Experimental report

02/10/2021

Proposal: 5-31-2574 **Council:** 4/2017

Title: Magnetic structure of the 4d honeycomb antiferromagnet MoSiP3O11

Research area: Physics

This proposal is a new proposal

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Samples: MoSiP3O11

Instrument	Requested days	Allocated days	From	To
D2B	1	1	18/06/2018	19/06/2018
D20	1	1	23/05/2018	24/05/2018

Abstract:

We propose to investigate crystal and magnetic structures of MoSiP3O11, a 4d honeycomb antiferromagnet that may potentially host exotic spin states with valence-bond-solid correlations. We will determine ordered magnetic moment on Mo3+ and assess its reduction with respect to the classical spin-only value. We will also explore the nature of magnetic order in this material, investigate underlying magnetic interactions, and analyze the role of the spin-orbit coupling. Our results will shed light on the scarcely investigated magnetism of Mo3+ and provide a useful reference for the ongoing research on honeycomb materials with 4d and 5d transition metals.

***Experimental report* on 5-31-2574**

Magnetic structure of the $4d$ honeycomb antiferromagnet $MoSiP_3O_{11}$

Neutron diffraction on MoP_3SiO_{11} has been measured at D2B ($T = 1.5, 10, 100, 295\,\mathrm{K}$) and D20 ($T = 1.5 - 12\,\mathrm{K}$). Above $T_N = 6.7\,\mathrm{K}$, the patterns could be refined in the $R\bar{3}c$ space group, which is higher in symmetry than $C2/c$ proposed previously [1]. This observation led us to perform a high-resolution x-ray diffraction measurement (at ID22, ESRF) that confirmed the absence of a monoclinic distortion and thus revised the crystallographic symmetry of MoP_3SiO_{11} as trigonal.

Below T_N, magnetic scattering with the propagation vector $\mathbf{k} = 0$ was observed. A subsequent refinement of the collinear antiferromagnetic model produced the size and direction of the Mo^{3+} magnetic moment. This magnetic structure is fully in line with the exchange couplings calculated *ab initio*.

The results of this study were published in [Phys. Rev. B 104, 094428 (2021)]. The paper was chosen as Editors' Suggestion.

[1] A. Leclaire and B. Raveau, J. Solid State Chem. 71, 283 (1987).

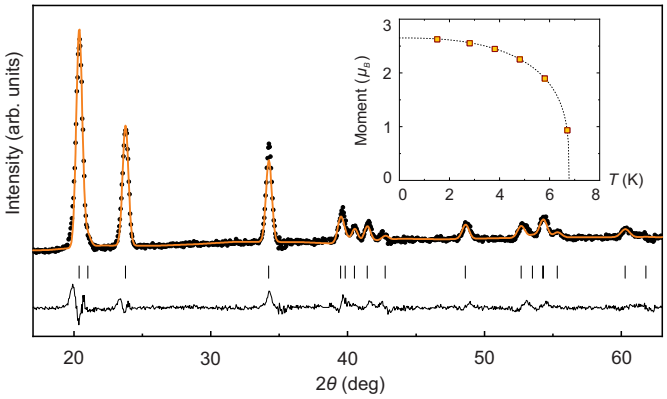

Figure 1. Rietveld refinement for the magnetic neutron scattering obtained by subtracting the 12 K data (above T_N) from the 1.5 K data (below T_N). The orange line is the fit with the covalent magnetic form factor calculated *ab initio*. The inset shows temperature dependence of the ordered magnetic moment and its empirical fit with $\mu = \mu_0[1 - (T/T_N)^\alpha]^\beta$ where $T_N = 6.78\,\mathrm{K}$, $\alpha = 2.5$, $\beta = 0.29$, and $\mu_0 = 2.65\,\mu_B$.