Experimental report

14/02/2025

Proposal: 5-31-2768 **Council:** 4/2020

Title: The magnetic structure of VPS3

Research area: Physics

This proposal is a new proposal

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Samples: V0.9PS3

Instrument	Requested days	Allocated days	From	To
D7	7	5	28/01/2021	02/02/2021

Abstract:

The family of compounds MPS3 (M = transition metal) are examples of quasi-two dimensional materials. The transition metal atoms lie on a honeycomb lattice in the ab planes, and the planes are weakly bound by van-der-Waals forces.
One compound that has received little attention is VPS3. It has the smallest electronic band gap of the family, making metallization under pressure more achievable; a study we recently carried out. The compound is not fully stoichiometric when synthesized and is deficient in vanadium. The magnetism of the compound is potentially interesting as theory suggests a honeycomb lattice of S = 3/2 moments might dimerize to form a Peierls-like structure. The compound also makes an interesting contrast with its sister antiferromagnets CoPS3 and NiPS3, with the same crystal structure and spins S=3/2 and S=1.
We propose to study the magnetic properties of V0.9PS3 as an example of low-dimensional model magnetism, and the role of charge and vacancy disorder on the magnetic properties. We require neutron scattering to determine the magnetic structure. Test measurements have suggested this structure to be an interesting contrast to the rest of the MPS3 family.

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The magnetic structure of VPS_3

D7 2020

5 days were allocated for this proposal, which followed on from 2 single crystal studies at the ILL (5-41-1002 on D10, 5-41-962 on D19). We were not able to resolve any magnetic Bragg peaks in the anticipated positions for MPS_3 in those runs. We also carried out a powder measurement on D20 (Easy-Access continuation to 5-41-1002), which showed no resolvable differences between high and low temperature diffraction plots, no magnetic signal.

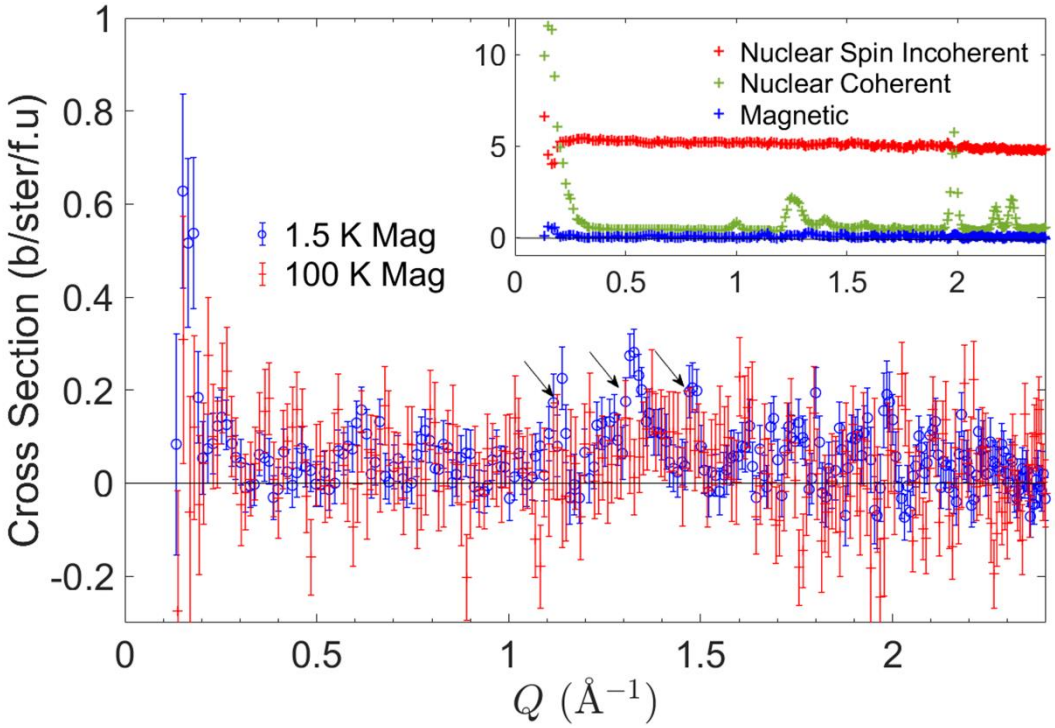

Fig 1 - Powder diffraction patterns of $V_{0.9}PS_3$ taken during previous test on D7 with less sample. Polarisation analysis has been used to extract only the magnetic contribution to the scattering. Blue datapoints were taken at 1.5 K, red at 300 K. Inset- relative small size of the magnetic scattering.

Measurements were done on as-grown powder sample from batch 17OctMJC06. The first day was used in alignment and calibration, then data were collected for 48 hours at 1.5 and 100 K, above and below magnetic transition temperature.

The polarisation analysis was, fundamentally, successful in separating out the scattering contribution from vanadium's nuclear spin incoherent response. This swamps the actual magnetic signal and would easily explain why no signal was resolvable on e.g. D20.

The data reveal possible hints of magnetic order peaks at low temperature. These peaks are at Q values not expected, not seen in other MPS_3 materials (they index at an estimated (1/3 1/3 0). The data are not conclusive and further work is required.

Retyring this experiment with ~10 times the volume of sample will get signal-background ratio down enough to reliably resolve these features. Crystal growth of these materials is a challenge, so the next step is producing a batch of sufficient mass to attempt this measurement again. The material is of pressing current interest and has many unanswered questions, and the magnetism seems unusual – from these first data and from magnetometry – so it seems well worth the effort.