Experimental Report

Proposal: **4-01-1377** **Council:** 4/2014

Title: The magnetic density of states in NiPS3

This proposal is a new proposal

Researh Area: Physics

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Experimental Team: LANCON Diane

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Samples: NiPS3

Instrument	Req. Days	All. Days	From	To
D7	5	5	11/09/2014	16/09/2014

Abstract:

NiPS3 belongs to a family of quasi-2D antiferromagnets on a honeycomb lattice. We have previously used neutron spectroscopy to establish that other members of the family are very good model magnets, namely: MnPS3, which is Heisenberg-like; and FePS3, which is Ising-like. NiPS3 shows novel effects in comparison, and we now wish to measure the magnetic density of states from a powder using time-of-flight spectroscopy. We already have data from a thermal three-axis spectrometer that shows a potential feature at ~6.5 meV and need a combination of IN4 and D7 to verify that this mode is indeed magnetic, and to search for magnetic features at larger energy transfers.

This is a preliminary report describing the results of experiment 4-01-1377 on D7:

The magnetic density of states in $NiPS_3$

carried out by Diane Lançon and Andrew Wildes on D7, 11 - 16 September 2014.

The experiment was conducted using 3.1 Å neutrons. The sample was composed of 10.6 g of powdered $NiPS_3$. Powdered samples of this material are notorious for having preferred orientation issues due to their two-dimensional nature. In an attempt to improve this, the sample mass was divided into three parts and pressed into cylindrical pellets. The pellets were then stacked such that their cylindrical axes were orthogonal.

Preliminary experiments showed that the sample contained water, giving significant nuclear spin incoherent scattering. Consequently, the sample was heated to 105°C in a dry nitrogen atmosphere for 5 days prior to the experiment.

Measurements were initially performed in diffraction mode. Data were taken at 300 K and 2 K, with associated quartz and vanadium calibration measurements and with measurements of an empty sample can and cadmium for background. The data showed that a substantial amount of water remains in the sample. This is a new discovery, although it does not appear to have implications for the magnetic properties of the material as magnetic and nuclear Bragg peaks were observed at the expected positions.

Figures showing the data from the diffraction mode measurements are in preparation.

The chopper was subsequently put in the incident beam and the scattering from the sample was measured in time-of-flight mode. The sample was measured for ~ 2 days at 2 K and ~ 1 day at 300 K. Measurements of an empty sample can (~ 12 hours) and vanadium (~ 12 hours) were performed for background and time-of-flight calibration.

Figure 1 shows preliminary data from $NiPS_3$. The data come from the total scattering time with a rudimentary background subtraction. A more sophisticated treatment of the data is forthcoming.

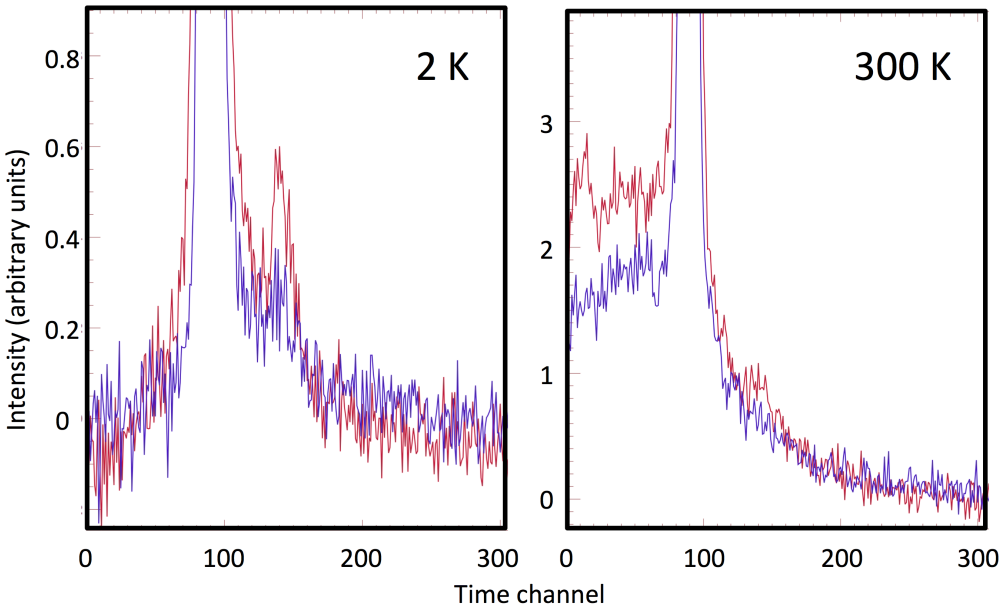

Figure 1: Data from a 10g sample of powdered $NiPS_3$, measured on D7 with fixed E_i = 8.5 meV. The red data correspond to non-spin flip intensities, while the blue correspond to spin flip.

The data appear to show a small feature at 2 K in time channel ~140, which corresponds to an energy transfer of ~3 meV. This may be due to a spin wave gap. If so, it would suggest that the anisotropy in $NiPS_3$ is substantially smaller than 1.39 meV, which was a value suggested from the literature [1]. The value may be based on poor data, however. The value was derived from susceptibility measurements, which showed some anisotropy above the Néel temperature. Our susceptibility measurements on single crystals of $NiPS_3$ show that the act of gluing a sample to a support will give a signal that appears to be anisotropic, while a sample that has not been glued shows isotropic susceptibility above the Néel temperature. Hence, it is feasible that a 3meV gap exists in $NiPS_3$. Figure 2 shows a comparison of the two susceptibilities.

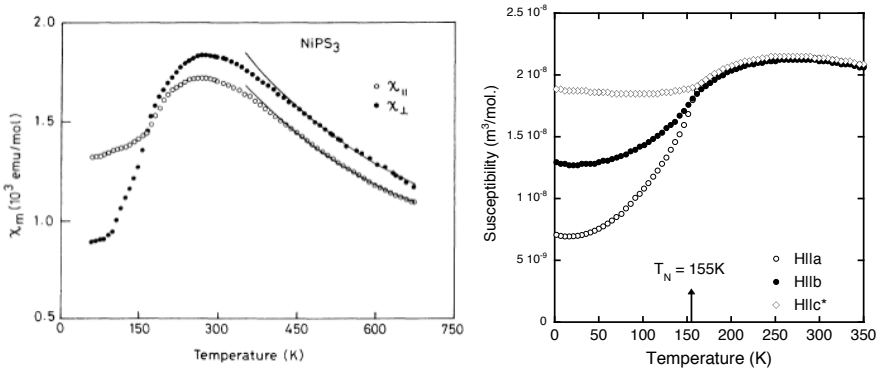

Figure 2: Susceptibilities of $NiPS_3$, as shown in reference [1] (left) and by our own work on single crystals that have not been glued to a sample support (right).

The experiment appears to represent the limits of what is reasonably achievable in using D7 as a spectrometer. The moment is small in this material, S = 1, and required a measuring time of 2 days to have something which requires significantly more statistics. Furthermore, there is no evidence of spin waves at the Brillouin zone boundary, which is not surprising as this is probably higher than the E_i = 8.5 meV incident energy used for the experiment, which is the maximum that can be reached on D7. We plan to ask for a continuation on IN4 to verify the existence of a mode at 3meV, and to attempt to fully measure the magnon density of states.

[1] P. A. Joy and S. Vasudevan, Phys. Rev. B **46** (1992) 5425