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## FERMI SURFACES AND EFFECTIVE MASSES IN $\text{LnB}_6$ , $\text{Ln} \equiv \text{La}$ , $\text{Ce}$ AND $\text{Pr}^*$

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### Summary

The Fermi surface has been compared for the three compounds  $\text{LnB}_6$  ( $\text{Ln} \equiv \text{La}$ ,  $\text{Ce}$  and  $\text{Pr}$ ) by measurement of the de Haas-van Alphen effect. The major part is observed to be similar in each compound, most likely consisting of X-centred ellipsoids with a total effective volume of about 1 electron per formula unit. Differences occur in the details of the shape of the FS, clearly seen for  $\text{PrB}_6$ .

Large effective masses,  $m^*$ , are observed for  $\text{CeB}_6$  and  $\text{PrB}_6$ ,  $m^* = 6$  and about 1.8, respectively. These have to be compared with  $m^* = 0.6$  for  $\text{LaB}_6$ .

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### Introduction

In metallic lanthanide systems many questions arise around the character of the 4f electrons, being localised on the ion core or assuming an itinerant character, through the formation of bands hybridised with the s and d states. From the experiments direct information can be obtained by studying Fermi surfaces (FS), their shape and derived properties, and comparing the FS for several Ln compounds of similar nature. When hybridisation takes place one expects to find large dissimilarities.

One such system has been investigated earlier by Johanson *et al.* [1]. From data obtained by the de Haas-van Alphen effect (dHvA) they concluded on large differences between the FS of  $\text{LaSn}_3$  and  $\text{CeSn}_3$ . In both compounds orbits are observed which belong to parts of the FS enclosing a substantial part of the Brillouin zone (BZ) volume, *i.e.*, containing a large number of electrons. From the very observation of such orbits they conclude

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that the behaviour of the electron states is coherent over several hundreds of unit cells.

The FS of  $\text{LaB}_6$  has been the subject of earlier investigations [2, 3]. Experiment (dHvA) and band theory agree on an FS having a total volume of one electron per formula unit, consisting of large, X-centred electron ellipsoids. The ellipsoids are interconnected by necks along the X-X directions; orbits around the necks and on the ellipsoids crossing the necks are observed over a limited angular range for directions around [100].

## Results and Discussion

Here we report data on the shape of the FS for other  $\text{LnB}_6$  compounds. The experimental procedure has been described elsewhere [4, 5]. The dHvA oscillations are detected in high magnetic fields, between 10 and 21 T for  $\text{LaB}_6$  and  $\text{PrB}_6$ , respectively, 25 and 33 T for  $\text{CeB}_6$ , at temperatures between 1.3 and 4.2 K.

$\text{CeB}_6$  shows several magnetic phases as functions of temperature and field [6, 7]; one infers from the magnetisation data that in the region where dHvA is measured, a ferromagnetic ordering is imposed by the magnetic field. For  $\text{PrB}_6$  the situation is less clear. From neutron scattering it was found [8] that two magnetic structures exist in zero field, a commensurate antiferromagnetic for  $T < 4.2$  K and an incommensurate for  $4.2 \text{ K} < T < 6.9$  K. The moment at  $T = 1.74$  K is  $1.77 \mu_B$ . We measured the magnetisation on a sample consisting of a large number of single crystals. At a temperature of 4.2 K it varies approximately linearly with magnetic field up to 15 T; at 15 T one finds  $0.7 \mu_B$  per Pr atom.

For  $\text{LaB}_6$ , dHvA frequencies are obtained as given earlier by Arko *et al.* [2]. Our results for the Ce and Pr compound are given in Fig. 1. For  $\text{PrB}_6$  the labels are given based on the merging of branches at high symmetry directions, indicating that the corresponding surfaces are connected through symmetry. For  $\text{CeB}_6$  the labels are attributed based on the similarity to  $\text{PrB}_6$ .

In all three compounds dHvA orbits are observed with frequencies ranging from 8 to  $10 \times 10^3$  T, labeled "a" in Fig. 1. For  $\text{LaB}_6$  they are the belly orbits on the X-centred ellipsoids,  $\chi$  in the notation of ref. 2. In a comparison of the a-branches in Fig. 1 with the data for  $\text{LaB}_6$  (ref. 2), a striking similarity is seen. For  $\text{PrB}_6$  and  $\text{LaB}_6$  the frequencies are nearly equal; for  $\text{CeB}_6$  they are 5 - 10% larger. The data for the Ce compound do not extend over the full (110) plane for experimental reasons rather than for the non-existence of dHvA orbits near [110].

For  $\text{PrB}_6$  two other sets of branches, labeled "b" and "c" are observed. Most of them are detected over the full (110) plane, indicating that the corresponding FS sheets are closed. This is in contrast to the  $\text{LaB}_6$  case, where the lower frequencies are due to orbits involving the X-X necks. The three-fold degeneracy of the b branches for the [111] orientation may have two causes; it can be due to a non-symmetry position in the BZ of the centre of

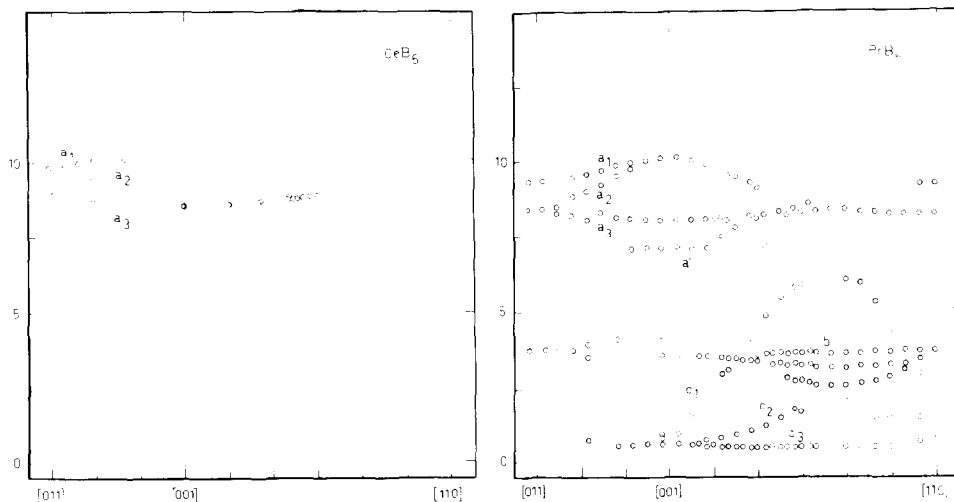


Fig. 1. Observed de Haas-van Alphen orbits in the (001) and (110) planes for  $\text{CeB}_6$  and  $\text{PrB}_6$ . The ordinate is in units of  $10^3$  Tesla. The orientation dependence of the high-frequency branches labeled a is similar to the one observed for  $\text{LaB}_6$ . The labels a, b, and c, are used with suffixes, based on the merging of the branches at the high-symmetry orientations only.

the corresponding sheets. In addition, it may stem from exchange splitting between the two spin directions. However, no such splitting is unambiguously resolved for the other sheets.

The effective mass,  $m^*$ , of the a branches has been determined by fitting the temperature dependence of the dHvA amplitude to the Lifshitz-Kosevich [9] expression. In  $\text{PrB}_6$  we find  $m^*$  equal to  $1.9 \pm 0.2$  and  $1.8 \pm 0.2$  for  $a_{1,2}$  and  $a_3$ , respectively, for the [001] orientation, using five temperatures between 1.3 and 4.2 K. No such accuracy is obtained in the case of  $\text{CeB}_6$ , as the signal is only observed for temperatures between 1.3 and 2.2 K. The value obtained is  $6 \pm 2$  for the  $a_3$  branch along [001]. For  $\text{LaB}_6$  the corresponding values are 0.65 and 0.61, respectively [2].

The a-branches shown in Fig. 1. have the highest frequency which varies only 25% over all orientations; they stem from orbits on the major FS sheets. When the a-branches have a common origin, the threefold degeneracy in the (001) plane places the centre of the sheets at the X point in the BZ, or M. The dominant part of the Fermi surfaces then has a strong similarity to the one of  $\text{LaB}_6$ . In this picture the f electrons are localised; they influence mainly the dispersion at  $E_F$ , increasing the effective masses above the value for  $\text{LaB}_6$ . The b- and c-branches for  $\text{PrB}_6$  may arise from distortions of the  $\text{LaB}_6$  bands near  $E_F$ . No obvious explanation is available for the a' branch.

## Conclusion

A direct interpretation of the FS data in terms of a band structure is not yet possible due to the lack of a sufficiently detailed calculation, allowing

for the magnetic structure of the materials. A nonmagnetic calculation has been carried out, treating the 4f electrons as itinerant for CeB<sub>6</sub> [10] and for CeB<sub>6</sub> and PrB<sub>6</sub> [11]. Both calculations indicate 4f states close to  $E_F$  and strongly mixed with the boron-derived band that is responsible for the Fermi surface of LaB<sub>6</sub>. The FS derived for the heavier Ln compounds do not resemble the one for LaB<sub>6</sub> at all. It is made up of sheets centred at  $\Gamma$  and R; their size is of the correct order of magnitude when compared with the a-branches. In this case the similarity between the three compounds is incidental. A comparison with the refined calculation will provide a better answer.

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