism in a chiral quantum magnet

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We have performed magnetic powder diffraction on a family of  $A(BO)Cu_4(PO_4)_4$  compounds that have varying amounts of crystal chiralities. Using the D20 diffractometer we obtained high-quality, high-resolution diffraction patterns using which we were able to solve the magnetic structures of the compounds.

Recent discovery of  $Ba(TiO)Cu_4(PO_4)_4$  (or BaTi) shows great promise to be a very exciting system to study novel quantum magnetism [1-3]. The crystal structure of BaTi is rather complicated consisting of corrugated  $CuO_4$  square planes separated by Ba,  $PO_4$  tetrahedra and  $TiO_{1+4}$  pyramids [1]. The compound crystallises in a tetragonal structure that can be described by the tetragonal  $P4_212$  space group with  $a = 9.60 \text{ \AA}$  and  $c = 7.12 \text{ \AA}$  lattice parameters. The crystal structure is non-centrosymmetric giving rise to crystal chiral domains. However, a closely related  $K(NbO)Cu_4(PO_4)_4$  (KNb) possesses a higher crystal symmetry of  $P4/nmm$  as demonstrated by the absence of  $(hk0)=\text{odd}$  reflections in powder X-ray diffraction and is therefore achiral.

Through careful study using polarized-light microscopy and X-ray diffraction, it was shown that substitution of  $A^{2+}$  cation controls the strength of the structural chirality in  $A(TiO)Cu_4(PO_4)_4$ , where  $A = Ba, Sr$  [3]. While more recently, KNb, has emerged as an important high-symmetry reference material. Having a tuneable crystal structure is an interesting arena to explore the fundamental interactions.

In order to obtain the magnetic structure of the compounds of interest, we have performed

high-resolution, high-statistics measurements of four systems: BaTi, PbTi, SrTi, and KNb using the D20 diffractometer. Approximately 5 g of each powder were recorded for 8 hours in the magnetically ordered and paramagnetic states for each compound. The data for KNb requires more detailed analysis. Our results of the BaTi, PbTi, and SrTi compounds is shown in Fig. 1. The magnetic moments on Cu ions are approximately the same in all three systems – with slightly different tilts of the moments in BaTi and SrTi. The SrTi and BaTi magnetic reflections can be indexed by  $(0,0,0.5)$  propagation wavevector. However, as shown in Fig. 1, the case of PbTi is different and instead we have ferromagnetically coupled planes stacked along the c-axis.

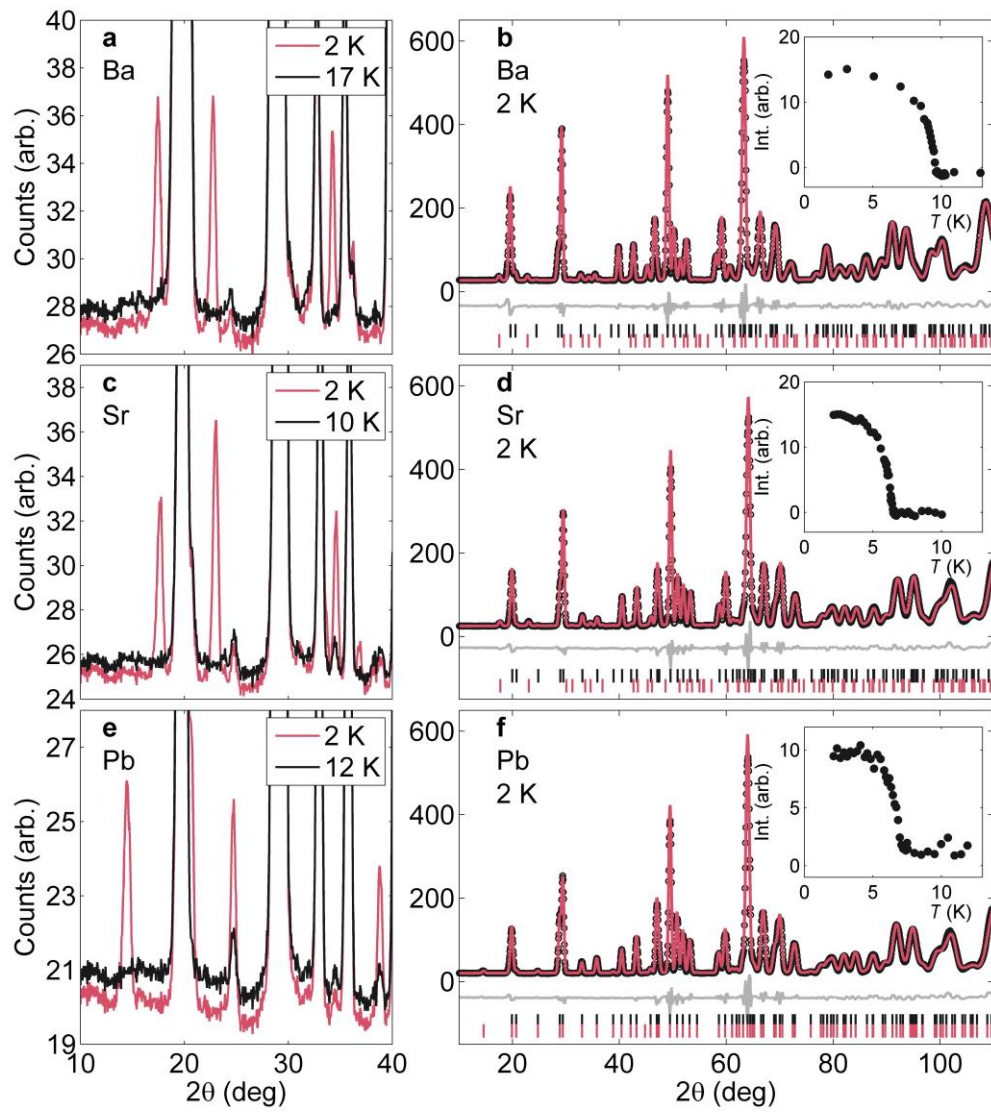
Ongoing efforts to characterise the magnetic interactions by means of inelastic neutron spectroscopy are ongoing.

[1] S. Meyer, and Hk. Müller-Buschbaum, Z. Anorg. Allg. Chem. 623, 1693 (1997)

[2] K. Kimura, M. Sera and T. Kimura, Inorg. Chem. 55(3), 1002 (2016)

[3] K. Kimura et al., Nat Comm. 7, 13039 (2016)

[4] K. Kimura et al., submitted to PRL



**Figure 1.** Powder diffraction patterns collected for BaTi, SrTi, and PbTi above and below magnetic ordering temperatures. The inset shows the development of magnetic intensity as the systems order. The solid lines in panels b, d, f are Reitveld refinements of the nuclear and magnetic structures. After [4].