Experimental report

18/06/2022

Proposal: 4-05-844 **Council:** 4/2021

Title: Magnetic excitation spectrum a thenew 3-dimensional frustrated quantum magnet

Research area: Physics

This proposal is a new proposal

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Samples: Sc2VO5

Instrument	Requested days	Allocated days	From	To
PANTHER	3	3	17/06/2021	20/06/2021

Abstract:

Frustration in isotropic magnetic compounds occurs where the magnetic ions are connected by antiferromagnetic interactions into triangular or tetrahedral motifs, or where first and further neighbor interactions give rise to competing magnetic structures. Three-dimensional frustrated magnets usually have a pyrochlore magnetic lattice (network of corner-sharing tetrahedra) or hyperkagome magnetic lattice (network of corner-sharing triangles). Here we propose to investigate a new frustrated three-dimensional lattice that consists of tetrahedral units of magnetic ions that are connected together by an intermediate magnetic ion into a three-dimensional network. No evidence for long-range magnetic order has been found down to T=0.3 K and the magnetic ions have spin-1/2 suggesting that it is a potentially highly frustrated quantum magnet.

Magnetic excitation spectrum a the new 3-dimensional frustrated quantum magnet

Introduction

The spin-liquids are a class of material where magnetic ground state does not develop a long-range ordered state or a frozen state but forms a magnetic liquid state where spins continues to fluctuates due to quantum mechanical oscillations and thus shows very intriguing quantum phenomena such as fractionalization of magnetic excitations and quantum entanglement[1]. Magnetic frustration due competing magnetic interactions from neighboring ions may lead to such a spin-liquid state in some compounds[2]. In isotropic compounds this frustration may occur due to the geometric position of the magnetic ions connected by antiferromagnetic interactions into triangular or tetrahedral arrangement[3]. Here we report a new type of three-dimensional magnetic lattice. The compound Sc_2VO_5 crystallize into a tetragonal structure with space group I -4[4], as shown in figure 1. The magnetic ions of V^{4+} with spin-$\frac{1}{2}$ are at two sites. One of which forms a tetrahedral motif with two different bond lengths. And the second types connects these tetrahedra together into a three-dimensional network. Due to these tetrahedral arrangement of the magnetic ions high magnetic frustration is expected in this coumpound.

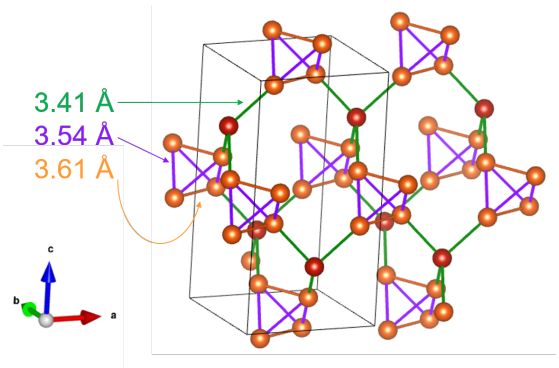

Figure 1: Crystal structure of Sc_2VO_5 showing only V^{4+} ions of which there are two types: In orange V^1 ions form tetrahedra with 2 different exchange strengths, orange and purple bonds; whereas, In red V^2 connect these tetrahedra together through the red bonds

Experimental Details

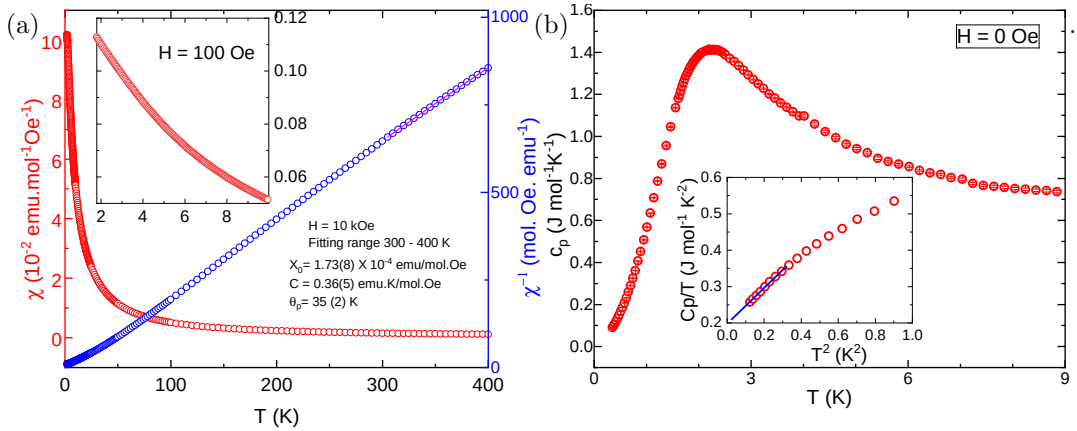

Figure 2: (a) Magnetic susceptibility $\chi(T)$ of Sc_2VO_5 are shown red circles. The reciprocal, $1/\chi(T)$ shown in blue circles, is fitted with Curie-Weiss law. Inset: low-field$\chi(T)$ shows no anomaly associated with any magnetic ordering. (b) Heat capacity $C_p(T)$ measured in zero external field. Inset: Low-T C_p Vs T^2, blue line is a linear fit.

A phase pure powder has been synthesized through solid state reaction of high purity stoichiometric mixture of Sc_2O_3 and VO_2 and then pressed into a pellet for bulk properties measurement. The Magnetization and specific heat measurements were done in a VSM-SQUID and in a PPMS, respectively at HZB. Low-T for specific heat measurements were attained using a He^3 setup. An inelastic neutron scattering experiment was done on the time of flight spectrometer at PANTHER, ILL on 5 grams of powder sample packed in a Cu can. Later a scan for empty can was also performed in order to subtract the contribution from the can and it's surroundings.

Results and discussion

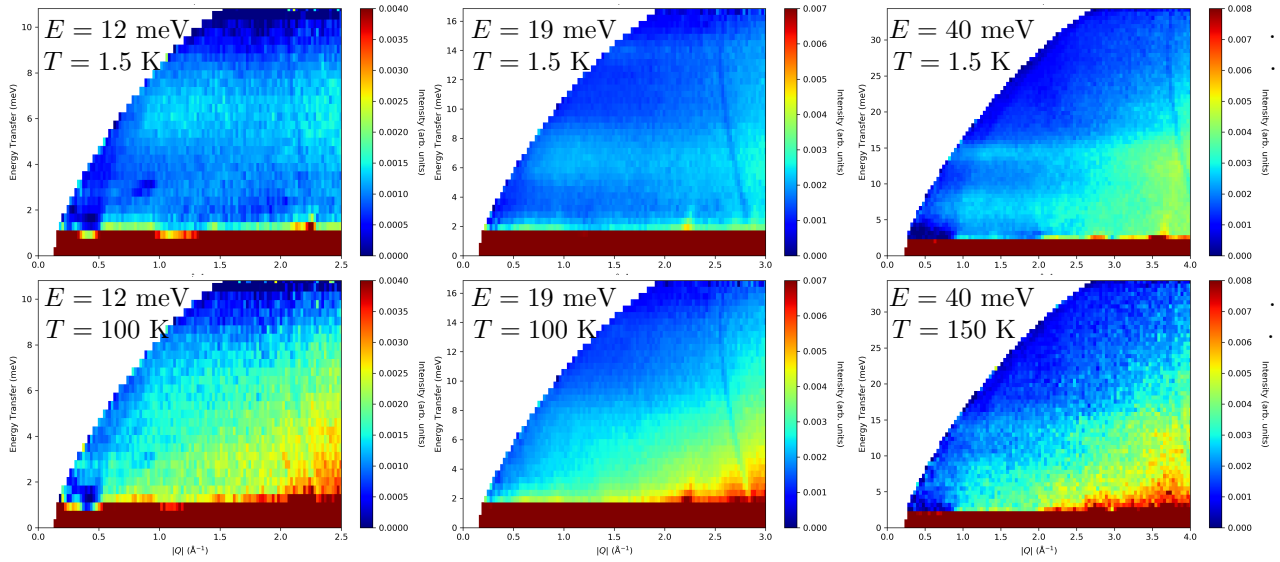

Figure 3: Background subtracted inelastic neutron scattering data collected on Sc_2VO_5 powder over 6-8h each. Empty can was measured for 6h to estimate the background.

Bulk magnetic susceptibility $\chi(T)$ at 10 kOe as well as at 100 Oe as shown figure 2(a) features no magnetic anomaly data down to $T = 1.8$ K corresponding to a magnetic order. The reciprocal $1/\chi(T)$ looks almost linear in temperature range $T > 100$ K. However, satisfactory fit to the Curie-Wiess law $[\chi(T) = \chi_0 + C/(T - \theta_p)]$ can only be obtained for fitting range $T > 300$ K. The obtained effective moment from the Curie parameter C amounts to $\mu_{\text{eff}} = 1.737\mu_B/V^{4+}$ consistent with spin-$\frac{1}{2}$ magnetic ions, hence, indicates that the orbital moment is quenched. The deduced value for the Curie-Wiess temperature $\theta_p = +35$ K, suggests and overall ferromagnetic interaction. Altogether we conclude that Sc_2VO_5 consists of both ferromagnetic and antiferromagnetic interactions where the ferromagnetic interactions are stronger giving rise to the positive Curie-Weiss temperature while the antiferromagnetic interactions compete with the ferromagnetic interactions suppressing long-range magnetic order. The absence of any magnetic ordering is may be due to strong magnetic frustration due to geometrical tetrahedral arrangement of magnetic ions around both V1 and V2 ions.

The absence of magnetic any long-range magnetic ordering is further confirmed down to base temperature of $T = 0.3$ K from the specific heat $C_p(T)$ measurements, shown in figure 2(b). Low temperature specific heat follow $\alpha T + \gamma T^3$ rule (shown in the lower inset of figure 2(b)), indicative to a gapless magnetic contribution.

The background corrected inelastic neutron scattering data collected for different incident energy have been shown in the colour plots of figure 3. In comparison to the data collected at higher temperature the low temperature data shows two clear bands at 14 meV and 7 meV and possibly near 2 meV. These bands may corresponds to magnetic excitations for different magnetic sub-systems present in the system.

To see them clearly $|Q|$ cuts were taken arround $0.5 <$

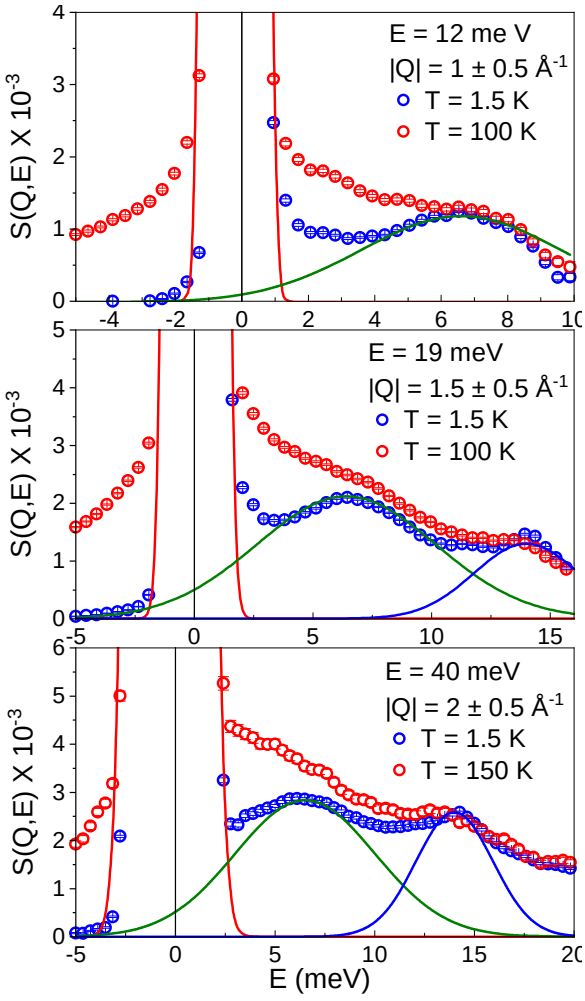

Figure 4: Cuts along $|Q|$ for both temperatures. Solid lines represent Gaussian fits to the humps.

$|Q| < 1.5$ Å^{-1} for $E = 12$ meV, $1 < |Q| < 2$ Å^{-1} for $E = 19$ meV and $1.5 < |Q| < 2.5$ Å^{-1} for $E = 40$ meV for both temperature data as shown in figure 4. Cuts are fitted to several Gaussian equations to calculate width of the different bands. The widths of the bands remains fairly unchanged for different incident energies. The excitation at 14 meV appears to be sharper in width and gapped in energy scale, and can be related to intra tetrahedral interactions between V1 ions. However, the excitation close to 7 meV is much wider and extends to zero energy transfer. This is in line with heat capacity data where it indicates a gapless magnetic contribution. This magnetic excitation, which is dispersive, may be related to exchange between the tetrahedras through V2 ions. The feature at $E \sim 2$ meV is not clearly visible even in the cuts due to its vicinity to the Braggs peaks. A neutron scattering experiment on single crystals will be help to understand different excitations present in the system.

Conclusions

Sc_2VO_5 possesses no magnetic ordering down to 0.3 K due to highly frustrated magnetic geometry and competing magnetic interactions. There are several magnetic excitations due to different magnetic exchange between the intra and inter-tetrahedral V4+ ions. The lowest magnetic excitation is gap less. This together with the absence of magnetic order in the system makes it a good candidate for the studies of spin-liquid systems. Growth of large single crystals are in progress and will be very helpful to understand further it's magnetic behaviour.

References

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3. Christian Balz *et al* J. Phys.: Condens. Matter 29, 225802 (2017)
4. Hengjiang Cong *et al* Crystal Growth & Design 10, 4389–4400 (2010)