Crystal Structure and Magnetic Ordering in $Ce^{11}B_6$ Revised by Neutron Diffraction

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Both unpolarised and polarised neutron diffraction studies were performed on CeB_6 at SINQ and at ILL. They reveal that the crystal structure of CeB_6 remains cubic in the antiferroquadrupolar and antiferromagnetic states. A new k-k' model of the AF magnetic structure of CeB_6 is proposed. The temperature evolution of antiferromagnetic intensity has a normal behaviour in the 700 mK – 2.3 K range.

The dense Kondo CeB_6 compound with a cubic CaB_6-type structure has an unusual phase diagram [1, 2]. At T_Q=3.3 K it undergoes a transition from the paramagnetic to the antiferroquadrupolar (AFQ) state associated with $\mathbf{k_q}$=[1/2 1/2 1/2]. At T_N=2.3 K the antiferro(AF)-magnetic ordering described by the wave vectors $\mathbf{k_1}$=[1/4,1/4,0], $\mathbf{k_2}$=[1/4,-1/4,0] and $\mathbf{k'_1}$=[1/4,1/4,1/2], $\mathbf{k'_2}$=[1/4,-1/4,1/2] takes place.
The crystal structure and zero-field magnetic structure of $Ce^{11}B_6$ have been revised by neutron diffraction including experiments at high-resolution and high-flux neutron powder diffractometers HRPT at SINQ and D20 at ILL, neutron single crystal diffractometer TriCS at SINQ and spherical neutron polarimetry (SNP) at IN20 at ILL.
The crystal structure remains cubic below T_Q=3.3 K in the AFQ and AF phases within the limit of detection. The change of the lattice constant *a* is very subtle within the 1.5 K– 8 K temperature interval, $Da/a<1.5\ e^{-5}$.
We derived a new **k-k'** model of the AF magnetic structure of CeB_6 based on 60 mK D20 data. It corresponds to the following combination of Fourier components:
$\mathbf{M}(\mathbf{R_n})=m_1/\sqrt{2}\cos\{\mathbf{k_1R_n}\}\mathbf{e_{1\text{-}10}}+m_2/\sqrt{2}\sin\{\mathbf{k'_2R_n}\}\mathbf{e_{110}}$

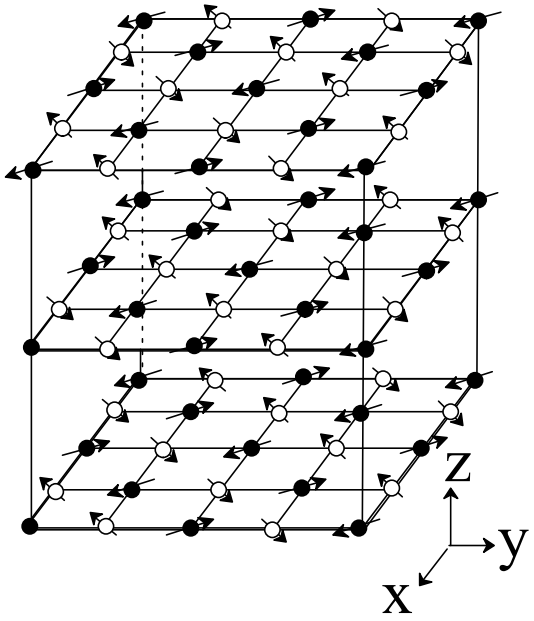

Figure 1: Proposed AF magnetic structure (I) of $Ce^{11}B_6$. Only Ce-atoms are presented. The atoms with magnetic moments associated to $\mathbf{k_1}$ and $\mathbf{k'_2}$ are shown by black and white circles, respectively.
Magnetic structure consists of four Ce sublattices with magnetic moments in the (xy0)-plane strictly along <110> (fig. 1). The magnetic moments along the [110] direction have ferromagnetic stacking along z and the moments pointing along [1-10] show AF coupling of neighboring planes along z. The resulting ordered magnetic Ce moments are 0.41(1) μ_B and 0.52(1) μ_B at 60 mK, respectively.
Several *hhl* reflections have been studied by SNP. Analysis of polarization of scattered neutrons indicates that the magnetic Ce moments associated with $\mathbf{k_1}$ and $\mathbf{k'_1}$ point strictly along a [1-10] direction. Moreover, there is no ferromagnetic component proposed by ref. [1]. These results allow to rule out several models: a helical structure with magnetic moments in the (001) plane and sine modulated structures with moments along <111> or <100> [1, 3].
The measured temperature dependency of intensity of several AF reflections in the 700 mK - 2.3 K range shows a normal behaviour (fig. 2), in contrast to the peculiar behaviour of some spontaneous μ^+ Larmor precession frequencies [4]. This indicates no change of the long-range order of the Ce magnetic moments below 1 K.

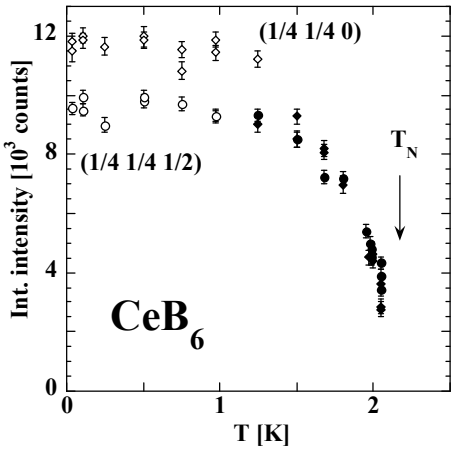

Figure 2: Temperature dependency of AF intensity of (1/4 1/4 0) and (1/4 1/4 1/2) reflections in the mK regime.

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Work partially performed at SINQ
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