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$Er_{36}Pt_{102-x}Si_{32}$ (x = 2.6), a new structure type of a ternary intermetallic silicide

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The title erbium platinum silicide compound represents a new structure type of intermetallic silicide with platinum and a heavy rare earth element (Tb–Tm). Four atoms exhibit disorder. Coordination polyhedra of most of the Pt atoms are distorted cuboctahedra; coordination polyhedra of the silicon atoms are distorted trigonal prisms with three additional atoms capping the square faces.

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Er–Si) = 0.004 Å
Disorder in main residue
R factor = 0.049
wR factor = 0.135
Data-to-parameter ratio = 27.5

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

Comment

We have shown that intermetallic compounds RPt_3Si of the light rare earths (R = La, Ce, Nd, Sm) crystallize with the $CePt_3B$ structure type (Sologub *et al.*, 2002) (space group $P4mm$, tP5) (Tursina *et al.*, 2003). The compounds with approximate composition RPt_3Si, where R is a heavy rare earth element (R = Tb–Tm), are found to belong to a new structure type. The present work reports the results of a crystal structure investigation of the first member of this new structural family of ternary intermetallic silicides. A view of the structure is shown in Fig. 1. In the structure of the title compound, atoms Si1, Pt4 and Pt10 deviate from the ideal positions on the symmetry elements. To account for the

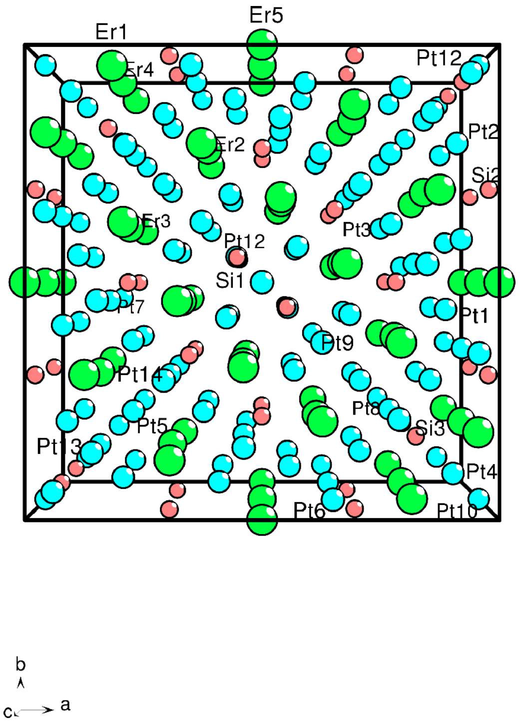

Figure 1
Perspective view of the unit-cell contents, with Er atoms shown as large green circles, Pt atoms as medium blue circles, and Si atoms as small purple circles. Atoms Si1, Pt4, and Pt10 are shown at the ideal positions on the symmetry elements. Atom Pt11 has been omitted.

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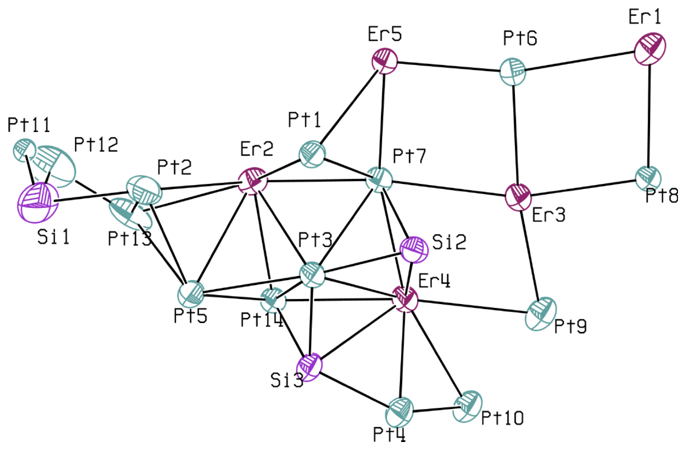

Figure 2
The asymmetric unit of the title compound, with atom labelling and displacement ellipsoids drawn at the 90% probability level.

corresponding very large atomic delocalization, these atoms have been refined with an occupancy of 50% in the positions 16*k* instead of 8*j* (for Si1 and Pt4) and in the position 4*g* instead of 2*b* (for Pt10). The Pt11 and Pt12 sites, with occupancies of 19.1 (7) and 80.9 (7)%, respectively, represent the unique atomic 4*f* position split into two 4*f* positions, the Pt11—Pt12 distance being equal to 0.733 Å. Owing to the existence of vacancies in the 4*f* position occupied by the Pt13 atoms, the formula of the compound is $Er_{36}Pt_{99.4}Si_{32}$, or $Er_{36}Pt_{102-x}Si_{32}$ (x = 2.6). Five crystallographically different Er atoms (Er1, Er2, Er3, Er4 and Er5) have high coordination numbers 13, 14, 14, 16 and 12, respectively, and rather distorted coordination polyhedra. The coordination polyhedra of most of the platinum atoms (excluding Pt4, Pt10, Pt11 and Pt12) are distorted cuboctahedra. Atoms Si1, Si2, and Si3 are surrounded in the first coordination sphere by tetragonal pyramids of five Pt atoms, located at the relatively short distances of 2.32–2.58 Å. Together with the four next-nearest neighbours, Er atoms lying at distances >3.0 Å, Pt atoms form distorted trigonal prisms with three additional atoms capping the square faces, coordination polyhedra typical for the group IV elements.

Experimental

The title compound was prepared by arc melting of the constituent elements (Er 98.0, Pt 99.9, Si 99.999 wt.% pure) under a high purity argon atmosphere on a water-cooled hearth. The arc-melted button with nominal composition $ErPt_3Si$ was turned over and remelted to ensure its homogeneity. The weight loss was less than 1%. The sample was annealed in an evacuated double quartz ampoule at 870 K over a period of 600 h and quenched in cold water. A single crystal was selected from the surface of the resulting alloy.

Crystal data

$Er_{36}Pt_{99.39}Si_{32}$
M_r = 26308.84
Tetragonal, $P4_2/mnm$
a = 18.6723 (1) Å
c = 8.1734 (1) Å
V = 2849.70 (4) Å^3
Z = 1
D_x = 15.330 Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 10500 reflections
θ = 2.4–42.1°
μ = 147.87 mm^{-1}
T = 293 (2) K
Prism, metallic dark grey
0.06 × 0.06 × 0.06 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: sphere (*WinGX*; Farrugia, 1998)
$T_{\min}$ = 0.009, $T_{\max}$ = 0.040
12 063 measured reflections
3795 independent reflections

3190 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.063
$\theta_{\max}$ = 36.5°
$h = -31 \rightarrow 31$
$k = -31 \rightarrow 31$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.135
S = 1.14
3795 reflections
138 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0717P)^2 + 50.7015P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 5.78 e Å^{-3}
$\Delta\rho_{\min}$ = −5.13 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.000061 (10)

The highest peak and deepest hole in the difference map are located 0.67 Å from Pt1 and 2.04 Å from Er5, respectively.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1998); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL*97 and STIDY (Parthé *et al.*, 1993).

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