Experimental report

01/08/2024

Proposal: 5-31-2958 **Council:** 4/2023

Title: Structure and magnetic ordering ofthe new layered oxide chalcogenideSr3Fe4S2O6

Research area: Chemistry

This proposal is a new proposal

Main proposer: Simon James CLARKE

Experimental team: Alexis GILLETTE
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Samples: Sr3Fe4S2O6

Instrument	Requested days	Allocated days	From	To
D2B	1	1	31/08/2023	01/09/2023
D1B	1	1	30/08/2023	31/08/2023

Abstract:

This proposal is to explore a new compound Sr3Fe4S2O6 devised using a building block approach and probe the magnetic ordering on the two Fe sublattices, and the evolution of this order and the subtleties of the distorted crystal structure as a function of temperature. Sr3Fe4S2O6 contains Fe3+ ions in FeO5 square-based pyramids sharing all their vertices with similar units, and Fe2+ ions in FeO2S4 distorted octahedra compressed along the axial Fe¿O bonds and sharing faces. The communication between the two magnetic sublattices and the correlation with the subtle structural distortion will be probed optimally using a D2B/D1B combination.

EXPERIMENTAL REPORT

EXPERIMENT N° 5-31-2958 INSTRUMENT D1B, D2B

DATES OF EXPERIMENT 30/08/2023 to 01/09/2023

TITLE Structure and magnetic ordering ofthe new layered oxide chalcogenideSr3Fe4S2O6

EXPERIMENTAL TEAM (names and affiliation)

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Date of report 01/08/24

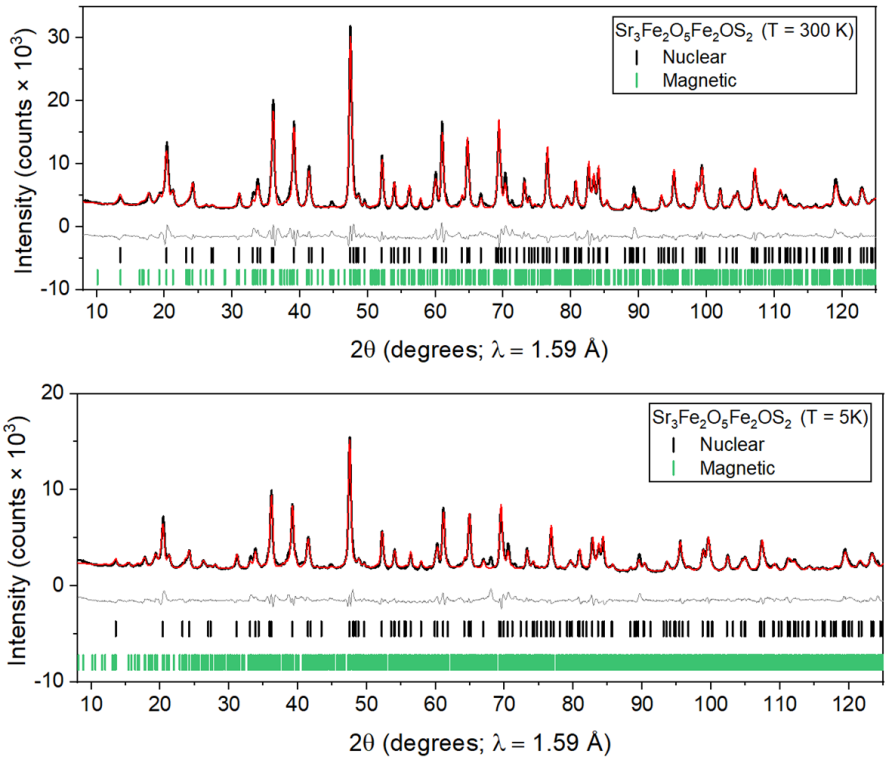

Fig. 1. NPD pattern of $Sr_3Fe_4O_6S_2$ measured at T = 300 K (top) and T = 5 K (bottom) on the D2B instrument at the ILL showing the observed (black), calculated (red) and difference (grey) curves. There are two Fe sublattices with magnetic ordering present one one of them at 300K and with the additional magnetic scattering appearing at 5K arising from order on the second sublattice. Some subtleties in the magnetic structures are under continued investigation.

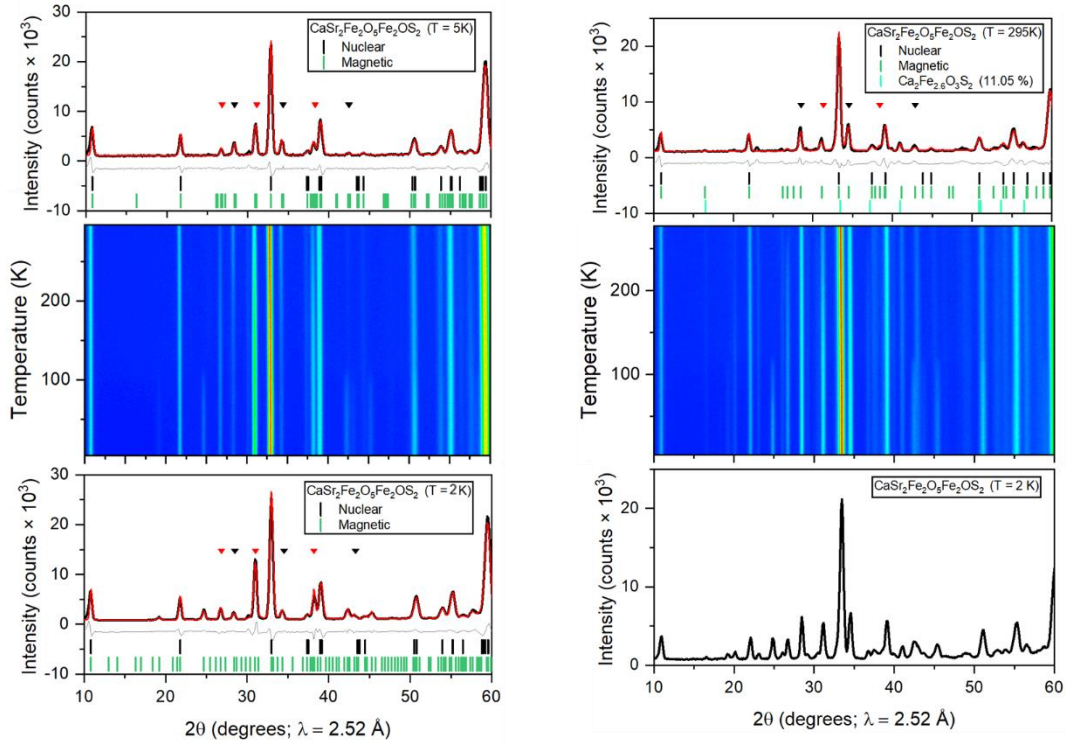

Fig. 2. Variable temperature NPD patterns of $CaSr_2Fe_4O_6S_2$ (left) and $Ca_2SrFe_4O_6S_2$ (right) measured on the D1B instrument at the ILL with Rietveld refinements at T = 300 K (top) and T = 2 K (bottom) showing the observed (black), calculated (red) and difference (grey) curves. The red and black triangles denote magnetic reflections from two distinct magnetic models.

The data gathered on the D2B instument were useful for the detailed structural refinement, whereas that gathered on D1B was important for the determination and analysis of the magnetic models, due to their high resolutions at the relevant d-spacings. The D1B data was particularly useful in determining the most likely magnetic model for the long-range ordering of Fe as there exist two distinct magnetic models that contain Fe^{3+}-containing layers either stacked directly atop one another or offest by ½ of a unit cell translation both at room and low temperatures.

Overall the experiment was a full success and we were able to have a prliminary look at the samples in which some Sr had been replaced by Ca. Remaining analyses are still in progress. The work carried out in this experiment will be published in an international journal and will form a significant part of the D.Phil thesis of Alexis Gillette.