Experimental report

18/09/2024

Proposal: 5-31-2957 **Council:** 4/2023

Title: Canted magnetic structure of a Honeycomb lattice NdPt6Al3 using neutron diffraction

Research area: Physics

This proposal is a new proposal

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Samples: NdPt6Al3

Instrument	Requested days	Allocated days	From	To
D1B	2	2	25/09/2023	27/09/2023
D20	2	0		

Abstract:

Honeycomb lattice magnets have attracted considerable attraction due to the bond dependent exchange interactions based on the exactly solvable Kitaev Honeycomb model, resulting in a quantum spin-liquid ground state. We have investigated honeycomb lattice CePt6Al3 using neutron diffraction and muon spin rotation, which revealed a paramagnetic ground state down to 90 mK, which is surprising and opens debate whether geometrical frustration supresses the magnetic ordering to T = 0 K. To understand this unusual behaviour, we have now synthesised NdPt6Al3, which exhibits a magnetic ground state as evident from the bulk measurements. In fact, the heat capacity reveals a sharp maximum at 1.2 K, indicating a long-range magnetic ordering. Furthermore, our single crystal magnetization shows easy-plane anisotropy with a spontaneous ferromagnetic moment of 0.26 ¿B/Nd for a field perpendicular to the c-axis. We expect that the small FM component in the AFM ordered state is caused by canting of the Nd moments by the Dzyaloshinski-Moriya interaction as recently suggested for GdPt6Al3. We propose to investigate the canted magnetic structure of NdPt6Al3 in the presence of DM interaction using D20.

Experimental report of neutron powder diffraction for $NdPt_6Al_3$ on D20/D1B, ILL (Exp No: 5-31-2957)

Honeycomb lattice compounds have been much interested in a wide field of magnetism and magnetic materials because magnetic frustration, Kitaev interaction, and Dzyaloshinskii-Moriya (DM) interaction induce unconventional magnetic orders and novel quantum states. As a new perfect honeycomb series with three-fold rotational symmetry, $RE Pt_6Al_3$ (RE = Ce, Pr, Nd, Sm, Gd, and Tb) series was reported in 2017 to crystallize in the trigonal structure with the centrosymmetric space group $R\bar{3}c$. Our previous study for single-crystalline samples suggested that $NdPt_6Al_3$ orders in a canted antiferromagnetic (AFM) structure at T_m = 1.2 K.

To determine the magnetic structure of $NdPt_6Al_3$, neutron powder diffraction (NPD) experiments were performed with the high-intensity D20 and D1B powder diffractometers at ILL. For the NPD, we prepared polycrystalline samples by arc melting stoichiometric quantities of the elements with subsequent annealing at 1100°C for 10 days. The powdered sample of 10 g was introduced in the cylindrical Cu sample holder (5 mm diameter) with He-exchange gas, which was set in a 3He-4He dilution cryostat. The diffraction measurements were carried out in zero field between 0.05 and 1.6 K. Rietveld refinements were done using the software FullProf.

Figure (a) displays the diffraction patterns at 1.6 K > T_m and 0.05 K < T_m with a neutron wavelength of 2.524 Å. The refinement of the crystal structure at 1.6 K yielded the trigonal lattice parameters a = 7.5141(6) Å and c = 39.091(3) Å. Note that the peak marked by the arrows in the pattern at 0.05 K are significantly enhanced compared with those at 1.6 K. Figure (b) represents the differential intensity obtained by subtracting the intensity at 1.6 K from that at 0.05 K. It is noteworthy that all the peaks can be indexed with a propagation vector **k** = [0, 0, 0].

Magnetic symmetry analysis using the program BASIREPS for Wyckoff site 12c of the Nd atoms with the centrosymmetric space group $R\bar{3}c$ returned six allowed irreducible representations (IR). Out of the above six IRs, one of the IRs with BVs within the honeycomb plane gives the best refinement shown in Fig. (b).

The proposed magnetic structure of $NdPt_6Al_3$ is depicted in Fig. 11(c), whose magnetic space group is #15.85 $C2/c.1$. The ordered moment of the Nd^{3+} ion was refined as 2.62(2) μ_B. As shown in the inset of Fig. (b), the NN Nd^{3+} moments are canted from antiparallel alignment by an angle of 15°. We propose that the canting of AFM moments results from the DM interaction between the nearest neighbor Nd^{3+} moments at the midpoint of which the inversion symmetry is broken by the presence of the Pt triangle inside the Nd hexagon.

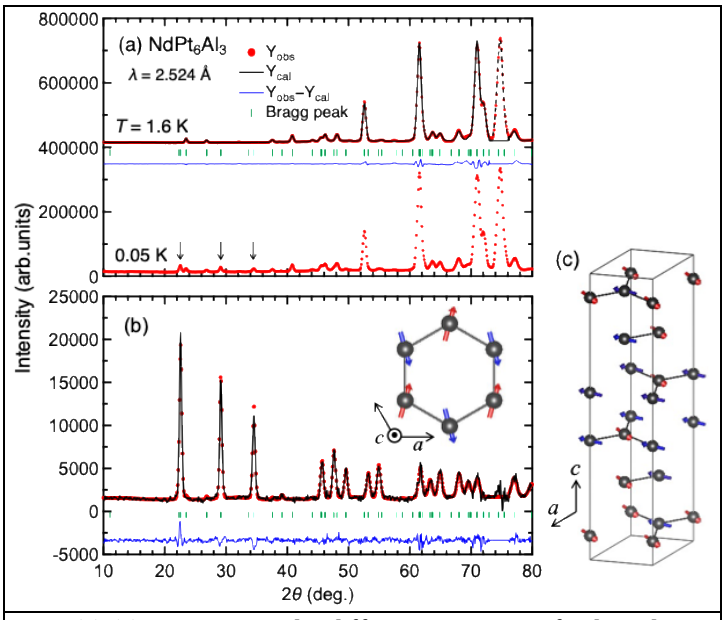

FIG. (a) (a) Neutron powder diffraction patterns of $NdPt_6Al_3$ at 1.6 and 0.05 K collected at the D1B diffractometer. (b) Rietveld refinement of the magnetic intensities obtained by subtracting the pattern at 1.6 K from that at 0.05 K. (c) The canted AFM structure of $NdPt_6Al_3$.