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Intermetallic CePdIn

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(In–Pd) = 0.002 Å
R factor = 0.040
wR factor = 0.112
Data-to-parameter ratio = 15.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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Cerium palladium indide, CePdIn, crystallizes in the hexagonal space group $P\bar{6}2m$ and belongs to the ZrNiAl structure type.

Comment

During systematic studies of the ternary cerium–palladium–indium system, the intermetallic compound CePdIn was obtained. In the Ce–Pd–In system, four ternary compounds have been investigated previously by single-crystal X-ray diffraction: $CePdIn_2$ (Ijiri *et al.*, 1996), $Ce_4Pd_{10}In_{21}$ (Zaremba *et al.*, 2003), $CePd_2In_4$ (Tursina *et al.*, 2003), and $CePd_3In_2$ (Nesterenko *et al.*, 2004).

CePdIn crystallizes in the ZrNiAl-type structure (Krypyakevich *et al.*, 1967), which is an ordered variant of the binary compound Fe_2P (Rundqvist & Jellinek, 1959). Up to now, only lattice parameters of CePdIn have been determined (Ferro *et al.*, 1974; Brück *et al.*, 1993). Each Ce atom is surrounded by five Pd and six In atoms, which form a distorted pentagonal prism with one additional atom [Pd_5In_6]. Atom Pd1 is coordinated by six Ce atoms forming a trigonal prism [at a distance of 3.0710 (8) Å] and three additional In atoms capping the square faces at 2.9484 (19) Å. Atom Pd2 is at the center of a similar polyhedron formed by six In atoms at 2.777 (2) Å and three Ce atoms at 3.183 (3) Å. The In atom is surrounded by a distorted tetragonal prism with four additional atoms [$Ce_6Pd_4In_2$] (Fig. 1).

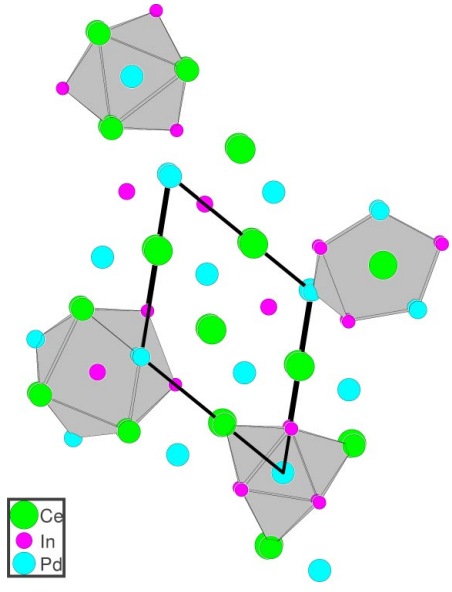

Figure 1
A view of the CePdIn structure along the c axis. Part of the structure is shown in the polyhedral representation.

Experimental

The title compound was prepared by direct arc melting of high purity components (Ce 98.0, Pd 99.9, In 99.9 wt% pure) under an argon atmosphere. The sample with nominal composition $Ce_{33}Pd_{34}In_{33}$ was annealed in an evacuated double quartz ampoule at 770 K over a period of 600 h and quenched in cold water. Weight loss was less than 1% of the total mass of 1.0 g. A single crystal was selected from the surface of the resulting alloy.

Crystal data

CePdIn
M_r = 361.34
Hexagonal, $P\bar{6}2m$
a = 7.7036 (15) Å
c = 4.0190 (14) Å
V = 206.56 (9) Å^3
Z = 3
D_x = 8.715 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 7.3–18.9°
μ = 30.63 mm^{-1}
T = 293 (2) K
Prism, metallic dark grey
0.09 × 0.03 × 0.03 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.285, T_{max} = 0.393
551 measured reflections
195 independent reflections
171 reflections with $I > 2\sigma(I)$
R_{int} = 0.077
θ_{max} = 27.1°
$h = 0 \rightarrow 9$
$k = -9 \rightarrow 8$
$l = 0 \rightarrow 5$
1 standard reflection
frequency: 120 min
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 0.80
195 reflections
13 parameters
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.59 e Å^{-3}
$\Delta\rho_{min}$ = −1.90 e Å^{-3}
Absolute structure: Flack (1983), 118 Friedel pairs
Flack parameter = 0.38 (14)

Table 1
Selected interatomic distances (Å).

In—Pd2	2.777 (2)	In—Ce^{iii}	3.4267 (18)
In—Pd1^{i}	2.9484 (19)	Ce—Pd1^{iv}	3.0710 (8)
In—Ce	3.290 (3)	Ce—Pd2^{v}	3.183 (3)
In—In^{ii}	3.319 (5)		

Symmetry codes: (i) $x, y-1, z$; (ii) $-x, -x+y, z$; (iii) $y, x-1, z$; (iv) y, x, z; (v) $1+x, y, z$.

Refinement of the structure, taking into account inversion twinning, did not result in a significant improvement. The highest peak and the deepest hole in the difference map are located 1.92 Å from In and 0.76 Å from Ce, respectively.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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References

Brandenburg, K. (1998). *DIAMOND*. Version 2.1*b*. Crystal Impact GbR, Bonn, Germany.
Brück, E., Nakotte, H., Bakker, K., de Boer, F. R., de Chatel, P. F., Li, J.-Y., Kuang, J. P. & Yang, F.-M. J.(1993). *J. Alloys Compd*, **200**, 79–86.
Enraf–Nonius (1994). *CAD*-4 *EXPRESS*. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Ferro, R., Marazza, R. & Rambaldi, G. (1974). *Z. Metallkd.* **65**, 37–39.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Harms, K. & Wocadlo, S. (1995). *XCAD*4. University of Marburg, Germany.
Ijiri, Y., DiSalvo, F. & Yamane, H. (1996). *J. Solid State Chem.* **122**, 143–147.
Krypyakevich, P. I., Markiv, V. Y. & Melnyk, Y. V. (1967). *Dopov. Akad. Nauk Ukr. RSR Ser. A*, **8**, 750–753.
Nesterenko, S. N., Tursina, A. I., Rogl, P. & Seropegin, Y. D. (2004). *J. Alloys Compd*. In the press.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Rundqvist, S. & Jellinek, F. (1959). *Acta Chem. Scand.* **13**, 425–432.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Tursina, A. I., Gribanov, A. V., Seropegin Y. D. & Nesterenko, S. N. (2003). 14*th International Conference on Solid Compounds of Transitional Elements*, Programme and Abstracts, Linz, Austria, p. PO II-20.
Zaremba, V. I., Rodewald, U. C., Kalychak, Y. M., Galadzhun Y. V., Kaczorowski, D., Hoffmann, R.-D. & Pöttgen, R. (2003). *Z. Anorg. Allg. Chem.* **629**, 434–442.