

Magnetic structure and crystal field states of the heavy fermion system YbPt₅B₂Leonid Salamakha^{1,2}, Oksana Sologub¹, Herwig Michor¹, Dmitry Khalyavin³, Manh Duc Le³, Devashibhai T. Adroja³ and Ernst Bauer^{1,*}¹*Institute of Solid State Physics, TU Wien, Wiedner Hauptstraße 8-10, A-1040 Wien, Austria*²*Department of Physics of Metals, L'viv National University, L'viv, Ukraine*³*ISIS Neutron and Muon Source, STFC, Rutherford Appleton Laboratory, Chilton, Oxfordshire OX11 0QX, United Kingdom*

(Received 22 May 2025; accepted 3 September 2025; published 26 September 2025)

Monoclinic compounds YbPt₅B₂ and LuPt₅B₂ [space group *C2/m* (No. 12), own structure type] have been studied by means of elastic and inelastic neutron scattering experiments. The heavy fermion system YbPt₅B₂ orders antiferromagnetically below $T_{N1} = 7.8$ K and exhibits an incommensurate magnetic structure with a temperature-dependent propagation vector, $\vec{k}_1 = (0.194, 0, -0.045; T = 6 \text{ K})$. Below $T_{N2} = 4.7$ K, a transition into a commensurate structure, $\vec{k}_2 = (0, 0, 0)$, takes place. The transition at T_{N2} turns out to be of first order, as obvious from commensurate and incommensurate contributions to the magnetic moments around $T = T_{N2}$. Rather large Yb moments, $m(\text{Yb}) > 3\mu_B$, yet reduced due to the Kondo effect, were obtained as a result of the splitting of the Yb³⁺ eightfold-degenerate ground state into four doublets, owing to crystalline electric field (CEF) effects. Such unusually large moments in Yb systems can be explained only by an appropriate wave function $\sum_{i=-7/2}^{i=7/2} \pm \alpha_i |i/2\rangle$, $\sum_i \alpha_i^2 = 1$, constituting the CEF ground state doublet, which indeed was concluded from the present inelastic neutron data, considering the crystalline electric field theory. The overall CEF splitting is on the order of 44 meV, while the first excited level is located ≈ 25 meV above the ground state.

DOI: [10.1103/pj8b-d5h9](https://doi.org/10.1103/pj8b-d5h9)**I. INTRODUCTION**

Among *f*-electron-based heavy fermion systems, Yb-based compounds and alloys form a wide variety of binary, ternary, or quaternary materials, which exhibit a broad diversity of mostly low-temperature features, associated with superconductivity [1–3], magnetic order with substantially reduced magnetic moments [4], Kondo-driven anomalies in transport properties [5], quantum criticality [6,7], intermediate valence behavior [8,9], paramagnetic ground states [10], or phase transitions triggered by abrupt changes of the valence state of the Yb ion, e.g., from Yb²⁺ toward Yb³⁺ [11], or vice versa.

Basically, three different kinds of interaction that exist in such materials, as well as their mutual balance, are responsible for the above-mentioned physical features. (i) Ruderman-Kittel-Kasuya-Yoshida (RKKY) interactions [12–14], where due to a distance-dependent interplay of the *f* moments with the spins of the conduction electrons, magnetic order tends to be established, both of ferro- or antiferromagnetic type. The strength of this interaction depends on a coupling constant (*J*) and the electronic density of states at the Fermi energy [*N*(*E_F*)], $T_{\text{RKKY}} \sim N(E_F)J^2$. (ii) The Kondo effect [15] results in a screening of the *f* moments owing to a cloud of

conduction electrons with opposite spins. In the optimal case, the total magnetic moment of such a quasiparticle vanishes, and the entire system adopts a paramagnetic ground state due to Kondo singlet formation. The strength of the Kondo effect is dependent on *JN*(*E_F*), too, however, in an exponential manner, $T_K \sim \exp\{-1/[2N(E_F)J]\}$. This causes that for small values of *JN*(*E_F*), the RKKY interaction dominates and the system orders magnetically. In the opposite case, the Kondo effect dominates so the system stays paramagnetic down to the lowest temperatures. (iii) Crystalline electric field (CEF) effects [16] provoke a lifting of the (2*j* + 1)-fold ground state degeneracy of the *f* moment, where *j* is the total angular momentum (e.g., *j* = 7/2 for Yb-4*f*¹³). This phenomenon results from the impact of electric charges of the atoms in the vicinity of a distinct *f* ion. Besides charges, the value of *j*, as well as the structural and symmetry properties of the material, define CEF features. Macroscopic properties, like the magnetic moment at low temperatures, are then a result of the ground state multiplet created by CEF effects.

The present study focuses on the magnetism of ternary YbPt₅B₂, exploring in detail the complex magnetic structure, as well as details of CEF effects by means of elastic and inelastic neutron investigations, which have been carried out at ISIS (UK). Although the magnetic moment associated with the Yb³⁺ state, $m(\text{Yb}^{3+}) = 4 \mu_B$, is larger than that of comparable Ce systems [$m(\text{Ce}^{3+}) = 2.14 \mu_B$], long-range magnetic ordering for the latter frequently happens at much higher temperatures, and ferromagnetism is reported for CeRh₃B₂ with *T_C* as high as 115 K [17]; many others can exceed *T_{ord}* = 10 K [18–20]. Note, the above-indicated moment values refer to a single isolated Yb or Ce ion. Because of CEF effects in solids, these values are reached, in general, only at very high

*Contact author: bauer@ifp.tuwien.ac.at

magnetic fields. On the other hand, the transition temperatures of binary and ternary Yb intermetallics are frequently constrained to values on the order of 1 K [21,22]. Some ternary Yb compounds order around 5 K [23–26] and Yb₂MgSi was found to order antiferromagnetically at around 9.5 K [27].

Recently, ternary compounds YbPt₅B₂ and isostructural nonmagnetic LuPt₅B₂ have been characterized for the first time and several bulk properties have been studied in detail [28]. YbPt₅B₂ exhibits two magnetic phase transitions at $T_{N1} = 7.8$ K and $T_{N2} = 4.7$ K. A substantial splitting of the CEF-generated excited levels from the ground state ($\Delta E_1 \approx 25$ meV) ensures that long-range magnetic order in YbPt₅B₂ is a phenomenon of the ground state doublet only.

II. EXPERIMENTAL DETAILS

Polycrystalline samples of YbPt₅B₂ and LuPt₅B₂ (8 g each) were prepared by argon-arc-melting appropriate amounts of the constituent elements using Ti as getter material. Yb-weight losses were compensated for by adding additional amounts of Yb before melting. For homogeneity, the samples were remelted several times. Subsequently, the samples were wrapped in Mo foil, sealed in evacuated silica tubes, and heat treated for 10 days at 1020 K. Phase purity and crystal structure of the various specimens were checked by x-ray diffraction, prior to our neutron studies. Details are summarized in the Supplemental Material (SM), Fig. S1 [29].

All neutron measurements were performed at ISIS (UK), using time-of-flight spectrometers.

The WISH diffractometer was used to perform neutron diffraction studies at temperatures from 1.5 K to room temperature. The samples were powdered and filled into vanadium cans before mounting in the cryostat.

For inelastic neutron scattering (INS) experiments, the MARI spectrometer with the gadolinium chopper was employed and various temperatures, from 5 K to room temperature, were applied. The incident neutron energies were set from $E_i = 10$ meV to 170 meV, with the chopper speed set at 200 or 400 Hz.

III. EXPERIMENTAL RESULTS AND DISCUSSION

In order to summarize the main results derived in our previous study [28], Fig. 1 renders the most important facts and figures known about YbPt₅B₂. Figure 1(a) sketches the crystalline unit cell of YbPt₅B₂, crystallizing in its own structure type. The monoclinic crystal structure is characterized by very large values of the lattice parameter $a \approx 15.5$ Å while b and c are almost identical (≈ 5.5 Å). Intrinsic anisotropic properties are thus expected. Various temperature and field dependent bulk properties of YbPt₅B₂ that were considered [28] revealed two temperature and at least two field-induced phase transitions below $T_{N1} = 7.8$ K and $T_{N2} = 4.7$ K, respectively. These magnetic phase transitions can be seen from the temperature-dependent specific heat and thermal expansion of YbPt₅B₂ shown in Fig. 1(b). Both thermodynamic properties exhibit distinct anomalies around T_{N1} and T_{N2} , unambiguously referring to magnetic phase transitions, which are present in magnetic susceptibility data at the very same temperatures, too. The heat capacity data, furthermore, in-

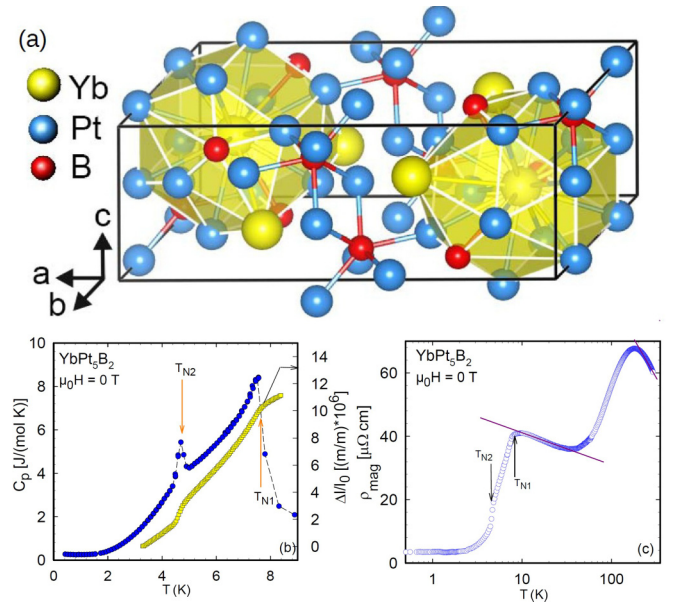


FIG. 1. (a) Sketch of the monoclinic crystalline unit cell of YbPt₅B₂. (b) Temperature-dependent specific heat C_p (left axis) and thermal expansion (right axis) of YbPt₅B₂. (c) Temperature-dependent magnetic contribution ρ_{mag} of YbPt₅B₂ plotted on a logarithmic temperature scale. The arrows mark the magnetic phase transition temperatures.

dicate that the phase transition at $T = T_{N2}$ is likely of a first-order type. Long-range magnetic order of Yb-based intermetallics is, in general, based on the RKKY interaction, where conduction electrons couple to the spins of the $4f$ electrons.

Due to the presence of the Kondo effect [compare the resistivity data in Fig. 1(c)], the magnetic moment is reduced from the expected value associated with isolated ytterbium ions, and the RKKY interaction is also weakened, which lowers the magnetic phase transition temperatures. A measure for the strength of the Kondo effect present in YbPt₅B₂ is the magnetic entropy released at $T = T_{N1}$, being below the expected value of $R \ln 2$ (about 85%). This value can be translated into a characteristic temperature, $T_K = 8$ K [30], which is comparable to the magnetic phase transition temperature ($T_{N1} = 7.8$ K). Thus, the Yb- $4f$ moments are expected to be smaller than $g_j j = 4 \mu_B$, where $j(\text{Yb}) = 7/2$ is the total angular momentum of Yb³⁺ and $g_j = 8/7$ is the respective Landé factor.

Besides this, CEF effects also play a most crucial role in determining the ground state properties of monoclinic YbPt₅B₂. The CEF lifts the eightfold-degenerate ground state of the $j = 7/2$ multiplet into four doublets with the energetically lowest doublet forming the ground state of the system. At $T = 0$, only the ground state is populated and this thus determines physical properties at low temperatures. As the temperature rises, CEF levels, which are separated energetically from the ground state, become populated. The physical properties are then modified accordingly. The impact of all three mechanisms present in YbPt₅B₂ can best be seen from the magnetic contribution to the temperature-dependent electrical resistivity, rendered in Fig. 1(c). There, resistivity

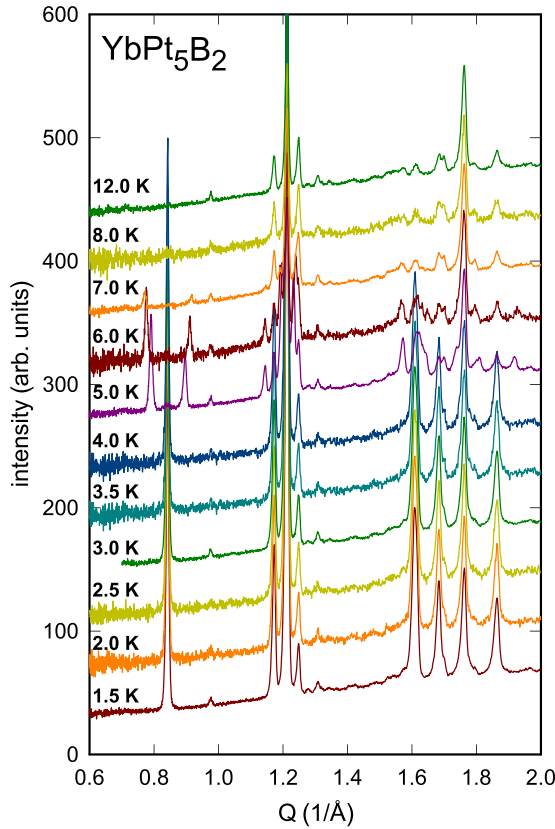


FIG. 2. Neutron powder diffraction data of YbPt_5B_2 collected in a range from 1.5 to 12 K at zero external magnetic field. For clarity, constant-temperature data are shifted vertically against each other.

data are plotted on a logarithmic temperature scale. The anomalies at low temperatures refer to magnetic phase transitions (marked by arrows at T_{N1} and T_{N2}); the negative logarithmic resistivity contributions at low and high temperatures (marked by solid lines) refer to the Kondo effect in the CEF ground state and excited states, respectively, and the maximum of $\rho_{\text{mag}}(T)$ around 150 K is a measure of the overall CEF splitting [31,32].

In the following, neutron experiments and their analyses will help to qualitatively and quantitatively understand the magnetic order, CEF effects, and Kondo interaction simultaneously present in YbPt_5B_2 .

A. Neutron powder diffraction

Figure 2 summarizes neutron powder diffraction (NPD) data of YbPt_5B_2 collected at zero field and different temperatures below $T = 12$ K. No preferred orientation of grains is present in the powdered sample, which is important for evaluating the proper magnetic structure and the size of the magnetic moments. For temperatures below $T_{N1} = 7.8$ K and $T_{N2} = 4.7$ K, the structural powder pattern (such as present at $T = 12$ K) becomes distinctly modified, as evident from Fig. 2 for data collected, e.g., at 6 and 1.5 K, respectively. It is natural to assign these modifications to the magnetic phase transitions as observed previously from our transport, magnetization, and specific data discussed above. While the

magnetic Bragg peaks at $T = 1.5$ K can be successfully accounted for using the nuclear unit cell and a magnetic propagation vector $\vec{k}_2 = (0, 0, 0)$, the set of additional reflections at $T = 6$ K can only be indexed using an incommensurate propagation vector $\vec{k}_1 = (0.194, 0, -0.0450)$.

In order to derive both the crystal and the magnetic structure of YbPt_5B_2 in detail, Rietveld refinements, assisted by symmetry analyses based on the space group representation theory, have been carried out, using the program package FullProf [33].

In the paramagnetic temperature range ($T > 7.8$ K), the monoclinic crystal structure [space group $C2/m$ (No. 12)], with no apparent foreign phases, is revealed [see Fig. 3(a)]. The lattice parameters obtained at $T = 12$ K are $a = 15.4555(2)$ Å, $b = 5.5158(1)$ Å, $c = 5.5496(1)$ Å; the monoclinic distortion $\beta = 105.4090(9)^\circ$. These values are in reasonable accordance with our room-temperature x-ray data, $a = 15.4746(4)$ Å, $b = 5.5216(1)$ Å, $c = 5.5511(1)$ Å, and $\beta = 105.342(1)^\circ$ (compare SM, Fig. S1 [29]).

The magnetic structure solution was done using group representation theory, assuming an irreducible nature of the magnetic order parameter, which is strictly only valid for second-order phase transitions. The Yb magnetic moments are expressed as a Fourier series and under the assumptions of Landau's theory; the Fourier coefficients are linear combinations of basis vectors determined from the point symmetry of the Yb atoms and the propagation vector.

The decomposition of the magnetic representation associated with the Wyckoff position $4i$ of Yb and $\vec{k}_1 = (0, 0, 0)$ yields $\Gamma_{\text{mag,Yb}} = 1\Gamma_1^1 + 2\Gamma_2^1 + 2\Gamma_3^1 + 1\Gamma_4^1$, where Γ_1^1 , Γ_2^1 , Γ_3^1 , and Γ_4^1 are one-dimensional representations in the little group.

Basis vectors of these irreducible representations (IRs) were tested against the experimental data with excellent fitting quality obtained for Γ_2^1 IR [see Fig. 3(c)]. The corresponding magnetic structure implies collinear ordering of the Yb moments confined within the a - c plane and antiferromagnetic coupling between the Yb sites related by spatial inversion (see Fig. 4, left panel). The value of the ordered moments at $T = 1.5$ K is $m(\text{Yb}) = 3.04(2) \mu_B$ and the moments make an angle of 43° with respect to the c axis. The magnetic space group, which describes the symmetry of this ground state, is $C2/m'$; this space group keeps the lattice vectors and origin of the parent paramagnetic structure.

The incommensurate structure at high temperatures was approached in a similar way [see Fig. 3(b)]. The magnetic representation associated with the propagation vector $\vec{k}_2 = (0.194, 0, -0.045)$ decomposes into $\Gamma_{\text{mag,Yb}} = 1\Gamma_1^1 + 2\Gamma_2^1$. IRs Γ_1^1 and Γ_2^1 correspond to spin density wave moments perpendicular and parallel to the a - c plane, respectively. Quantitative refinement [Fig. 3(b)] revealed that, similarly to the ground state configuration, the moments in the incommensurate phase are also confined within the a - c plane, making 45° with the c axis. The amplitude of the spin density wave at $T = 6$ K is $2.34(4) \mu_B$ and the relative magnetic phase between the Yb sites, related by the spatial inversion, was refined to be $0.405(9)$ in units of 2π .

In order to visualize the magnetic structures in both regimes, Fig. 4 sketches conditions at $T = 1.5$ K (left panel) and $T = 6$ K (right panel), respectively [34]. In both cases the crystalline unit cell is drawn without Pt and B atoms.

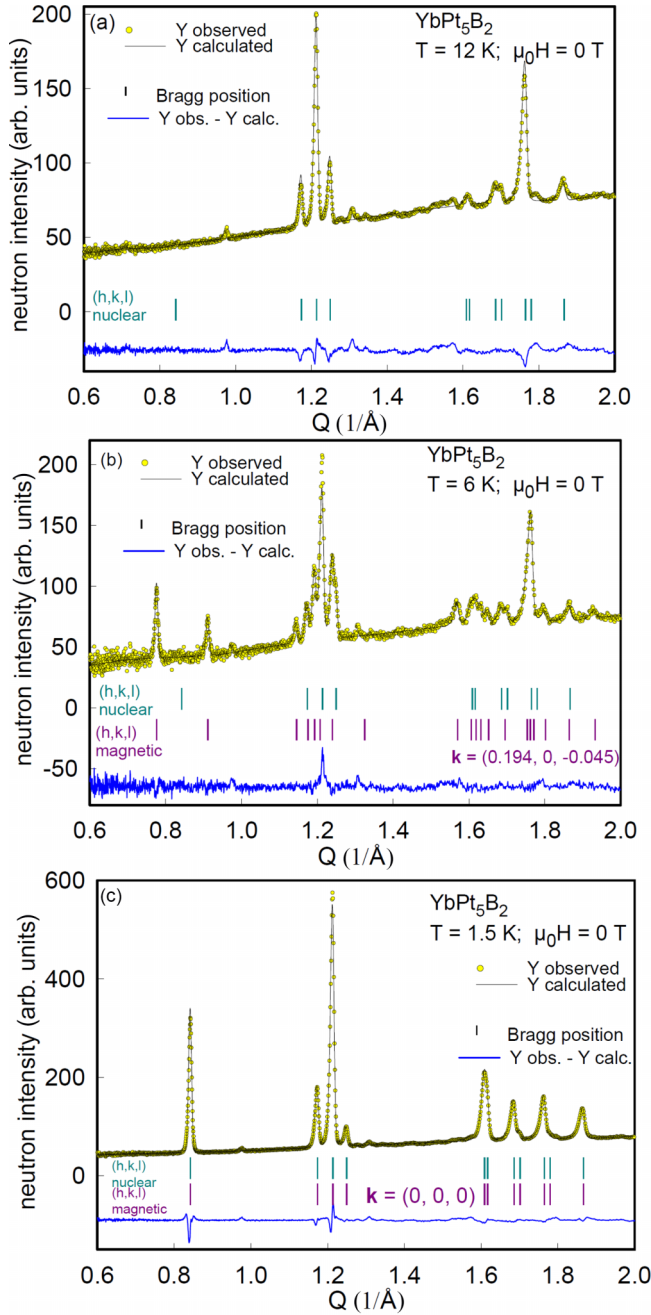


FIG. 3. Neutron diffraction data of YbPt_5B_2 collected at $T = 12, 6, 1.5$ K at zero external magnetic field. Data are analyzed in terms of a Rietveld refinement employing the program package FullProf. All experimental data are represented by yellow filled circles, while the theoretical results are given by black solid lines. The differences between experimental and model data are shown on the bottom of each panel as blue solid lines. The positions of the revealed nuclear and magnetic Bragg peaks are represented by colored vertical lines.

Yb ions are located at the lattice sites $4i$, with $x = 0.32746$, $y = 0.00000$, and $z = 0.67044$ (Yb1). The remaining Yb ions shown in this figure are revealed from symmetry operations associated with the monoclinic crystal structure, space group $C/2m$. The relevant space group operations are $-x, -y, -z$;

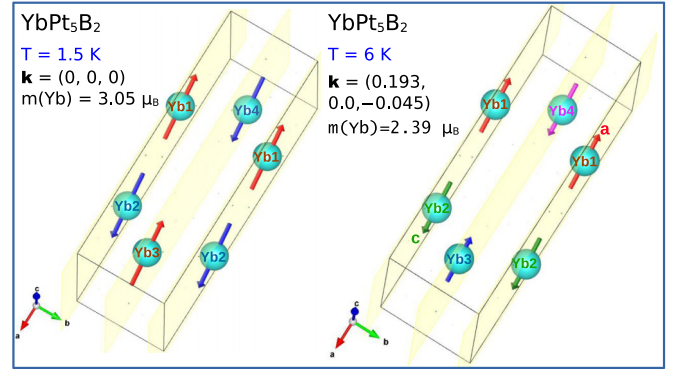


FIG. 4. Sketch of the magnetic structures at $T = 1.5$ K (commensurate phase, left panel) and $T = 6$ K (incommensurate phase, right panel). Here, the unit cell, for simplicity, contains only Yb ions. The various positions of the Yb ions are revealed from symmetry operations as explained in the text. The color, length, and orientation of the arrows represent the size and the direction of the Yb-4*f* magnetic moments in both panels. All moments are arranged in the a - c plane. This is emphasized by light yellow planes in a $(0,1,0)$ configuration.

$x + 1/2, y + 1/2, z$; and $-x + 1/2, -y + 1/2, -z$; resulting in three additional ions at $x = 0.67254, y = 0.00000, z = 32956$ (Yb2); $x = 0.82746, y = 0.50000, z = 0.67044$ (Yb3); and $x = 0.17254, y = 0.50000, z = 0.32956$ (Yb4).

The left panel of Fig. 4 reveals the commensurate case of antiferromagnetic order of the Yb-4*f* magnetic moments, where all moments are locked in the a - c plane in a simple collinear antiferromagnetic structure with the propagation vector $\vec{k}_2 = (0, 0, 0)$. At $T = 1.5$ K, the absolute value of the magnetic moment is equal for each Yb ion in the unit cell, which is $m_{\text{Yb}} = 3.04 \mu_B$. Because of the impact of crystalline electric field splitting, this rather large value of the ordered Yb moments requires a suitable CEF ground state wave function as pointed out in Eq. (4). More quantitative details are discussed in Sec. III B.

The right panel of Fig. 4 summarizes the magnetic structure of the Yb ions in the incommensurate case at $T = 6$ K, for which the propagation vector was evaluated as $\vec{k}_1 = (0.194, 0, -0.045)$. A more extended view on the incommensurate magnetic phase in YbPt_5B_2 is presented in the SM, Fig. S3 [29]. Still, all magnetic moments are lying in the a - c plane, as in the case of the commensurate regime. In the incommensurate structure regime, the moments take all possible values between $2.39 \mu_B$ and $-2.39 \mu_B$ ($T = 6$ K) upon propagation through the crystal. As sketched in Fig. 4, the magnetic phase is arbitrarily set to zero for Yb1 at the $4i$ site of the crystalline unit cell. Inverting the above site (resulting in Yb2) reveals a magnetic moment of $1.97 \mu_B$, with a phase shift $\Delta\varphi = 0.405$ [$m_{\text{Yb2}} = m_{\text{Yb1}} \cos(2\pi \Delta\varphi)$].

The moment sizes on the remaining Yb sites (Yb3 and Yb4) are determined by a Fourier transform associated with the C-centered translation [$m_{\text{Yb3}} = m_{\text{Yb1}} \exp[-2\pi(\vec{k}_1 \vec{t})]$ and $m_{\text{Yb4}} = m_{\text{Yb2}} \exp[-2\pi(\vec{k}_1 \vec{t})]$, where $\vec{k}_1$ is the propagation vector and $\vec{t} = (1/2, 1/2, 0)$]. When propagating through the crystal, the moment sizes on the four Yb sites are changing, taking all possible values in the spin density wave. Note, however, the relative magnetic phases at these sites are preserved.

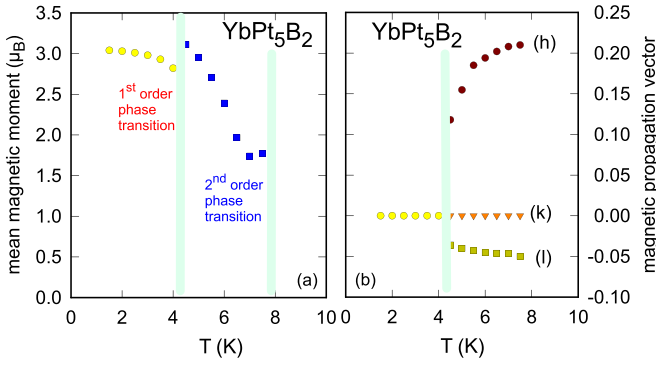


FIG. 5. (a) Temperature-dependent Yb-4*f* magnetic moment of YbPt₅B₂ as obtained from NPD measurements at zero external magnetic field in both the commensurate and incommensurate ordered regime. (b) Temperature dependence of the magnetic propagation vector for both the commensurate and incommensurate ordered phase.

Figures 5(a) and 5(b) summarize the outcome of all NPD measurements carried out at low temperatures. In Fig. 5(a) the observed magnetic moments of the Yb ions are shown as a function of temperature. At temperatures below $T_{N2} = 4.7$ K, a smooth, Brillouin-like decrease of $m(T)$ with increasing temperatures is revealed, with no change of the commensurate propagation vector $\vec{k}_2 = (0, 0, 0)$. For $4.7 < T < 7.8$ K, the Yb-4*f*¹³ moments decrease further upon an increasing temperature, vanishing at $T = T_{N2}$. The propagation vector $\vec{k}_1$, however, exhibits a strong temperature dependence [except the component (k)], which is opposite for the component (h) compared to (l), again different from the temperature-independent behavior of $\vec{k}_2$.

As already concluded earlier from heat capacity data [28], the phase transition at T_{N2} appears to be of a first-order type. This becomes obvious, if carefully checking the NPD data in the proximity of T_{N2} ; compare Fig. 6. There, data are collected from 4 K ($T < T_{N2}$) to 5.5 K ($T > T_{N2}$). While for the Q range from about 0.75 to 0.95 Å⁻¹ the latter exhibits just incommensurate magnetic Bragg peaks, the former shows only a commensurate peak, in coincidence to $\vec{k}_2 = (0, 0, 0)$. For $T = 4.5$ K, which is just below T_{N2} , however, both commensurate and incommensurate Bragg peaks are present. Even at $T = 5$ K a shallow contribution around 0.84 Å⁻¹ is observable. This indicates a coexistence of both commensurate and incommensurate phases and thus confirms the phase transition being of a first-order type.

B. Inelastic neutron scattering

An inelastic neutron scattering study on YbPt₅B₂ has been carried out primarily to derive appropriate insight into the impact of crystalline electric field (CEF) effects, acting on the Yb-4*f* electrons. It is well known that CEF is responsible for lifting the ground state degeneracy, $N = 2j + 1$, of the total angular momentum j . Details of this effect are dependent on the symmetry of the crystal structure, on the point symmetry of the rare earth ion, i.e., Yb, as well as on the absolute value of j . While half-integral values of j cause only a partial lifting

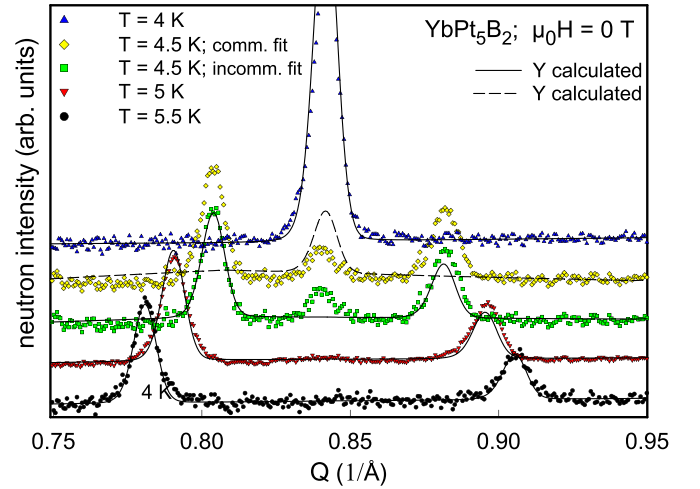


FIG. 6. NPD data of YbPt₅B₂ at various temperatures near to $T_{N2} = 4.7$ K, in a narrow q range ($0.75 \leq q \leq 0.95$ Å⁻¹). Data are shifted vertically against each other. Symbols are experimental data, while the solid and dashed lines represent Rietveld refinements [carried out for the entire experimental q range (from 0.5 to 6.5 Å⁻¹)]. Powder data taken at $T = 4.5$ K clearly exhibit both commensurate and incommensurate contributions, illustrating the ambiguous fit results.

of the degeneracy (into doublets and quartets), integers of j can cause a lifting into singlets, doublets, triplets, and quartets.

A theoretical description of this phenomenon is based on an appropriate crystal field Hamiltonian H_{CEF} [35–37],

$$H_{\text{CEF}} = -|e| \sum_{i=1}^N V_c(\vec{r}_i), \quad V_c(\vec{r}) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d^3r', \quad (1)$$

where the potential $V_c(\vec{r})$, created by the neighboring ions, acts on the 4*f* ions at position $\vec{R}$. $\rho(\vec{r})$ is the respective charge density and $|e|$ the absolute value of the elementary charge. This potential satisfies Laplace's equation and thus allows an expansion in terms of spherical harmonic functions [38]. As a result, a much simpler model Hamiltonian follows,

$$H_{\text{CEF}} = \sum_{l,m} B_l^m O_l^m, \quad (2)$$

with O_l^m being so-called Stevens operators, which are tabulated for all rare earth ions. B_l^m are parameters, which can be calculated (e.g., in terms of the point-charge model), or deduced from experimental data, like inelastic neutron spectra [36,37] or single-crystal susceptibility.

For a monoclinic crystal structure with a local site symmetry C_{2v} of the Yb ions, Eq. (2) can be represented as

$$H_{\text{CEF}} = B_2^0 O_2^0 + B_2^2 O_2^2 + B_4^0 O_4^0 + B_4^2 O_4^2 + B_4^4 O_4^4 + B_6^0 O_6^0 + B_6^2 O_6^2 + B_6^4 O_6^4 + B_6^6 O_6^6, \quad (3)$$

with nine independent parameters B_l^m . These parameters have to be deduced such that all physical properties, which are dependent on CEF effects, are reasonably well described. Owing to the Yb-site symmetry, with a mirror plane perpendicular to the monoclinic b axis as the twofold rotation axis, the quantization axis z is along b . In the following, the INS data

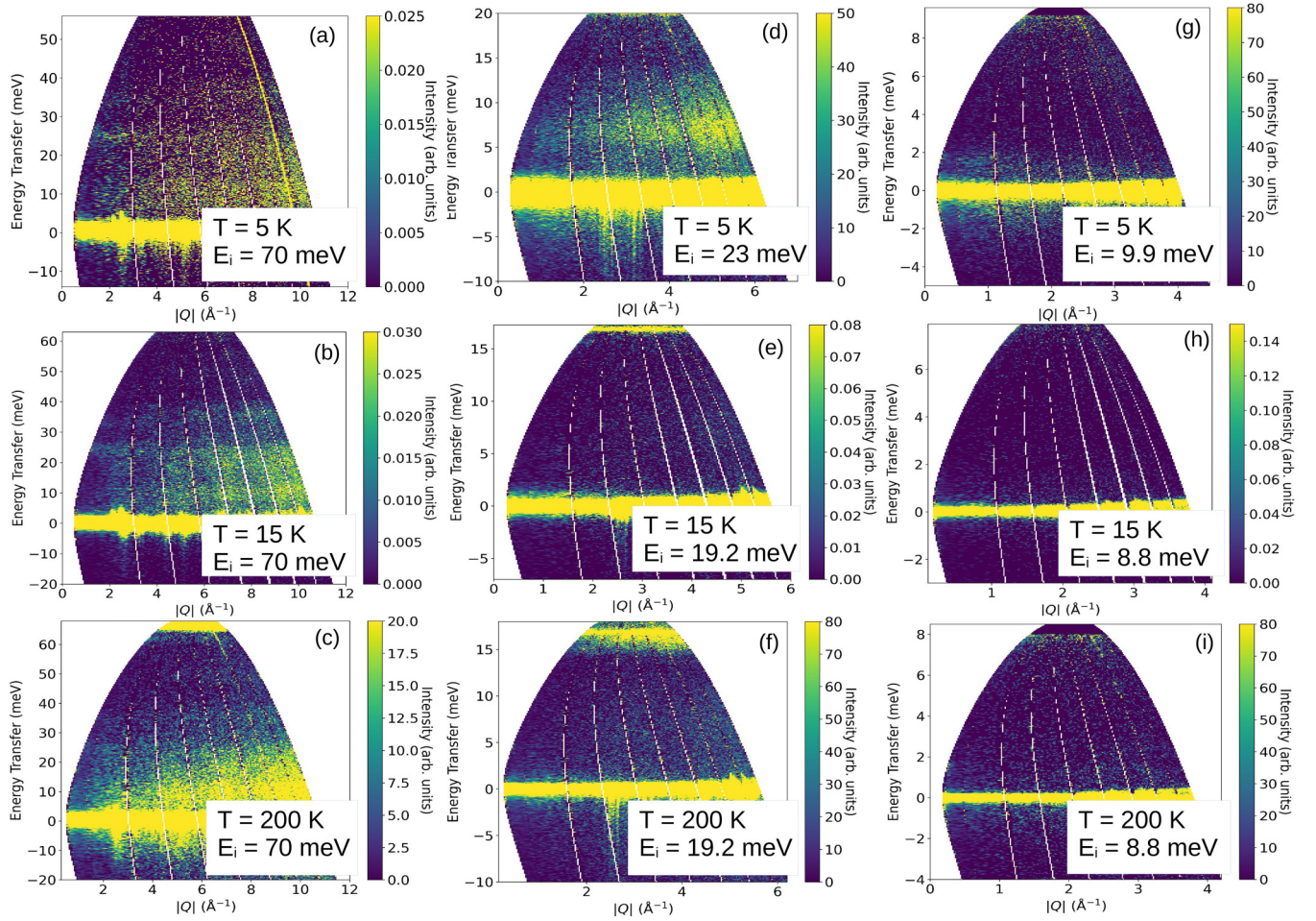


FIG. 7. Energy and wave vector dependent inelastic neutron scattering intensities of YbPt_5B_2 taken at different temperatures and incident neutron energies.

are accounted for in the context of magnetic susceptibility data of this ternary compound. The latter is debated in detail in the SM; see Fig. S5 [29]. In addition, constraints on the position of the first excited CEF level above the ground state ($\Delta E_1 > 20$ meV) are revealed from the previously derived specific heat data [28]. Equation (3) describes the splitting of the eightfold-degenerate ground state ($N = 2j + 1 = 8$) into four doublets with distinct eigenenergies ΔE_i above the ground state doublet. Each of these doublets is characterized by a specific wave function, compiled of states from $j_z = -|7/2\rangle$ to $j_z = +|7/2\rangle$. These wave functions allow, among others, the calculation of the respective magnetic moments.

An overview on INS data obtained for YbPt_5B_2 at different temperatures ($T = 5, 15, 200$ K) as well as different neutron incident energies ($E_i \approx 8.8$ to 70 meV) are collected in Fig. 7. While temperatures increase from top to bottom, the incident neutron energy decreases from left to right. For the data with high incident neutron energies (left column, Fig. 7), several inelastic excitations with different Q dependence are present. Besides the dominating quasielastic line, weaker intensities are present for small values of $|Q|$ above 20 meV and below 40 meV, while at the high momentum transfer side growing intensity is visible at about $10, 20$, and 40 meV (details are revealed in Fig. 8 for the case of $T = 5$ K and $E_i = 70$ meV). On the opposite, in the

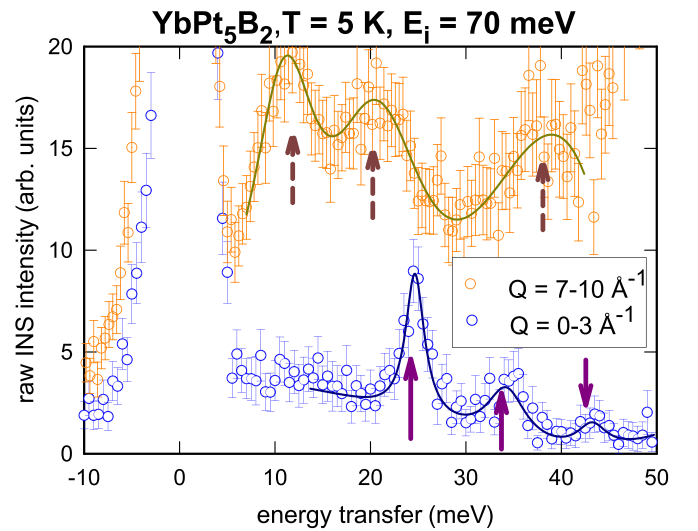


FIG. 8. Energy-dependent inelastic neutron scattering of YbPt_5B_2 taken at 5 K for $E_i = 70$ meV. The blue-colored data set represents INS data for small momentum transfer ($0 < Q < 3 \text{ \AA}^{-1}$); the orange-colored one summarizes data for $7 < Q < 10 \text{ \AA}^{-1}$. The solid lines are least-squares fits as described in the text.

paramagnetic temperature range, i.e., $T = 15$ K, no features (i.e., phonons and CEF excitations) are present for small neutron incident energies (right column, middle). For the magnetically ordered range ($T = 5$ K), the low neutron energy case originates modest intensity at low $|Q|$ values, likely due to spin waves in the incommensurately ordered regime.

To identify the nature of all inelastic excitations obtained from the experimental MARI data, two procedures were chosen: (i) Considering different moment transfers ΔQ allows us to roughly discriminate between magnetic excitations, being dominant for small values of Q and phonons, being prominent for large values of Q . (ii) A comparison can be made between YbPt_5B_2 and isostructural LuPt_5B_2 . Since the latter is nonmagnetic ($j = 0$), no magnetic excitations are present and the INS spectrum observed is originated by phonons only. Moreover, since the atomic masses of Yb and Lu are very similar, the phonon spectrum of LuPt_5B_2 is expected to be almost identical to the Yb-based sample.

As an example of the moment transfer sensitivity, INS data of YbPt_5B_2 , collected at $T = 5$ K, are shown in Fig. 8 for incident neutron energies $E_i = 70$ meV. Obviously, there is a distinct difference for data for $0 < Q < 3 \text{ \AA}^{-1}$ and $7 < Q < 10 \text{ \AA}^{-1}$, reflecting the difference between crystal field excitations (low Q) and phonons (high Q). To quantitatively account for the excitation energies, the intensity data are described by Lorentzians for the former (blue solid line) and damped harmonic oscillators (orange solid line), as pointed out in Ref. [39], for the latter (details regarding the phonons are discussed in the SM, Ref. [29]). This initial analysis clearly discriminates between CEF excitations and phonons. For the former, CEF energies are obtained at $\Delta E_{\text{CEF}} \approx 25, 34$, and 43 meV. Phonons are roughly located at $\Delta E_{\text{ph}} \approx 10, 20$, and 39 meV. The CEF energy scheme derived here is in excellent agreement with heat capacity data, where the magnetic entropy suggests the first excited CEF level being located > 20 meV above the ground state [28].

In order to derive a reliable set of CEF parameters for YbPt_5B_2 , the difference of INS data of YbPt_5B_2 and LuPt_5B_2 , obtained in the paramagnetic temperature range ($T = 15$ K), was employed and analyzed according to the crystal field theory outlined above. Additionally, data collected at $T = 5$ K, i.e., in the magnetically ordered regime, were analyzed as well by including an internal magnetic field on the order of 18 T.

Figure 9(a) shows the difference INS data $\{\text{Yb}, \text{Lu}\}\text{Pt}_5\text{B}_2$ for $T = 15$ K and incident neutron energies $E_i = 70$ meV. Besides the dominating quasielastic line, revealed from Yb-4f and its interaction with conduction electrons (e.g., Kondo effect) or unresolved spin waves (in the $T = 5$ K study only), three distinct inelastic features are present in Fig. 9. The usage of low- Q data underscores the magnetic nature of these excitations. Note that, on the other hand, high- Q data rather trace phonons, as the square of the 4f magnetic form factor and hence the magnetic scattering signal becomes negligibly small. Thus, excitations present at $\Delta E = 23.95, 33.1$, and 43.6 meV (see Fig. 9) are expected to be of magnetic origin, only.

To quantitatively account for CEF effects and to derive the numeric B_l^m values as indicated in Eq. (3), least-squares fits were carried out, using the program package CrystalField of the Mantid Workbench [40]. In order to enhance the reliability

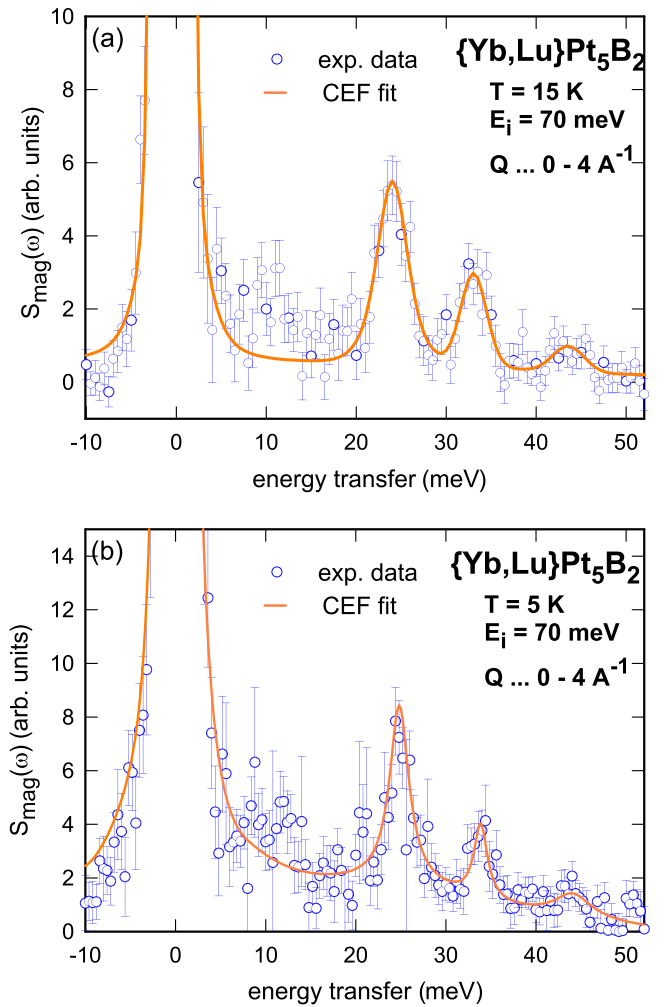


FIG. 9. Energy-dependent magnetic inelastic neutron scattering data $S_{\text{mag}}(\omega)$ of $\{\text{Yb}, \text{Lu}\}\text{Pt}_5\text{B}_2$ (a) at 15 and (b) 5 K, $E_i = 70$ meV; data are summed up for a momentum transfer Q from 0 to $4 \text{ \AA}^{-1}$. Experimental data are derived by subtracting the spectrum of isostructural LuPt_5B_2 from YbPt_5B_2 at the very same parameter sets. The solid line is a least-squares fit employing Eq. (3) in the scope of the CEF theory.

of the results obtained, fits are done simultaneously in combination with temperature-dependent magnetic susceptibility data of YbPt_5B_2 , employing the very same set of B_l^m values for both physical quantities. Fine agreement is obtained between theory and experiment [solid orange line, Fig. 9(a)] with a set of crystal field parameters B_l^m as collected in Fig. 10, left panel. These parameters confirm the splitting of the CEF doublets from the ground state (compare Fig. 10, central panel) and allow us to derive the wave functions of these states as well (see Table S1 in SM, [29]). Using the B_l^m 's as collected in Fig. 10, the temperature-dependent magnetic susceptibility can be revealed reasonably well (compare SM, Fig. S5, [29]). This coincidence allows us to state fair reliability of the crystal field parameters currently derived.

To further substantiate the appropriateness of the above-derived CEF parameters, additional analyses of INS data have been carried out. $T = 5$ K data are selected for this purpose. Shown in Fig. 9(b) are difference INS data for $E_i = 70$ meV

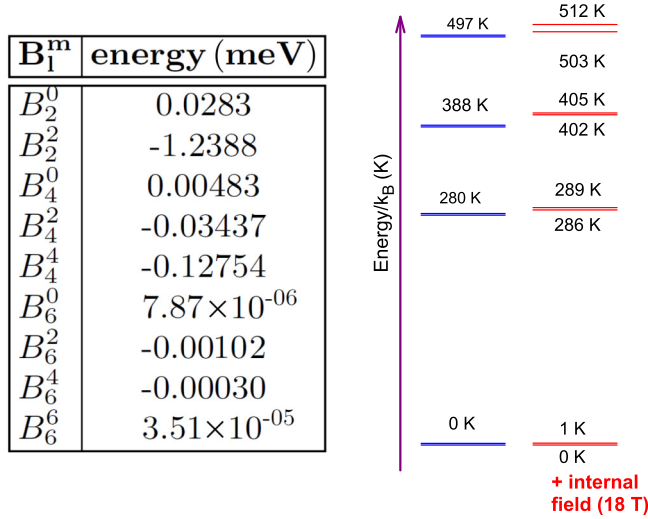


FIG. 10. The left panel summarizes all CEF parameters B_l^m as obtained from the CEF fit according to Eq. (3). The right panel is a sketch of the splitting of the CEF states in the presence of an internal magnetic field $B_{\text{int}} = 18$ T. The central panel presents the case for $B_{\text{int}} = 0$ T.

and $\mathbf{Q} = 0\text{--}4 \text{ \AA}^{-1}$. Because YbPt_5B_2 is magnetically ordered at this temperature, the related internal magnetic field triggers a further splitting of the CEF doublets (Zeeman effect), as, indeed, is obvious from the INS spectrum of Fig. 9(b). Taking into account an internal magnetic field, $B_{\text{int}} = 18$ T, and the crystal field parameters as summarized in Fig. 10, sound congruence is obtained between theoretical and experimental data [solid line, Fig. 9(b)]. As already noted, the Zeeman effect leaves behind eight singlet states (see Fig. 10, right panel); the ground state doublet becomes split by about 0.1 meV.

Some discrepancy between the experimental data and the accurate CEF-based description is obvious in Figs. 9(a) and 9(b) around 10 meV. This is likely originated from a phonon with about this energy, as obvious from the qualitative analysis of Fig. 8. These phonons were identified from INS measurements on nonmagnetic isostructural LuPt_5B_2 , too, obtained at various temperatures, for several incoming neutron energies and momentum transfers $\mathbf{Q}$. Details of this study and relevant analyses are discussed in the SM part of this work [29].

The substantial splitting of the first excited doublet from the ground state ($\Delta E_1 \approx 25$ meV) means that magnetic ordering of the $\text{Yb-}4f$ electrons at low temperatures is solely determined from the wave function of the ground state doublet. Coupling with excited CEF levels is then of minor importance and can thus be neglected. The resulting eigenvectors and eigenvalues, corresponding to the CEF parameters listed in Fig. 10, are summarized in Tables S1 and S2 of the SM [29] for the paramagnetic and the magnetically ordered regime, respectively. Since three inelastic CEF excitations from the ground state with different intensities are obtained experimentally at low temperatures, appropriate matrix elements, $|\langle \Gamma_i | J | \Gamma_j \rangle| > 0$ (according to the dipole selection rules), are required and, in fact, revealed from the eigenstates of Table S1. In order to compare the ground state wave functions with the ordered magnetic moments as observed from

the refinement of the magnetic structure (compare Sec. III A), the coordinate system of the CEF Hamiltonian is rotated such that the quantization axis aligns with the easy axis of CEF. This is achieved by a 90° rotation ($z \rightarrow x$) using the McPhase software [41], i.e., by rotating the quantization axis from the b axis into the a - c plane. Thereby, the ground state wave functions are transformed to

$$\begin{aligned} |\Gamma_0^+\rangle &\simeq 0.90|+7/2\rangle - 0.43|+3/2\rangle, \\ |\Gamma_0^-\rangle &\simeq 0.90|-7/2\rangle - 0.43|-3/2\rangle, \end{aligned} \quad (4)$$

with negligible components $|\pm 5/2\rangle$ and $|\pm 1/2\rangle$.

The magnetic moment associated with the ground state doublet [Eq. (4)] in the $\hat{z}$ direction follows from $m_z = g_j \mu_B \langle \Gamma_i | J_z | \Gamma_i \rangle$. For the $\hat{x}$ and $\hat{y}$ directions the moments are obtained employing $m_x = (1/2)g_j \mu_B \langle \Gamma_i | (J_+ + J_-) | \Gamma_i \rangle$ and $m_y = -(1/2)ig_j \mu_B \langle \Gamma_i | (J_+ - J_-) | \Gamma_i \rangle$. J_+ and J_- are ladder operators as defined by $J_{\pm} = J_x \pm iJ_y$.

Evaluating the magnetic moment of the Yb^{3+} ion accordingly reveals $m_{\text{Yb}} = 3.55 \mu_B$. NPD data taken at 1.5 K, on the other hand, indicate an ordered moment $m_{\text{Yb}}^{\text{NPD}} = 3.04 \mu_B$, while the free saturated moment value of Yb^{3+} is $4 \mu_B$. This hierarchy of moment values is the result of a combination of CEF effects ($m_{\text{Yb}} = 3.55 \mu_B$) and Kondo interaction ($m_{\text{Yb}}^{\text{NPD}} = 3.04 \mu_B$, $T_K \approx 7$ K, $T = 1.5$ K), with a very plausible variation of moment values.

In order to calculate the magnetization associated with the various CEF levels, specifically of the CEF ground state, besides H_{CEF} , the Zeeman term $H_z = \mu_B \mathbf{H} \cdot (g_j \hat{\mathbf{J}})$ has to be taken into consideration. The magnetization may then be calculated from the expectation value of the magnetic moment operator $\hat{J}$ with $\hat{J} = \hat{L} + 2\hat{S} = (\hat{J}_x, \hat{J}_y, \hat{J}_z)$ [42]:

$$M(H, T) = \frac{1}{Z} \sum_n \langle \Gamma_n(\vec{H}) | \hat{J} | \Gamma_n(\vec{H}) \rangle \exp \left(\frac{-E_n(\vec{H})}{k_B T} \right). \quad (5)$$

$Z = \sum_n \exp[-E_n(H)/k_B T]$ is the partition function. $|\Gamma_n(\vec{H})\rangle$ is the wave function (eigenvector) of the Hamiltonian, containing CEF and Zeeman terms. E_n are the eigenvalues of the different CEF levels.

Results derived in terms of Eq. (5) are presented in Fig. 11(a) for temperatures $T = 1.5$ K. It should be noted that internal magnetic fields due to long-range magnetic order are not considered in this evaluation.

While the moments along z are very large, those in x and y are small in the low-field region. It would take large externally applied fields to compensate the Kondo effect, or even larger fields (on the order of 100 T) to overcome the impact of CEF splitting, recovering the free Yb^{3+} moment of $m(\text{Yb}^{3+}) = 4 \mu_B$. The former is expected to impact the field-dependent magnetization measurements carried out in the paramagnetic temperature range of YbPt_5B_2 [filled symbols, Fig. 11(b)] on polycrystalline samples. Based on Eq. (5) and the CEF parameters obtained from the CEF fit, $M(\mu_0 H)$ is obtained for $T > T_{N1}$ [solid lines, Fig. 11(b)]. Besides some uncertainties regarding the accuracy of the CEF parameters derived, and the averaging process of polycrystalline materials, the Kondo effect present in YbPt_5B_2 is a rational mechanism that decreases the experimentally observed magnetic moments. A recovery

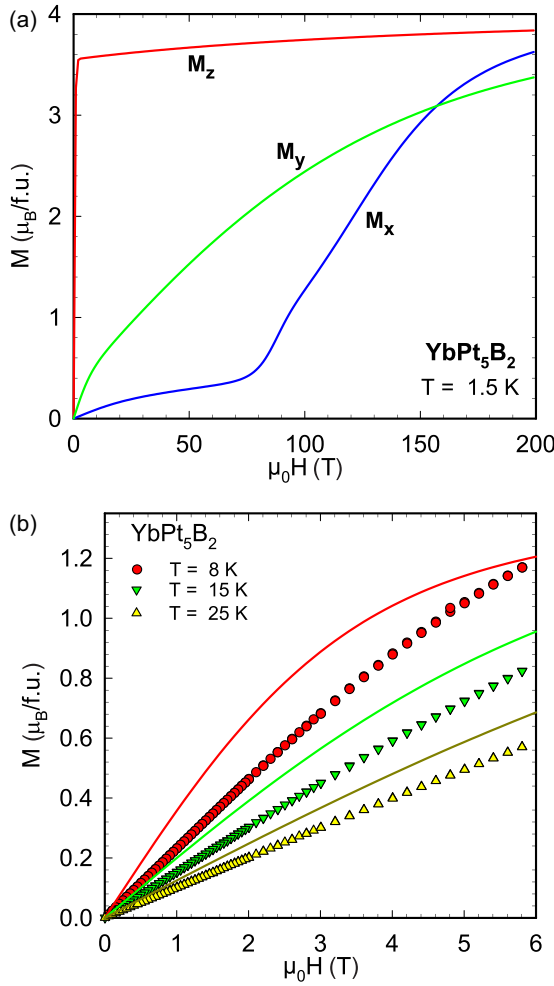


FIG. 11. (a) Field and direction dependent magnetization M of YbPt_5B_2 at $T = 1.5$ K derived from the CEF model Eq. (4), i.e., calculated as a single-ion response to the applied magnetic field. (b) Field-dependent isothermal magnetization curves of polycrystalline YbPt_5B_2 in comparison to CEF-derived magnetization data.

of the pure CEF-related values is only expected after the suppression of the Kondo effect by reasonably strong applied magnetic fields.

IV. CONCLUSIONS

Elastic (NPD) and inelastic (INS) neutron scattering experiments have been carried out on polycrystalline $\{\text{Yb}, \text{Lu}\}\text{Pt}_5\text{B}_2$. These studies allowed us to derive for the former the magnetic structure and the magnetic moments associated with the $\text{Yb-}4f^{13}$ electronic configuration, both as a function of temperature and externally applied magnetic fields. In the case of INS, the splitting of the eightfold-degenerate ground state of the $j = 7/2$ total angular momentum was obtained, revealing a separation of the CEF ground state from the first excited level of about 25 meV. This implies that the entire magnetic ordering scenario present in YbPt_5B_2 below $T_{\text{N1}} = 7.8$ K is due to the ground state doublet only [compare Eq. (3)], with negligible contributions from excited states. The uppermost CEF level is about 44 meV above the ground state. Magnetic order sets in when cooling down YbPt_5B_2 below 7.8 K. For temperatures $4.7 < T < 7.8$ K, the magnetic structure obtained is of an incommensurate antiferromagnetic type, with a propagation vector $\vec{k}_1 = (0.194, 0, -0.045)$ ($T = 6$ K), which, however, is strongly temperature dependent. At a first-order type of phase transition, $T_{\text{N2}} = 4.7$ K, a spin reorientation is observed, revealing commensurate magnetic order with $\vec{k}_2 = (0, 0, 0)$. At lowest temperatures ($T = 1.5$ K), the ordered moment reaches values $m_{\text{Yb}} \approx 3.04 \mu_{\text{B}}$, which has to be compared with the Yb^{3+} moment of $4 \mu_{\text{B}}$. This requires a CEF ground state wave function $|\Gamma_0^\pm\rangle \simeq 0.90|\pm 7/2\rangle - 0.43|\pm 3/2\rangle$ as derived with respect to the easy axis of CEF from our analyses of INS data collected for YbPt_5B_2 .

ACKNOWLEDGMENTS

O.S. acknowledges financial support by Project No. FWF P31979-N36. Experiments at the ISIS Neutron and Muon Source were supported by beamtime allocations RB2220762 and RB2220763 from the Science and Technology Facilities Council. E.B. would like to thank C. Ritter (ILL Grenoble, France) for helpful discussions.

DATA AVAILABILITY

The data that support the findings of this article are openly available [43].

- [1] J. Remeika, G. Espinosa, A. Cooper, H. Barz, J. Rowell, D. McWhan, J. Vandenberg, D. Moncton, Z. Fisk, L. Wolf, H. Hamaker, M. Maple, G. Shirane, and W. Thomlinson, A new family of ternary intermetallic superconducting/magnetic stanides, *Solid State Commun.* **34**, 923 (1980).
- [2] S. Nakatsuji, K. Kuga, Y. Machida, T. Tayama, T. Sakakibara, Y. Karaki, H. Ishimoto, S. Yonezawa, Y. Maeno, E. Pearson, G. G. Lonzarich, L. Balicas, H. Lee, and Z. Fisk, Superconductivity and quantum criticality in the heavy-fermion system $\beta\text{-YbAlB}_4$, *Nat. Phys.* **4**, 603 (2008).
- [3] E. Schuberth, M. Tippmann, L. Steinke, S. Lausberg, A. Steppke, M. Brando, C. Krellner, C. Geibel, R. Yu, Q. Si, and

F. Steglich, Emergence of superconductivity in the canonical heavy-electron metal YbRh_2Si_2 , *Science* **351**, 485 (2016).

- [4] E. Bauer, E. Gratz, R. Hauser, L. Tuan, A. Galatanu, A. Kottar, H. Michor, W. Perthold, G. Hilscher, T. Kagayama, G. Oomi, N. Ichimiya, and S. Endo, Pressure- and field-dependent behavior of YbCu_4Au , *Phys. Rev. B* **50**, 9300 (1994).
- [5] C. Rossel, K. N. Yang, M. B. Maple, Z. Fisk, E. Zirngiebl, and J. D. Thompson, Strong electronic correlations in a new class of Yb-based compounds: YbXCu_4 ($X = \text{Ag}, \text{Au}, \text{Pd}$), *Phys. Rev. B* **35**, 1914 (1987).
- [6] P. Gegenwart, J. Custers, C. Geibel, K. Neumaier, T. Tayama, K. Tenya, O. Trovarelli, and F. Steglich, Magnetic-field induced

- quantum critical point in YbRh_2Si_2 , *Phys. Rev. Lett.* **89**, 056402 (2002).
- [7] J. Custers, P. Gegenwart, H. Wilhelm, K. Neumaier, Y. Tokiwa, O. Trovarelli, C. Geibel, F. Steglich, C. Pépin, and P. Coleman, The break-up of heavy electrons at a quantum critical point, *Nature (London)* **424**, 524 (2003).
 - [8] D. M. Rowe, V. L. Kuznetsov, L. A. Kuznetsova, and G. Min, Electrical and thermal transport properties of intermediate-valence YbAl_3 , *J. Phys. D* **35**, 2183 (2002).
 - [9] E. Bauer, R. Hauser, L. Keller, P. Fischer, O. Trovarelli, J. G. Sereni, J. J. Rieger, and G. R. Stewart, Onset of magnetic order in $\text{YbCu}_{5-x}\text{Al}_x$, *Phys. Rev. B* **56**, 711 (1997).
 - [10] E. Bauer, R. Hauser, E. Gratz, K. Payer, G. Oomi, and T. Kagayama, Pressure dependence of the electrical resistivity of YbCu_4Ag , *Phys. Rev. B* **48**, 15873 (1993).
 - [11] I. Felner, I. Nowik, D. Vaknin, U. Potzel, J. Moser, G. M. Kalvius, G. Wortmann, G. Schmiester, G. Hilscher, E. Gratz, C. Schmitzer, N. Pillmayr, K. G. Prasad, H. de Waard, and H. Pinto, Ytterbium valence phase transition in $\text{Yb}_x\text{In}_{1-x}\text{Cu}_2$, *Phys. Rev. B* **35**, 6956 (1987).
 - [12] M. A. Ruderman and C. Kittel, Indirect exchange coupling of nuclear magnetic moments by conduction electrons, *Phys. Rev.* **96**, 99 (1954).
 - [13] T. Kasuya, A theory of metallic ferro- and antiferromagnetism on Zener's model, *Prog. Theor. Phys.* **16**, 45 (1956).
 - [14] K. Yosida, Magnetic properties of Cu-Mn alloys, *Phys. Rev.* **106**, 893 (1957).
 - [15] J. Kondo, Resistance minimum in dilute magnetic alloys, *Prog. Theor. Phys.* **32**, 37 (1964).
 - [16] D. Newman, Theory of lanthanide crystal fields, *Adv. Phys.* **20**, 197 (1971).
 - [17] A. Yaouanc, P. Dalmas de Réotier, J.-P. Sanchez, T. Tschentscher, and P. Lejay, CeRh_3B_2 : A ferromagnet with anomalously large Ce $5d$ spin and orbital magnetic moments, *Phys. Rev. B* **57**, R681 (1998).
 - [18] S.-i. Kimura, T. Iizuka, H. Miyazaki, A. Irizawa, Y. Muro, and T. Takabatake, Electronic-structure-driven magnetic ordering in a Kondo semiconductor $\text{CeOs}_2\text{Al}_{10}$, *Phys. Rev. Lett.* **106**, 056404 (2011).
 - [19] P. Fischer, G. Meier, B. Lebech, B. D. Rainford, and O. Vogt, Magnetic phase transitions of CeSb . I. Zero applied magnetic field, *J. Phys. C* **11**, 345 (1978).
 - [20] A. Thamizhavel, T. Takeuchi, T. D. Matsuda, Y. Haga, K. Sugiyama, R. Settai, and Y. Ōnuki, Unique magnetic phases in an antiferromagnet CeCoGe_3 , *J. Phys. Soc. Jpn.* **74**, 1858 (2005).
 - [21] E. Morosan, S. Bud'ko, P. Canfield, M. Torikachvili, and A. Lacerda, Thermodynamic and transport properties of RAgGe ($\text{R} = \text{Tb-Lu}$) single crystals, *J. Magn. Magn. Mater.* **277**, 298 (2004).
 - [22] J. Thompson, P. Canfield, A. Lacerda, M. Hundley, Z. Fisk, H.-R. Ott, E. Felder, M. Chernikov, M. Maple, P. Visani, C. Seaman, M. Lopez de la Torre, and G. Aeppli, Physics of YbBiPt , *Phys. B: Condens. Matter* **186-188**, 355 (1993).
 - [23] B. K. Rai, S. Chikara, X. Ding, I. W. H. Oswald, R. Schönmann, V. Loganathan, A. M. Hallas, H. B. Cao, M. Stavinoha, T. Chen, H. Man, S. Carr, J. Singleton, V. Zapf, K. A. Benavides, J. Y. Chan, Q. R. Zhang, D. Rhodes, Y. C. Chiu, L. Balicas *et al.*, Anomalous metamagnetism in the low carrier density Kondo lattice YbRh_3Si_7 , *Phys. Rev. X* **8**, 041047 (2018).
 - [24] S. Dhar, S. Singh, P. Bonville, C. Mazumdar, P. Manfrinetti, and A. Palenzona, Magnetic behavior of $\text{Yb}_3\text{Cu}_4\text{Ge}_4$ and $\text{Gd}_3\text{Cu}_4\text{Ge}_4$, *Phys. B: Condens. Matter* **312-313**, 846 (2002).
 - [25] K. Katoh, Y. Mano, K. Nakano, G. Terui, Y. Niide, and A. Ochiai, Magnetic properties of YbTGe ($\text{T} = \text{Rh, Cu, Ag}$), *J. Magn. Magn. Mater.* **268**, 212 (2004).
 - [26] M. Avila, S. Bud'ko, C. Petrovic, R. Ribeiro, P. Canfield, A. Tsvyashchenko, and L. Fomicheva, Synthesis and properties of YbB_2 , *J. Alloys Compd.* **358**, 56 (2003).
 - [27] K. V. Shah, P. Bonville, P. Manfrinetti, F. Wrubl, and S. K. Dhar, The $\text{Yb}_2\text{Al}_{1-x}\text{Mg}_x\text{Si}_2$ series from a spin fluctuation ($x = 0$) to a magnetically ordered ground state ($x = 1$), *J. Phys.: Condens. Matter* **21**, 176001 (2009).
 - [28] L. Salamakha, O. Sologub, A. Riss, H. Michor, H. Müller, B. Stöger, G. Giester, P. Rogl, A. Sakai, P. Gegenwart, and E. Bauer, Complex transport and magnetism of the ternary boride YbPt_5B_2 , *Phys. Rev. B* **105**, 205112 (2022).
 - [29] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/pj8b-d5h9> for more details on elastic and inelastic neutron scattering on $\{\text{Yb, Lu}\}\text{Pt}_5\text{B}_2$ and analyses, which also contains Refs. [33,34].
 - [30] J. A. Blanco, M. de Podesta, J. I. Espeso, J. C. Gómez Sal, C. Lester, K. A. McEwen, N. Patrikios, and J. Rodríguez Fernández, Specific heat of $\text{CeNi}_x\text{Pt}_{1-x}$ pseudobinary compounds and related dilute alloys, *Phys. Rev. B* **49**, 15126 (1994).
 - [31] B. Cornut and B. Coqblin, Influence of the crystalline field on the Kondo effect of alloys and compounds with cerium impurities, *Phys. Rev. B* **5**, 4541 (1972).
 - [32] Y. Lassailly, A. K. Bhattacharjee, and B. Coqblin, Low-temperature resistivity and magnetoresistivity of cerium compounds, *Phys. Rev. B* **31**, 7424 (1985).
 - [33] J. Rodríguez-Carvajal, FULLPROF: A program for Rietveld refinement and pattern matching analysis, in *Abstracts of the Satellite Meeting on Powder Diffraction of the XV Congress of the IUCr* (Toulouse, France, 1990), p. 127.
 - [34] K. Momma and F. Izumi, VESTA: A three-dimensional visualization system for electronic and structural analysis, *J. Appl. Crystallogr.* **41**, 653 (2008).
 - [35] M. Hutchings, Point-charge calculations of energy levels of magnetic ions in crystalline electric fields, *Solid State Phys.* **16**, 227 (1964).
 - [36] P. Fulde, Chapter 17: Crystal fields, in *Handbook on the Physics and Chemistry of Rare Earths* (Elsevier, 1979), Vol. 2, pp. 295–386.
 - [37] P. Fulde and M. Loewenhaupt, Magnetic excitations in crystal-field split 4f systems, *Adv. Phys.* **34**, 589 (1985).
 - [38] K. Stevens, Matrix elements and operator equivalents connected with the magnetic properties of rare earth ions, *Proc. Phys. Soc. London Sect. A* **65**, 209 (1952).
 - [39] B. Fåk and B. Dorner, Phonon line shapes and excitation energies, *Phys. B: Condens. Matter* **234-236**, 1107 (1997).

- [40] O. Arnold, J. Bilheux, J. Borreguero, A. Buts, S. Campbell, L. Chapon, M. Doucet, N. Draper, R. F. Leal, M. Gigg, V. Lynch, A. Markvardsen, D. Mikkelsen, R. Mikkelsen, R. Miller, K. Palmen, P. Parker, G. Passos, T. Perring, P. Peterson *et al.*, Mantid: Data analysis and visualization package for neutron scattering and μ SR experiments, *Nucl. Instrum. Methods Phys. Res., Sect. A* **764**, 156 (2014).
- [41] M. Rotter, Using McPhase to calculate magnetic phase diagrams of rare earth compounds, *J. Magn. Magn. Mater.* **272-276**, E481 (2004).
- [42] J. Jensen and A. R. Mackintosh, *Rare Earth Magnetism* (Clarendon Press, Oxford, 1991).
- [43] Data are available at <https://doi.org/10.5286/ISIS.E.RB2220762> and <https://doi.org/10.5286/ISIS.E.RB2220763>.