Experimental report

24/10/2016

Proposal: 5-23-681 **Council:** 4/2015

Title: Topochemically Reduced Iridium Double Perovskite Phases

Research area: Chemistry

This proposal is a new proposal

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Samples: Sr2FeIrO4
Sr2CoIrO6

Instrument	Requested days	Allocated days	From	To
D2B	2	2	02/12/2015	04/12/2015
D20	0	0		

Abstract:

We propose to collect neutron powder diffraction data from Sr2FeIrO4 and Sr2CoIrO4 at room temperature to determine their anion-deficient crystal structures. We also propose to collected data at low temperature to determine their magnetically ordered structures. Magnetisation measurements indicate the two phases should be formulated as Sr2M(II)Ir(II)O4 (M=Fe, Co) and as such they represent the first examples of Ir(II) in an extended oxide phase.

Neutron powder diffraction data were collected from $LaSrNiIrO_6$ at room temperature and 5K. Analysis of the data collected at room temperature (Figure 1) confirmed that $LaSrNiIrO_6$ has a pseudo-cubic monoclinic structure. A model with space symmetry $P2_1/n$ and B-site cation order was refined against the data collected and gave an excellent statistical fit. The crystallographic unit cell obtained from this analysis is shown in Figure 2.

Neutron powder diffraction data collected at 5K had addition peaks compared to the room temperature data. These extra peaks could be attributed to long range magnetic order. A series of models were constructed with highs spin Ni^{2+} (d^8 s=1) and diamagnetic Ir^{5+} (d^4 J_{eff}= 0) were constructed. The best fit was obtained with a unit cell related to the crystallographic unit cell by a 2x1x2 expansion with G-type antiferromagnetic ordering. In this model the spin vectors are aligned parallel to the crystallographic *c*-axis. The refinement of this model against the data gave an excellent fit and is shown in Figure 3.

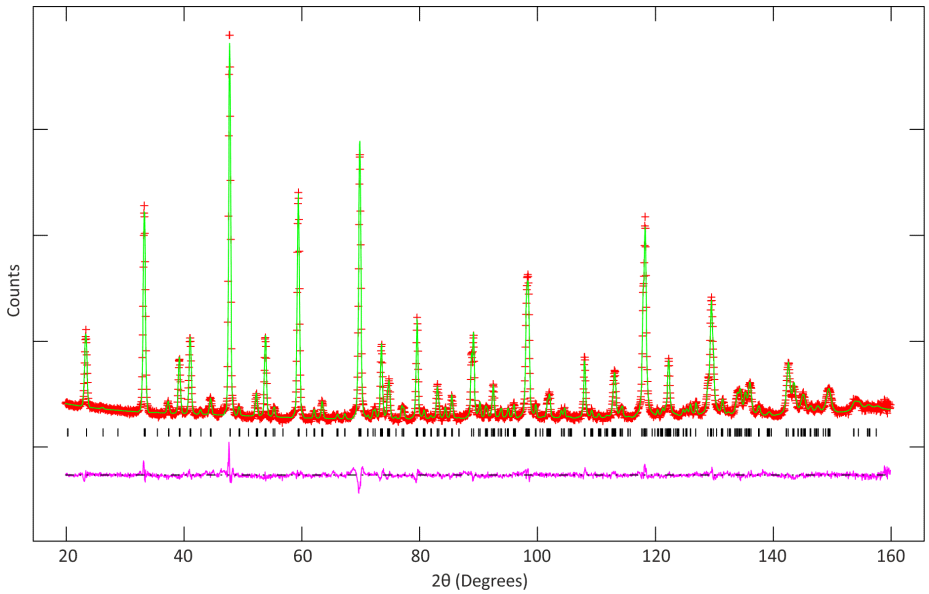

Figure 1. Observed, calculated and difference plots from the refinement of a $P2_1/n$ model against neutron data collected from $LaSrNiIrO_6$ at room temperature

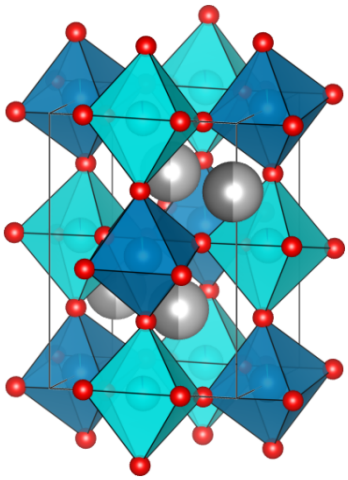

Figure 2. Crystallographic unit cell of $LaSrNiIrO_6$

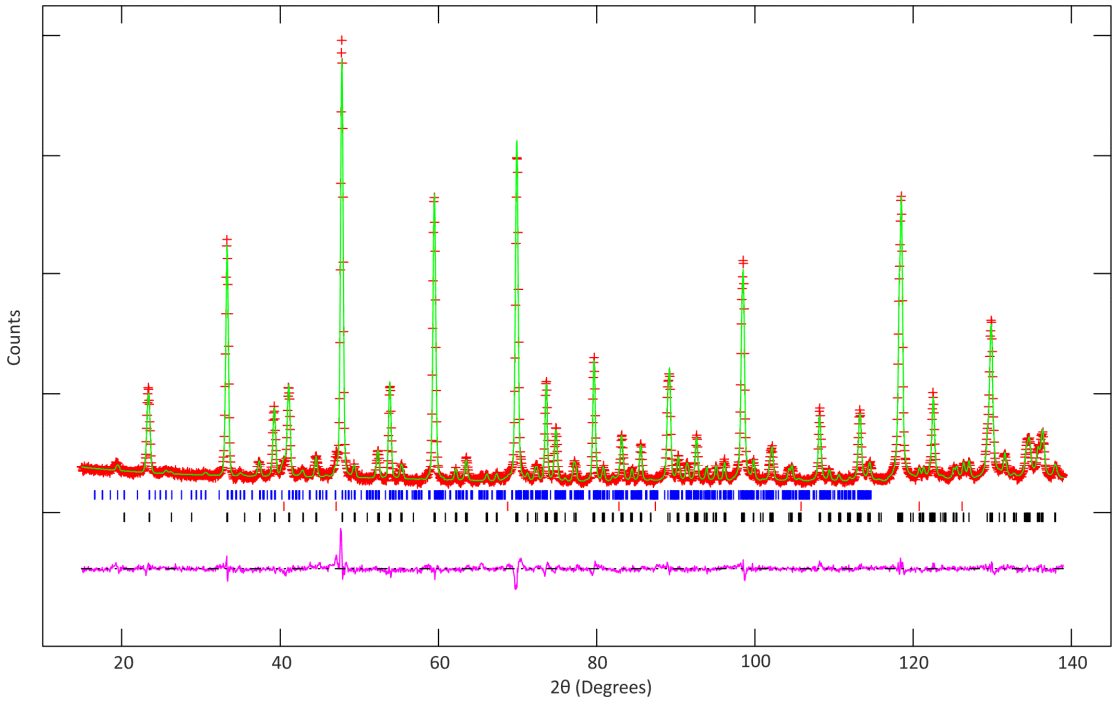

Figure 3. Observed, calculated and difference plots from the refinement of a $P2_1/n$ model against neutron data collected from $LaSrNiIrO_6$ at 5K. Black tick marks are structural peaks, blue tick marks are magnetic peaks and red tick marks are the unknown cubic phase.

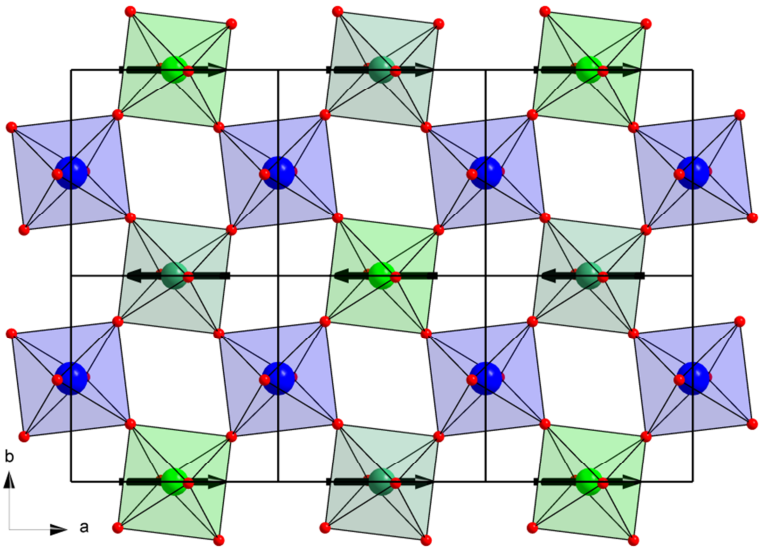

Figure 4. The refined magnetic structure of LaSrNiIrO6. Green octahedra represent Ni^{2+}, blue octahedra represent Ir^{5+}