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	Experiment title: Magnetic and Quadrupolar Order in PrB_6	**Experiment number**: 28-01-695
Beamline: BM28	**Date of experiment**: from: 2 February 2005 to: 8 February 2005	**Date of report**: April 2005
Shifts: 18	**Local contact(s)**: Danny Mannix	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

*Keith A McEwen, *Desmond F McMorrow, * Helen C Walker, *Matthias Bleckmann
(all University College London, UK)

*Je-Geun Park, *Seongsu Lee (both SungKyunKwan University, Suwon, Korea)

Report:

The cubic **RB_6** rare-earth hexaboride compounds display a rich variety of magnetic phenomena. The most investigated compound of this series is **CeB_6**, whose properties remain incompletely understood, despite many x-ray and neutron scattering studies. In an earlier experiment on XMaS we made the first resonant x-ray scattering study of **GdB_6**, which had not been studied with neutrons due to the high absorption of both Gd and B [1]. Our single crystal of GdB_6 was prepared by Seongsu Lee and Je-Geun Park, who have also been successful in producing crystals of other RB_6 compounds. In February 2005, we made the first resonant x-ray scattering study of **PrB_6** on XMaS.

Bulk property measurements indicate that PrB6 exhibits phase transitions at T_1=7K and T_2=4.2K. In their neutron diffraction study, Burlet et al [2] proposed that the transition at T_1 was to an antiferromagnetically (AFM) ordered state with an incommensurate wave vector of $q_1=(^1/_4-\delta, {}^1/_4, {}^1/_2)$, where $\delta \sim 0.05$. Below T_2, the structure was found to be commensurate, with $q_2=(^1/_4, {}^1/_4, {}^1/_2)$, with the moments directed along [110] directions. . The ordered moment below T_2 is only $1.2\mu_B$/Pr ion, significantly less than the $2.0\mu_B$/Pr ion of a Γ_5 ground state, indicated by inelastic neutron scattering [3] This discrepancy can be understood if antiferroquadrupolar (AFQ) ordering coexists with the magnetic ordering below T_2. The magnetic structure suggests that the most likely AFQ order parameter is O_{xy}, with an ordering wave vector of probably either $q_3=(^1/_2, {}^1/_2, 0)$, or $q_4=(^1/_2, {}^1/_2, {}^1/_2)$ – the latter being the wave vector of the AFQ phase in CeB_6.

In experiment 28-01-695, we used a single crystal of PrB_6, mounted in the XMaS He flow cryostat that allowed temperatures down to 2K to be obtained reliably. The crystal was cut with a face normal to the [011] direction, and oriented to give a [011] – [100] vertical scattering plane. Almost all measurements were made with an x-ray energy of 6.440 keV, corresponding to the Pr L_{II} edge. Polarisation analysis was carried out with a Cu (220) analyser crystal.

We observed and measured the temperature dependence of several magnetic reflections characteristic of the phases in the incommensurate phase below T_1, at for example ($^1/_2$,$^7/_4$ +δ, $^7/_4$), and at ($^1/_2$,$^7/_4$,$^7/_4$) in the commensurate phase below T_2. Resonant scattering was observed in both σ–σ and σ–π channels at the Pr L_{II} edge. In the time available we were able to measure the azimuthal dependence of the σ–σ and σ–π intensities at ($^1/_2$,$^7/_4$+δ,$^7/_4$), i.e. in the incommensurate phase. The results are shown in Fig. 1. Over the 110° range measured, the σ–π channel data exhibit a relatively straightforward ψ-dependence. However, the σ–σ channel data are more complex. Our θ-scans showed a subsidiary peak about 0.05^0 away from the main peak, for ψ angles between 10° and –40°, where it almost vanishes. This peak does not appear in the σ–π channel, and requires further investigation – these azimuthal scans were taken on the last night of our experiment.

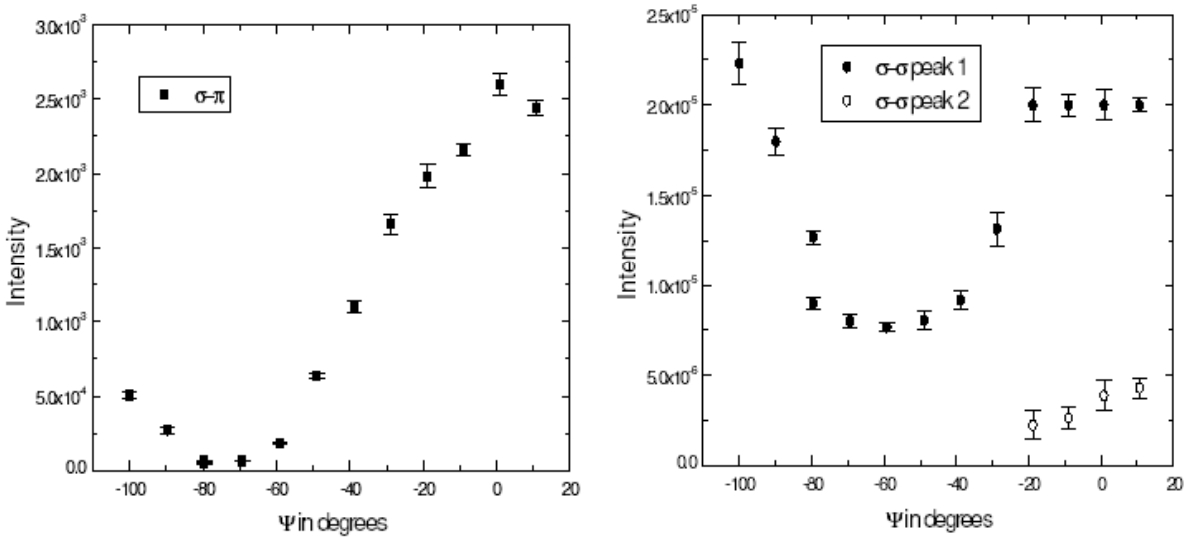

Fig.1. Azimuthal dependence of σ–π and σ–σ intensities at ($^1/_2$,$^7/_4$+δ,$^7/_4$), at T=5K

Earlier in our experiment, we discovered a **new first-order structural transition in PrB_6**, coexisting with the magnetic transition to the commensurate phase at T_2. Bragg peaks such as (0,1,1) and (2,2,2) were observed to split into 4 peaks below T_2. We believe that this splitting is most likely due to the anticipated distortion of boron octahedra, which appears to be much larger in PrB_6 than in CeB_6, where a structural transition of this nature has not been detected. Verifying this new transition in PrB_6, and measuring its temperature dependence for two reflections, left us little time to make a detailed search for possible quadrupolar reflections with wave vectors of either q_3=($^1/_2$, $^1/_2$, 0) or q_4=($^1/_2$, $^1/_2$, $^1/_2$).

In conclusion, the experiment was extremely fruitful. Detailed analysis is in progress and our results will be presented at the International Conference on Strongly Correlated Electron Systems (SCES2005) in Vienna in July 2005. However, many questions about this most interesting compound remain, and a continuation proposal is being submitted.

References

[1] D.F. McMorrow, K.A. McEwen et al., Physica B **345** 66 (2004)
[2] P. Burlet et al., J. Phys. (Paris) C **8** 459 (1988)
[3] M. Loewenhaupt and M. Prager, Z. Phys. **62** 195 (1986)