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TITLE: LOW-ENERGY EXCITATIONS, SYMMETRY BREAKING AND SPECIFIC HEAT IN YbBiPt

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LOW-ENERGY EXCITATIONS, SYMMETRY BREAKING AND SPECIFIC HEAT IN YbBiPt

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Abstract

The heavy fermion compound YbBiPt has a very large linear coefficient of specific heat $\gamma = 8$ $Jmol^{-1}K^{-2}$ and this is understood, to first order, in terms of the observed low-energy neutron scattering response. However, at low temperatures, symmetry forbidden splittings at 1 and 2 meV respectively are observed. These levels give good qualitative agreement with the measured specific heat, but poor quantitative agreement. Indeed, the specific heat drops more rapidly with temperature than can be acounted for assuming a temperature-independent density of states. We also present new low-temperature crystallographic data, which rule out any significant structural distortions.

Key Words: YbBiPt, Crystal-Field Levels, Specific Heat

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The cubic heavy-fermion compound YbBiPt was discovered in 1991 by Canfield et al. [1,2] and has a very large linear specific-heat coefficient $\gamma = 8$ J mol^{-1} K^{-2}. YbBiPt forms in the $C1_b$ or MgAgAs structure type (space group $F\bar{4}$ 3m), which is a common Heusler-alloy structure, with only one formula unit per primitive unit cell. The atoms are distributed on 3 of the 4 sites along the [111] long body diagonal of the cell. All four sites have tetrahedral point-group symmetry $\bar{4}$ 3m. The cubic crystal-field environment should split the eight-fold degenerate J=7/2 state for the Yb^{3+} ion should be split into 3. At high temperature (>10K), the neutron inelastic scattering spectra[3] can be understood in these terms, albeit with very strong damping, and a heavily damped three-component crystal-field model gives remarkably good agreement with the measured low-temperature values for C and γ. However, at low temperatures, additional structure appears in the broad quasielastic component that might be associated with a lifting of the Γ_8 quartet degeneracy. It appears that this scattering splits into two excitations at approximately 1 and 2 meV. If these excitations can be thought of as excitations to Kramers-doublet crystal-field states, as shown by the density of states in the inset to Fig. 1, the specific heat (and γ) can be calculated using the same recipe as in Ref. 3, and the results of such a calculation are shown as a solid line in Fig. 1. Comparing the present result with Fig. 4 of Ref. 3, we still reproduce the experimental value of γ, though this time, it is predominantly due to the broadened Γ_7 ground state, with no contribution from the 1 and 2 meV levels. Of course, one cannot hope to reproduce the features at 0.4 K and just below, which are associated with a magnetic phase transition[4]. In Fig. 1(b), our model now gives features in the specific heat below 1K and at around 6K, in qualitative agreement with the measured specific heat. The comparison between the measured and calculated specific heats illustrates an additional problem

in describing the 6K specific-heat peak. Its shape is much sharper than a Schottky anomaly and C falls off more rapidly than $1/T^2$ on its high-temperature side. This means that the peak cannot be described in terms of excitations involving any temperature-independent density of states.

A possible explanation for this unusual property would be that there is a small temperature-dependent lattice distortion away from cubic symmetry of the Yb ions which develops below ~6 K. If the anomaly at ~6 K is associated with this "gradual" distortion, the thermodynamics of this process are peculiar because the anomaly is much broader than a phase transition which would normally accompany a Jahn-Teller type distortion [5]. The distortion may also be periodic over a long range since a decrease in the scattering rate is observed in the electrical resistivity at temperatures around the specific heat peak. Finally, the entropy at 20 K, obtained by integrating the magnetic contribution to the specific heat, is ~12.5 J/mol K, which is less than the amount expected from the observed CEF levels. It is possible that a varying hybridization of the Yb ions occupying different crystallographic sites may give an entropy between R ln(4) and R ln(6).

Such distortions could also give rise to the splitting of the 1 and 2 meV levels which is forbidden in cubic symmetry and sets in well above the 0.4K magnetic transition. If the distortions have long-range order, one might hope to see them in a diffraction experiment, and in a previous experiment[6] we looked for distortions to the obvious tetragonal (I4m2) and rhombohedrally (R3m) distorted structures. No splittings or broadenings of crystallographic lines were seen down to 0.45K, and full Rietveld refinements were performed down to 27K. The latter method is more sensitive, especially to the internal displacements allowed in R3m. We have therefore made additional powder diffraction experiments at 1.5K on the high-resolution neutron powder diffractometer (NPD) at Los Alamos. Again Rietveld refinements were performed in the cubic,

tetragonal and rhombohedral space groups, with no evidence for any deviation from cubic symmetry.

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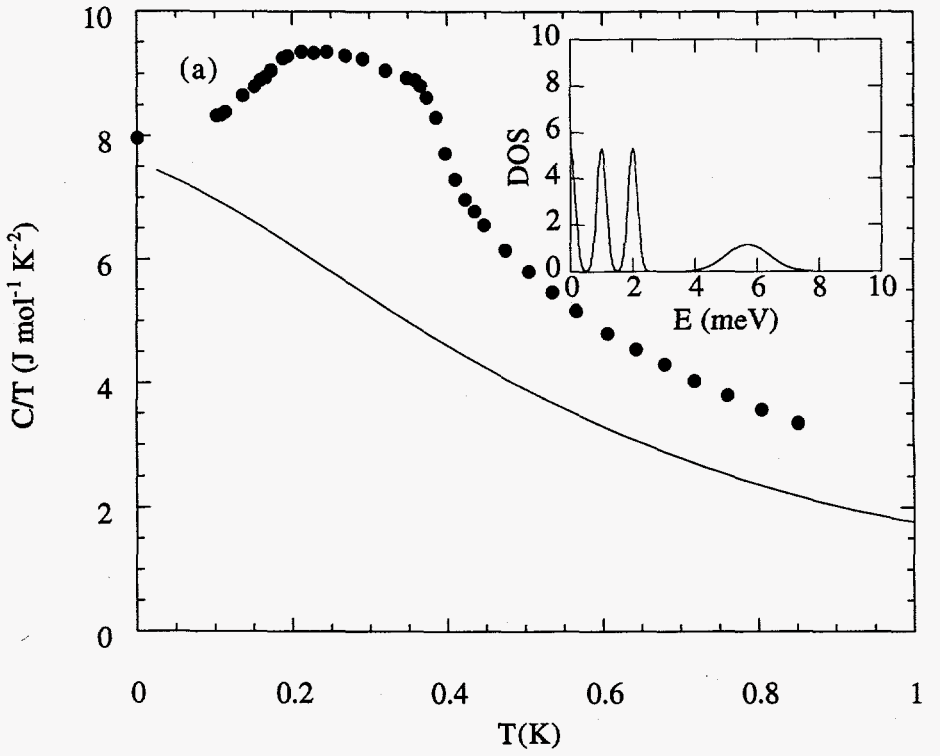
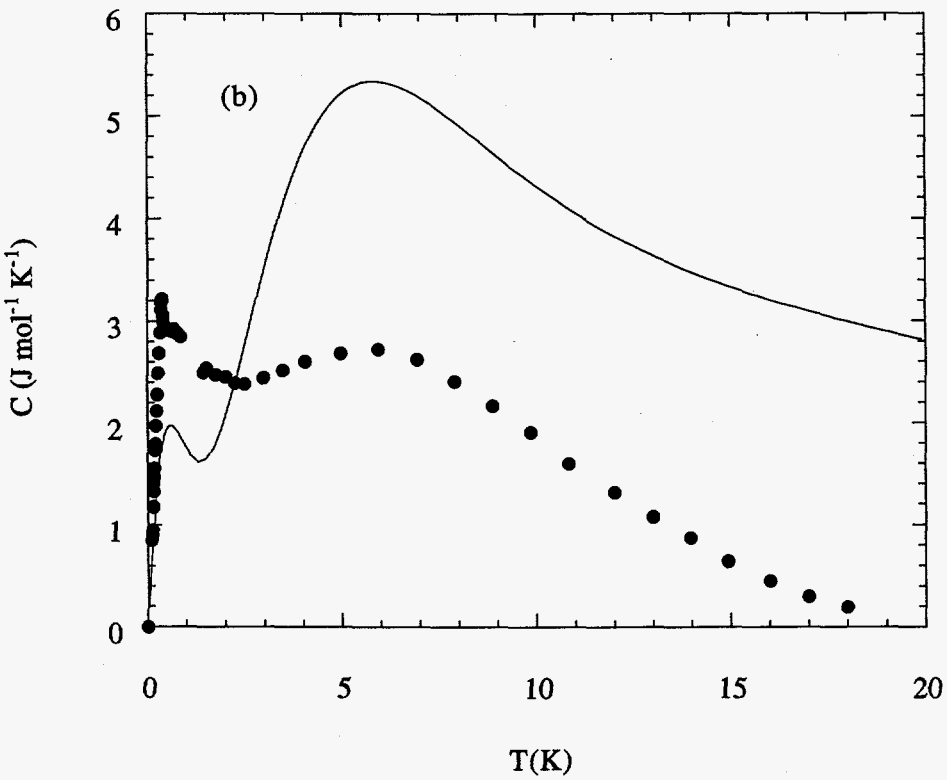
FIGURE CAPTIONS

Fig. 1 C/T and specific-heat values calculated assuming a temperature-dependent four-component lineshape including the "forbidden" splitting that can be associated with the Γ_8 level. We assume the three lowest components have the same Gaussian width with σ = 0.15+ 0.013T, roughly following the T-dependence of σ given in Ref. 3. The inset shows the corresponding density of excited states. The solid line is calculated from this model, while the points are the experimental specific-heat data, after subtraction of the lattice contribution, from Ref. 2. This figure is directly comparable to Fig. 4 of Ref. 3, in which the simpler three-component density of states is assumed.


(a)
C/T (J mol^{-1} K^{-2})
T(K)
DOS
E (meV)


(b)
C (J mol^{-1} K^{-1})
T(K)