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**Structural, Magnetic and Electrical Properties
of the New Ternary CePdIn₂**

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ABSTRACT

CePdIn₂ is found to crystallize in the orthorhombic space group *Cmcm* (*Z*=4) with *a* = 4.6210(9) Å, *b* = 10.694(2) Å, and *c* = 7.455(2) Å. Single crystal X-ray data were refined to *R* = 0.0459 (*wR*₂ = 0.0666), with 255 independent reflections and 16 variables. The structure adopts the BRe₃ structure type and is the first known Ce-containing member. Magnetic measurements indicate that CePdIn₂ undergoes a ferromagnetic phase transition with a *T*_c near 10 K. The electrical resistivity of CePdIn₂ shows metallic behavior with a small anomaly at the magnetic phase transition.

INTRODUCTION

Over the past 20 years, research in ternary cerium intermetallics has grown substantially as interesting strongly correlated electron systems have been observed (1,2,3). While much progress has been made in understanding the origin of these effects, this knowledge is insufficient to predict new compounds which exhibit these phenomena.

However, as discussed by Fisk et al. (4), the chemical composition of the interesting Ce compounds includes mostly elements in the late transition metal and early p block columns. In particular, in the Ce-Pd-In ternary phase diagram, there are a number of interesting correlated electron materials such as CePd_3 (5), CeIn_3 (6), and CePdIn (7).

Motivated by the unusual materials found in this system as well as more recently discovered compounds (8), we have been searching for other new ternaries in this phase space (9). Here, we report the structure and properties of a new compound, CePdIn_2 .

EXPERIMENTAL

Sample Preparation

CePdIn_2 was synthesized by arc-melting stoichiometric amounts of the elements on a water-cooled, Ta coated copper hearth under a flow of Ti-gettered Ar (Centorr Furnaces, Model 2B-20). The arc-melted beads were flipped over and remelted repeatedly to increase homogeneity. Mass losses after arc-melting were less than 0.5%.

The elements used were all at least of purity 99.9%. The cerium was further purified by vacuum melting into a water-cooled copper cup, leaving behind much of the outer oxide coat often present on Ce pieces.

The arc-melted beads were then placed in tantalum tubing and sealed in quartz under vacuum. The beads were then heated at 825 °C for one week.

Structure determination

Preliminary structure characterization was done with electron and x-ray diffraction of finely ground powder. Electron diffraction patterns were obtained using powder suspended on holey carbon coated grids in a double tilt holder in a JEOL 1200 EX transmission electron microscope. The powder was also studied by X-ray diffraction using a Scintag XDS 2000 diffractometer with Cu K α radiation. The diffraction data indicated an orthorhombic cell of approximate dimensions 4.621 x 10.692 x 7.450 Å and C-centering.

Shards of lightly cracked beads were mounted and screened for crystal quality using precession camera photos. Single crystal data were collected on a Siemens P4 four-circle diffractometer in the θ -2 θ mode from $-1 \leq h \leq 6$, $-1 \leq k \leq 13$, and $-1 \leq l \leq 9$. The lattice constants for the cell were $a = 4.6210(9)$ Å, $b = 10.694(2)$ Å, and $c = 7.455(2)$ Å, in good agreement with the powder data. Three check reflections were measured every 50 reflections, and they showed no evidence of crystal decomposition or movement on the fiber. An empirical psi-scan absorption correction was applied to the data, yielding an $R_{int} = 0.0305$. The semi-invariants representation program SIR92 (10) was used to generate a model for the structure which was refined with XL from the SHELXTL

version 5 γ program (11). The final structure R values were $wR_2 = 0.0666$ and $R_1 = 0.0459$ for all data and $wR_2 = 0.0614$ and $R_1 = 0.0310$ for $I > 2\sigma(I)$. The MISSYM algorithm (12) detected no further symmetry elements than those expected for Cmc m .

Crystal structure data, values of the atomic parameters, and anisotropic displacement parameters are listed in Tables 1, 2, and 3. The atomic positions are presented both in accordance with previous BRe_3 structure literature and also in the standard format as determined by the program STRUCTURE TIDY (13). This program standardizes inorganic structures to help identify similar structures, obscured by differences in the reporting of crystal data.

Additional structure information, including structure amplitudes, is available as supplementary material.¹

Physical property measurements

The magnetic susceptibility of $CePdIn_2$ was measured using a Faraday balance on coarsely ground, loose powder. The field dependence of the susceptibility at room temperature from 2.1 kG to 14.6 kG showed variations of less than 1%, indicating the absence of ferromagnetic impurities. Temperature dependent data from 4 to 325 K were collected in a field of 10 kG. Platinum was used as a calibration standard. The measured room temperature susceptibility of Pt $\chi(293\text{ K})$ was 1.030×10^{-6} emu/g, in good agreement with a literature value of 1.035×10^{-6} emu/g (14).

Electrical resistivity was measured using standard four probe AC techniques. The contacts were ohmic by linearity of the I-V curve. The

resistivity sample was bar-shaped, cut with a string saw from a bead after heat treatment.

RESULTS AND DISCUSSION

Structural Aspects

The structure of CePdIn_2 is isotypic with the rare earth intermetallics $(\text{Y, Gd, Tb, Dy})\text{NiIn}_2$ (15), $(\text{Y, Tb-Lu})\text{NiGa}_2$ (16), $(\text{Y, Tb-Lu})\text{PdGa}_2$ (17), and $(\text{Y, Tb-Lu})\text{NiAl}_2$ (18). Thus, the structure type was previously known only for compounds containing the smaller rare earth atoms.

As shown in Figure 1, the structure can be described as a staggered net of trigonal prisms. Each prism is composed of four In atoms and two Ce atoms centered by a Pd atom.

Selected bond distances are listed in Table 4. The bond distances indicate that the chemical environment of the atoms is more complicated than emphasized in Figure 1. Figure 2 shows the coordination polyhedra around each of the atoms as determined by the principle of maximal gap in near neighbor distances (19). All resulting distances are short enough to be considered as bonding to the central atom.

As shown in Figure 2a, the 13-coordinate environment around the Ce can be described as a distorted pentagonal prism of eight In atoms and two Pd atoms with two In atoms and one Pd atom capping three square faces of the prism. The Pd environment of nine neighbors, shown in Figure 2b, consists of a trigonal prism of four In atoms and two Ce atoms, tricapped by two In

atoms and one Ce atom. The coordination geometry of In to its 12 neighbors is irregular and is depicted in Figure 2c. It consists roughly of Ce atoms in square pyramidal coordination and In atoms in tetrahedral coordination about the central In. Three Pd atoms complete the coordination polyhedron.

The complicated polyhedra suggest that size constraints strongly limit the formation of the BRe_3 structure type. An unsuccessful attempt at making $CeNiIn_2$ underscores this probable steric limitation. The larger Pd and In atoms are perhaps necessary to stabilize the structure for the larger rare earth Ce atom. To date, the presented structure is the only known Ce or Pd-In example for this structure type.

Magnetic properties

Figure 3 shows the inverse magnetic susceptibility for $CePdIn_2$ upon heating the powder sample from 4.2 K. The data were fit to the Curie-Weiss

$$\text{law: } \chi = \chi_0 + \frac{C}{T - \theta} .$$

The fit parameters were selected by choosing a temperature range of fit, fixing θ , and then determining C and χ_0 using standard analysis techniques (20). θ was varied, and for each choice, a fractional variance σ was calculated. The final parameters were chosen to minimize σ over the largest temperature range.

These parameters were found to be $\chi_0 = 2.6 \pm 0.4 \times 10^{-7}$ emu/g, $C = 1.60 \pm 0.02 \times 10^{-3}$ emu-K/g, and a ferromagnetic $\theta = 16.5 \pm 1.5$ K for the temperature

range of 75 to 325 K with a $\sigma = 1.5 \times 10^{-3}$. At temperatures below 75 K, some deviations from the Curie-Weiss law occur, most likely due to crystal field effects. The Curie constant corresponds to a moment of $2.47 \pm 0.02 \mu_B$ which is very close to the free ion value of $2.54 \mu_B$ for Ce^{+3} . Hence, it appears that in $CePdIn_2$, the Ce is trivalent, with ferromagnetic exchange. We can estimate a transition temperature of ≈ 10 K from the inflection point of the χ vs temperature curve.

As shown in Figure 4, the field dependence of the low temperature susceptibility is consistent with a ferromagnetically ordered material. Fitting the χ vs $1/H$ curve to a straight line, we obtain a magnetization at 4.2 K of $1.6 \mu_B$ vs the expected $gJ = 2.14 \mu_B$ for completely oriented Ce^{+3} ions in a $J=5/2$ state. The deviation from the expected value may indicate that there is some canting of the spins in the ordered state or more likely that crystal field splitting reduces the ground state moment.

The existence of ferromagnetism in this system agrees well with the empirical observations of Sereni and Kappler (21). They found that ferromagnetic behavior is often present in systems with Ce-Ce nearest neighbor distances between 3.7 and 4.1 Å. In $CePdIn_2$ this distance is 4.063 Å.

Electrical properties

Resistivity data from room temperature to 4.2 K are shown in Figure 5. The magnitude of the resistivity and its monotonic decrease with temperature down to ≈ 20 K indicate metallic conduction. At roughly 10 K,

there is a kink in the resistivity, most likely due to a coupling of the carriers to the ordering Ce moments.

Note that the resistivity decreases more rapidly below 10 K than just above, indicating that spin-disorder scattering may be playing a role at higher temperatures. Below the ferromagnetic transition, this extra scattering is expected to die out as the moments order. This behavior is similar to that observed in other rare earth intermetallic compounds such as NdAuAl (22) and GdNiGe (23).

CONCLUSIONS

We have synthesized a new ternary intermetallic compound, CePdIn₂, the first known Ce containing member of the BRe₃ structure type. From the magnetic and electrical properties, we conclude that CePdIn₂ is a ferromagnet with a T_c of about 10 K. It appears that the Ce moments do not interact strongly with the conduction electrons, as we see little evidence of Kondo-like magnetic or transport behavior.

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TABLE 1

Crystal Data and Structure Refinement for CePdIn₂

Empirical formula	CePdIn ₂
Formula weight	476.16
Diffractometer type	Siemens P4 four-circle
Radiation	Graphite monochromated MoK _α , λ=0.71073 Å
Temperature	293(2) K
Scan type	θ-2θ
Crystal system	Orthorhombic
Space group	Cmcm (No. 63)
Unit cell dimensions	a = 4.6210(9) Å b = 10.694(2) Å c = 7.455(2) Å
Volume	368.40(13) Å ³
Z	4
Density (calculated)	8.585 g/cm ³
Absorption coefficient	29.012 mm ⁻¹
F(000)	808
Crystal size	0.19 x 0.05 x 0.04 mm
θ range for data collection	3.81° to 27.48°
Index ranges	-1 ≤ h ≤ 6, -1 ≤ k ≤ 13, -1 ≤ l ≤ 9
Reflections collected	391
Independent reflections	255 (R _{int} = 0.0305)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.984 and 0.509
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	255/0/16
Goodness-of-fit on F ²	1.089
Final R indices (I>2σ(I))	R ₁ = 0.0310, wR ₂ = 0.0614
R indices (all data)	R ₁ = 0.0459, wR ₂ = 0.0666
Largest diff. peak and hole	2.547 and -1.546 eÅ ⁻³

TABLE 2

Atomic Coordinates^a and Equivalent Isotropic
Displacement Parameters ($\text{\AA}^2 \times 10^3$) for CePdIn₂

	x	y	z	U(eq)
In in 8(f)	0.0 [0.0]	0.3612(1) [0.1388]	0.0506(1) [0.0506]	11(1)
Ce in 4(c)	0.0 [0.0]	0.0756(1) [0.4244]	0.25 [0.25]	10(1)
Pd in 4(c)	0.0 [0.0]	0.7931(2) [0.7069]	0.25 [0.25]	11(1)

^aCoordinates in brackets are in STRUCTURE TIDY format.

TABLE 3

Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for CePdIn₂

	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃ =U ₁₂
Pd	9(1)	12(1)	10(1)	0	0
Ce	10(1)	11(1)	11(1)	0	0
In	11(1)	13(1)	8(1)	1(1)	0

TABLE 4

Interatomic Bond Distances (\AA)
for CePdIn₂

Ce	1Pd	3.021(3)
	2Pd	3.278(2)
	4In	3.2891(9)
	2In	3.396(2)
	4In	3.5786(13)
Pd	1Ce	3.021(3)
	2Ce	3.278(2)
	2In	2.783(2)
	4In	2.8421(9)
In	2Ce	3.2891(9)
	1Ce	3.396(2)
	2Ce	3.5786(13)
	1Pd	2.783(2)
	2Pd	2.8421(9)
	1In	2.973(2)
	1In	3.064(2)

LIST OF FIGURE CAPTIONS

FIG. 1. Structure of CePdIn_2 illustrating trigonal prismatic coordination around the Pd atoms.

FIG. 2. Local coordination environments around a) Ce b) Pd and c) In atoms. The dark lines indicate the pentagonal and trigonal prismatic units in the Ce and Pd coordination polyhedra.

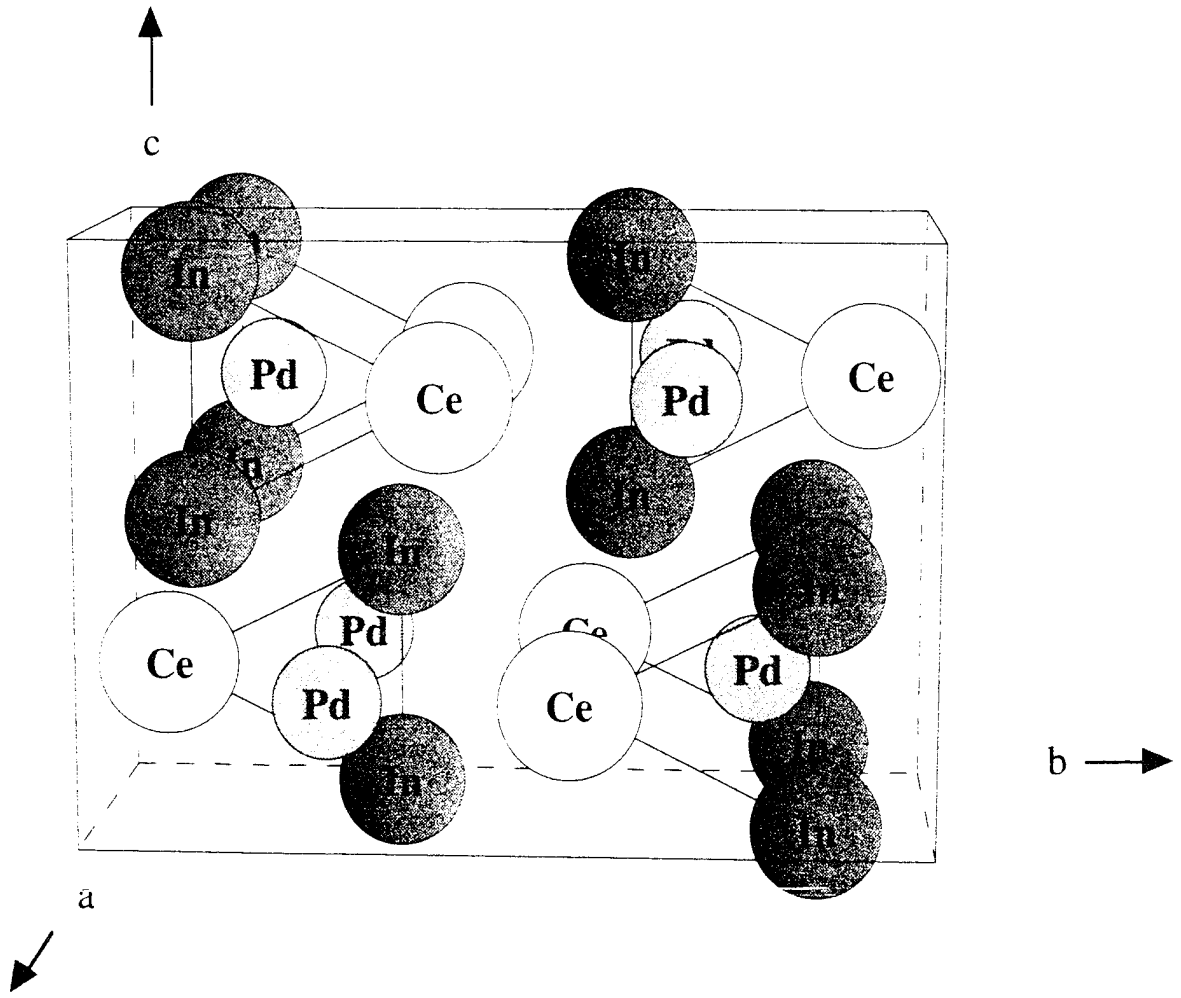
FIG. 3. Inverse magnetic susceptibility as a function of temperature. Inset shows susceptibility vs temperature for $T < 50$ K.

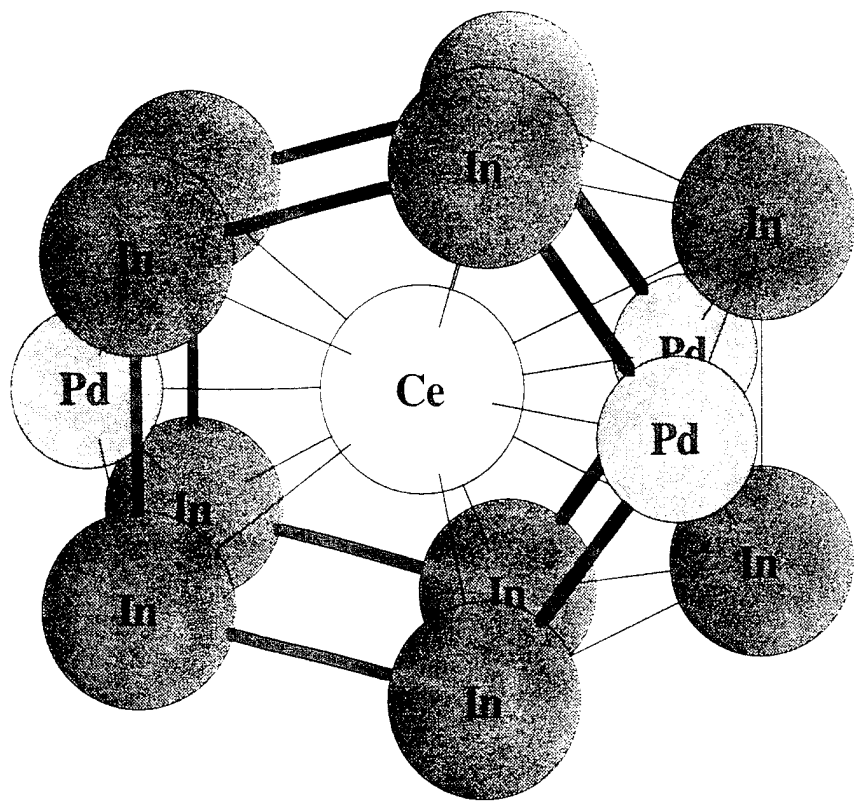
FIG. 4. Magnetic susceptibility vs inverse field at 4.2 K.

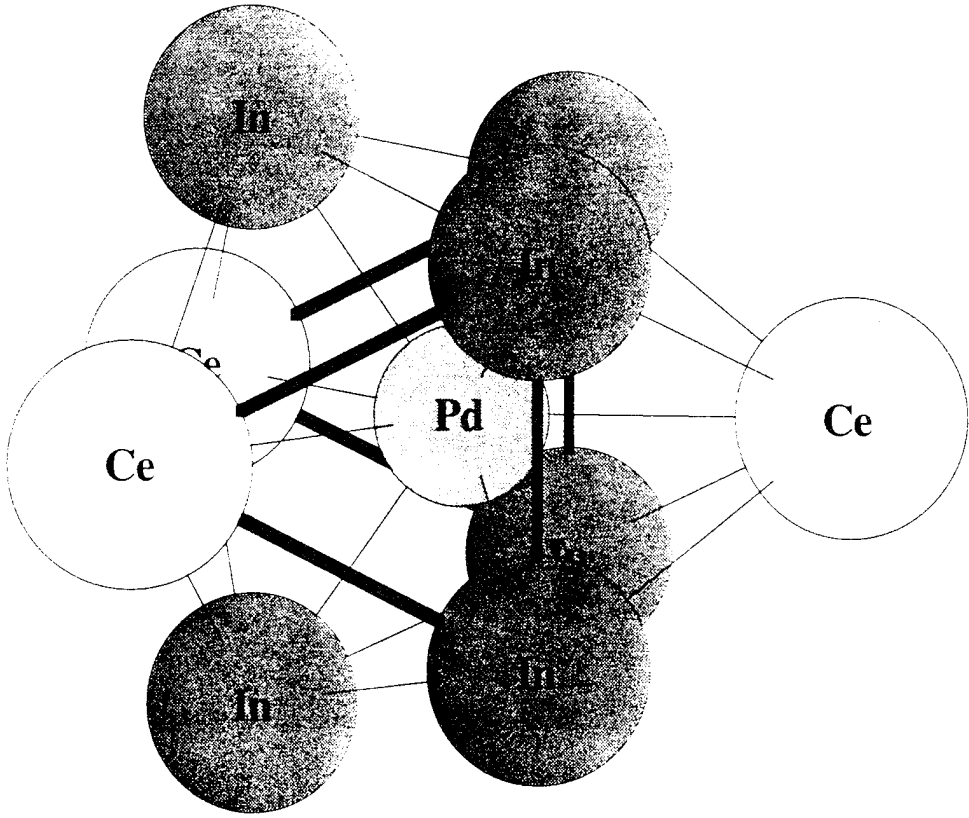
FIG. 5. Electrical resistivity as a function of temperature. Inset shows resistivity for $T < 25$ K.

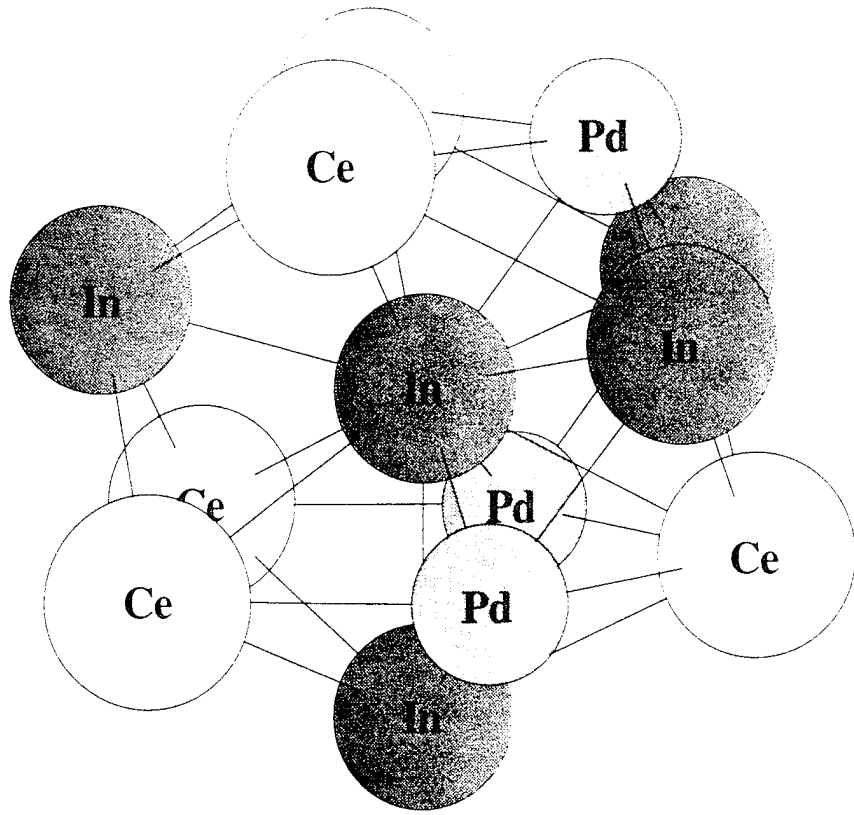
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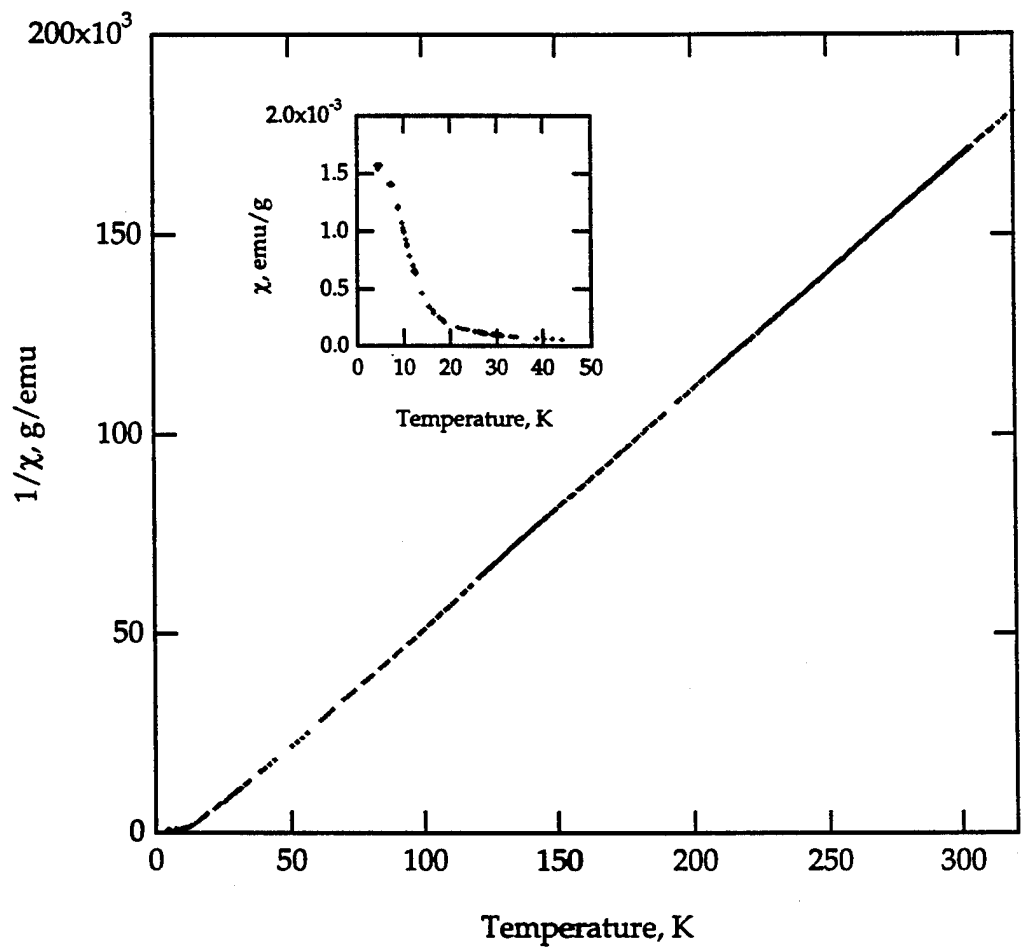
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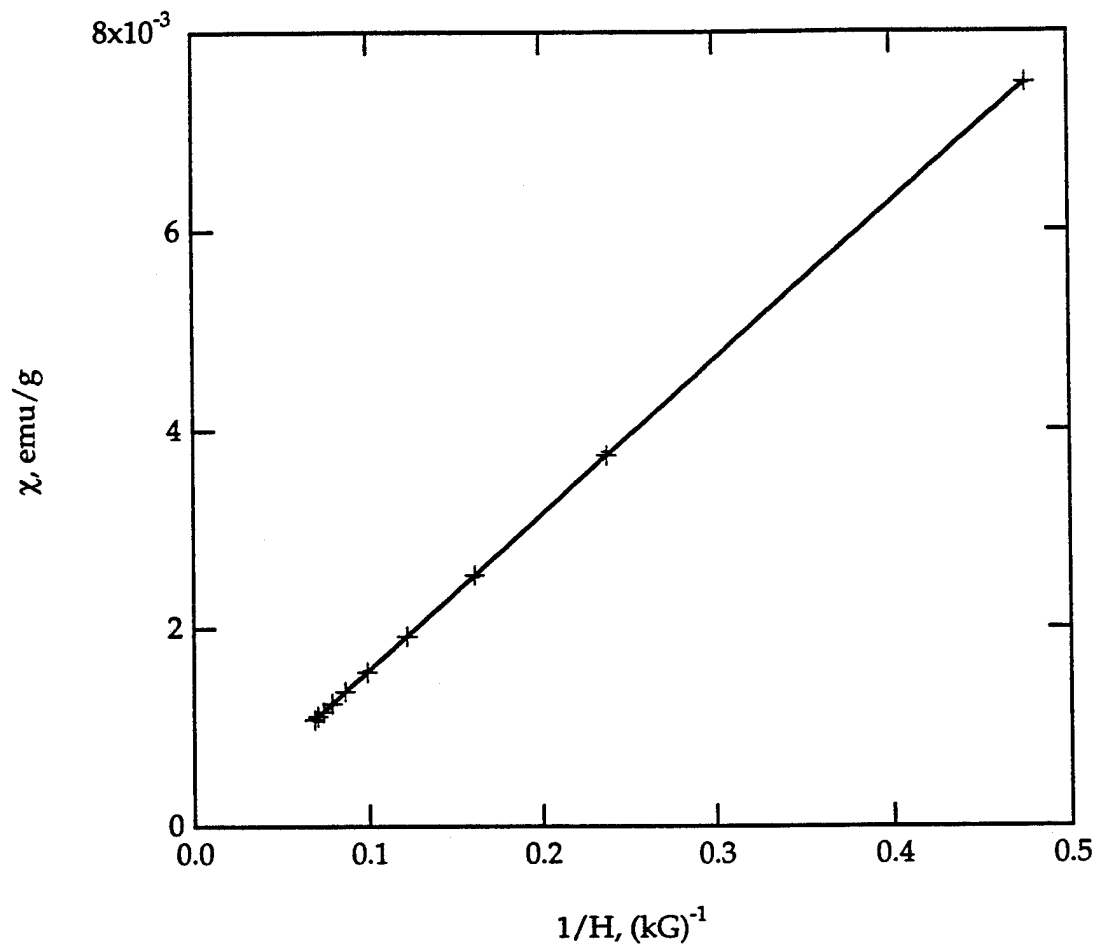


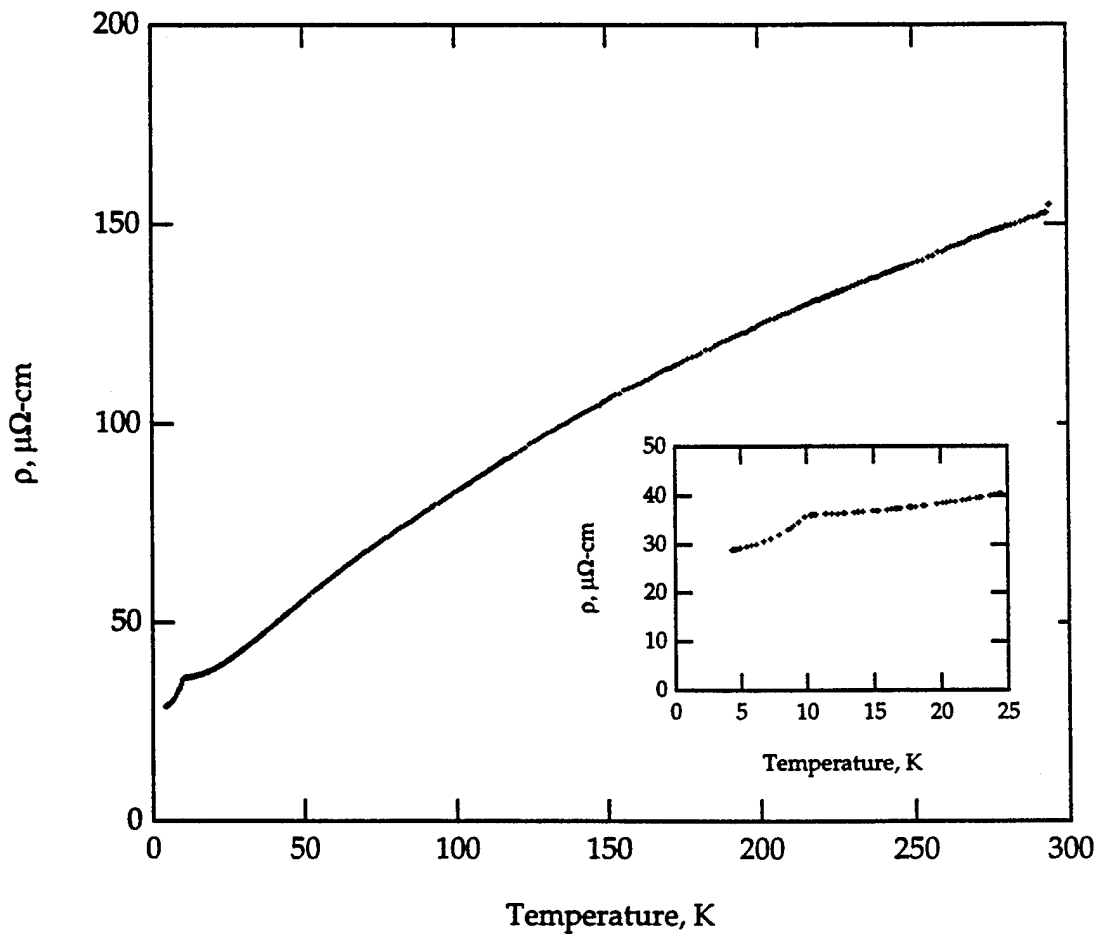












Supplementary information: additional bond lengths (Å) and angles (°)

In-Pd#1	2.783(2)	In-Pd#2	2.8421(9)
In-Pd#3	2.8421(9)	In-In#4	2.973(2)
In-In#5	3.064(2)	In-Ce#6	3.2891(9)
In-Ce#7	3.2891(9)	In-Ce#8	3.396(2)
In-Ce#2	3.5786(13)	In-Ce#3	3.5786(13)
Ce-Pd	3.021(3)	Ce-Pd#9	3.278(2)
Ce-Pd#10	3.278(2)	Ce-In#11	3.2891(9)
Ce-In#12	3.2891(9)	Ce-In#13	3.2891(9)
Ce-In#14	3.2891(9)	Ce-In#15	3.396(2)
Ce-In#8	3.396(2)	Ce-In#2	3.5786(13)
Ce-In#16	3.5786(13)	Ce-In#17	3.5786(13)
Pd-In#18	2.783(2)	Pd-In#4	2.783(2)
Pd-In#17	2.8421(9)	Pd-In#2	2.8421(9)
Pd-In#3	2.8421(9)	Pd-In#16	2.8421(9)
Pd-Ce#19	3.278(2)	Pd-Ce#20	3.278(2)
Pd#1-In-Pd#2	105.63(3)	Pd#1-In-Pd#3	105.63(3)
Pd#2-In-Pd#3	108.77(5)	Pd#1-In-In#4	143.65(4)
Pd#2-In-In#4	58.47(2)	Pd#3-In-In#4	58.47(2)
Pd#1-In-In#5	112.10(6)	Pd#2-In-In#5	112.15(5)
Pd#3-In-In#5	112.15(5)	In#4-In-In#5	104.26(4)
Pd#1-In-Ce#6	64.73(4)	Pd#2-In-Ce#6	168.55(4)
Pd#3-In-Ce#6	80.67(2)	In#4-In-Ce#6	132.95(2)
In#5-In-Ce#6	68.46(3)	Pd#1-In-Ce#7	64.73(4)
Pd#2-In-Ce#7	80.67(2)	Pd#3-In-Ce#7	168.55(4)
In#4-In-Ce#7	132.95(2)	In#5-In-Ce#7	68.46(3)
Ce#6-In-Ce#7	89.25(3)	Pd#1-In-Ce#8	79.60(4)
Pd#2-In-Ce#8	62.67(4)	Pd#3-In-Ce#8	62.67(4)
In#4-In-Ce#8	64.05(2)	In#5-In-Ce#8	168.30(6)
Ce#6-In-Ce#8	118.89(3)	Ce#7-In-Ce#8	118.89(3)
Pd#1-In-Ce#2	135.59(2)	Pd#2-In-Ce#2	54.69(5)
Pd#3-In-Ce#2	118.15(4)	In#4-In-Ce#2	65.46(2)
In#5-In-Ce#2	58.75(3)	Ce#6-In-Ce#2	127.21(3)
Ce#7-In-Ce#2	72.40(2)	Ce#8-In-Ce#2	113.23(3)
Pd#1-In-Ce#3	135.59(2)	Pd#2-In-Ce#3	118.15(4)
Pd#3-In-Ce#3	54.69(5)	In#4-In-Ce#3	65.46(2)
In#5-In-Ce#3	58.75(3)	Ce#6-In-Ce#3	72.40(2)
Ce#7-In-Ce#3	127.21(3)	Ce#8-In-Ce#3	113.23(3)
Ce#2-In-Ce#3	80.43(4)	Pd-Ce-Pd#9	135.19(3)
Pd-Ce-Pd#10	135.19(3)	Pd#9-Ce-Pd#10	89.62(6)
Pd-Ce-In#11	101.87(3)	Pd#9-Ce-In#11	50.14(2)
Pd#10-Ce-In#11	110.44(4)	Pd-Ce-In#12	101.87(3)
Pd#9-Ce-In#12	110.44(4)	Pd#10-Ce-In#12	50.14(2)
In#11-Ce-In#12	156.27(6)	Pd-Ce-In#13	101.87(3)
Pd#9-Ce-In#13	50.14(2)	Pd#10-Ce-In#13	110.44(4)
In#11-Ce-In#13	85.90(3)	In#12-Ce-In#13	89.25(3)
Pd-Ce-In#14	101.87(3)	Pd#9-Ce-In#14	110.44(4)
Pd#10-Ce-In#14	50.14(2)	In#11-Ce-In#14	89.25(3)
In#12-Ce-In#14	85.90(3)	In#13-Ce-In#14	156.27(6)
Pd-Ce-In#15	154.05(2)	Pd#9-Ce-In#15	50.36(3)
Pd#10-Ce-In#15	50.36(3)	In#11-Ce-In#15	61.11(3)
In#12-Ce-In#15	96.51(3)	In#13-Ce-In#15	96.51(3)
In#14-Ce-In#15	61.11(3)	Pd-Ce-In#8	154.05(2)
Pd#9-Ce-In#8	50.36(3)	Pd#10-Ce-In#8	50.36(3)
In#11-Ce-In#8	96.51(3)	In#12-Ce-In#8	61.11(3)

In#13-Ce-In#8	61.11(3)	In#14-Ce-In#8	96.51(3)
In#15-Ce-In#8	51.91(4)	Pd-Ce-In#2	50.15(2)
Pd#9-Ce-In#2	155.46(2)	Pd#10-Ce-In#2	89.98(3)
In#11-Ce-In#2	150.26(4)	In#12-Ce-In#2	52.79(3)
In#13-Ce-In#2	107.60(2)	In#14-Ce-In#2	87.78(2)
In#15-Ce-In#2	139.28(2)	In#8-Ce-In#2	113.23(3)
Pd-Ce-In#16	50.15(2)	Pd#9-Ce-In#16	155.46(2)
Pd#10-Ce-In#16	89.98(3)	In#11-Ce-In#16	107.60(2)
In#12-Ce-In#16	87.78(2)	In#13-Ce-In#16	150.26(4)
In#14-Ce-In#16	52.79(3)	In#15-Ce-In#16	113.23(3)
In#8-Ce-In#16	139.28(2)	In#2-Ce-In#16	49.08(4)
Pd-Ce-In#17	50.15(2)	Pd#9-Ce-In#17	89.98(3)
Pd#10-Ce-In#17	155.46(2)	In#11-Ce-In#17	52.79(3)
In#12-Ce-In#17	150.26(4)	In#13-Ce-In#17	87.78(2)
In#14-Ce-In#17	107.60(2)	In#15-Ce-In#17	113.23(3)
In#8-Ce-In#17	139.28(2)	In#2-Ce-In#17	100.30(5)
In#16-Ce-In#17	80.43(4)	In#18-Pd-In#4	107.29(7)
In#18-Pd-In#17	124.96(3)	In#4-Pd-In#17	74.37(3)
In#18-Pd-In#2	74.37(3)	In#4-Pd-In#2	124.96(3)
In#17-Pd-In#2	150.32(9)	In#18-Pd-In#3	74.37(3)
In#4-Pd-In#3	124.96(3)	In#17-Pd-In#3	63.07(4)
In#2-Pd-In#3	108.77(5)	In#18-Pd-In#16	124.96(3)
In#4-Pd-In#16	74.37(3)	In#17-Pd-In#16	108.77(5)
In#2-Pd-In#16	63.07(4)	In#3-Pd-In#16	150.32(9)
In#18-Pd-Ce	126.35(4)	In#4-Pd-Ce	126.35(4)
In#17-Pd-Ce	75.16(4)	In#2-Pd-Ce	75.16(4)
In#3-Pd-Ce	75.16(4)	In#16-Pd-Ce	75.16(4)
In#18-Pd-Ce#19	65.13(3)	In#4-Pd-Ce#19	65.13(3)
In#17-Pd-Ce#19	138.99(5)	In#2-Pd-Ce#19	66.97(3)
In#3-Pd-Ce#19	138.99(5)	In#16-Pd-Ce#19	66.97(3)
Ce-Pd-Ce#19	135.19(3)	In#18-Pd-Ce#20	65.13(3)
In#4-Pd-Ce#20	65.13(3)	In#17-Pd-Ce#20	66.97(3)
In#2-Pd-Ce#20	138.99(5)	In#3-Pd-Ce#20	66.97(3)
In#16-Pd-Ce#20	138.99(5)	Ce-Pd-Ce#20	135.19(3)
Ce#19-Pd-Ce#20	89.62(6)		

Symmetry transformations used to generate equivalent atoms:

#1 $x, y, z+1$ #2 $-x-1/2, -y+1/2, -z+1$ #3 $-x+1/2, -y+1/2, -z+1$
#4 $x, y, -z+3/2$ #5 $-x, -y, -z+2$ #6 $x+1/2, y-1/2, z+1$
#7 $x-1/2, y-1/2, z+1$ #8 $-x, -y+1, -z+1$ #9 $x+1/2, y+1/2, z$
#10 $x-1/2, y+1/2, z$ #11 $x+1/2, y+1/2, -z+3/2$ #12 $x-1/2, y+1/2, z-1$
#13 $x+1/2, y+1/2, z-1$ #14 $x-1/2, y+1/2, -z+3/2$ #15 $-x, -y+1, z-1/2$
#16 $-x-1/2, -y+1/2, z-1/2$ #17 $-x+1/2, -y+1/2, z-1/2$ #18 $x, y, z-1$
#19 $x-1/2, y-1/2, z$ #20 $x+1/2, y-1/2, z$

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