Experimental report

15/05/2024

Proposal: 5-31-2960 **Council:** 4/2023

Title: Metamagnetism in Sr2MnO2Na1.7Se2

Research area: Chemistry

This proposal is a resubmission of 5-31-2931

Main proposer: Simon James CLARKE

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Souvik GIRI

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Samples: Sr2MnO2Na1.7Se2

Instrument	Requested days	Allocated days	From	To
D20	1	0		
D2B	1	1	08/11/2023	09/11/2023

Abstract:

This proposal is to explore the magnetic ordering in the metastable mixed-valent Mn2+/3+ oxide chalcogenide prepared using soft chemical synthesis. Measurements using 2.4 Å neutrons of the magnetic scattering in zero field and in an applied magnetic field will enable us to fully characterise the material. This follows a preliminary 1.6 A D2B experiment (5-31-2880) to show that there exist magnetic Bragg peaks. Magnetometry shows the antiferromagnetic ordering and the metamagnetism in applied fields. The behaviour is distinct in its details from that of other members of this class and characterisation of this phase will give a fuller understanding of the complexity of these mixed-valent manganese oxide chalcogenides.

EXPERIMENTAL REPORT

EXPERIMENT N° 5-31-2960 INSTRUMENT D2B

DATES OF EXPERIMENT 8/11/2023 to 9/11/2023

TITLE Metamagnetism in Sr2MnO2Na1.7Se2

EXPERIMENTAL TEAM (names and affiliation)

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Date of report 15/05/24

We have determined the magnetic ordering in a layered manganese oxide sulfide in zero field and in an applied field. This shows that the sample is metamagnetic and at zero field at 5K it has ferromagnetic MnO_2 sheets coupled antiferromagnetically. Above 2 Tesla there is a transition to a fully ferromagnetis state. This is part of work on the synthesis series of metastable new materials using soft chemistry as well as an investigation of the fundamental chemistry. Measurements were done on D2B instrument using 1.6 Å neutrons in the cryomagnet. The sample was physically constrained within the vanadium can using Cd discs. This work has been accepted for publication in *Chemistry of Materials* for the CNR Rao 90th Birthday special issue, and forms an important part of the PhD thesis of Souvik Giri.

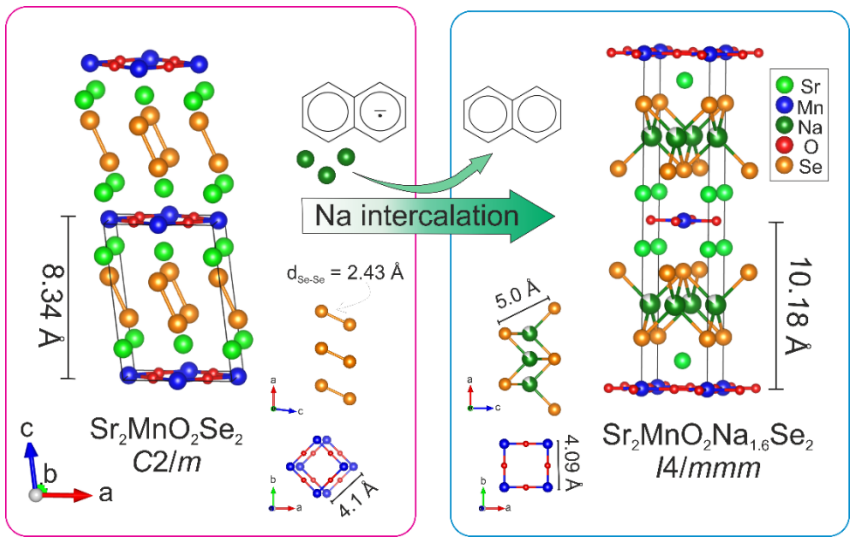

Fig 1: Schematic of topochemical Na intercalation into $Sr_2MnO_2Se_2$ structure with $[Se_2]^{2-}$ dimers, using $Na^+[C_{10}H_8]^-$ as reductant. Na intercalation leads to cleavage of the Se-Se bond, forming $[Na_{2-x}Se_2]$ layers. The measurements of D2B confirmed that the product initially formed has x = 0.3, but rapidly oxidises to the sample characterised in this experiment which is $Sr_2MnO_2Na_{1.6}Se_2$

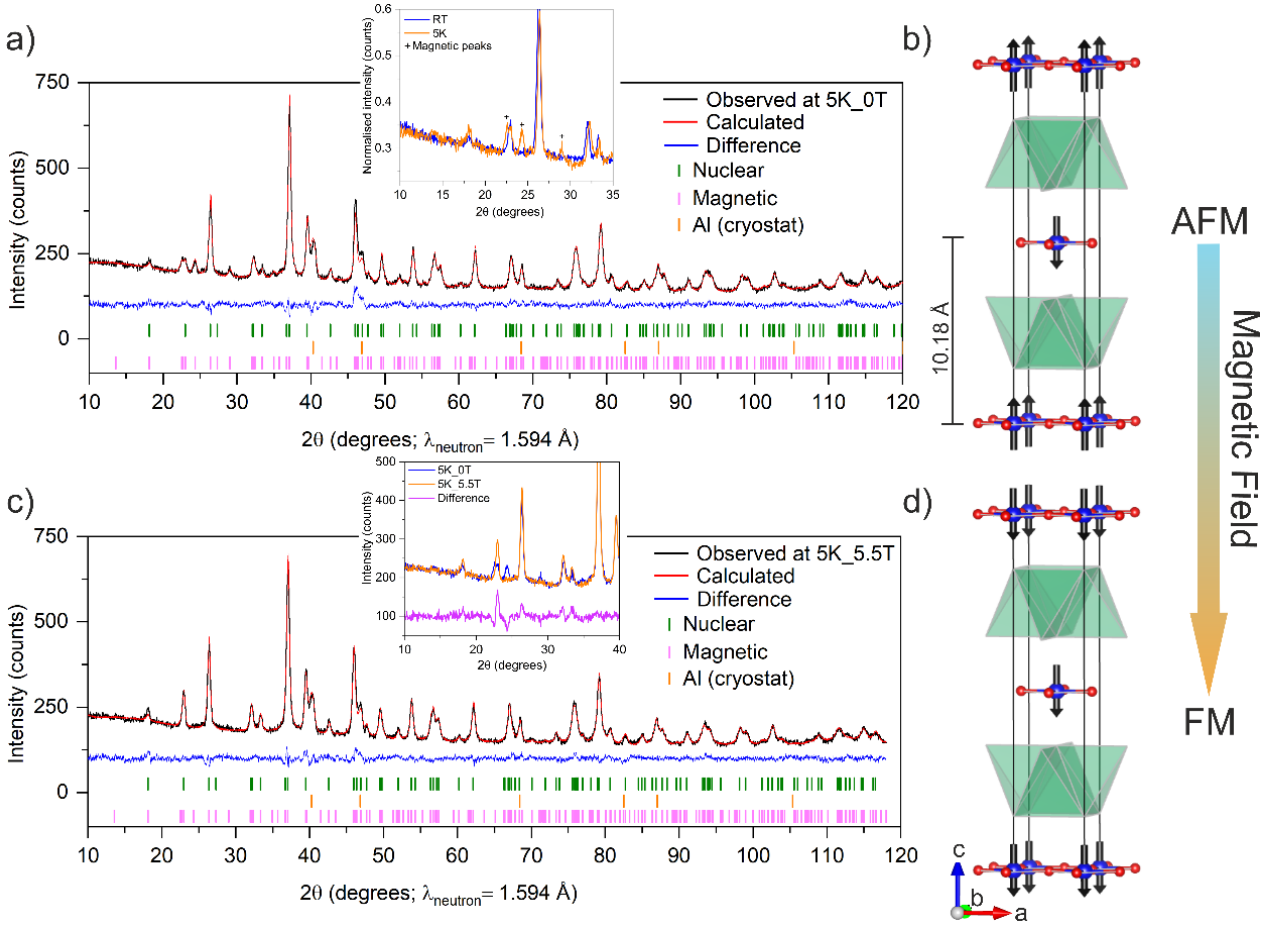

Fig 2: a) Rietveld refinement against NPD data at 5 K without magnetic field R_{wp} = 3.47 % and χ^2 = 1.3. Inset: highlighting the appearance of magnetic Bragg reflections at 5 K compared with the room temperature pattern. b) the magnetic structure of $Sr_2MnO_2Na_{1.6}Se_2$ at zero magnetic field where Mn moments interact ferromagnetically within MnO_2 planes and antiferromagnetically between two adjacent MnO_2 planes. c) Rietveld refinement against PND data at 5K at 5.5 T magnetic field R_{wp} = 3.07 % and χ^2 = 1.34. Inset: highlighting the disappearance of magnetic Bragg reflections and the emergence of magnetic intensity on top of the nuclear peaks. d) The magnetic structure of $Sr_2MnO_2Na_{1.6}Se_2$ in a 5.5 T magnetic field where the compound has undergone the metamagnetic transition and is in the ferromagnetic regime.