Proposal:	4-05-7	/64	Council: 10/2019				
Title:	Excita	Excitations in the paramagnetic phase of dioptase					
Research area: Physics							
This proposal is a new proposal							
Main proposer: Irina SAFIULINA							
Experimental t	eam:	Irina SAFIULINA					
Local contacts: Mechthild ENDERLE							
		Ursula Bengaard HAN	SEN				
Samples: CuSiO3.H2O							
Instrument			Requested days	Allocated days	From	То	
IN3			1	1	04/09/2020	05/09/2020	
IN20			8	6	10/09/2020	19/09/2020	

Abstract:

The gem-stone mineral green dioptase, CuSiO3.H2O, crystallizes in the space group R3. Hexagonal rings of silica tetrahedra interconnect the magnetic Cu2+ ions with spin 1/2. The Cu2+ are surrounded by axially-elongated oxygen octahedra [1, 2]. The copper-oxygen network forms corner-sharing spirals along the hexagonal c-axis, neighbouring copper sites along the spiral are displaced by c/3. The spiral chains have a honeycomb arrangement in the ab-plane.

The small amount of entropy involved in the phase transition, and the small size of the ordered moment point to dominant quantum fluctuations and a close-by spin-liquid phase. Moreover, dioptase is quasi-one dimensional with dominant AF-intrachain interactions. We therefore wonder if the broadened features in the inelastic spectra are related to remainders of spinon-continua as in the ordered phase of KCuF3 (TN =39 K). To prove this idea we propose to explore the inelastic spectrum above the Neel temperature, at about 20 K, up to twice the 1D-spin-wave zone boundary energy (11meV) on IN20.

Experimental report 4-05-764: Excitations in the paramagnetic phase of dioptase

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1 Aim of the experiment

The gem-stone mineral green dioptase, $\text{CuSiO}_3.\text{H}_2\text{O}$, crystallizes in the space group R $\overline{3}$. Hexagonal rings of silica tetrahedra interconnect the magnetic Cu^{2+} ions with spin 1/2. The Cu^{2+} are surrounded by axiallyelongated oxygen octahedra [1, 2]. The copper-oxygen network forms corner-sharing spirals along the hexagonal c-axis, neighbouring copper sites along the spiral are displaced by c/3. The spiral chains have a honeycomb arrangement in the ab-plane. The small amount of entropy involved in the phase transition, and the small size of the ordered moment point to dominant quantum fluctuations and a close-by spin-liquid phase. Moreover, dioptase is quasi-one dimensional with dominant AF-intrachain interactions. We therefore wonder if the broadened features in the inelastic spectra are related to remainders of spinon-continua as in the ordered phase of KCuF₃ ($T_N = 39K$ [3]). To prove this idea we propose to explore the inelastic spectrum above the Neel temperature, at 22 K, up to twice the 1D-spin-wave zone boundary energy (11meV) on IN20.

2 Experimental details

The experiment was performed on IN20 from the 10th to the 19th of September 2020. The experimental setup was equipped with Helmholtz coils for the XYZ-polarization analysis. The spectrometer was used in W-configuration. The neutron energy was selected by a doubly focusing polarizing Heusler(111) monochromator, and analyzed with Heusler(111) operating at fixed k_f =2.662 Å⁻¹. The beryllium filter was positioned at k_f . No collimation was used. The diaphragms were placed next to the sample. The sample was mounted into the Orange Cryostat. The data was collected at 1.5K and 22K. We've used the (hhl)-oriented crystal previously used for the D3 (5-54-252) and Thales (4-01-1574) experiments. We measured SF and NSF xx, yy, zz cross-sections at the constant energy transfer.

3 Preliminary results

We measured the inelastic spectrum at the constant energy transfer 7 meV near the 1D AF zone center (0 0 1.5) above T = 22K and below T = 1.5K the Néel temperature. We obtain the pure magnetic scattering (free of background) using the linear combination of the following cross-sections:

$$|M_{\perp}|^{2} = \frac{\sigma_{NSF}^{yy} + \sigma_{NSF}^{zz} - 2\sigma_{NSF}^{xx} + 2\sigma_{SF}^{xx} - \sigma_{SF}^{yy} - \sigma_{SF}^{zz}}{2}$$

The main result of the experiment is shown in the Fig.1. We observed the magnetic scattering at both temperatures near the AF zone center from $(0\ 0\ 0.9)$ till $(0\ 0\ 2)$. At low temperature one can expect to have stronger scattering due to the system's ordering.



Figure 1: Magnetic scattering $|M_{\perp}|^2$ at 1.5K (blue) and 22K (red) in a constant energy scan along (00l) at 7 meV. The solid blue line was added at E = 0 meV was added for the better visualization of the magnetic scattering strength.

4 References

- [1] W. Eysel and K.-H. Breuer, Z. Deutsch. Gemmol. Ges. 30, 219 (1981).
- [2] E. L. Belokoneva et al., phys. chem. minerals 29, 430 (2002).
- [3] e.g. B. Lake et al., Nat. Mat. 4, 329 (2005).