Experimental report

25/01/2024

Proposal: **5-31-2961**

Council: 4/2023

Title: Magnetic ground state of the quasi-one-dimensional S= 1/2 chain compound AgCuVO4

Research area: Physics

This proposal is a new proposal

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Experimental team:

Local contacts: Clemens RITTER

Samples: AgCuVO4

Instrument	Requested days	Allocated days	From	To
D20	3	3	10/11/2023	13/11/2023

Abstract:

We propose to investigate the magnetic ground state of a quasi-one-dimensional S = 1/2 chain compound AgCuVO4 at millikelvin temperatures. Its exchange interactions along the chain are bridged by Cu-O-Cu bonding angles of 113°, leading to an antiferromagnetic exchange interaction amounting to ~300 K. Moreover, DFT calculations imply additional frustrated interchain interactions, which promise a rich magnetic phase diagram consisting of complex magnetic phases that may exhibit intriguing magnetic excitations. Indeed, the specific heat has a magnetic anomaly at 2.5 K, but even at 0.13 K only very weak magnetic reflections has been detected in our preceding study. We are confident that additional measurements with significantly higher statistics will allow us determining the size of the ordered magnetic moment and hopefully to single-out the exact magnetic ground state of AgCuVO4.

Magnetic ground state of the quasi-one-dimensional S= 1/2 chain compound $AgCuVO_4$

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Scientific background

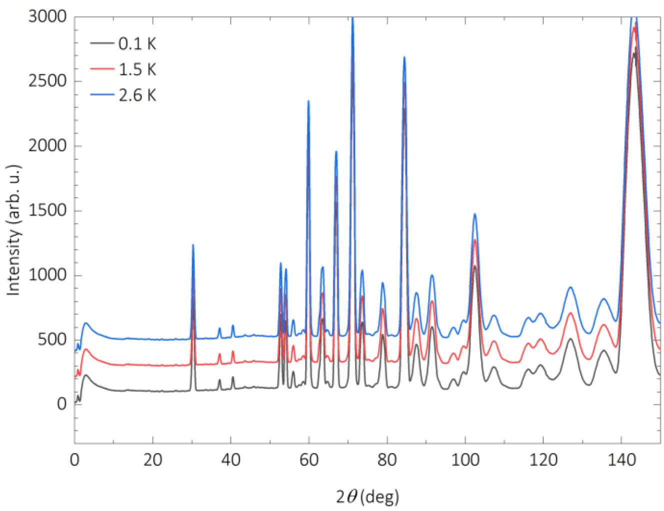
Spin chains exhibit many remarkable features that are rarely found in higher dimensions, the most prominent of them being their elementary excitations – the spinons – that are spatially confined and have a fractional-spin quantum number [1]. As such, they give rise to a plethora of fascinating phenomena, ranging from a broad excitation continuum to enhanced ballistic heat transport. Moreover, when exchange interactions are frustrated, a variety of exotic ground states with even more complex elementary excitations can emerge.

An intriguing quasi-one-dimensional S = 1/2 chain compound is $AgCuVO_4$ [2]. In contrast to the cuprate compounds mentioned above, here the bridging Cu-O-Cu angle amounts to 113°. This suggests significantly reduced, yet still antiferromagnetic interactions along the chains. Moreover, density-functional-theory (DFT) calculations predict that besides the dominant nearest-neighbour intrachain interaction several interchain interactions exist, which are frustrated. In addition, the chain structure allows for alternating Dzyaloshinskii-Moriya interaction that invariably leads to a staggered component of the magnetization.

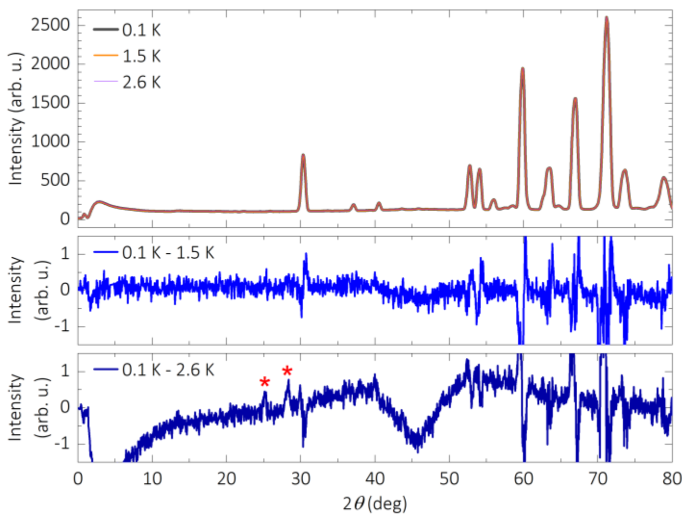
$AgCuVO_4$ crystalizes in the orthorhombic space group Pnma with lattice parameters a = 9.255(1) Å, b = 6.778(1) Å, and c = 5.401(1) Å. The spin chains are formed out of corner-sharing [CuO_4] plaquettes that run along the b axis, which are interconnected via nonmagnetic [VO_4] tetrahedra and separated from each other by nonmagnetic Ag^+ ions (Fig. 1). The broad maximum in the magnetic susceptibility (Fig. 2) is well described by the Bonner-Fisher model for the S = 1/2 chain with the antiferromagnetic interaction $J \sim 335$ K [2]. This is in reasonable agreement with the DFT calculations yielding $J = 280 \pm 35$ K. These calculations suggest also several competing interchain interactions of the order J/100 [2].

Summary of results

To determine magnetic structure of $AgCuVO_4$ we performed high-statistic measurements using dilution refrigerator and neutron wavelength of 2.4 Å at D20 instrument at ILL, measuring ~24 h per scan. The results show almost no difference in diffraction patterns measured at 0.1, 1.5 and 2.6 K.



Detailed comparison of 0.1 K and 1.5 K data still shows almost no difference, while the difference between 0.1 K and 2.6 K reveals the two weak magnetic reflections. Clearly, the high background stemming from the dilution setup hinders the detection of magnetic reflections at higher 2θ. Our neutron results show that the majority of magnetic intensity develops between 1.5 and 2.6 K.



[1] M. Mourigal et al., *Nature Physics* **9**, 435 (2013).
[2] A. Möller et al., *Phys. Rev. B* **80**, 125106 (2009).