International Conference on Strongly Correlated Electron Systems (SCES 2011) IOP Publishing
Journal of Physics: Conference Series **391** (2012) 012055 doi:10.1088/1742-6596/391/1/012055

Magnetic order in non-centrosymmetric $CePt_3B$

D Rauch[1], S Süllow[1], M Bleckmann[2], A Buchsteiner[3], N Stüßer[3], H-H Klauss [4], H Luetkens[5] and E Bauer[6]

[1] Institute of Physics of Condensed Matter, Technical University of Braunschweig, D-38106 Braunschweig, Germany
[2] Wehrwissenschaftliches Institut für Werk- und Betriebsstoffe WIWeB, D-85435 Erding, Germany
[3] Berlin Neutron Scattering Center, Helmholtz Zentrum Berlin, D-14109 Berlin, Germany
[4] Institute of Solid State Physics, University of Technology Dresden, D-01069 Dresden, Germany
[5] Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen, Switzerland
[6] Institute of Solid State Physics, Vienna University of Technology, A-1090 Vienna, Austria

E-mail: `d.rauch@tu-bs.de`

Abstract.
$CePt_3B$ exhibits two magnetic phases, an antiferromagnetic and a weak ferromagnetic one. To determine these magnetic structures of $CePt_3B$, neutron diffraction and μSR experiments have been carried out. Neutron diffraction experiments provided no evidence of either antiferromagnetic or ferromagnetic order. In contrast, in zero field muon-spin relaxation (μSR) experiments, magnetic transition temperatures $T_N = 7.8$ K and $T_C \sim 6$ K are observed from the onset of spontaneous muon precession.

In recent years, the observation of heavy fermion superconductivity in non-centro symmetric intermetallics such as $CePt_3Si$ [1] has initiated a multitude of experimental and theoretical studies. Especially, in terms of superconductivity the nature of the pairing states has been of interest [2]. Conversely, the lack of inversion symmetry gives rise to an additional magnetic exchange term, the Dzyaloshinsky-Moriya (DM) interaction [3, 4]. This term tends to align spins perpendicular to each other, which combined with the common (for instance Heisenberg like) magnetic exchange effectively gives rise to spin canting or complex magnetic structures.

Already for $CePt_3Si$, which crystallizes in a tetragonal lattice with the space group $P4mm$ [1], the DM interaction could be a relevant issue for the magnetic behaviour, since the system orders antiferromagnetically below $T_N = 2.2$ K. However, it has been shown that the antiferromagnetically ordered state is collinear ($Q = (0, 0, 1/2)$), with small magnetic moments $\mu_{ord} = 0.16\ \mu_B$ [5]. In contrast, $CePt_3B$, which is isostructural and related in electron count to $CePt_3Si$ [6, 7, 8, 9], exhibits a complex magnetically ordered state at low temperatures, with an antiferromagnetic phase below $T_N = 7.8$ K and a second weakly ferromagnetic transition below $T_C \sim 6$ K. While the weak ferromagnetism might point to the relevance of the DM interaction, the microscopic nature of these magnetic phases has not been revealed so far. Here, we present a first study of these magnetic phases by means of neutron diffraction and μSR experiments.

The polycrystalline sample $CePt_3B$, using ^{11}B in the production, was prepared by melting high-purity elements in a water-cooled copper crucible using a high frequency generator under argon atmosphere. Subsequently the sample was annealed at 880°C for 14 days. The magnetization and susceptibility was measured employing a commercial SQUID magnetometer. Neutron diffraction experiments were performed using the E6 spectrometer of the Berlin Neutron Scattering Center (BENSC) of the Helmholtz Zentrum Berlin, with a neutron wave length of $\lambda = 2.444$ Å in a standard Orange cryostat ($T \geq 1.6$ K). The μSR experiments were carried out at the Swiss Muon Source of the Paul Scherrer Institute. Measurements were performed on the GPS instrument using a He-flow cryostat ($T \geq 1.7$ K).

For sample characterization, magnetization measurements on $CePt_3B$ at low temperatures $T = 1.8 - 8$ K have been carried out (Fig. 1). A ferromagnetic hysteresis below $T = 5$ K is observable, and which has vanished for 8 K. In the limit of zero temperature, an extrapolated remanent magnetization of $\mu \approx 0.09\mu_B$/Ce atom is obtained, in agreement with Ref. [6] (inset of Fig. 1). Further, at low temperatures the inverse susceptibility χ^{-1} indicates two magnetic phase transitions into long range ordered states, an antiferromagnetic and a weak ferromagnetic one (Fig. 2). The antiferromagnetic T_N and ferromagnetic temperatures T_C for $CePt_3B$ are determined as $T_N = 7.8$ K and $T_C \sim 6$ K from χ^{-1}, in good agreement with the Refs. [6, 8].

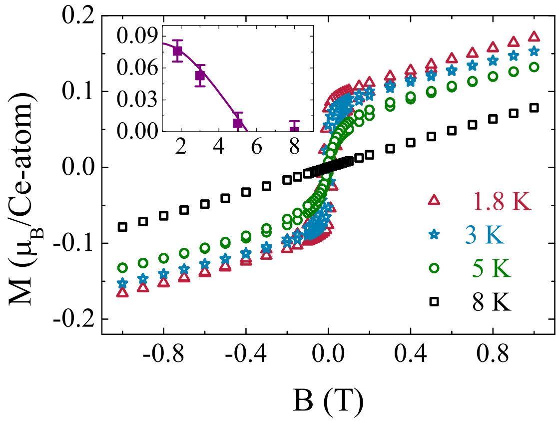

Figure 1. The magnetization of $CePt_3B$, as function of temperature. Inset: The remanent ferromagnetic moment as function of temperature of $CePt_3B$; solid line as guide to the eye.

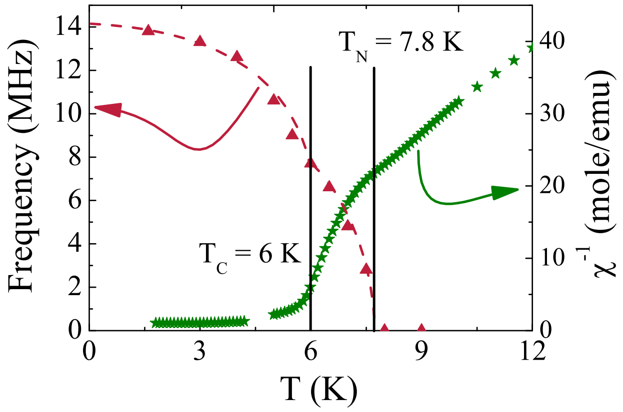

Figure 2. Oscillation frequencies of the muon signal (red), together with the inverse susceptibility χ^{-1} (green) of $CePt_3B$; lines are guides to the eye, for details see text.

Neutron diffraction patterns of $CePt_3B$, taken at 1.6, 6.6 and 15.3 K are depicted in Fig. 3. The data at 15.3 K are successfully fitted with the tetragonal structure model (space group *P4mm*) of Sologub *et al.* [7] (not shown in the plot for clarity). In these fits, a few minor peaks could not be associated to this structure, indicating the presence of a second phase (volume fraction ∼ 10 %). In the refinement, by excluding the secondary phase peaks a value $R_{Bragg} = 6.2$ % is obtained. In Tab. 1 we summarize the result of our refinement. All parameter are in a good agreement with the values obtained of Sologub *et al.* [7]. The smaller lattice parameters are reflecting a shrinking of the lattice due to the lower temperature used in our experiments, as compared to the room temperature experiments carried out by Sologub *et al.* [7].

A comparison of the spectra at 1.6, 6.6 and 15.3 K and the difference spectra (lower panel) at 1.6 K/15.3 K and 6.6 K/15.3 K are also shown in Fig. 3. All the data are normalized to a secondary phase peak, which should not change intensity upon transition into the magnetically ordered state. Surprisingly, within experimental solution no additional diffraction intensity has been found for any of our examined Bragg peaks, nor have additional peaks been observed.

To estimate the magnetic moment that ought to be detectable in our experiment, magnetic

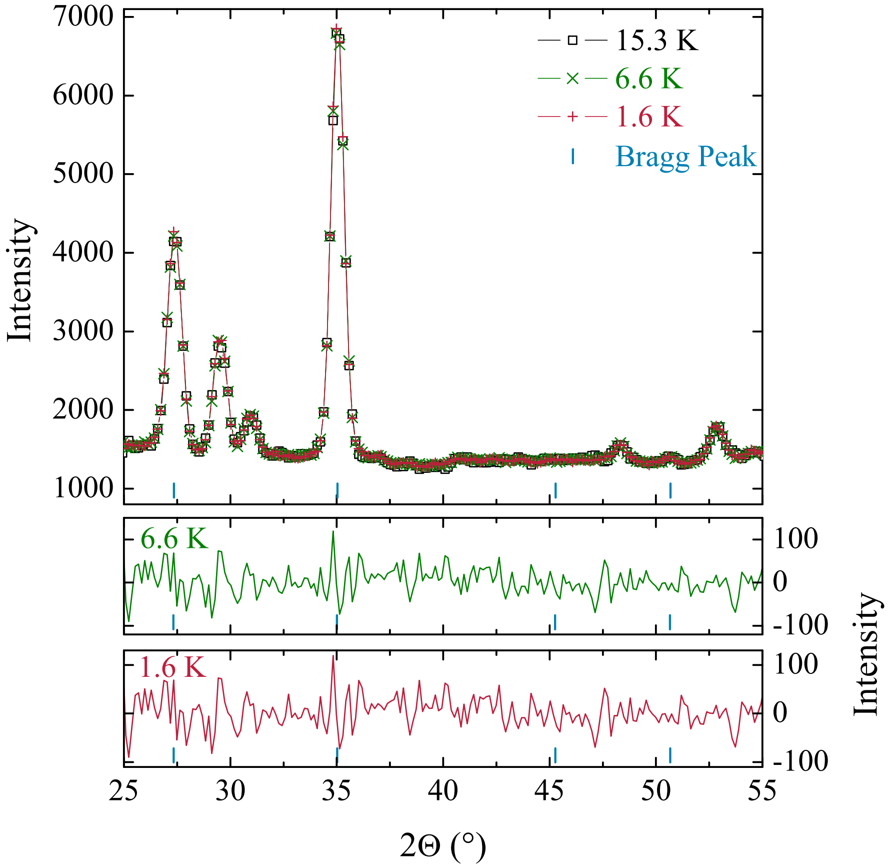

Figure 3. Neutron diffraction pattern of $CePt_3B$, taken at 1.6 (red), 6.6 (green) and 15.3 K (black). In the lower panels, the difference between the data at 1.6/6.6 K and the 15.3 K data are shown.

Table 1. Results of a refinement of powder neutron diffraction data on $CePt_3B$ at $T = 15$ K, in comparison to x-ray powder diffraction at room temperature carried out by Sologub *et al.* [7]. Here, the lattice parameter a, b and c and the positional parameter x, y, z are summarized.

	15.3 K			**Sologub** *et al.* **[7]**		
a (Å)	3.9943(4)			4.0031(3)		
b (Å)	3.9943(4)			4.0031(3)		
c (Å)	5.0620(1)			5.0736(4)		
R_{Bragg} (%)	6.2			4.8		
Ce	0	0	0	0	0	0
Pt(1)	0	0.5	0.522(1)	0	0.5	0.5132(13)
Pt(2)	0.5	0.5	0.131(3)	0.5	0.5	0.1174(11)
B	0.5	0.5	0.713(8)	0.5	0.5	0.688 (17)

structure simulations with magnetic moments of different size and arrangement have been performed. In particular, a ferromagnetic arrangement of the magnetic moments and an antiferromagnetic one with a doubling of the unit cell in a direction have been assumed. These simulations indicate that a magnetic moment of 0.5 μ_B in the ferromagnetic and 0.2 μ_B in the antiferromagnetic case should be observable.

Since the neutron diffraction experiments did not deliver information about the magnetic phases, zero field μSR measurements were carried out on the same sample. In these experiments a distinctive μSR oscillatory signal below the antiferromagnetic transition temperature T_N is observed, clearly indicating the presence of static magnetic fields from long range magnetic order in the bulk of the sample (Fig. 4). In a next step, we determined the temperature dependence of the muon oscillation frequencies.

These zero field spectra have been analyzed using a sum of three precession signals associated with different muon sites in the lattice. Plotted is the highest frequency as a function of temperature, the other frequencies are proportional to it. The results are depicted in Fig. 2, together with the inverse susceptibility χ^{-1}.

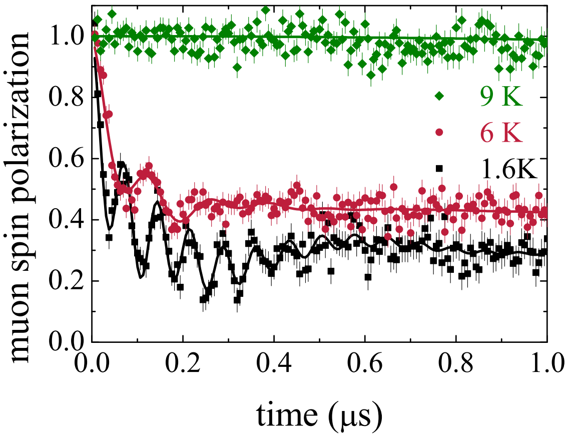

Figure 4. Time dependence of the μ^+ spin polarization of CePt$_3$B for temperatures $T = 1.6$ K (black), 6 K (red) and 9 K (green).

Both transition temperatures T_N and T_C can also be identified in the μSR measurements. From Fig. 2 it is seen that T_N denotes the temperature of onset of spontaneous muon precession, while at T_C there is a change of slope of the temperature dependence of the muon oscillation frequency. The weak ferromagnetic behavior likely is formed by canting of magnetic moments of the antiferromagnetic structure of CePt$_3$B.

In conclusion, the structural properties, investigated by neutron diffraction experiments, are in good agreement with those reported in Sologub *et al.* [7]. Further, we have unsuccessfully attempted to identify scattering intensity in our neutron study upon transition into the magnetically ordered phases. However, our μSR experiments clearly show the existence of long range magnetic order in the bulk of our sample. Taken together, neutron diffraction and μSR experiments suggest that the magnetically ordered phases in CePt$_3$B carry magnetic moments of medium size, probably with an ordering vector different from the one in CePt$_3$Si.

Altogether, CePt$_3$B exhibits an antiferromagnetic and a weak ferromagnetic phase, with $T_N = 7.8$ K and $T_C \sim 6$ K. In view of the data presented here, a possible explanation for the weak ferromagnetic behavior below T_C could be the canting of antiferromagnetic ordered spins with decreasing temperature. The DM interaction might be, most likely, the cause for this canting of magnetic moments in non-centro symmetric CePt$_3$B.

References

[1] Bauer E et al. 2004 *Phys. Rev. Lett.* **92** 2
[2] Fujimoto S 2007 *J. Phys. Soc. Jpn.* **76** 051008
[3] Dzyaloshinsky I 1958 *J. Phys. Chem. Sol.* **4** 241
[4] Moriya T 1960 *Phys. Rev.* **120** 91
[5] Metoki N et al. 2004 *J. Phys.: Condens. Matter* **16** L207-212
[6] Süllow S et al. 1994 *Physica B* **199 & 200** 644
[7] Sologub O et al. 2002 *J. Alloys Comp.* **337** 10
[8] Lackner R et al 2005 *J. Phys.: Condens. Matter* **17** S 905
[9] Vejpravov J, Prokleš J, Sechovsk V 2006 *J. Alloys Comp.* **408** 54