A new ternary aluminide, CePt$_3$Al$_5$

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The intermetallic title compound, cerium triplatinum penta-aluminium, crystallizes in a site-exchange variant of the YNi$_5$Si$_3$-type structure.

Comment

To date, the crystal structures of three ternary intermetallics from the Ce–Pt–Al system have been determined, namely CePtAl (Xue & Schwer, 1994), Ce$_{0.67}$Pt$_2$Al$_5$ and Ce$_{1.33}$Pt$_3$Al$_8$ (Murashova *et al.*, 2005). Here, we present the structure of the new title compound with a high aluminium content, CePt$_3$Al$_5$, exhibiting a site-exchange variant of the YNi$_5$Si$_3$ structure type (Aksel'rud *et al.*, 1976).

A view of the structure is presented in Fig. 1. All atoms have significantly distorted coordination polyhedra. The Ce atom is surrounded by 12 Al atoms [distance range 3.218 (4)–3.857 (4) Å] and six Pt atoms [distance range 3.2393 (7)–3.2670 (8) Å], which form a hexagonal prism with six addi-
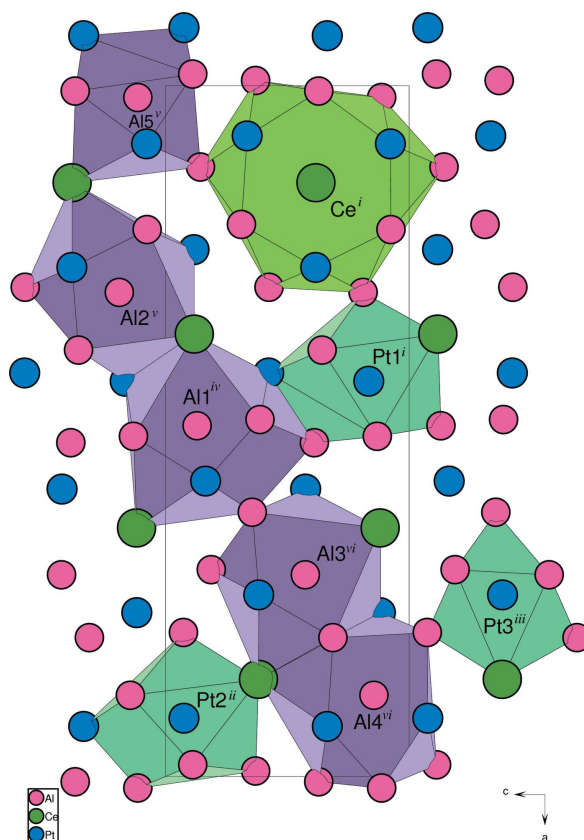

Figure 1
A view, along the *b* axis, of the CePt$_3$Al$_5$ structure. Part of the structure is shown in the polyhedral representation. [Symmetry codes: (i) $\frac{1}{2} - x, 1 - y, -\frac{1}{2} + z$; (ii) $1 - x, \frac{1}{2} + y, 1 - z$; (iii) $1 - x, \frac{1}{2} + y, -z$; (iv) $\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} + z$; (v) $\frac{1}{2} - x, 1 - y, \frac{1}{2} + z$; (vi) $\frac{1}{2} + x, \frac{3}{2} - y, \frac{1}{2} - z$.]
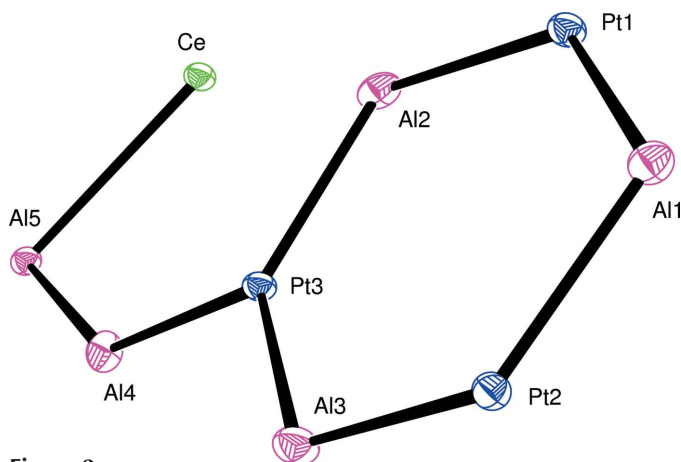
Figure 2
The asymmetric unit of CePt$_3$Al$_5$, with displacement ellipsoids drawn at the 90% probability level.

tional atoms capping the square faces. The prism is completed by two Ce atoms capping the hexagonal faces of the prism, the Ce···Ce distance being 4.1381 (8) Å. The coordination polyhedra of the Pt atoms can be regarded as trigonal prisms with four (Pt1 and Pt2) and three (Pt3) additional atoms. For the Al atoms, three types of coordination polyhedra are observed. Atoms Al1, Al2 and Al3 are at the centres of cuboctahedra. The pentagonal prism around atom Al4 is capped on four tetragonal faces. The coordination polyhedron of atom Al5 is a tetragonal prism with two additional atoms capping two lateral faces of the prism.

The interatomic distances in the structure of CePt$_3$Al$_5$ are in the typical range for intermetallic compounds (Table 1).

Experimental

A single crystal was taken from the surface of an ingot of nominal composition 10% Ce, 30% Pt and 60% Al prepared by arc melting under an argon atmosphere. High-purity elements were used as starting materials: Ce 99.85%, Pt 99.9% and Al 99.999%. Homogenization annealing was performed at 770 K for 720 h.

Crystal data

CePt$_3$Al$_5$	Mo $K\alpha$ radiation
$M_r = 860.29$	Cell parameters from 25
Orthorhombic, $Pnma$	reflections
$a = 20.651$ (4) Å	$\theta = 15.5–20.6°$
$b = 4.1381$ (8) Å	$\mu = 74.96$ mm^{-1}
$c = 7.2842$ (15) Å	$T = 291$ (2) K
$V = 622.5$ (2) Å^3	Prism, metallic light grey
$Z = 4$	$0.04 \times 0.04 \times 0.04$ mm
$D_x = 9.180$ Mg m^{-3}	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.058$
ω scans	$\theta_{max} = 32.5°$
Absorption correction: ψ scan	$h = 0 \rightarrow 31$
(North *et al.*, 1968)	$k = -6 \rightarrow 4$
$T_{min} = 0.065$, $T_{max} = 0.073$	$l = 0 \rightarrow 11$
2062 measured reflections	1 standard reflection
1259 independent reflections	frequency: 120 min
1041 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	$(\Delta/\sigma)_{max} < 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.034$	$\Delta\rho_{max} = 3.95$ e Å^{-3}
$wR(F^2) = 0.084$	$\Delta\rho_{min} = -5.87$ e Å^{-3}
$S = 0.99$	Extinction correction: *SHELXL97*
1259 reflections	(Sheldrick, 1997)
56 parameters	Extinction coefficient: 0.00169 (14)
$w = 1/[\sigma^2(F_o^2) + (0.0516P)^2$	
$+ 2.6515P]$	
where $P = (F_o^2 + 2F_c^2)/3$	

Table 1
Selected interatomic distances (Å).

Ce—Al5	3.218 (4)	Pt2—Al5^{viii}	2.500 (4)
Ce—Pt1^i	3.2393 (7)	Pt2—Al5^{ix}	2.506 (2)
Ce—Pt2^{ii}	3.2529 (8)	Pt2—Al3	2.566 (4)
Ce—Pt3^{ii}	3.2670 (8)	Pt2—Al1	2.655 (4)
Ce—Al2^i	3.290 (3)	Pt2—Al4^{ix}	2.707 (3)
Ce—Al3^{ii}	3.356 (3)	Pt3—Al4	2.478 (4)
Ce—Al3^{iii}	3.424 (4)	Pt3—Al3	2.512 (4)
Ce—Al1^i	3.435 (3)	Pt3—Al3^i	2.566 (2)
Ce—Al1^{iv}	3.553 (4)	Pt3—Al2	2.567 (4)
Ce—Al4^{iii}	3.488 (4)	Pt3—Al2^{ix}	2.617 (3)
Ce—Al2	3.568 (4)	Al1—Al5^{ix}	2.797 (4)
Ce—Ce^v	4.1381 (8)	Al1—Al1^x	2.827 (6)
Pt1—Al5^{vi}	2.457 (4)	Al2—Al3^{iii}	2.816 (6)
Pt1—Al1	2.532 (4)	Al2—Al3^i	2.912 (4)
Pt1—Al2	2.658 (4)	Al2—Al4^{ii}	2.956 (4)
Pt1—Al1^{vii}	2.661 (4)	Al4—Al5	2.793 (6)
Pt1—Al4^i	2.664 (3)	Al5—Al5^{xi}	2.730 (5)
Pt1—Pt2^{iii}	3.0092 (9)		

Symmetry codes: (i) $-x+\frac{1}{2}, -y+1, z+\frac{1}{2}$; (ii) $-x+\frac{1}{2}, -y, z+\frac{1}{2}$; (iii) $x, y, z+1$; (iv) $x+\frac{1}{2}, y, -z+\frac{3}{2}$; (v) $x, y-1, z$; (vi) $x-\frac{1}{2}, y, -z+\frac{3}{2}$; (vii) $-x, -y, -z+1$; (viii) $x-\frac{1}{2}, y, -z+\frac{3}{2}$; (ix) $-x+\frac{1}{2}, -y, z-\frac{1}{2}$; (x) $-x, -y+1, -z+1$; (xi) $-x+1, -y, -z+1$.

The atomic parameters were standardized with the program *STRUCTURE TIDY* (Gelato & Parthé, 1987). The highest peak and deepest hole in the final difference map are located 1.54 Å from Al3 and 0.97 Å from Al4, 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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