Experimental report

13/02/2019

Proposal: 5-32-862 **Council:** 4/2018

Title: Geometrical Frustration in Metal–Organic Frameworks based on the Trillium Net

Research area: Chemistry

This proposal is a new proposal

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Samples: sodium cobalt formate
sodium manganese formate

Instrument	Requested days	Allocated days	From	To
D7	7	7	18/10/2018	22/10/2018

Abstract:

We propose to study the interplay between compositional and magnetic disorder in the frustrated trillium-net metal-organic frameworks NaM(DCOO)3 (M = Mn, Co). As part of the study we will develop the spinvert code to enable magnetic refinement for systems with inhomogeneous distributions of magnetic species. The project is also associated with a 3-month Stagaire position supported by the ILL.

Preliminary Report

Due to technical problems, we were unable to synthesise a pure powder sample of $NaMn(DCO_2)_3$ or $NaCo(DCO_2)_3$.Thankfully, we were able to use an already synthesised and characterised sample – 0.41g of undeuterated $NaMn(HCO_2)_3$ – but have been unable to source any $NaCo(DCO_2)_3$. For these reasons, the decision was taken to split the (7-day) experiment into two 4-day experiments – one of which occurred during the scheduled dates and the other is planned for the next cycle. What follows is the report for the former experiment on $NaMn(HCO_2)_3$.

We were able to measure at two temperatures with sufficient statistics, the lowest of which (1.5 K) was the base temperature for the standard D7 cryostat. We used the 10 point method to separate magnetic from nuclear scattering and spin incoherent scattering and magnetic scattering was normalised by fitting a scale factor to the nuclear diffuse scattering (an internal standard). Results after normalisation are shown in Figure 1.

The presence of a diffuse hump in the 1.5 K data at ~ 0.8$Å^{-1}$ is in line with theoretical predictions for a trillium anti-ferromagnet and its disappearance at 20 K demonstrates that this temperature is in the paramagnetic limit. We hope to publish these results with a rigorous analysis in the near future.

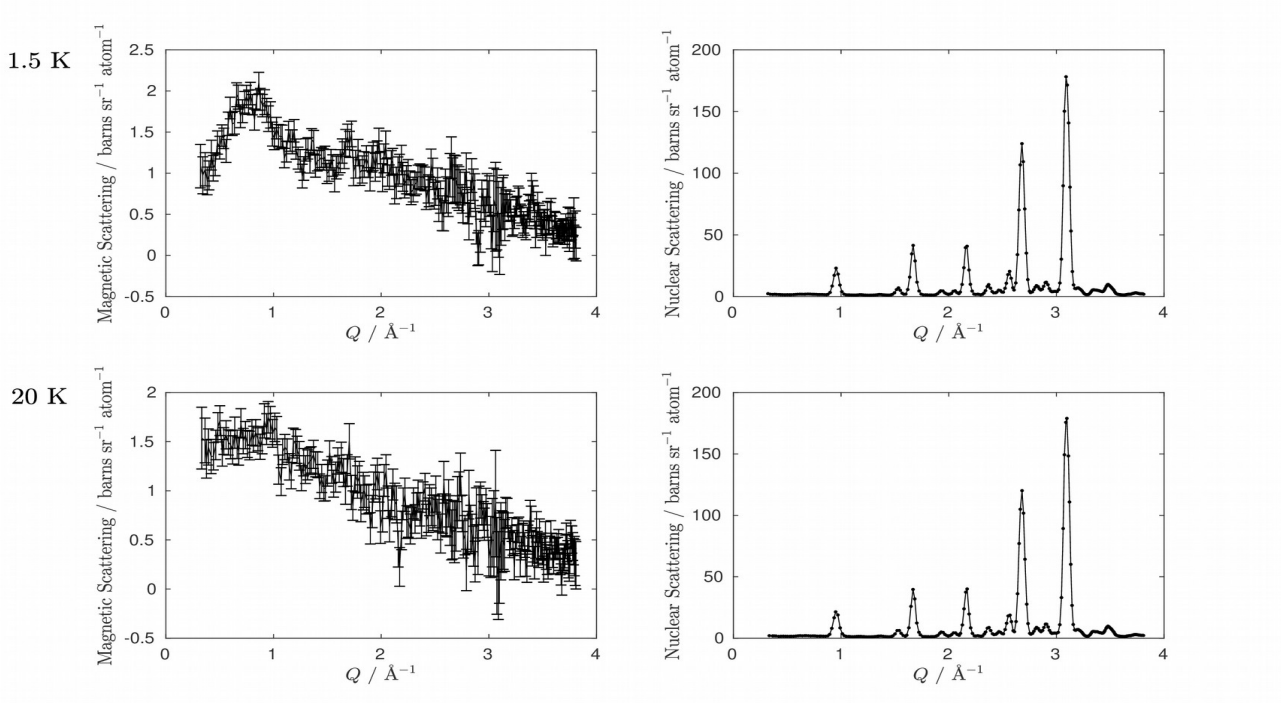

Figure 1 – Normalised and processed data showing both nuclear and magnetic scattering at two temperatures – 1.5 K (top) and 20 K (bottom). Error bars on the nuclear scattering are too small to show.