Thermal, magnetic and electronic properties of non-centrosymmetric YbPt$_2$B

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Abstract

Ternary YbPt$_2$B crystallizes in the non-centrosymmetric hexagonal CePt$_2$B-type structure (space group $P6_222$). Electrical resistivity, specific heat and magnetic measurements reveal a magnetic instability at 5.6 K. Furthermore, a spin-reorientation of presumably a ferromagnetic type occurs around 1.5 K. The behaviour at low temperature is governed by a rather weak Kondo effect, $T_K \approx 1$ K, in the presence of strong crystalline electric field splitting, with a doublet ground state. Besides, the complex magnetic behaviour presumably results from a Dzyaloshinskii–Moriya interaction triggered by the absence of inversion symmetry in the crystal structure. Scaling according to the de Gennes factor traces back magnetic ordering in YbPt$_2$B to the Rudermann–Kittel–Kasuya–Yoshida (RKKY) interaction and the smooth evolution of the lattice constants and the unit cell volume of REPt$_2$B (RE = rare earths) refers to the $4f^{13}$ electronic configuration of Yb in YbPt$_2$B.

Keywords: ferromagnetic order, non-centrosymmetric crystal structure, Dzyaloshinskii–Moriya interaction

(Some figures may appear in colour only in the online journal)

1. Introduction

Ternary rare earth (alkaline earth)—noble metal—metalloid (B, Si, Ge) systems have been extensively explored, evidencing a variety of interesting ground states. Among them is heavy fermion superconductivity in absence of inversion symmetry in CePt$_3$Si [1], BCS superconductivity without inversion symmetry in BaPt$_3$Si$_2$ [2] or a diversity of magnetically ordered states in RE$_2$Pd$_{14-x}$B$_x$ [3].

In order to extend the knowledge of such compounds and to continue our systematic investigations of RE-Pt-B systems, the Yb-Pt-B phase diagram has been examined in some detail. These studies revealed a novel ternary compound, YbPt$_2$B, being isostructural to the hexagonal CePt$_2$B type [4]. In previous studies [5–7] physical properties of REPt$_2$B have been probed. CePt$_2$B orders antiferromagnetically at $T_N \approx 2.1$ K [6]. Besides the RKKY interaction, responsible for long range magnetic order, Kondo and crystalline electric field (CEF) effects determine the ground state properties. PrPt$_2$B was characterised as a metallic antiferromagnet with $T_N = 4.6$ K. NdPt$_2$B, however, was found to exhibit two consecutive phase transitions upon cooling: an antiferromagnetic instability at $T_N = 18$ K followed by ferromagnetism below 10 K [5]. A recent study regarding TmPt$_2$B evidenced a quite complicated magnetically ordered phase below $T_C = 12.5$ K with predominant ferromagnetic character followed by a spin re-orientation below 6 K [7].

The aim of the present work is to identify physical properties of YbPt$_2$B by means of x-ray, resistivity, magnetisation and heat capacity measurements. Results obtained should allow to classify the magnetic behaviour of this compound and, moreover, assess the electronic configuration (EC) of Yb, which, in general, can fluctuate between the magnetic $4f^{13}$ and the non-magnetic $4f^{14}$ state. Interesting ground states are expected due to the presence of various mutual interactions (Kondo effect, RKKY interaction, CEF...
effect) on similar or different energy scales. A comparison will be made with isostructural CePt$_2$B as an opportunity to consider the occasionally stressed electron—hole symmetry of Ce and Yb compounds. LuPt$_2$B will provide information on the lattice dynamics in this ternary and serves to filter out the magnetic contribution in YbPt$_2$B.

The absence of inversion symmetry in a magnetically ordered compound might be the reason for the occurrence of quite complex magnetic phases, like canted structures or spirals. This is due to an additional magnetic interaction term, the so-called Dzyaloshinskii–Moriya (DM) interaction [8, 9]. Here, the magnetic exchange term $S_1 \times S_2$ between two spins $S_1$ and $S_2$ on sites without inversion symmetry—in the context of magnetic exchange coupling (antiferro- or ferromagnetic)—can provoke rather intricate magnetic phases.

2. Experimental

Polycrystalline samples with a weight of about 1 g were prepared by argon arc-melting elemental pieces of rare earth (purity > 99.9 mass %, Auer Remy, D), platinum foil (99.9%, Ögussa, A) and crystalline boron (98%, Alfa Aesar, D). For homogeneity, the samples were re-melted several times without significant weight losses (< 1 mass%). Both YbPt$_2$B and LuPt$_2$B were found to form directly from melts with nominal composition R$_2$Pt$_5$B$_5$ (in at.%). X-ray diffraction data were collected employing a Guinier–Huber image plate system with monochromatic CuK$_\alpha$ radiation ($\theta < 20 < 100^\circ$). Precise lattice parameters were calculated by least squares fits to the indexed 20 values calibrated with Ge as internal standard ($d_{Ge} = 0.565791$ nm). Single crystals suitable for x-ray structure determination were broken from alloys with nominal composition YbPt$_2$B and LuPt$_2$B. Inspection on an AXS-GADDS texture goniometer assured high crystal quality, unit cell dimensions and Laue symmetry of the specimens, prior to an x-ray intensity data collection on a four-circle Nonius Kappa diffractometer equipped with a CCD area detector employing graphite monochromated MoK$_\alpha$ radiation ($\lambda = 0.071069$ nm). The orientation matrix and unit cell parameters were derived using the program DENZO [10]. No additional (beside Psi-scans) absorption corrections were necessary because of the rather regular crystal shape and small dimensions of the investigated specimens. The structures were solved by direct methods and were refined with the SHELX-97 program [11]. A variety of standard techniques were employed to study electronic transport, thermodynamic and magnetic properties [12, 13].

3. Results and discussion

3.1. Structural properties

Single crystal x-ray intensity data for YbPt$_2$B and LuPt$_2$B (crystal size < 50 $\mu$m) revealed a primitive hexagonal unit cell for both crystals. Structure solution by direct methods and employing difference Fourier syntheses for the boron atoms confirmed the atom arrangement, which was proposed for CePt$_2$B. The refinements smoothly converged to the satisfactorily low values of reliability factors for both compounds. Structure data are summarized in table 1. The crystal structure of YbPt$_2$B was also confirmed from powder x-ray diffraction data employing a full profile Rietveld refinement (program FULLPROF [14], see figure 1).

Summarized in figure 2 are the lattice parameters, $a$, $c$ and the unit cell volume, $V$, of already known members of the series REP$_2$B (see [5–7]), together with the respective values of YbPt$_2$B. The monotonic variation of both $a$ and $c$ with rising ordinal number of the rare earths complies with a decreasing unit cell volume, i.e. the lanthanoid contraction.

The crystal structure of YbLu$_x$Pt$_{2-x}$B$_2$ is shown in figure 3. As described earlier for CePt$_2$B [4, 6], the structure of YbPt$_2$B represents a layered planar arrangement of Yb$_2$Pt$_2$ tetra-corner nets, located parallel to the basal plane, forming the top and ground faces of unfilled and B-filled tetragonal antiprisms Yb$_2$Pt$_4$ (figure 3(b)). In addition, a non-centrosymmetric arrangement of Yb ions is present with respect to the $c$-axis of the unit cell. While the in-plane distances between Yb ions are about 0.542 nm, shortest distances between Yb ions are perpendicular to the basis plane with $d_{Yb-Yb} = 0.371$ nm. Magnetic exchange between adjacent layers might then be responsible for the resulting spin structure. Both the absence of inversion symmetry of the crystal structure and the strong spin–orbit coupling of the heavy elements Yb and Pt possibly leads to exchange interactions of the DM type. As a result, rather complicated magnetic structures like spirals, cones or canted spin arrangements, as well as various temperature induced phase transitions can occur.

According to the lanthanoid contraction (see figure 2) atom distances between Yb-atoms, $d_{Yb-Yb} = 0.371$ nm, range between those of Tm ($d_{Tm-Tm} = 0.371$ 59(1) nm) and Lu ($d_{Lu-Lu} = 0.370$ 54(2) nm) suggesting a 2$F_{7/2}$ ground state for the Yb-atoms. No boron–boron contacts exist in the structure.

3.2. Ground state properties of YbPt$_2$B

Figure 4 focuses on the low temperature physical behaviour of YbPt$_2$B as derived from temperature dependent electrical resistivity measurements, $\rho(T)$ and heat capacity measurements, $C_p(T)$. In agreement with both measurements, a magnetic phase transition occurs at $T_{m1} \approx 5.6$ K, with minor differences in temperature between the electrical resistivity and the specific heat data. A further anomaly in both quantities appears around 1.5 K, signifying another phase transition, most likely of magnetic origin. This would imply that the magnetic structure adopted at 5.6 K re-orients at $T_{m1} \approx 1.5$ K upon cooling. For temperatures below $\approx$500 mK, an upturn of $C_p(T)$ due to core contributions occurs, which has been corrected in a standard manner assuming $C_{core}/T \propto T^{-2}$. The solid line in figure 4 represents the magnetic entropy $S_{mag}$ derived by integrating $C_{mag}/T$ from zero to temperatures above $T_{m1}$. $C_{mag}$ was obtained from the difference of the heat capacities of YbPt$_2$B and of isostructural, nonmagnetic LuPt$_2$B. Data on the latter are shown in figure 4, too. A detailed analysis of $C_p(T)$ of LuPt$_2$B was presented in [7], revealing the Sommerfeld value $\gamma = 2.2$ mJ molK$^{-2}$ and a Debye temperature $\theta_D^{LT} = 250$ K.
Table 1. Crystal structure data (standardized using the program Structure Tidy) for YbPt₂B and LuPt₂B (CePt₂B-type, space group P6₂22; No. 180) collected on Nonius KappaCCD with MoKα radiation.

| Nominal composition              | YbPt₂B                | LuPt₂B                |
|----------------------------------|-----------------------|-----------------------|
| Formula from refinement          | YbPt₂B               | LuPt₂B               |
| Range for data collection        | 2.24 < 2θ < 72.60     | 2.24 < 2θ < 72.70     |
| Crystal size                     | 35 × 35 × 50 μm³     | 30 × 30 × 45 μm³     |
| a [nm]                           | 0.52498(2)           | 0.52417(2)           |
| c [nm]                           | 0.78672(3)           | 0.78583(4)           |
| a [nm] (Rietveld refinement)     | 0.524576(5)          | 0.523885(9)          |
| c [nm] (Rietveld refinement)     | 0.786488(9)          | 0.78582(1)           |
| Reflections in refinement        | 307 Fo > 4σ(Fo) of 313 | 289 Fo > 4σ(Fo) of 301 |
| Mosaicity                        | <0.4                 | <0.3                 |
| Number of variables              | 12                   | 12                   |
| R²                              | 0.0265               | 0.0281               |
| GOF                             | 1.136                | 1.107                |
| Extinction (Zachariasen)         | 0.0132(9)            | 0.0071(7)            |
| M                               | 3c (1/2,0,0)         | 3c (1/2,0,0)         |
| Occupancy                       | 1.00Yb               | 1.00Lu               |
| U₁₁, U₂₂                        | U₁₁w = 0.0024(3)ᵇ    | 0.0042(2); 0.0051(3) |
| U₃₃, U₁₂                        | 0.0068(3); 0.0025(4) |                     |
| Pt                              | 6i (x,2x,0); x = 0.151 36(6) | 6i (x,2x,0); x = 0.151 46(6) |
| Occupancy                       | 1.00Pt               | 1.00Pt               |
| U₁₁, U₂₂                        | U₁₁w = 0.0024(3)ᵇ    | 0.0052(2); 0.0049(2) |
| U₃₃, U₁₂, U₁₃, U₁₂              | 0.0067(2); 0.0012(1); 0.0024(1) |                     |
| B                               | 3d (1/2,0,1/2);      | 3d (1/2,0,1/2);      |
| Occupancy                       | 1.00B                | 1.00B                |
| U₁₁w                            | 0.0012(23)           | 0.008(3)             |
| Residual electron density c max; min | 3.783;−4.839 | 4.13; −5.71          |

a Anisotropic atomic displacement parameters Uᵢᵢ in [10² nm²].

b Isotropic atomic displacement parameter Uᵢᵢw in [10² nm²].

c In [electrons nm⁻³] × 1000.

Figure 1. X-ray diffraction pattern of YbPt₂B. The solid line derives from the Rietveld refinement (on the basis of single crystal data). Yobs.–Ycalc. is the intensity difference between experimental data and Rietveld calculations. The inset on the left shows the metal coordination around the boron atom (Archimedian antiprism; Yb-atoms in yellow, Pt in blue and B in red).

Sₘₐₕ(T) of YbPt₂B increases continuously up to T = Tₘ₂, where a fraction of about 95% of R ln 2 is released. For T > Tₘ₂ only a weak temperature dependent behaviour is evident from the experimentally derived data. This behaviour allows drawing the following conclusions: (a) magnetic ordering happens in a crystalline electric field (CEF) doublet ground state and (b) the first excited CEF doublet is well separated from the ground state; therefore no substantial contributions from excited CEF levels to the magnetic features at low temperatures are expected.

The jump of the specific heat anomaly right at Tₘ₂ (δCₘₕ) is about 9.5 J mol K⁻¹, thus slightly below the value expected for an effective spin 1/2 system, where mean field results indicate δC₁/₂ₘₕ = 12.5 J mol K⁻¹. This discrepancy might be a consequence of specific mechanisms or a combination of them. Besides the second phase transition at Tₘ₁, short range order effects above the phase transition and/or the Kondo effect transfer entropy above the phase transition temperature. As a consequence, both δCₘₕ and Sₘₕ will be reduced below the simple mean field values.
3.3. Kondo and crystalline electric field effects in YbPt$_2$B

Kondo type interactions cause, in theory [15], a progressive diminution of $\delta C_{\text{mag}}$ versus $T_K/T_{\text{mag}}$, where $T_K$ is the Kondo temperature and $T_{\text{mag}}$ the ordering temperature of the system. Applying $T_{\text{mag}} = T_{m2} \approx 5.6 \text{ K}$ to this model reveals $T_K \approx 1.8 \text{ K}$. Further evidence for Kondo type interaction with a small characteristic temperature follows from a roughly 5% reduction of the entropy at $T = T_{m2}$, in comparison to magnetic ordering within a simple CEF doublet as ground state [16].

To account for the temperature dependent specific heat at low temperatures, a phenomenological model is employed, which involves long range magnetic ordering in terms of the molecular field theory together with the Kondo effect [15, 17–19] (for details see e.g. [20]). Convincing agreement between model assumptions and the experimental data is obtained for a Kondo temperature $T_K \approx 1 \text{ K}$ and a coupling constant between magnetic Yb ions $J \approx 12.1 \text{ K}$ (solid line, figure 5(a)). The latter takes into account next-nearest neighbour interactions and would reveal a magnetic instability at $T_{\text{mag}} = 6.05 \text{ K}$ in absence of the Kondo effect ($T_{\text{theo}} = J/2$). Simultaneously, the competition of long range magnetic order and the Kondo effect not only decreases the ordering temperature (by about 0.5 K), but, in addition, the spontaneous magnetisation is expected to be reduced by 5%.

A fit with about the same agreement (dashed–dotted line, figure 5(a)) is obtained in terms of the mean field theory only, where ordering sets in at $T_{\text{mag}} = 5.6 \text{ K}$. Different to the previous case, however, the magnetic contribution to the heat capacity entirely vanishes right at the phase transition temperature, while in the case of a Kondo contribution entropy is spread to higher temperatures. Thus, the finite values of $C_p$ at $T_{\text{mag}}$ are well reproduced in terms of the combined model. For temperatures above about 10 K, the Kondo contribution is almost negligible. The coincidence between the experimental data and the model employed also confirms the close match of the phonon contributions in both YbPt$_2$B and LuPt$_2$B.

Except for small fields ($\mu_0H < 1 \text{ T}$), the application of a magnetic field causes a response of the heat capacity data typical of ordered ferromagnetic systems: increasing fields smear out the jump of $C_p$ right at $T = T_{\text{mag}}$. The maximum of the resulting anomaly shifts to higher temperatures before it vanishes at very high fields. Altogether, externally applied magnetic fields shift entropy to higher temperatures. An attempt was made to theoretically describe these temperature and field dependencies of the heat capacity at low temperatures. Based on the model discussed above involving the Kondo effect and long range magnetic order in terms of the molecular field theory, the externally applied magnetic field was added. Results are shown in figure 5(a) as solid lines, revealing good agreement with the experimentally observed results without changing the parameters used above.

Figure 5(b) displays $C_{\text{mag}}(T)$ of YbPt$_2$B for temperatures up to about 150 K. Since the crystalline electric field, CEF, exerted on the Yb ions in this hexagonal compound causes a lifting of the $2J + 1$-fold degenerate ground state, 4 CEF doublets are created. In terms of specific heat, this causes the occurrence of a Schottky anomaly. A least squares fit (solid line, figure 5(b)) considering a ground state doublet and 3 excited levels reveals reasonable agreement for $\Delta_1 \approx 160 \text{ K}$, $\Delta_2 \approx 290 \text{ K}$ and $\Delta_3 \approx 310 \text{ K}$. This allows to conclude, in agreement with the entropy released at low temperatures,
A much more complex resistivity behaviour is evident for YbPt$_2$B. A pronounced curvature of $\rho(T)$ characterises the ordered region of YbPt$_2$B, a model developed in [21] is applied, yielding an analytic expression regarding the temperature dependent electrical resistivity:

$$\rho = BT\Delta \left( 1 + \frac{2T}{\Delta} \exp(-\Delta T) \right).$$

(1)

This expression is based on scattering of conduction electrons on ferromagnetic magnons with a dispersion relation $\hbar \omega = \Delta + C_0 k^2$, where $\Delta$ is the spin wave gap and $C_0$ is the spin wave stiffness. $B$ is a material dependent constant related to the spin disorder. It provides the well known $T^2$ behaviour of the temperature dependent electrical resistivity of ferromagnets in the gapless case. Applying equation (1) to the experimental data yields a spin wave gap $\Delta \approx 1.1$ K.

Despite the data set being limited to the narrow temperature range below the low temperature phase transitions (0.4 < $T < 1.5$ K), the spin wave gap obtained is quite reasonable with respect to the magnitude of the ordering temperature.

Figure 5. (a) Temperature dependent magnetic contribution to the specific heat $C_{\text{mag}}$ for various applied magnetic fields. The solid lines are least squares fits as explained in the text. The dashed line is a fit using the molecular field model only. (b) Temperature dependent magnetic contribution to the specific heat $C_{\text{mag}}$ for temperatures up to 150 K. The low temperature anomaly is accounted for as explained in the text; the high temperature contribution is described employing a Schottky anomaly with CEF doublets separated from the ground state by 160, 290 and 310 K, respectively.

Figure 6. (a) Temperature dependent electrical resistivity $\rho$ of YbPt$_2$B and LuPt$_2$B normalized to the respective room temperature values. The dashed line illustrates the negative logarithmic $\rho(T)$ behaviour. (b) Low temperature details of $\rho(T)$ (left axis) and its temperature derivative $d\rho/dT$ (right axis, dashed line). The solid line is a least squares fit according to equation (1).

$S_{\text{mag}}(T = 10\,\text{K}) \approx 5.8\,\text{J}\,\text{mol}\,\text{K}^{-1}$, that ordering of the Yb moments occurs in the doublet ground state without substantial contributions from excited levels. Of course, inelastic neutron scattering experiments would be needed to precisely determine the wave function and the respective energies of the CEF scheme of YbPt$_2$B.

3.4. Electronic transport in YbPt$_2$B

Figure 6(a) displays the temperature dependent electrical resistivity $\rho$ of both YbPt$_2$B and LuPt$_2$B. Because of microcracks and fractures in the specimens, the data in figure 3 are normalised to the respective values at room temperature. LuPt$_2$B is characterized by a metallic behaviour with a smooth increase of $\rho$ with increasing temperatures.

A much more complex resistivity behaviour is evident for YbPt$_2$B. A pronounced curvature of $\rho(T)$ characterises the paramagnetic temperature range of this compound, being a result of CEF effects, where the total angular momentum of Yb, $j = 7/2$, is split into 4 doublets owing to the electric fields of charges in hexagonal symmetry. In the absence of single crystals and/or inelastic neutron scattering data, an estimation of an appropriate CEF scheme is all but impossible. Upon cooling, a weak minimum in the 10 K range and a logarithmic behaviour is observed, followed by a drop of $\rho(T)$ below 5 K. In accordance with the heat capacity data, this anomaly is interpreted as the onset of long range magnetic order. A closer inspection of low temperature details of the electrical resistivity (compare figure 6(b), open symbols), clearly evidences a further magnetic phase transition, again in agreement with specific heat data. Both magnetic phase transitions are revealed in more detail from the first derivative of $\rho$ with respect to temperature (dashed line, figure 6(b), right axis).

In an attempt to quantitatively describe the magnetically ordered region of YbPt$_2$B, a model developed in [21] is applied, yielding an analytic expression regarding the temperature dependent electrical resistivity:
A ferromagnetic scenario was chosen here because of the conclusions made from magnetisation data (compare figure 8).

The application of magnetic fields causes substantial changes in the temperature dependent electrical resistivity of YbPt$_2$B at low temperatures (see figure 7(a)). Primarily, the anomaly at $T_m$ becomes gradually washed-out and slightly shifts for larger fields to higher temperatures. Additionally, $T_m$ vanishes and a simple power-law behavior becomes obvious for magnetic fields in the 8–12 Tesla range. Analyzing the data at these fields according to $\rho = \rho_0 + A \cdot T^n$ reveals $n = 1.14$ and $n = 1.17$ for the 8 and the 12 Tesla run, respectively. Obviously, the non-Fermi liquid behavior observed results from the proximity of a quantum phase transition owing to the suppression of magnetic order by externally applied magnetic fields.

The application of hydrostatic pressure (figure 7(b)) does not significantly change the overall resistivity behavior of YbPt$_2$B. The vertical dashed line in this figure evidences that the phase transition at $T_m$ stays almost unaffected in the low pressure range. The phase transition at lower temperatures, however, seems to become suppressed.

3.5. Magnetic properties of YbPt$_2$B

Magnetic measurements have been carried out on YbPt$_2$B to collect information about the electronic configuration of the Yb ions, their interaction and analyse the ordered state below about 6 K. Different kinds of samples from the same batch of YbPt$_2$B were used for these measurements. The first run was made with an appropriate piece (about 30 mg) of polycrystalline...
material. In the second run we used the same, but powdered material which could freely rotate in the sample ampulla inside of the SQUID magnetometer. The last run was made on statistically oriented, fixed powder. Figure 8(a) displays isothermal magnetization data of two different polycrystalline samples (A, B) taken at \( T = 1.3 \) and 2.8 K in fields up to 6 T. While the former temperature is below \( T_{m1} = 1.5 \) K, the latter is below \( T_{m2} = 5.6 \) K, referring to measurements in the two magnetically ordered phases of YbPt2B. The solid line is again a fit using the molecular field model. The dashed line represents the same model, but Kondo interaction (\( T_K = 1 \) K) is added. There are several interesting features:

(i) Spontaneous magnetisation is likely in both regimes and measurements carried out at small positive and negative fields revealed a weakly hysteretic behaviour as a consequence of ferromagnetic-like ordering at \( T_{m2} = 5.6 \) K and \( T_{m1} = 1.5 \) K. Depending on the state of the sample, different values of the magnetisation at 6 T are found. If the sample is measured on the freely rotating powder, magnetisation reaches about 3.1 \( \mu_B \) Yb\(^{-1}\), while the polycrystalline sample attains 1.7 \( \mu_B \) Yb\(^{-1}\) at \( T = 2.8 \) K. The magnetisation of the fixed powder sample is just in-between both. The \( M(H) \) curve at \( T = 1.3 \) K observed on the polycrystalline material has a larger magnetisation than the 2.8 K run, but the overall behaviour does not change. This run was made in a different, \(^3\)He based set-up of the SQUID magnetometer. An entirely identical orientation of the polycrystalline piece of YbPt2B was not achieved. While the similar overall shapes of \( M(H) \) unambiguously refer to a predominantly ferromagnetic state, the slight changes in absolute magnetisation can be, at least partly, a consequence of a minor change of the sample-orientation, too. The polycrystalline sample used in the present study obviously has some texture and the preferred orientation at the magnetic measurement primarily pointed into the direction of the hard magnetic axis. This can be seen from the susceptibility data as well (figure 8(b)).

(ii) The deviation of the calculated and measured isotherms can be attributed to magneto-crystalline anisotropy in this hexagonal compound. It was shown that a substantial uniaxial magneto-crystalline anisotropy causes a remarkable downturn of the Arrott plots below \( T_c \) [22]. In this model the negative curvature of the Arrott plots below \( T_c \) (compare figure 9(a), fixed powder sample) can be accounted for as a result of domain rotations in the non-oriented crystallites against the random but uniaxial anisotropy fields \( H_A \). A rather simple way to estimate \( H_A \) in terms of this model is to extrapolate the linear part of the Arrott plot backwards to obtain the spontaneous magnetisation (dashed lines, figure 9(a)). Taking 91.3% of that value gives with a parallel forward extrapolation an intersection with the experimental Arrott plot, yielding a value for \( H/M \) where this particular field corresponds to the anisotropy field \( H_A \) (dashed–dot lines (figure 9(a))). For further details see [22]. Using this simple estimate we obtain an anisotropy field of about 0.9 T which arises from the uniaxial anisotropy of the building blocks. Accordingly, one would expect a coercivity of about 0.08 T as mentioned above, however, the measured coercivity of about a few mT is rather small in particular with respect to the estimated anisotropy field. On the other hand a complex structure such as a conical one reduces the coercivity remarkably due to the easy rotation of the magnetic moment along the cone. Such a ferromagnetic cone structure may also be a precursor for spin-reorientation at lower temperatures.

Figure 9(b) illustrates the results of temperature dependent a.c. susceptibility measurements taken at \( \nu = 100 \) Hz and at a field amplitude of 325 A m\(^{-1}\). While the in-phase component \( \chi' \) clearly reveals a sharp maximum near \( T = T_{m2} \), the out-of-phase part \( \chi'' \) definitely reveals a hysteretic behaviour below \( T_{m2} \), thus confirming the ferromagnetic nature of the magnetic phase in the low field limit (compare e.g. [13]). The sharp maximum arises...
Magnetisation at 6 T on the freely rotating sample reaches about 3.1 $\mu_B$ Yb$^{3+}$. This is a rather large value compared to other Yb compounds but is still smaller than the magnetic moment of the free Yb$^{3+}$ ion ($M_{\text{eff}} = g_j \cdot j = 8/7 \cdot 7/2 = 4 \mu_B$). Both, the Kondo and CEF effects can be made responsible for such a behaviour. The Kondo effect with $T_K$ being of the order of 1 K will cause only a minor reduction of the spontaneous magnetisation. Thus, the CEF ground state doublet possesses—at least—a moment of about 3.1 $\mu_B$. Hence, in terms of an effective spin-1/2 state, the modified Landé-factor needs to be of the order of $g_{1/2}^{\text{eff}} \approx 6.2$. A CEF in hexagonal symmetry causes, in general, a mixing of $|5/2\rangle$ and $|7/2\rangle$ states, while the $|1/2\rangle$ and $|3/2\rangle$ state can occur as pure eigenstates. In order to explain the large magnetic moment observed in the ground state in terms of the CEF theory, the weight factors $\alpha$ and $\beta$ in the wave function $|\alpha|5/2\rangle \pm |\beta|7/2\rangle$ are expected as $\alpha \ll \beta$.

Shown in figure 8(b) is the the temperature dependent inverse magnetic susceptibility $1/\chi$ for the three different kinds of samples. Experimental data exhibit good scaling for various fields (0.1 T, 1 T and 3 T) above 20 K. As expected from the isothermal magnetisation data, the susceptibility at the three different conditions of measurement reflect the CEF anisotropy. While the polycrystal behaves likely as a material oriented along the hard axis, the freely rotating powder is oriented by the applied field towards the easy axis. The blocked powder represents then a statistical average of Oriented by the applied field towards the easy axis. The blocked powder represents then a statistical average of

Figure 10. (a) Magnetic phase transition temperatures of REPt$_2$B versus the de Gennes factor. (b) Preliminary magnetic phase diagram of YbPt$_2$B. The asterix should indicate that both ferromagnetic phases appear to be complex.

from the fact that the anisotropy field (estimated as about 0.9 T, see above), largely exceeds the amplitude of the applied a.c. field (about 0.4 mT).

(iii) Magnetisation at 6 T on the freely rotating sample reaches about 3.1 $\mu_B$ Yb$^{3+}$. This is a rather large value compared to other Yb compounds but is still smaller than the magnetic moment of the free Yb$^{3+}$ ion ($M_{\text{eff}} = g_j \cdot j = 8/7 \cdot 7/2 = 4 \mu_B$). Both, the Kondo and CEF effects can be made responsible for such a behaviour. The Kondo effect with $T_K$ being of the order of 1 K will cause only a minor reduction of the spontaneous magnetisation. Thus, the CEF ground state doublet possesses—at least—a moment of about 3.1 $\mu_B$. Hence, in terms of an effective spin-1/2 state, the modified Landé-factor needs to be of the order of $g_{1/2}^{\text{eff}} \approx 6.2$. A CEF in hexagonal symmetry causes, in general, a mixing of $|5/2\rangle$ and $|7/2\rangle$ states, while the $|1/2\rangle$ and $|3/2\rangle$ state can occur as pure eigenstates. In order to explain the large magnetic moment observed in the ground state in terms of the CEF theory, the weight factors $\alpha$ and $\beta$ in the wave function $|\alpha|5/2\rangle \pm |\beta|7/2\rangle$ are expected as $\alpha \ll \beta$.

Shown in figure 8(b) is the the temperature dependent inverse magnetic susceptibility $1/\chi$ for the three different kinds of samples. Experimental data exhibit good scaling for various fields (0.1 T, 1 T and 3 T) above 20 K. As expected from the isothermal magnetisation data, the susceptibility at the three different conditions of measurement reflect the CEF anisotropy. While the polycrystal behaves likely as a material oriented along the hard axis, the freely rotating powder is oriented by the applied field towards the easy axis. The blocked powder represents then a statistical average of $\alpha$- and $c$-axes contributions. Analysing the latter (above about 50 K) in terms of a modified Curie Weiss law, i.e. $\chi = \chi_0 + C/(T - \theta_p)$, the experimental data can be accurately accounted for. Here, $\chi_0$ represents a temperature independent Pauli-like susceptibility, $C$ is the Curie constant, related to the $\mu_{\text{eff}}$ and $\theta_p$ is the paramagnetic Curie temperature. The results of a least squares fit (solid line, inset figure 8) yield $\chi_0 = 0.0006$ emu mol$^{-1}$, an effective moment $\mu_{\text{eff}} = 4.51 \mu_B$ and a paramagnetic Curie temperature $\theta_p = -3$ K. The value obtained for $\mu_{\text{eff}}$ is very close to the theoretical value of 4.54 $\mu_B$ associated with the Yb$^{3+}$ state. This unambiguously allows to conclude that Yb in YbPt$_2$B is in its 4$f^{13}$ EC, being the magnetic EC of Yb.

3.6. Magnetic phase diagram of YbPt$_2$B

As mentioned above, the Yb ions in the crystalline unit cell form a 3D network of triangular-like structures with varying Yb–Yb distances; the smallest one is 0.3701 nm, arranged roughly in a zig–zag manner along the hexagonal c-axis. A coupling of magnetic moments along these Yb–Yb nearest neighbour paths is rather likely. Coupling of next-nearest Yb ions, i.e. within the basal planes, might happen by assistance of the Pt electron density. One may speculate that the Dzyaloshinskii–Moriya type interaction in this non-centrosymmmetric compound finally drives a non-collinear spin structure which then provides the basis for a further moment re-orientation of the initial magnetic phase.

The REPt$_2$B compounds summarized in the introduction (except the case of non-magnetic La and Lu) exhibit long range magnetic order, which, in the case of metallic rare earth compounds are expected to be based on the RKKY interaction. In order to check the same background of magnetic order under similar circumstances, the respective ordering temperatures are plotted as a function of the de Gennes factor, $(g - 1)^2|j + 1|$. Summarized in figure 10 are the ordering temperatures previously established, together with YbPt$_2$B. Overall, the transition temperatures follow fairly well the general trend determined by the Landé factor and the total angular momentum. Yb as well as Pr deviate slightly from this linear dependence. Two facts can be considered being responsible: (a) The de Gennes factor implicitly takes into account the total angular momentum of the rare earth ion;
CEF effects, however, fix a certain ground state and the wave function associated with this multiplet might result in a magnetic moment which is quite different from the free ion value. As a result, ordering temperatures can deviate significantly from the expected one. (b) Pr as well as Tm are so-called non-Kramers ions, allowing singlet and triplet states, which can be non-magnetic, in contrast to those of Ce, Nd and Yb.

A comparison of YbPt$_2$B and CePt$_2$B shows that both ternary systems exhibit a weak Kondo effect in the presence of long range magnetic order which evolves in a CEF doublet as ground state. While the former reveals two magnetic instabilities above 300 mK, the latter shows just a single magnetic phase transition. In many isostructural Ce and Yb compounds it has been observed that in Yb systems with transition metal elements having unfilled $d$-shells, the larger Yb valence is stabilized. Consequently, such systems can order magnetically. In the case of Ce systems, the larger valence causes a nonmagnetic ground state. If the transition metal elements have already filled $d$-shells, an entirely reversed behaviour occurs. A very good example here is CeCu$_5$ and YbCu$_5$, matching perfectly these empirical rules (compare e.g. [23]). The fact that both YbPt$_2$B and CePt$_2$B exhibit long range magnetic order indicates a stable 3$^\text{rd}$ state of the Ce and the Yb ions, respectively, in contradiction to the above indicated phenomenological rules. It might refer to boron which possibly acts as electron donor instead of Ce.

A preliminary magnetic phase diagram (figure 10(b)) has been compiled using resistivity and heat capacity data. The field dependent transition temperature $T_{n2}$ decreases slightly at low fields; a further field increase broadens the field-induced ferromagnetic state, where the crossover temperature has been taken from the smooth maxima of the field dependent heat capacity data (compare figure 5). Note that the range of decrease of $\rho(T)/\mu_0 H$ roughly coincides with the negative magnetoresistance observed at low temperatures and low fields. The second phase transition around 1.5 K, deduced from $\rho(T)$ data, appears to be only weakly field dependent before the magnetic signal vanishes in the background at $\mu_0 H \approx 4$ T. YbPt$_2$B with a magnetic phase transition temperature $T_{n2} = 5.6$ K is among those Yb compounds showing relatively large values of magnetic instabilities like YbRu$_2$Ge$_2$ [24], YbMgSi$_2$ [25], Yb$_2$Cu$_4$Ge$_4$ [26], or YbRhGe [27].

The complex form of ferromagnetic order at $T_{n2} = 5.6$ K, e.g. like that of a cone or a spiral and subsequently a spin-reorientation at $T_{n1} = 1.5$ K would be in line with the Dzyaloshinskii–Moriya interaction. This interaction, driven by spin–orbit coupling, is made responsible for spin fluctuation like that elaborated for MnSi, a cubic compound (space group $P2_13$, #198) without inversion symmetry [28].

4. Summary

The already explored members of REPt$_2$B compounds with light (La, Ce, Pr, Nd) and heavy (Tm, Yb, Lu) rare earth elements are characterised by a monotonic decrease of the lattice parameters due to the well known lanthanide contraction. This smooth behaviour refers to a 3$^\text{rd}$ state of the rare earth ions and thus to a magnetic EC for the respective Ce and the Yb compounds. In fact, detailed investigations of bulk properties of YbPt$_2$B reveal two consecutive magnetic instabilities at 1.5 and 5.6 K, respectively. RKKY interactions in the presence of a rather weak Kondo effect and CEF effects are responsible for long range magnetic order in a CEF doublet as ground state. Contributions from excited levels are negligible for this ternary compound. The complex ferromagnetic phase ($T_{n2} = 5.6$ K) and a spin-reorientation at about 1.5 K is suspected to be a consequence of the Dzyaloshinskii–Moriya interaction, established because of the absence of inversion symmetry in the crystal structure of YbPt$_2$B.

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