Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

A new ternary indide, Ce$_{20}$Pd$_{36}$In$_{67}$

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Received 7 April 2005
Accepted 25 April 2005
Online 14 May 2005

The intermetallic compound, cerium palladium indide, Ce$_{20}$Pd$_{36}$In$_{67}$, crystallizes in a new structure type in which atoms have significantly distorted polyhedra with coordination numbers CN 15–18 for Ce and CN 8–13 for Pd and In.

Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(In–In) = 0.002 Å
R factor = 0.034
wR factor = 0.079
Data-to-parameter ratio = 10.6

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

Comment

Crystal structures of five ternary compounds from the Ce–Pd–In system have been reported previously: CePdIn$_2$ (Ijiri *et al.*, 1996), Ce$_4$Pd$_{10}$In$_{21}$ (Zaremba *et al.*, 2003), CePd$_2$In$_4$ (Nesterenko, Tursina, Gribanov *et al.*, 2004), CePd$_3$In$_2$ (Nesterenko, Tursina, Rogl & Seropegin, 2004) and CePdIn (Tursina *et al.*, 2004). We present here the ternary compound Ce$_{20}$Pd$_{36}$In$_{67}$ exhibiting a new structure type.

In this structure, all atom sites are fully occupied, except for Pd1, Pd2, In1 and In2. The Pd1 and Pd2 sites represent closely spaced split positions (96*i*), with occupancies of 0.66 (2) and 0.34 (2), respectively, and a Pd1—Pd2 separation of

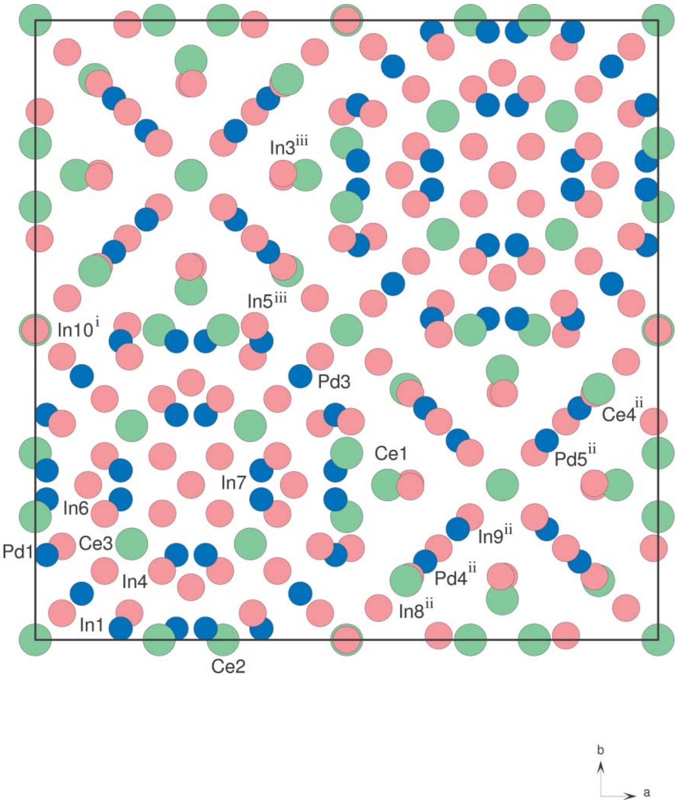

Figure 1
Projection of Ce$_{20}$Pd$_{36}$In$_{67}$, with Ce atoms shown as green circles, Pd atoms as blue circles and In atoms as pink circles. One half of the unit-cell content is presented, $0 \le z \le \frac{1}{2}$. Atoms Pd2 and In2 have been omitted for clarity. [Symmetry codes: (i) $x, \frac{1}{2}+y, \frac{1}{2}+z$; (ii) $x, y-\frac{1}{2}, z-\frac{1}{2}$; (iii) $\frac{1}{2}-x, z, \frac{1}{2}-y$.]

doi:10.1107/S1600536805013048

0.579 (7) Å. Likewise, the In1 and In2 sites represent split positions (48*h*), with occupancies of 0.68 (1) and 0.32 (1), respectively, and an In1—In2 separation of 0.893 (6) Å.

All atoms have significantly distorted coordination polyhedra. Atoms Ce1 and Ce2 are at the centres of pentagonal prisms with five and eight additional atoms, respectively. The coordination polyhedra around atoms Ce3 and Ce4 are essentially distorted hexagonal prisms with additional atoms, *viz*. $Ce3[Pd_6In_{12}]$ and $Ce4[Pd_7In_9]$. Most of the Pd and In atoms have a distorted icosahedral environment, with coordination numbers in the range 9–13. The Ce atoms are among the nearest neighbours of all Pd and In atoms with Ce—Pd(In) distances not exceeding 3.610 (2) Å (Table 1). Only Pd4—Ce distances considerably exceed the sum of the metallic radii of Ce and Pd (>4 Å). Consequently, atom Pd4 is surrounded by eight In atoms [2.693 (2)–2.858 (2) Å], which form a slightly distorted cube.

Fig. 1 shows the complex three-dimensional network of the structure and Fig. 2 shows the asymmetric unit.

Experimental

An ingot of nominal composition $Ce_{17}Pd_{32}In_{51}$ was prepared by arc melting under argon from Ce (99.85%), Pd (99.9%) and In (99.9%). The sample was annealed at 770 K in a silica tube under argon for 700 h. A single crystal was obtained from the crushed ingot. From EMPA analyses (Jeol JSM 6400 scanning electron microscope equipped with an Si/Li energy dispersive analyser), the composition of the new phase was estimated to be $Ce_{16.5}Pd_{30.4}In_{53.1}$, in good agreement with the composition of the $Ce_{20}Pd_{36}In_{67}$ compound in atomic percent, *viz*. $Ce_{16.26}Pd_{29.27}In_{54.47}$.

Crystal data

$Ce_{20}Pd_{36}In_{67}$
$M_r = 14325.74$
Cubic, $F\bar{4}3m$
$a = 21.8382$ (8) Å
$V = 10414.8$ (7) Å^3
$Z = 4$
$D_x = 9.136$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 23 reflections
$\theta = 14.2$–$16.4°$
$\mu = 29.04$ mm^{-1}
$T = 291$ (2) K
Prism, metallic light grey
0.12 × 0.05 × 0.03 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.207$, $T_{max} = 0.418$
9710 measured reflections
958 independent reflections
897 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$
$\theta_{max} = 31.9°$
$h = 0 \rightarrow 32$
$k = 0 \rightarrow 32$
$l = -32 \rightarrow 8$
2 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.079$
$S = 1.26$
958 reflections
90 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0194P)^2 + 1250.5768P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.97$ e Å^{-3}
$\Delta\rho_{min} = -2.81$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0000133 (11)
Absolute structure: Flack (1983), 2 Friedel pairs
Flack parameter = 0.16 (7)

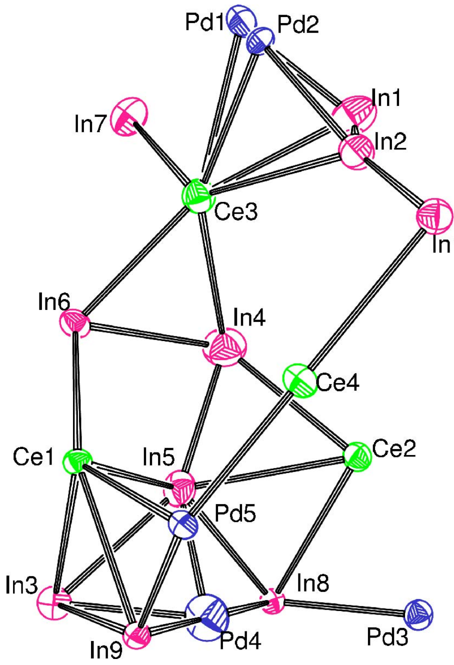

Figure 2
The asymmetric unit of $Ce_{20}Pd_{36}In_{67}$, with displacement ellipsoids drawn at the 90% probability level.

Table 1
Selected bond lengths (Å).

Ce1—Pd1^{i}	3.120 (6)	Pd2—In1	2.157 (14)
Ce1—In6^{ii}	3.296 (3)	Pd2—Pd2^{xiv}	2.542 (9)
Ce1—In9^{iii}	3.3002 (14)	Pd2—In2	2.737 (15)
Ce1—Pd5^{iv}	3.3040 (12)	Pd2—In3^{xxi}	2.833 (5)
Ce1—In3^{v}	3.3228 (9)	Pd2—In4	2.866 (8)
Ce1—In5^{vi}	3.4096 (17)	Pd2—Pd2^{xxiii}	3.202 (14)
Ce1—Pd2^{vii}	3.490 (11)	Pd2—In6	3.298 (11)
Ce2—In3^{viii}	3.3713 (16)	Pd2—In5^{xxii}	3.319 (14)
Ce2—In5^{ix}	3.4171 (9)	Pd3—In8^{xxiv}	2.841 (2)
Ce2—Pd2^{x}	3.429 (4)	Pd3—In5^{xxv}	2.8773 (19)
Ce2—Pd1^{xi}	3.430 (2)	Pd3—In4^{ii}	3.030 (3)
Ce2—In4^{x}	3.437 (2)	Pd4—In5^{xxvi}	2.693 (2)
Ce2—In1^{x}	3.544 (3)	Pd4—In9	2.710 (4)
Ce2—Pd3^{xii}	3.5560 (13)	Pd4—In8	2.831 (4)
Ce2—In8^{xiii}	3.5862 (16)	Pd4—In3^{xxvi}	2.858 (2)
Ce3—Pd2^{xiv}	3.244 (5)	Pd5—In9^{xxvii}	2.765 (2)
Ce3—In6	3.3141 (14)	Pd5—In3^{xvii}	2.7937 (18)
Ce3—In4	3.3812 (19)	In1—In1^{xxviii}	2.654 (6)
Ce3—Pd1^{xv}	3.392 (4)	In1—In2^{vi}	2.756 (5)
Ce3—In7^{vii}	3.442 (2)	In1—In1^{vi}	3.332 (5)
Ce3—In1	3.451 (3)	In2—In2^{xxviii}	2.716 (10)
Ce4—Pd5	3.142 (3)	In2—*In*10	2.760 (6)
Ce4—In2^{xvi}	3.261 (3)	In3—In9^{xxix}	3.186 (2)
Ce4—In3^{xvii}	3.324 (2)	In3—In5^{xxx}	3.2524 (16)
Ce4—In1^{xviii}	3.4519 (18)	In4—In4^{xxii}	2.840 (3)
Ce4—Pd2^{xix}	3.495 (10)	In4—In7^{ii}	2.863 (3)
Ce4—*In*10^{xx}	3.610 (2)	In4—In5^{xxii}	2.9569 (18)
Pd1—In4	2.607 (4)	In4—In6	3.2491 (13)
Pd1—In1	2.690 (9)	In5—In8^{xxix}	3.134 (2)
Pd1—Pd1^{xiv}	2.770 (6)	In6—In7^{vii}	2.9618 (18)
Pd1—In3^{xxi}	2.774 (2)	In7—In7^{vii}	2.845 (5)
Pd1—In5^{xxii}	2.806 (8)	In8—In8^{xxiv}	3.174 (4)
Pd1—In6	2.913 (6)	In9—In9^{xxvii}	3.218 (4)
Pd1—In2	3.305 (10)		

Symmetry codes: (i) $\frac{1}{2}-x, \frac{1}{2}-z, y$; (ii) $\frac{1}{2}-x, \frac{1}{2}-y, z$; (iii) $x, 1-y, 1-z$; (iv) $\frac{3}{2}-x, y-\frac{1}{2}, 1-z$; (v) $\frac{1}{2}+y, 1-z, \frac{1}{2}-x$; (vi) z, y, x; (vii) $\frac{1}{2}-x, y, \frac{1}{2}-z$; (viii) $1-z, -y, x$; (ix) $\frac{1}{2}-y, \frac{1}{2}-z, x$; (x) $z, -y, -x$; (xi) $z, -x, -y$; (xii) $x, \frac{1}{2}-y, \frac{1}{2}-z$; (xiii) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$; (xiv) x, z, y; (xv) y, z, x; (xvi) $1-z, 1-y, 1+x$; (xvii) $z, 1-y, 1-x$; (xviii) $1+x, 1-y, 1-z$; (xix) $1+x, 1-z, 1-y$; (xx) $1+x, 1+y, 1+z$; (xxi) $-x, y, 1-z$; (xxii) $\frac{1}{2}-z, y, \frac{1}{2}-x$; (xxiii) y, x, z; (xxiv) $1-x, y, 1-z$; (xxv) $z, \frac{1}{2}-y, \frac{1}{2}-x$; (xxvi) $z, \frac{1}{2}+y, \frac{1}{2}+x$; (xxvii) $\frac{3}{2}-x, y, \frac{3}{2}-z$; (xxviii) $-x, -y, z$; (xxix) $x-\frac{1}{2}, y-\frac{1}{2}, z$; (xxx) $z-\frac{1}{2}, y, \frac{1}{2}+x$.

The atomic parameters were standardized with the program *STRUCTURE-TIDY* (Gelato & Parthé, 1987). The highest peak and the deepest hole in the final difference map are located 0.66 Å from In6 and 0.28 Å from In7, respectively.

Data collection and cell refinement: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); data reduction: *XCAD4* (Harms & Wocadlo, 1995); structure solution: *SHELXS97* (Sheldrick, 1997); structure refinement: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1998) and *ORTEP-3* (Farrugia, 1997); publication material: *WinGX* publication routines (Farrugia, 1999).

This work was supported by the RFBR project No. 05-03-33045. We are greatful to A. V. Mironov for help with the X-ray experiment and for discussion.

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