Experimental Report

06/03/2015

Proposal: **5-31-2343** **Council:** 4/2014

Title: Magnetic phase transition in the new double-perovskite Ca2CoOsO6

This proposal is a new proposal

Researh Area: Physics

Main proposer: **PRINCEP Andrew**

Experimental Team: PRINCEP Andrew
RAHN Marein

Local Contact: SUARD Emmanuelle

Samples: Ca2CoOsO6

Instrument	Req. Days	All. Days	From	To
D2B	1	1	27/09/2014	28/09/2014

Abstract:

Osmates in the perovskite-like structure are very topical. For example, recent discoveries include Slater transitions, and "ferroelectric-like" structural transitions. These arise because of structural distortions, geometric frustration, magnetism and strong spin-orbit coupling. We have recently synthesised a new monoclinic (P21/n) double perovskite material Ca2CoOsO6 using a high pressure method. Bulk measurements show evidence for a ferrimagnetic phase transition at approximately 130K. We propose to determine the magnetic and crystal structure of ca2CoOsO6 as a function of temperature between 10 and 300K, with a particular view to disentangling the sublattice contributions to the magnetic structure and investigating the contribution of the osmium orbital moment to the magnetic properties.

Experimental report 5-31-2343 (instrument D2B)

Magnetic phase transition in the new double-perovskite Ca_2CoOsO_6

Scientific Background

Osmates in the perovskite-like structure are very topical. For example, recent discoveries include Slater transitions [1], and „ferroelectric-like“ structural transitions [2]. These arise because of structural distortions, geometric frustration, magnetism and strong spin-orbit coupling. We have recently synthesised a new double perovskite material Ca_2CoOsO_6 .

Aim of the experiment

To determine the magnetic and crystal structures of double perovskite Ca_2CoOsO_6 as a function of temperature between 300 and 10K. This will identify the nature of the phase transitions (magnetic/structural, first/second order) and establish the role of the 5d electrons in these transitions.

Technical

We filled 4.62 g of sample powder in a standard V can and measured powder histograms of 450000 monitor counts (ca. 7 h) at 350 K, room temperature (λ = 1.6 A), as well as one higher resolution dataset at base temperature (10 K, λ = 2.4 A).

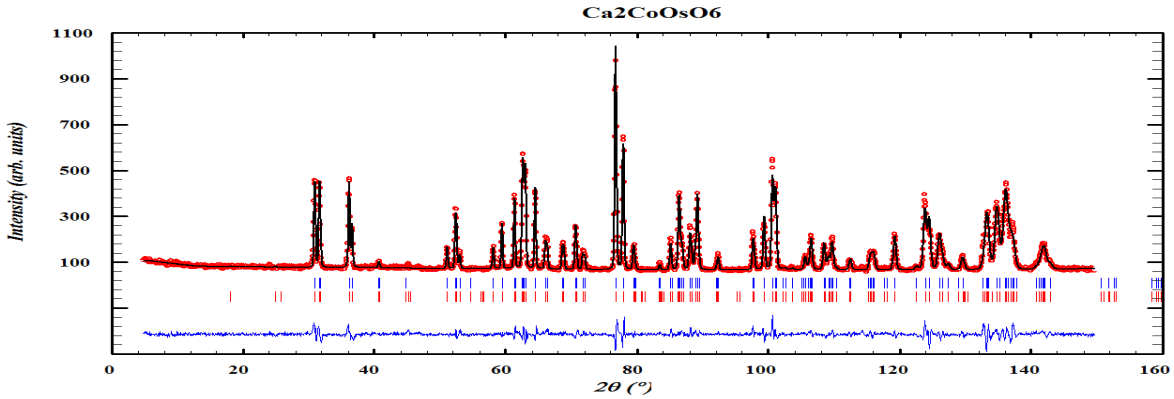

Figure 1. *Refined powder histogram of Ca2CoOsO6 (FullProf suite).*

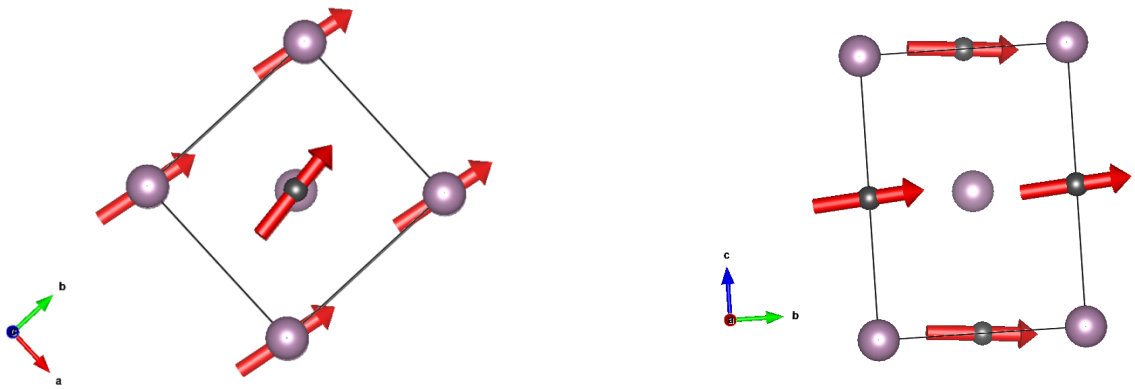

Figure 2. *Refined magnetic structure of Ca_2CoOsO_6 . Osmium moments lie in the ab plane at 90 degrees to the cobalt moments.*

Instrument performance

We experienced no technical difficulties with the instrument or sample environment. The control interface of D2B is very user friendly and we also benefited from the analysis software LAMP made available by the ILL. The instrument responsible Dr. Emmanuelle Suard was extremely helpful and contributed crucial experimental advice, also out of hours. As we performed this experiment in turn with our other experiments **5-31-2343** and **5-31-2344**, the rotating sample table of D2B came in as invaluable tool which rendered our beamtime highly efficient.

Key results

We have successfully refined all acquired powder histograms (R-factors $\leq$ 5, FullProf Suite). By means of representational analysis we have unequivocally determined the magnetic space group and refined this magnetic phase in our data. This reveals an ordering of Co and Os moments in a canted antiferromagnetic structure.

Overall evaluation

Our experiment 5-31-2343 has been highly successful. We lost no beamtime to technical difficulties, acquired the necessary data as planned and obtained the desired results. We would like to acknowledge the efficient instrumental setup at D2B and the useful experimental advice given by the local contact. We expect to publish our results within the year in the context of a comparative study of osmium prevskites.

References

[1] S. Calder et. al. Phys. Rev. Lett. 108, (2012) 257209

[2] Y Shi et. al. Nature Materials DOI: 10.1038/nmat3754 (2013).