# Experimental report

31/08/2017

**Proposal:** **5-41-858** **Council:** 4/2016

**Title:** Magnetic structure of the new heavy fermion compound $CePt_2In_7$

**Research area:** Physics

**This proposal is a new proposal**


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**Samples:** $CePt_2In_7$

| Instrument | Requested days | Allocated days | From | To |
|---|---|---|---|---|
| D10 | 7 | 7 | 20/09/2016 | 28/09/2016 |
| D23 | 7 | 0 | | |

## Abstract:


$CePt_2In_7$, a new antiferromagnetic heavy fermion compound, is a member of $CeM_xIn_{3+2x}$ family (among them $CeIn_3$ and $CeCoIn_5$). It demonstrates novel and unusual physical properties, such as a pressure-induced quantum critical point and unconventional superconductivity.
Previous NQR studies performed on single crystals suggest a coexistence of an incommensurate and commensurate antiferromagnetic components, whereas only commensurate phase was observed in polycrystalline samples. So far, no neutron diffraction experiments on $CePt_2In_7$ have been reported. Such measurements are crucial for resolving this apparent controversy.
A rapid one-day test on the D23 diffractometer on our very high quality sample suggests the existence of a commensurate propagation vector at 1.5 K. Built on these preliminary results, we propose to determine the details of the magnetic structure by single crystal neutron diffraction. To this end, the measurements will be performed over a temperature range from 1.5 K to above $T_N$ = 5.5 K in order to check carefully the existence of an incommensurate antiferromagnetic order and determine the value and orientation of the magnetic moments and their temperature dependence.

The coexistence and competition between unconventional superconductivity and antiferromagnetic order remains the key question in the physics of Ce-based heavy fermion compounds. Indeed, the appearance of superconductivity is intrinsically connected to the suppression of the magnetic order. $CePt_2In_7$ undergoes an antiferromagnetic (AF) transition at $T_N$ = 5.5 K [1,2]. Recent electrical resistivity and ac-calorimetry measurements under pressure on single crystals of $CePt_2In_7$ revealed a quantum critical point at a critical pressure $P_c \approx 3.2$ GPa, where the AF order is completely suppressed [3]. In $CePt_2In_7$, the magnetic structure of its AF ground state is still an open question. The existing reports on this matter are controversial. Indeed, NQR studies performed on polycrystalline samples [4] suggest that antiferromagnetism is commensurate in this material. The same conclusion was drawn from positive muon-spin rotation and relaxation ($\mu^+$SR) measurements also performed on polycrystalline samples [5]. On the contrary, the NQR spectra obtained on single crystals are consistent with the coexistence of an incommensurate (IC) and commensurate (C) AF component of the magnetic structure [6,7]. The C-AF order first occurs just below $T_N$, then, at lower temperatures of about 3 K, IC-AF order gradually grows in. This probably accounts for the observation of only commensurate magnetism in polycrystalline NQR measurements, which were performed at temperatures down to 4 K [2]. At 1.6 K, the volume fraction of the incommensurate order is about 75%. However, the C-AF order is stabilized by hydrostatic pressure: Its volume fraction becomes nearly 100% at 2.4 GPa, the pressure where superconductivity first occurs and f electrons change from localized to itinerant. All the NQR experiments [2,6,7] lead to the same conclusion: The magnetic propagation vector is (1/2, 1/2, δ), although the value of δ is not predicted. In this present experiment we have attempted to fully determine the antiferromagnetic structure of $CePt_2In_7$.

In a first step, a powder neutron diffraction experiment has been performed on the D1B spectrometer on $CePt_2In_7$ by using a pyrolytic graphite (002) monochromator providing a beam with a wavelength of 2.52 Å and a 128° multidetector. A great number of single crystals were ground into 1.6 g of fine powder. These measurements did not reveal any magnetic peaks below $T_N$ in spite of 10-hour-long acquisitions at both 1.5 and 10 K, mostly due to high neutron absorption of In. This puts an upper limit for the magnetic moment at about 0.8 $\mu_B$/Ce. Both the crystal structure and the lattice parameters remain unchanged in the AF state. Then, a one-day test experiment was performed on the D23 on the biggest available $CePt_2In_7$ single-crystal (2 x 2 x 0.1 mm$^3$). A weak magnetic peak appeared with the propagation vector **Q** = (1/2, 1/2, 1/2). This test strongly suggested that a commensurate propagation vector exists at 1.5 K. Finally, single-crystal neutron diffraction measurements were performed on the D10 keeping the same single-crystal sample. The instrument was used in a four-circle configuration with an additional triple-axis energy analysis. The latter was used in the elastic mode with a single detector to increase the signal-to-noise ratio. A vertically focusing pyrolytic graphite monochromator and analyzer were used, fixing the incident and analyzed wavelength at 2.36 Å. A pyrolytic graphite filter was used to reduce the higher harmonic contamination to $10^{-4}$ of the primary beam intensity. In order to reach temperatures down to 2 K, we used a four-circle cryostat with helium circulation.

The measured lattice parameters at T = 2 K are a = 4.595(2) Å and c = 21.558(5) Å, as obtained from the analysis of 30 nuclear Bragg peaks. We then performed scans across of 24 magnetic peaks at 2 K. This experiment confirmed the test on the D23 by showing a clear commensurate magnetic peak at **Q** = (1/2, 1/2, 1/2) (Figure 1). The temperature dependence of the (1/2, 1/2, 1/2) magnetic Bragg peak intensity yields a Néel temperature $T_N$ = 5.7 K (Figure 2). The refinement of these data suggested the magnetic structure shown in Figure 3, where magnetic moments are in-plane and turn by 90° from one $CeIn_3$ plane to another. In addition, the magnetic moment is estimated at 0.45(1) $\mu_B$/Ce which is in agreement with our previous experiment on D1B. However, the existence of the IC phase is still an open question. Indeed two complete **Q**-scans have revealed a satellite peak $\mathbf{Q_S}$ = (1/2, 1/2, 0.47) at 2

K which disappears at 4 K (Figure 4). This phenomenon seems partially in agreement with NQR measurements [6,7]. Unfortunately, the collected data are not sufficient to confirm this IC phase.

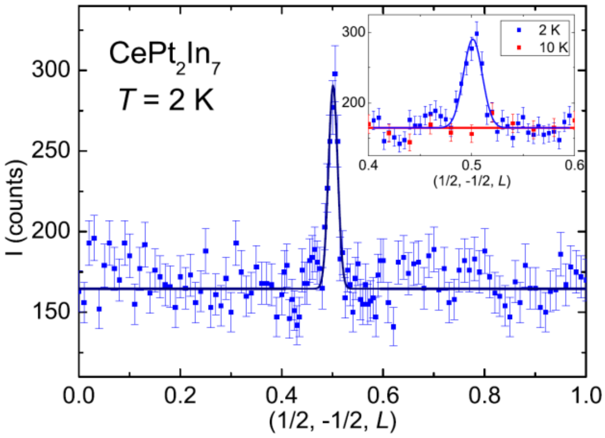


*Figure 1. **Q**-scan performed along the [0, 0, 1] direction at 2 K. The inset shows a zoom of the same **Q**-scan near **Q** = (1/2, −1/2, 1/2) at 2 and 10 K. The intensity is in number of counts per 4 × $10^6$ monitor counts, which corresponds roughly to 7 min. The solid lines are Gaussian fits of the peaks.*

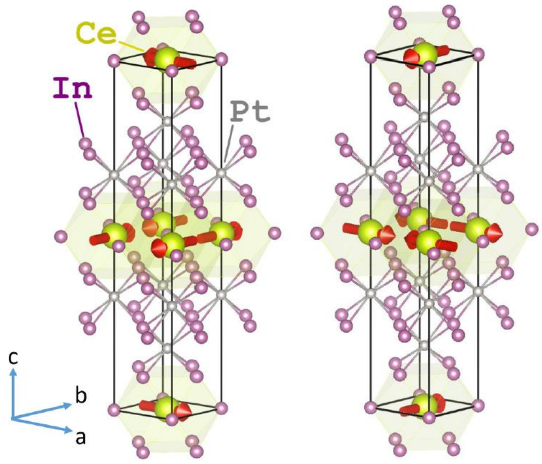


*Figure 3. Magnetic structure of $CePt_2In_7$ in a structural unit cell. The magnetic moment, schematically shown by arrows, is 0.45$\mu_B$ per Ce and it is aligned in the basal plane. Both magnetic domains are shown.*

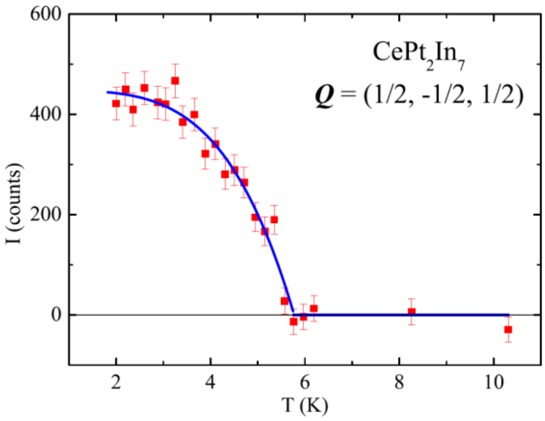


*Figure 2. Temperature dependence of the (1/2, −1/2, 1/2) magnetic Bragg peak intensity after subtracting the background. The intensity is in number of counts per 1.6 × $10^7$ monitor counts, which corresponds roughly to 27 min. The line is a phenomenological fit.*

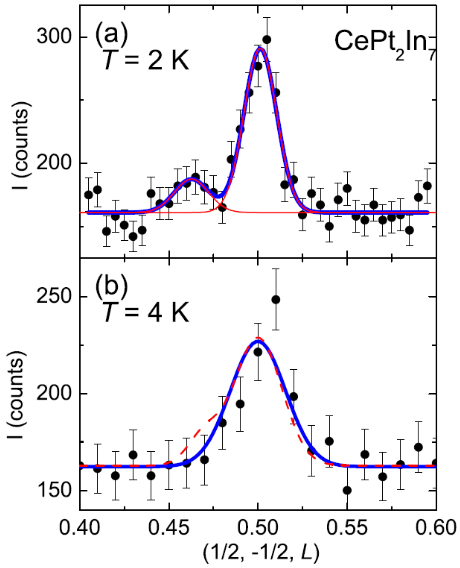


*Figure 4. Detailed **Q**-scans performed along the [0, 0, 1] direction at (a) 2 K and (b) 4 K. The intensity is in number of counts per 4 × $10^6$ monitor counts, which corresponds roughly to 7 min. The lines are Gaussian fits of the peaks. The data obtained at 2 K are well fit by two Gaussian peaks centered at (1/2, −1/2, 1/2) and (1/2, −1/2, 0.47). At 4 K, an attempt to fit the data by two Gaussian peaks while fixing the position of the second peak and the integrated intensity ratio of the two peaks (dashed line) does not yield a satisfactory result. The data are much better fitted by a single Gaussian peak (solid line).*

The results of this work were published in PRB Rapid Communication [8]. Another experiment has to be carried out using a $^3$He cryostat in order to reach lower temperatures for studying the temperature dependence of **Q** and $\mathbf{Q_S}$ peaks. Only a neutron diffraction experiment on either D10 or D23 could answer this question. Such an experiment is planned for the near future.

**References:**


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