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A new ternary indide, $Ce_5Pt_2In_4$, with the $Lu_5Ni_2In_4$ structure type

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The intermetallic title compound, pentacerium diplatinum tetraindide, crystallizes in space group *Pbam* and adopts the $Lu_5Ni_2In_4$ structure type. One Ce atom exhibits site symmetry $2/m$ and all other atoms (two Ce, one Pt and two In) are located on mirror planes.

Comment

Recent single-crystal X-ray investigations on ternary compounds of the Ce–Pt–In system revealed five indides: Ce_2Pt_2In (Galadzhun & Pöttgen, 1999) with the Mo_2FeB_2 structure type, $Ce_{12}Pt_7In$ (Galadzhun *et al.*, 1999) with a superstructure of the Gd_3Ga_2 structure type, $CePt_2In_2$ (Zaremba *et al.*, 2000) with a unique structure type, $CePt_2In_4$ (Nesterenko *et al.*, 2004) with the $NdRh_2Sn_4$ structure type, and $Ce_6Pt_{11}In_{14}$ (Stèpién-Damm *et al.*, 2004) with its own structure type. We present here a new ternary indide, $Ce_5Pt_2In_4$, that adopts the $Lu_5Ni_2In_4$ (Zaremba *et al.*, 1991) structure type.

The structure of $Ce_5Pt_2In_4$ can be considered as being built up of two layers. The first layer is composed of Ce atoms at z =
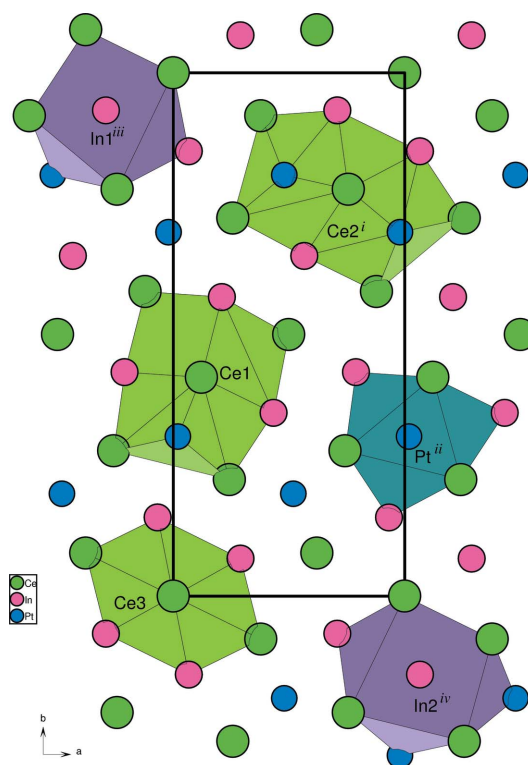

Figure 1
$Ce_5Pt_2In_4$ viewed along the *c* axis. Part of the structure is shown in a polyhedral representation. [Symmetry codes: (i) $1 - x, 1 - y, z$; (ii) $1 + x, y, z$; (iii) $-x, 1 - y, z$; (iv) $\frac{3}{2} - x, \frac{1}{2} + y, 1 - z$.]

0, and the second layer is composed of Pt and In atoms at $z = 0.5$. A projection of the stucture is presented in Fig. 1. Coordination numbers (CN) of the three crystallographically independent Ce atoms amount to 14, 16, and 12. Atom Ce1 is coordinated by two Pt and six In atoms, forming a distorted cube [2.9606 (7)–3.5131 (10) Å]. Six additional Ce atoms cap all faces of the cube [3.4609 (8)–4.0597 (11) Å]. Four Pt and six In atoms form a distorted pentagonal prism around atom Ce2 [3.0130 (8)–3.4521 (10) Å]. The next nearest neighbours, six Ce atoms, cap all but one rectangular face of the prism [3.7623 (12)–4.0597 (11) Å]. The fifth rectangular face is capped by atom Ce3 with a Ce2···Ce3 separation of 4.5892 (11) Å. The coordination environment of Ce3 does not include Pt atoms. The first coordination sphere around Ce3 consists of eight In atoms [3.3315 (8)–3.4233 (9) Å], the second one is made up of four Ce atoms [3.4609 (8)–3.8188 (8) Å]. Together, In and Ce atoms form a distorted cuboctahedron around Ce3. A trigonal–prismatic coordination is an appropriate description for the atom of the smallest radius, *viz.* Pt. The trigonal prism around Pt is formed by six Ce atoms, and three remote In atoms cap the faces of the prism [2.9599 (11)–3.4952 (12) Å]. Coordination polyhedra around In1 [CN = 10; 2.9703 (10)–3.5131 (10) Å] and In2 [CN = 11; 2.9599 (11)–3.4952 (12) Å] can be considered as distorted tetragonal prisms with, respectively, two and three additional atoms capping the lateral faces. This type of coordination is typical for middle-sized atoms in many ternary intermetallic compounds.

Fig. 2 shows the asymmetric unit of the title compound.

Experimental

An ingot of nominal composition $Ce_{45}Pt_{15}In_{40}$ (at. %) was prepared by arc melting under argon from Ce (99.85 wt% pure), Pt and In (99.9 wt% pure). The sample was annealed at 1220 K in a silica tube under Ar for 3 h. A lath-like single crystal was obtained from the crushed ingot. From EMPA analyses (Jeol JSM 6400 scanning electron microscope with an Si/Li energy-dispersive analyser), the composition of the phase was estimated to be $Ce_{46.2}Pt_{16.8}In_{37.0}$ with an uncertainty of about 1% for each element.

Crystal data

$Ce_5Pt_2In_4$	Mo $K\alpha$ radiation
$M_r = 1550.06$	Cell parameters from 25
Orthorhombic, $Pbam$	reflections
$a = 8.2088 (14)$ Å	$\theta = 18.2–23.1°$
$b = 18.579 (4)$ Å	$\mu = 50.69$ mm^{-1}
$c = 3.8188 (8)$ Å	$T = 291 (2)$ K
$V = 582.4 (2)$ Å^3	Lath, metallic light-grey
$Z = 2$	$0.07 \times 0.04 \times 0.01$ mm
$D_x = 8.839$ Mg m^{-3}	

Data collection

Enraf–Nonius CAD-4	1149 reflections with $I > 2\sigma(I)$
diffractometer	$\theta_{max} = 35.0°$
ω scans	$h = -13 \rightarrow 0$
Absorption correction: ψ scan	$k = 0 \rightarrow 29$
(North *et al.*, 1968)	$l = 0 \rightarrow 6$
$T_{min} = 0.090$, $T_{max} = 0.602$	1 standard reflections
1430 measured reflections	frequency: 120 min
1430 independent reflections	intensity decay: none

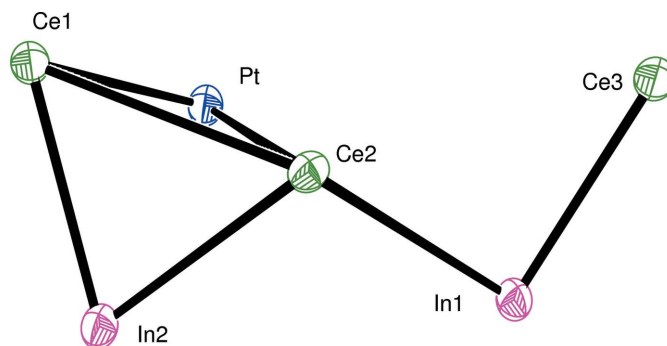**Figure 2**
The asymmetric unit of $Ce_5Pt_2In_4$, with displacement ellipsoids drawn at the 90% probability level.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.115$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.82$	$\Delta\rho_{max} = 2.46$ e Å^{-3}
1430 reflections	$\Delta\rho_{min} = -4.63$ e Å^{-3}
36 parameters	Extinction correction: *SHELXL97*
	Extinction coefficient: 0.0017 (3)

Table 1
Selected bond lengths (Å).

Ce1—Pt[i]	2.9606 (7)	Ce2—In1[i]	3.4132 (11)
Ce1—In1[ii]	3.3288 (10)	Ce2—In2[ii]	3.4521 (10)
Ce1—In2	3.4313 (10)	Ce2—Ce2[vi]	3.8188 (8)
Ce1—Ce3[iii]	3.4609 (8)	Ce3—In1[viii]	3.3315 (8)
Ce1—In1[iv]	3.5131 (10)	Ce3—In2[ix]	3.4233 (9)
Ce1—Ce1[v]	3.6474 (14)	Ce3—Ce3[vi]	3.8188 (8)
Ce1—Ce2	3.7623 (12)	Pt—In2[ix]	2.9599 (11)
Ce1—Ce1[vi]	3.8188 (8)	Pt—In1[ix]	2.9703 (10)
Ce1—Ce2[ii]	4.0597 (11)	Pt—In2	3.4952 (12)
Ce2—Pt[vii]	3.0130 (8)	In1—In2[ix]	3.2734 (13)
Ce2—Pt[i]	3.0530 (7)		

Symmetry codes: (i) $x, y, z - 1$; (ii) $x - \frac{1}{2}, -y + \frac{1}{2}, -z$; (iii) $x + \frac{1}{2}, -y + \frac{1}{2}, -z$; (iv) $-x + \frac{1}{2}, y + \frac{1}{2}, z$; (v) $-x, -y + 1, -z$; (vi) $x, y, z + 1$; (vii) $x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (viii) $-x, -y, -z$; (ix) $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$.

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 0.26 Å from In1 and 1.49 Å from Pt, respectively.

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

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