

Formation and low temperature physics of CePt₂Si

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Abstract

CePt₂Si crystallizes in the inverse CeNiSi₂-type structure. Magnetic properties are dominated by a mutual interaction of the RKKY interaction, the Kondo effect and crystalline electric field splitting, resulting in long range magnetic order below about 7 K. A slightly enhanced Sommerfeld value $\gamma = 42 \text{ mJ/mol K}^2$ and a distinct temperature dependence of the electrical resistivity refers to Kondo interaction in presence of strong crystalline electric field splitting.

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Heavy fermion superconductivity in absence of inversion symmetry, recently discovered in CePt₂Si [1], directed our interest to a systematic exploration of compounds in the Ce–Pt–Si phase diagram. Among other novel ternary compounds, CePt₂Si has been identified and firstly prepared. CePt₂Si was synthesized via argon-arc melting and from X-ray Rietveld refinements was found to crystallize in the inverse CeNiSi₂-type ($a = 0.40987(1)$, $b = 1.8032(2)$, $c = 0.41677(3) \text{ nm}$; space group Cmc₂; $R_F = 0.035$, $R_P = 0.047$). The aim of the present work is a thorough investigation of thermodynamic, magnetic and transport properties of CePt₂Si. To define the phonon contributions to the total measured effects, the corresponding quantities have also been investigated for isostructural, non-magnetic LaPt₂Si ($a = 0.41721(4)$, $b = 1.7894(2)$, $c = 0.42378(4) \text{ nm}$; $R_F = 0.065$).

Fig. 1 shows the temperature dependent magnetic susceptibility χ plotted as χ^{-1} vs. T for CePt₂Si from 2 to

300 K. Above about 50 K a Curie Weiss like behaviour indicates a simple paramagnetic state. A least squares fit to the modified Curie Weiss law, i.e., $\chi = \chi_0 + C/(T - \theta_p)$ yields an effective moment $\mu_{\text{eff}} = 2.32 \mu_B$ and a paramagnetic Curie temperature $\theta_p = -47 \text{ K}$. The effective magnetic moment is close to the theoretical value associated with the Ce³⁺ state, while the slight curvature of the inverse magnetic susceptibility observed below 50 K is attributed to crystal electric field (CEF) effects. A distinct upturn of $1/\chi(T)$ below about 7 K refers to the onset of long range magnetic order, of, presumably, an antiferromagnetic type. This would be in accordance to the negative paramagnetic Curie temperature, indicating antiferromagnetic interactions between conduction electrons and the almost localized 4f electrons. A closer inspection of the low temperature range (see inset, Fig. 1), reveals two consecutive phase transitions at $T_{m1} \approx 7 \text{ K}$ and $T_{m2} \approx 4 \text{ K}$, respectively. Two magnetic phase transitions at about the same temperatures have been found recently in CePt₃B [2].

The temperature dependent specific heat C_p of CePt₂Si is shown in Fig. 2 together with the non-magnetic isostructural reference compound LaPt₂Si. The latter defines the

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phonon contribution and is characterized by a Sommerfeld value $\gamma = 5.5 \text{ mJ/mol K}^2$ and a Debye temperature $\theta_D = 225 \text{ K}$. Heat capacity at zero external fields also evidences two successive phase transitions, at 6.6 and 5.6 K, respectively. The latter transition, however, is efficiently eliminated by external magnetic fields as small as 1 T. Isothermal magnetization measurements (not shown here), reveal, most likely, antiferromagnetism in both phases, and a metamagnetic transition takes place at 3.5 T at $T = 1.7 \text{ K}$.

In order to qualitatively account for the ordered region of CePt_2Si , a model developed by Continentino et al. [3] is

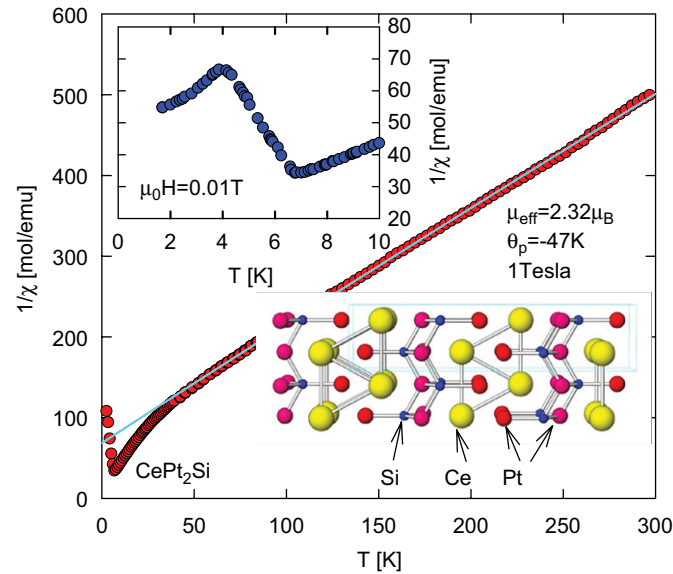


Fig. 1. (a): Temperature dependent magnetic susceptibility χ of CePt_2Si plotted as $1/\chi$ vs. T . The solid line is a least squares fit according to the modified CW-law. The inset shows low temperature details. The lower panel sketches the crystallographic unit cell of CePt_2Si .

applied, considering gapped antiferromagnetic spin waves. A least squares fit reveals for $T \ll T_{m2}$ a spin wave gap $\Delta \approx 4.8 \text{ K}$ together with a Sommerfeld constant $\gamma = 42 \text{ mJ/mol K}^2$ (solid line, Fig. 2).

The magnetic entropy associated with both phase transitions attains about $4.8 \text{ J/mol} \cdot \text{K}$ at $T = T_{m1}$, which is about 15% below the entropy release of a magnetically ordered state in an unperturbed crystal field ground state doublet. $R \ln 2$ is reached at about 16 K. This discrepancy is considered as a consequence of the Kondo effect, screening, at least partly, the Ce moments and spreading entropy to higher temperatures. In terms of a Bethe ansatz calculation [4], the Kondo temperature follows from these entropy data as $T_K \approx 2 \text{ K}$. Since $T_{m1} \gg T_K$, Kondo type

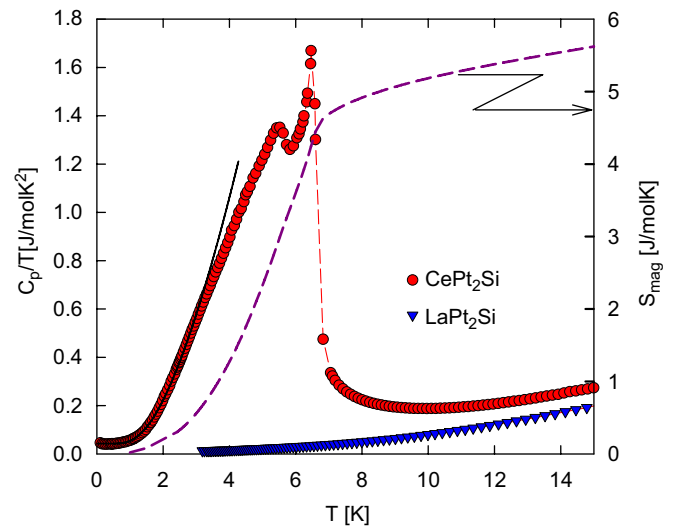


Fig. 2. Temperature dependent specific heat C_p of CePt_2Si and LaPt_2Si plotted as C_p/T vs. T (left axis). The solid line is a least squares fit using the model Ref. [3]. The magnetic entropy associated with CePt_2Si is shown as dashed line (right axis).

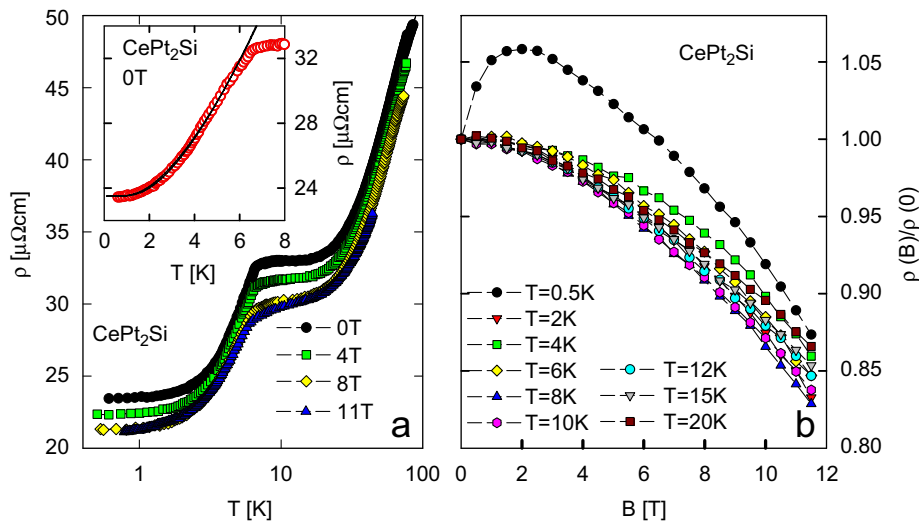


Fig. 3. (a) Temperature dependent electrical resistivity ρ of CePt_2Si measured at various externally applied magnetic fields. The inset shows low temperature features of $\rho(T)$ and the solid line is a least squares fit using the model Ref. [3]. (b) Isothermal magnetoresistance of CePt_2Si .

interaction appears to be weak in comparison to the RKKY interaction strength, placing this compound far left in Doniach's phase diagram of Kondo lattices. As a further consequence, the ordered moments should be almost unaffected and basically governed by the crystal field level scheme.

Fig. 3(a) displays the temperature dependent electrical resistivity ρ of CePt₂Si for various fields. A distinct kink in $\rho(T)$ around 7 K indicates the onset of long range magnetic order, which softens if magnetic fields are applied.

Employing the above model [3] allows a description of $\rho(T)$ well below T_m . A least squares fit (solid line, inset Fig. 3) yields a gap of 5.8 K, in fair agreement with the specific heat analysis. Isothermal magnetoresistance data are shown in Fig. 3(b). Data taken at 500 mK is initially positive, and exhibiting a maximum around 2 T, referring to a critical field, where the magnetic structure reorients. Above that field, magnetoresistance diminishes, referring to a ferromagnetic-like arrangement of the magnetic moments and a quenching of spin fluctuations as the field

strength further increases. Above T_{m1} , $\rho(B)/\rho(0)$ decreases and the s-shaped dependence reminds to Kondo type interaction.

In conclusion, the new ternary Ce compound, CePt₂Si has been synthesized and structurally characterized. The almost localized Ce-4f moments order antiferromagnetically below $T_{m1} = 6.6$ K followed by a spin-reorientation at $T_{m2} = 5.6$ K. The spin wave structure is gapped with $\Delta \approx 5$ K. Kondo type interactions are responsible for a moderately high Sommerfeld value $\gamma = 42$ mJ/mol K².

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