# Experimental report

21/06/2016

**Proposal:** 5-31-2431 **Council:** 4/2015

**Title:** Magnetic structure of spin orbit coupled transition metal chains in Ca4RhO6 and Sr4IrO6

**Research area:** Physics

**This proposal is a resubmission of 5-31-2363**


**Main proposer:** **Marein RAHN**

**Experimental team:** Andrew PRINCEP
Marein RAHN

**Local contacts:** Thomas HANSEN


**Samples:** Sr4 Ir O6
Ca4 Rh O6

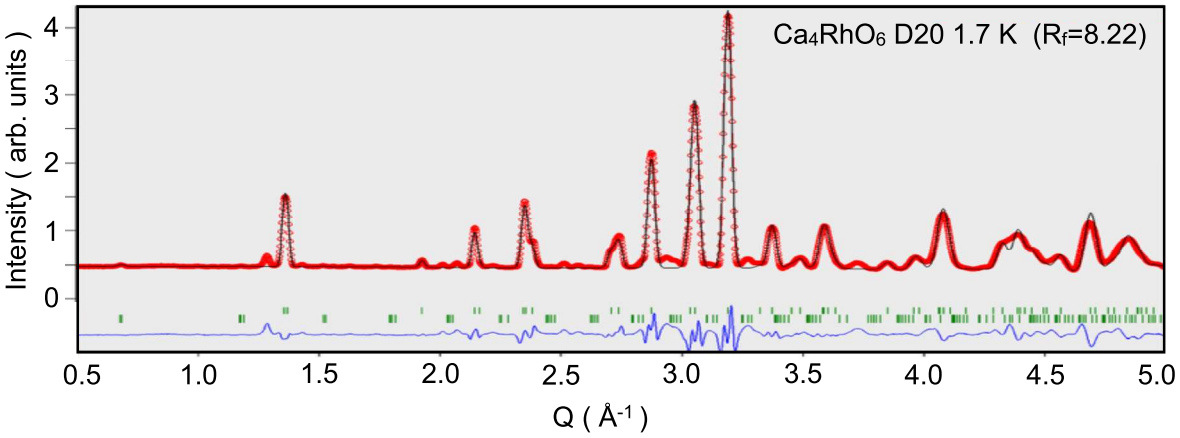
| Instrument | Requested days | Allocated days | From | To |
|---|---|---|---|---|
| D20 | 2 | 2 | 31/10/2015 | 03/11/2015 |

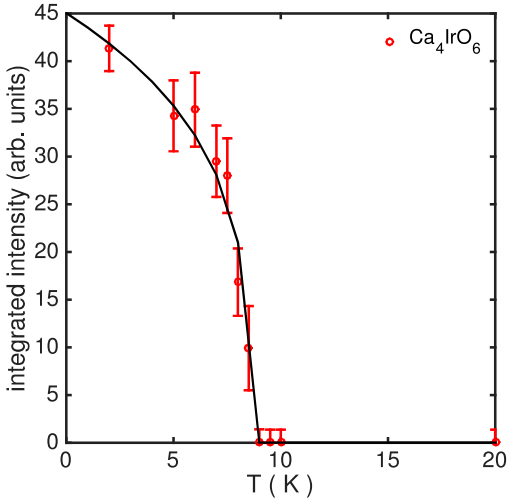

## Abstract:

It is difficult to predict the ground states of 5d transition metal oxide, as their electrons may be strongly correlated, sensitive to the surrounding crystal field symmetry and their spin- and orbital angular momentum strongly coupled. We propose to study two new compounds from this family, which combine this complex situation with low dimensionality. We have synthesised two isostructural and isoelectronic compounds Ca4IrO6 and Sr4IrO6. Their electronic ground states should represent the same electronic situation with different strengths of spin orbit coupling - which would yield an important comparison. To this end, we propose to characterise the antiferromagnetic order in our two samples (setting in at 10 and 12 K, respectively) by magnetic neutron powder diffraction.

An equivalent previous proposal to D2B (#5-31-2363) had been rejected on grounds of the magnetic moment being too small. We here follow the panel's recommendation to re-submit to D20. We expect a magnetic moment of 0.3 to 0.5 Bohr magnetons, which should yield an appreciable signal on D20.

# D20: Magnetic structure of $Ca_4RhO_6$




- On D20, several powder diffraction patterns were obtained at temperatures betweeon 1.7 and 20 K.
- A good refinement can be achieved using the structural parameters obtained from the D2B dataset.
- Several magnetic peaks appear below $T_N$= 8.0 ±0.1 K
- The thermal evolution of the integrated magnetic intensity can be fitted to a power law.

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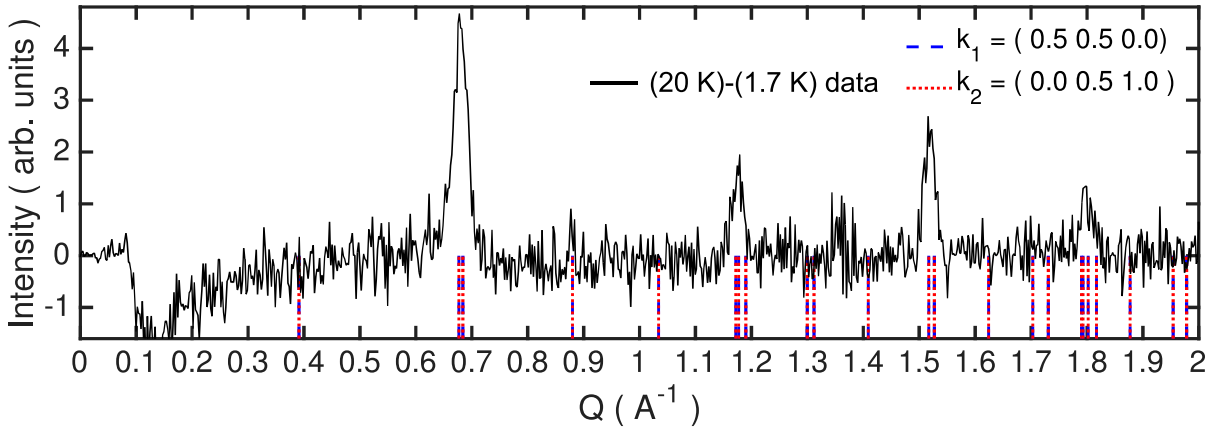
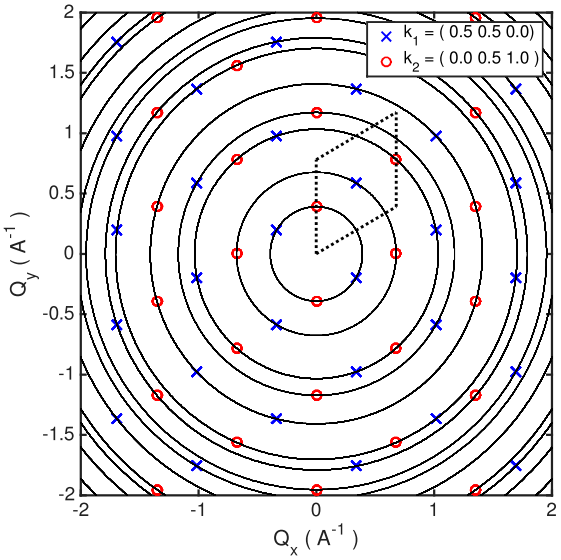
## Indexing Ca416 difference pattern



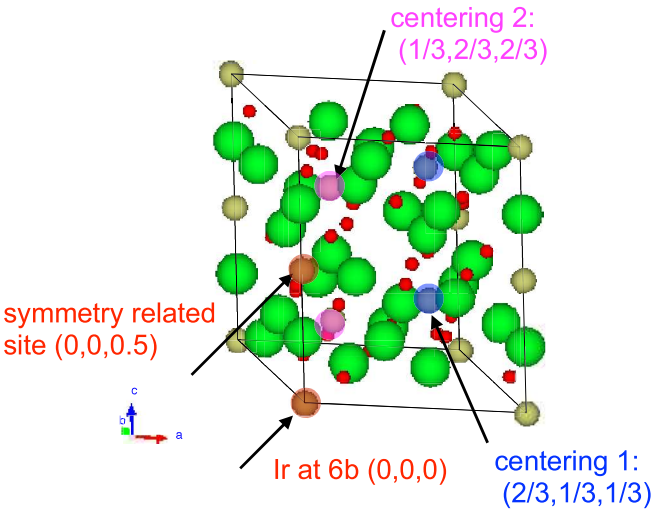

- In the trigonal Brillouin zone, the propagation vectors $k_1$=(1/2 1/2 0) and $k_2$=(0 1/2 1) correspond to the same modulus of momentum transfer. This means that they cannot be distinguished in powder averaged data.
- $k_1$ has previously been evidenced in a single crystal resonant x-ray diffraction study.

(Calder et al., PRB **89**, 081104(R), 2014)

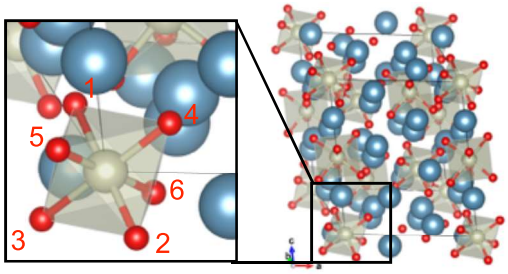
# Magnetic refinement & representational analysis

- the trigonal (R-3c) unit cell of these compounds contains six magnetic ions
- ordering of the Rh magnetic moments on this 6b (0,0,0) Wyckoff site was considered with either propagation vectors

  $\boldsymbol{k_1}$**=(1/2 1/2 0)** or $\boldsymbol{k_2}$**=(0 1/2 1)**
- each of these propagation vectors yields two irreducible representations, $\Gamma_1$ and $\Gamma_3$




- DFT (GGA/PAW) calculations for the corresponding iridate had determined the Ir-O bond directions as magnetic easy axes. (Calder et al., PRB **89**, 081104(R), 2014)
- the present data was fitted in the four irreducible representations ($k_1$ / $k_2$ ; each $\Gamma_1$ / $\Gamma_3$ ) with the Rh magnetic moment directed along the three axes of the $RhO_6$ octahedron ( 1-2; 3-4; 5-6; *cf*. figure)

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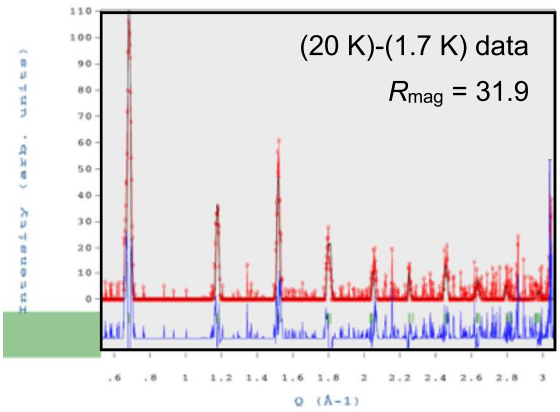
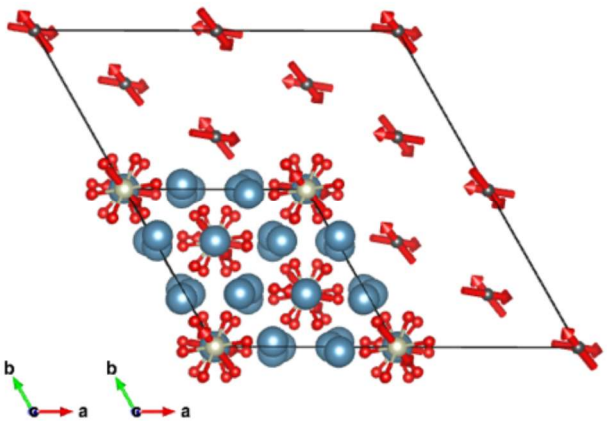
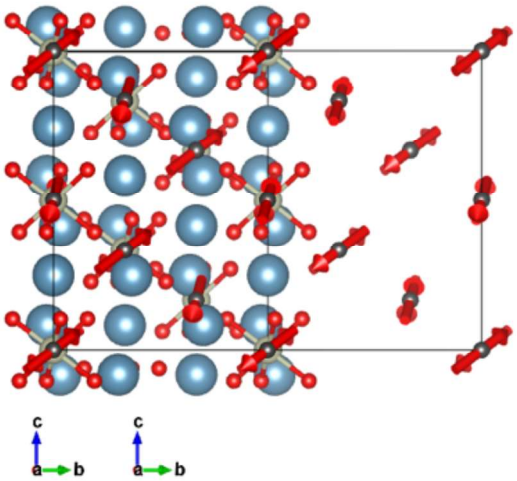
- The best fit is achieved in the setting $k_1/\Gamma_1$, with the magnetic moment oriented along the 1-2 axis (*cf*. figure above).
- This magnetic structure corresponds to the model proposed for $Sr_4IrO_6$.

  (Calder et al., PRB **89**, 081104(R), 2014)

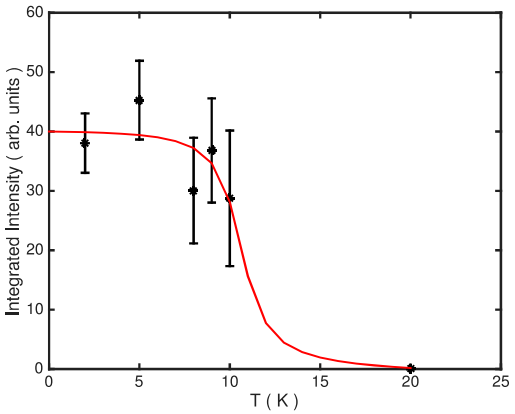


# D20: Magnetic structure of $Sr_4IrO_6$

- As for $Ca_4RhO_6$, several powder diffraction patterns were obtained at temperatures between 1.5 and 20 K.
- In the case of the iridate, the experiment is impeded by the strong neutron absorption and smaller moment size of Ir.
- Several magnetic peaks appear below $T_N$~11 K




- additional datasets between 7 K and 12 K have been obtained very recently (*data analysis in progress).*

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# Magnetic refinement & representational analysis

- The analysis of the magnetic phase in $Sr_4IrO_6$ is fully analogous to that of $Ca_4RhO_6$.
- Also in this case, the choice of $k_1/\Gamma_1$ with magnetic moment along the 1-2 Ir-O bonds (cf. figure above) produced the best fit. However, fits with $k_2/\Gamma_1$ and the moment oriented along the 3-4 axis are only marginally inferior.