# Experimental report

29/10/2023

**Proposal:** 5-31-2989 **Council:** 4/2023

**Title:** Clarifying the pressure induced phases in the Q1D compound K2Cr8O16

**Research area:** Physics

**This proposal is a new proposal**


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**Samples:** K2Cr8O16

| Instrument | Requested days | Allocated days | From | To |
|---|---|---|---|---|
| D20 | 3 | 3 | 22/09/2023 | 25/09/2023 |


## Abstract:

The title compound, K2Cr8O16, belongs to a series of quasi-1D compounds synthesized using a high-pressure/-temperature technique. The system reveals a metal to insulator transition (MIT) at 95 K which does not affect the ferromagnetic (FM) order emerging below TC = 180 K. The microscopic mechanism of this MIT is still under debate but one of the prominent scenarios includes a Peierls transition. Externally applied pressure on K2Cr8O16 stabilises a variety of different ground states. Previous pressure dependent magnetisation studies suggested a transition from a FM ground state to, via an intermediate ferromagnetic phase, a paramagnetic insulator (PI) or an anti-ferromagnetic insulator (AFI). However, our recent muSR measurements proposed this intermediate phase to be more of an anti-ferromagnetic (rather than FM) in nature and the high pressure regime to be a PI. With this proposal, we aim to clarify the debated magnetic phase diagram through pressure dependent neutron diffraction up to 40 kbar.

*Experimental report for 5-31-2989*

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## 1. Introduction

Low dimensional magnets represent model materials, in which a deep intertwining between electronic degrees of freedom lead to strongly correlated ground states. Experimental realizations feature an enhanced interplay between quantum and thermal fluctuations, that are tuneable via external parameters, such as pressure or chemical substitution. The hollandite family is a series of compounds exhibiting a quasi-1D structure. Hollandite compounds display various intriguing electronic and magnetic ground states, including metal- insulator transitions (MIT). In contrast to other members of the family, the transition in $K_2Cr_8O_{16}$ cannot be explained by the classical Mott-Hubbard model. The material is a 1D magnet where the formation of the magnetic ground state originates from competing nearest- and next-nearest neighbour interactions **[1 – 3]**. Intriguingly, the system reveals a metal-to-insulator transition (MIT) at $T_{MIT}$ = 95 K, which does not affect the ferromagnetic order emerging below $T_C$ = 180 K **[4]**. While ferromagnetism at $T_C$ = 180 K was concluded to be established by a double exchange interaction of the itinerant *d* electrons **[4]** the microscopic mechanism behind the MIT is heavily debated. While many models have been proposed **[1 – 4]**, one prominent scenario includes Peierls instability along the 1D Cr chains **[5]**.

The FM below and above MIT was proposed to be stabilized by the double exchange (DE) interaction. While DE mechanism by itinerant d-electrons is not intuitive for an insulating sample, a theoretical study based on the density matrix renormalisation group method on the 1D-DE model supports such scenario **[6]**. In fact, three ground states as a function of J/t and δ were found where J/t is Hunds coupling/conduction band width and δ is the Peierls gap. According to such study, a spin polarised FM state with a Peierls gap, a paramagnetic insulating state with a Mott gap and an intermediate state with partial spin polarisation should be stabilised as a function of the parameters. These findings motivated pressure dependent studies to experimentally tune J/t and δ.

## 2. Experiment

The goal of the experiment was to clarify high pressure and low temperature magnetic phases. Previous studies suggested there may be a supression of the magnetic order under pressure. To tackle this question, we utilised a Paris Edingbugh cell to reach pressure up to 40 kbar at temperatures down to 5 K. The avilable smaple space was fillied with powder $K_2Cr_8O_{16}$, inserted together with lead as a pressure caliber. Several neutron difraction patterns were collected as a functino of temperature for three different pressures. The collected patterns were analyzed during the experiment using the software package Fullprof.

## 3. Results

The neutron diffraction pattern collected at intermediate pressure were consistent with previous muon spin relaxation study, which predicted an antiferromagnetic phase. While we have not fully been able to refine the data yet, we seem to be converging towards an antiferromagnetic order, ordered within the plane with k = (0.25, 0.25, 0). As the pressure was increased, we expected a suppression of this order. Contrary to our expectation, Tn was increase with pressure. Moreover, the magnetic order seems to become incommensurate with perhaps multi-k structure. In our data analysis process, we are at the moment trying to refine the measured structures at T = 5 K for all measured pressures. Once refined the base temperature patterns is refined, we will also analyze the temperature dependence.

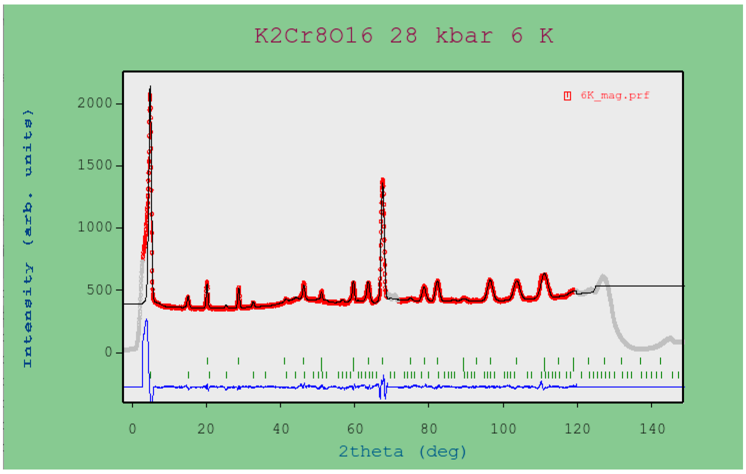


Figure 1. Neutron diffraction pattern collected at T = 5 K and p = 28 kbar. A clear and strong new magnetic peak is visible at 2theta ≈ 3 degrees, together with smaller weaker peaks. The magnetic pattern is indexed with k = (0.25, 0.25, 0). Basireps was used to evaluate the possible magnetic structures.

## 4. Conclusion

The main goal of the experiment was to unveal the detailed spin structure of the magnetic order at low temperature. The formation of an AF order under pressure was confirmed in this study. While we were expecting a supression of this AF order, to our surprise, this AF seem to stabilise under pressure. Moreover, an multi-k incommensuarte order seem to be formed at even higher pressures. We are currently analysing the data and hope to be able to publish the results in the near future.

## 5. References


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