ESRF	**Experiment title:** ***Spin density in CeB_6***	**Experiment number**: HE-1787
Beamline: ID15a	**Date of experiment**: from: 17***/11/04*** ***to:*** ***22/11/04***	**Date of report**: 20/08/05
Shifts: 15	**Local contact(s)**: Nozumi Hiraoka	*Received at ESRF:*

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Report:

The spin density of CeB_6 induced by a 1.0T magnetic field was measured at T = 2.0K using spin-polarised Compton scattering. The data show evidence of a delocalised 5*d*-like spin moment, but very little 4*f*-like spin contribution. The data suggest that the spin moment is itinerant in this material.

The heavy Fermion metal CeB_6 displays magnetic order below 3.3K, which arises from the single Ce 4*f* electron. CeB_6 possesses two magnetically ordered states at low temperature. Below 2.5K it is antiferromagnetic, and between 2.5K and 3.3K the ordering is probably antiquadrupolar, or octupolar, although this issue is still contentious. In an applied magnetic field, a small induced ferromagnetic component is created. This has been exploited in polarised neutron diffraction measurements to study the real space magnetisation density. These data, which relate to the *total*, spin plus orbital, magnetisation, are consistent with a localised 4*f*-like induced moment. There has, however, been much suggestion that the magnetisation in CeB_6 has some itinerant character. The goal of the spin-polarised Compton scattering experiment reported here was to study this directly.

Spin polarised Compton scattering samples the spin-dependent electron momentum density through the use of circularly polarised synchrotron radiation. The technique involves

high-energy inelastic scattering of a monochromatic beam of circularly polarised photons E_I=200-250keV. The energy dispersion of the scattered beam is directly related to the electron momentum distribution. In this case, an energy of ~219keV was used, with a scattering angle of 174 degrees, which gives the optimal resolution and countrate. The 13 element Ge detector was employed, of which 12 elements were usable. In order to extract the spin polarised signal two measurements are made with parallel and antiparallel applied field directions with respect to the scattering vector. The magnetic field was applied using the 1.0T electromagnet installed on ID15a, and an "orange" cryostat was used, with kapton windows to minimise background scattering.

The profiles in both the [100] and [110] directions, measured at 2K, show a spin moment more like the RHF free atom Ce 5*d* electron moment than that of the Ce 4*f* electrons expected, and little anisotrpoy was observed. The [100] data are shown in figure 1: note that the spin moment is antiparallel to the net magnetisation of the sample. It is interesting that very little, in any, of the large 4*f* moment observed in polarised neutron diffraction experiments is observed here. This suggests that the total magnetic moment in this compound is dominated by a large Ce 4*f* orbital moment. From these spin moment measurements and magnetisation data the magnitude of the orbital moments are estimated to be 0.52±0.05 μ_B[f.u.]$^{-1}$ and 0.53±0.06 μ_B[f.u.]$^{-1}$ in the [100] and [110] directions respectively, approximately a factor of 6 greater than the spin moment, as predicted by Hund's rules. That the neutron diffraction experiments have not previously identified this itinerant spin moment is not surprising as it is just 1/7th of the magnitude of the measured signal and would only be seen in reflections at low sin θ/λ where diffraction experiments are not particularly sensitive.

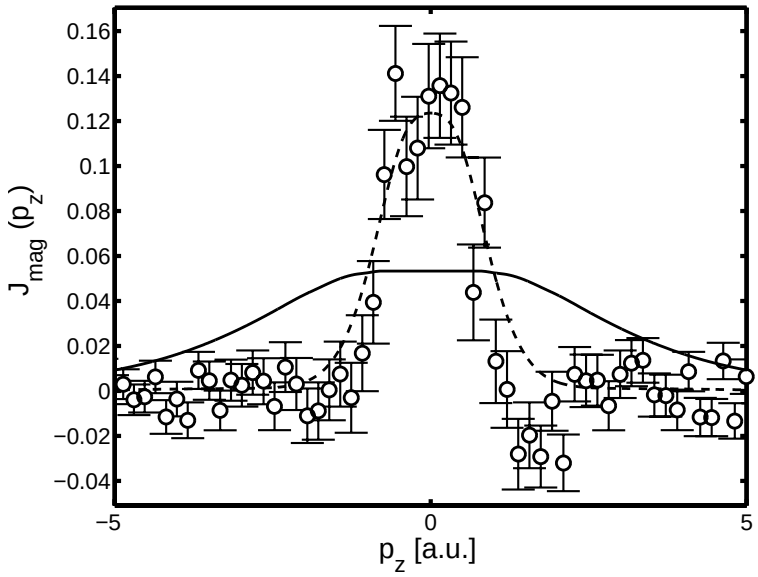

Figure 1. Spin-polarised Compton profile of CeB_6, resolving the [100] direction. The profile is normalised to 1 and has a momentum bin width of 0.2 a.u.. RHF free atom profiles of a Ce 4*f* (—) and Ce 5*d* (--) electron are also plotted for comparison.