

Experimental report

19/06/2026

Proposal: 5-31-3073

Council: 10/2024

Title: Spin correlations of the highly-frustrated centred-pyrochlore latticemagnet Mn(ta)₂

Research area: Physics

This proposal is a new proposal

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Samples: Mn(N₃C₂D₂)₂

Instrument	Requested days	Allocated days	From	To
D20	2	2	30/06/2025	02/07/2025

Abstract:

The centred pyrochlore lattice is extremely highly frustrated lattice, and we have recently shown that it has a spin liquid phase even more degenerate than the canonical pyrochlore and kagome lattices when considering nearest and next nearest neighbour Heisenberg interactions . It also also is described by an emergent Coulomb gauge field theory coupled to gauge charges, that can be seen as a "three-dimensional slab" of a four-dimensional structure.

We have recently uncovered the first example of a material that realises this model: the metal-organic framework Mn(II) triazolate (Mn(ta)₂). Mn(ta)₂ is highly frustrated ($T_{CW}/T_c \sim 50$, $T_c = 430$ mK) and bulk property measurements suggest this material will have a spin liquid phase around 1-2K before ordering into a complex structure in its ground state. We therefore propose to carry out the first neutron diffraction study of the ordered state of this compound to determining the magnetic ground state.

Experimental Report – Proposal 5-31-3073

Spin correlations of the highly-frustrated centred-pyrochlore lattice magnet $\text{Mn}(\text{ta})_2$

The experiment was successfully completed on D20 using a 2 g deuterated powder sample of $\text{Mn}(\text{ta})_2$. The primary objective was to determine the magnetic ground state of this highly frustrated centred-pyrochlore lattice magnet and to investigate the evolution of magnetic correlations across its ordering transition at $T_N \approx 0.43$ K. The experiment also aimed to characterise diffuse magnetic scattering associated with the predicted spin-liquid regime and to study the influence of helium adsorption on the magnetic and structural properties.

Neutron diffraction data were collected over a broad temperature range extending from approximately 70 mK to 200 K. Long counting measurements were performed at key temperatures including 70 mK, 0.5 K, 0.75 K, 1 K, 1.25 K, 2 K, 5 K, 10 K, 25 K and 200 K. Additional cooling and warming ramps were measured through the ordering transition to follow the temperature evolution of the magnetic scattering and order parameter. Complementary measurements under helium and under vacuum were also performed to investigate helium uptake within the framework and its associated phase transition.

The experiment successfully achieved its main objective. High-quality low-temperature diffraction data revealed the magnetic ground state of $\text{Mn}(\text{ta})_2$ for the first time. Analysis of the data is currently underway and has enabled the determination of the magnetic structure and the nature of the ordered state. Temperature-dependent measurements clearly capture the evolution of the magnetic correlations through the ordering transition.

The dataset is also being combined with complementary inelastic neutron scattering measurements and theoretical modelling to determine the magnetic Hamiltonian of the centred-pyrochlore lattice. The results provide the first experimental characterisation of magnetism on this lattice topology and will be compared with theoretical predictions for the highly frustrated Heisenberg model previously proposed for $\text{Mn}(\text{ta})_2$.

Data analysis is ongoing using Rietveld refinement, magnetic symmetry analysis and modelling of the magnetic correlations. The results obtained from this experiment form the basis of a manuscript currently in preparation in collaboration with experimental and theoretical partners.

