Experimental report

27/02/2025

Proposal: 5-41-1237 **Council:** 10/2023

Title: Determination of the magnetic structure in layered trihalide VBr3

Research area: Physics

This proposal is a continuation of 4-01-1759

Main proposer: Milan ORLITA

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Local contacts: Oscar Ramon FABELO ROSA

Samples: VBr3

Instrument	Requested days	Allocated days	From	To
D10	6	5	04/04/2024	09/04/2024

Abstract:

Magnetic van der Waals (vdW) crystals show promising potential for high-tech magnetic, magnetoelectric, and magneto-optic applications. The discovery of 2D ferromagnetism in a monolayer CrI3 at elevated temperatures has greatly promoted research in these materials. The large family of transition metal halides offers a large playground for systematic theoretical and experimental investigation of 2D magnetism.

At present, we focus on the vdW antiferromagnet VBr3, a member of the trihalide family. Our recent Raman spectroscopy experiment has detected the antiferromagnetic magnon in VBr3 at an energy 20 cm-1 (= 2.5 meV) similar to that of the FM counterpart VI3. Our very recent inelastic neutron experiment on VBr3 at ThALES aimed just at the dispersion of this magnetic excitation. However, the experimental setup did not allow us to unambiguously verify the propagation vector and reveal the magnetic structure. The proposed experiment is focused on the determination of the magnetic structure of VBr3. The results will be discussed in the frame of other vdW materials and will considerably support the interpretation of ThALES inelastic neutron scattering data.

Experimental report

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Proposal number: **5-41-1237**

Instrument: **D10**

Date of experiment: 4. – 9.4. 2024

Local contact: Oscar Ramon Fabelo Rosa

Experimental team: Milan Orlita, Milan Klicpera, Ondřej Michal

Abstract:
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Experiment and results:
To reveal the AFM structure of VBr_3 experimentally, we performed a single-crystal neutron diffraction study on a large high-quality single crystal. The collected data confirmed a slight monoclinic distortion of the high-temperature rhombohedral structure below 90 K. The magnetic structure was, nevertheless, investigated within the *R-3* model. The antiferromagnetic structure propagation vector k = (1, 0, ½) was revealed. In an attempt to determine the magnetic structure, 72 non-equivalent magnetic reflections were recorded. The experimental data were confronted with the magnetic space groups dictated by the *R-3* lattice symmetry and propagation vector. The best agreement between the experimental data and the magnetic structure model was obtained for the space group *P-1.1'_c*. The magnetic unit cell of the proposed unique antiferromagnetic structure with periodicity 6c is built from two identical triple layers antiferromagnetically coupled along the c axis. Each triple layer comprises a Néel antiferromagnetic monolayer sandwiched between two antiferromagnetically coupled ferromagnetic monolayers (see Figure 1).

The results of the study have already been published in peer-reviewed journal:

Unique magnetic structure of the vdW antiferromagnet VBr_3,
M. Klicpera, O. Michal, D. Hovančík, K. Carva, O.R. Fabelo Rosa, M. Orlita, V. Sechovský, J. Pospíšil,
Journal of Alloys and Compounds **1008** (2024) 176544
DOI: 10.1016/j.jallcom.2024.176544

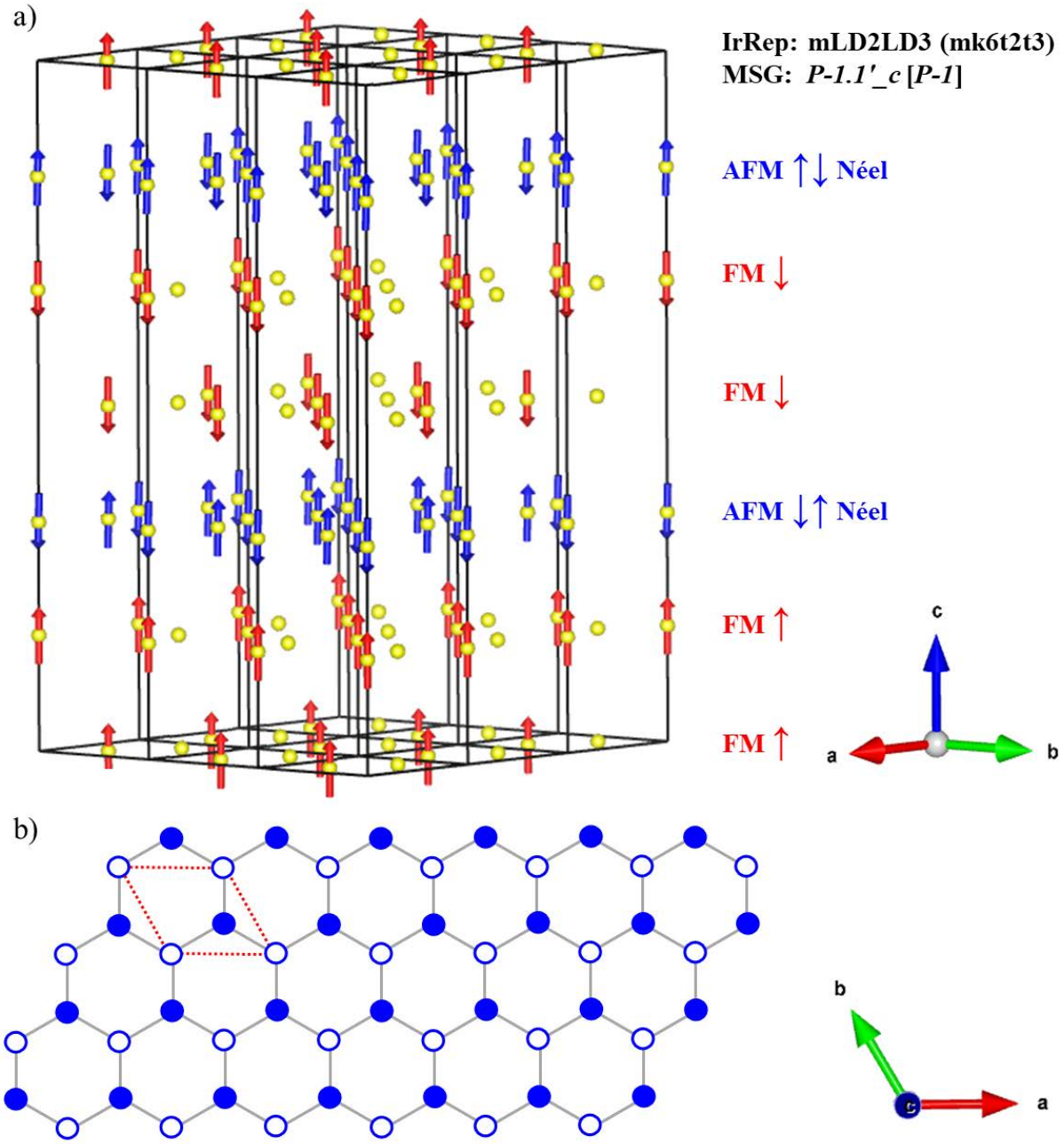

Figure 1 – The magnetic structure proposed in VBr_3. a) 9 magnetic unit cells are depicted to illustrate the nature of individual layers. Vanadium magnetic orbits V^{I} (zero moments), V^{II} (red arrows) and V^{III} (blue arrows) are color-distinguished, creating respective AFM Néel and FM layers. b) the *c*-axis projection of a single Néel layer is provided. Red dashed lines highlight the single unit cell, while the hexagonal array better illustrates the interatomic distances and arrangement of magnetic moments. The directions of moments pointing up and down of the *ab*-plane are distinguished by full and empty circles, respectively.