Experimental report

09/10/2019

Proposal: **CRG-2448** **Council:** 4/2017

Title: Magnetic phase transition in quasi-one-dimentional system BaMn2V2O8: a neutron powder diffraction study

Research area:

This proposal is a new proposal

Main proposer: **Beatrice GRENIER**

Experimental team: Yann ALEXANIAN
Beatrice GRENIER
Virginie SIMONET
Quentin FAURE

Local contacts: Claire COLIN

Samples: BaMn2V2O8

Instrument	Requested days	Allocated days	From	To
D1B	1	1	23/04/2018	24/04/2018

Abstract:

Report on the CRG-2448 experiment on D1B entitled:
"Magnetic phase transition in quasi-one-dimensional system $BaMn_2V_2O_8$: a neutron powder diffraction study"

$BaMn_2V_2O_8$ is a compound of the $AM_2V_2O_8$ family [1, 2] of quasi-one-dimensional antiferromagnets. It exhibits a magnetic phase transition at a relatively large Néel temperature of 37 K, supposed to be a canted antiferromagnetic phase from susceptibility measurements. This compound has a crystallographic structure very similar to that of the remarkable, and thus extensively studied, Ising-like compound $BaCo_2V_2O_8$ [3-7], and therefore it is of great interest to study the low temperature magnetic phase of the Mn compound, to highlight the effect of the isotropic nature of the $S = 5/2$ Mn^{2+} spins as compared to the Ising-like nature of the $S = 3/2$ Co^{2+} spins.

In this context, we have done a powder neutron diffraction experiment on D1B, using a 2.52 Å wavelength, to determine the low temperature magnetic structure of $BaMn_2V_2O_8$ and to study the magnetic phase transition.

Powder patterns were recorded first at room temperature, to check the experimental conditions and set up, then at 50 K, i.e. slightly above the Néel temperature T_N, and well below T_N at 2 K, both with a 1 hour acquisition time. A series of patterns, recorded while warming from 2 K up to 50 K, with a 1 K step and a 2 minutes acquisition time for each pattern, additionally confirmed the Néel temperature corresponding to a drop of intensity at 2θ positions indexed with the propagation vector $\vec{k} = (0,0,0)$.

The crystallographic structure could be well fitted from the patterns recorded above T_N and allowed to confirm the published structure. These also provided us with all the necessary information (instrument parameters, scale factor, refinable atomic coordinates and Debye-Waller factors) prior to the magnetic structure refinement.

The powder pattern recorded in the Néel phase at $T = 2$ K was then successfully fitted (see Figure) with the following model: the Mn^{2+} magnetic moments, aligned along the a axis (or along the equivalent b axis), are ferromagnetically coupled in the (a, b) plane and antiferromagnetically along the c axis. A magnetic moment amplitude of 3.85(2) μ_B/Mn^{2+} was refined, with an agreement R_F-factor of 7.32%. This reduced value (as compared to 5 μ_B expected for spins 5/2) is probably due to quantum effects, enhanced by the quasi-one dimensional structure of the $BaMn_2V_2O_8$ antiferromagnet. The ferromagnetic component was tentatively refined but with no success due to the small value of the ferromagnetic component. Note that the orientation of the magnetic moments in the (a, b) plane cannot actually be solved with this sole powder diffraction experiment and an experiment on a single-crystal diffractometer under magnetic field is planned to settle this issue.

The next step will indeed be to use a magnetic field to determine both the magnetic domain selection and the orientation of the in-plane magnetic moment in a $BaMn_2V_2O_8$ single-crystal (proposal submitted on D23), that was successfully grown at Institut Néel [8].

References

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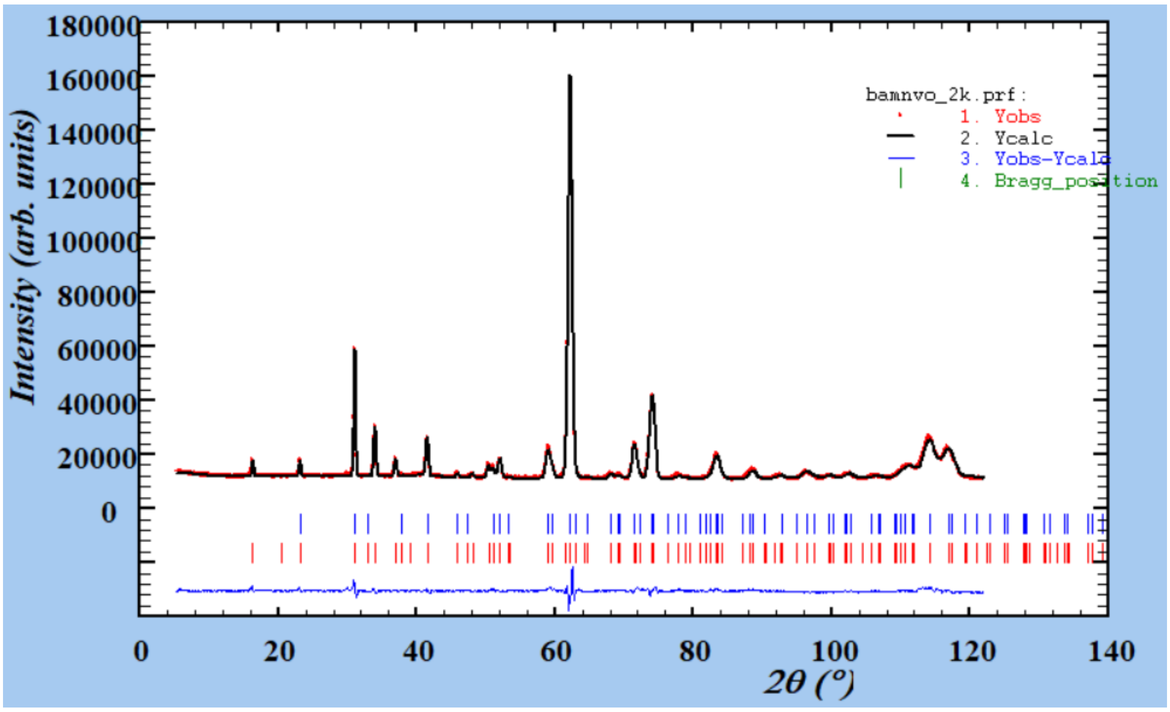

Figure: Nuclear and magnetic structure refinements in the Néel phase of $BaMn_2V_2O_8$ at $T = 2$ K, performed with FullProf. The blue and red ticks correspond to the nuclear and magnetic Bragg reflections, respectively. The difference (blue line) between the observed (red line) and calculated (black line) patterns emphasizes the good quality of the refinement.