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The new ternary compound $Ce_2Rh_{15}Si_7$

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The title compound, dicerium pentadecarhodium heptasilicon, includes two crystallographically independent Ce atoms, Ce1 having an ideal cubooctahedron polyhedron and Ce2 having a distorted polyhedron with 14 apices and an anomalously short Ce—Rh distance of 2.432 (3) Å.

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Si–Si) = 0.014 Å
R factor = 0.047
wR factor = 0.148
Data-to-parameter ratio = 16.3

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

Comment

Intermetallic compounds consisting of Ce, Rh(Pd) and Si exhibit many interesting physical properties, for example, magnetism, superconductivity, heavy-electron behavior and valence fluctuations (Buschow, 1993; Trovarelli *et al.*, 1998; Gomez-Berisso *et al.*, 1999). For this reason, we have been investigating ternary Ce–Rh–Si systems looking for new intermetallic compounds (Gribanov, Yatsenko, Seropegin, Kurenbaeva, Glazkova & Bodak, 2000; Gribanov, Yatsenko, Seropegin, Kurenbaeva, Kocherov & Bodak, 2000; Tursina *et al.*, 2001). Herein, we report the crystal structure of the new ternary compound, $Ce_2Rh_{15}Si_7$, (I).

The coordination polyhedra of the Ce atoms are cubooctahedron [Rh_{12}] for Ce1 and a distorted polyhedron with 14 apices [Rh_{14}] for Ce2. Coordination polyhedra of the Rh atoms are rather irregular, with 9 and 10 apices: Rh3 [$Ce_1Rh_4Si_4$], Rh4 [$Ce_2Rh_4Si_4$] and Rh5 [Rh_6Si_4]. The Si atoms have slightly distorted polyhedra with 10 and 9 apices: double-capped square antiprisms [$Ce_1Rh_8Si_1$] for Si6 and trigonal prisms with three additional atoms [Rh_9] for Si7. All interatomic distances in (I) are typical for such compounds except two Ce2—Rh3 distances [2.432 (3) Å] which are significantly shorter than the sum of the metallic radii *d*(Ce—Rh) = 3.18 Å. This peculiarity of (I) makes the probability of the existence of isostructural compounds very low, as any change in the composition must cause the changes in crystal structure providing more appropriate Ce—Rh interatomic distances. This can be demonstrated through the comparison of the two crystal structures, (I) and $Ce_4Pd_{29}Si_{14}$, (II) (Tursina *et al.*, 2001), which may be considered as a derivative of the crystal structure of (I) (Fig. 2).

The Pd substitution for Rh causes negligible changes in the mutual positions of all atoms in the structure of (II) except two Pd atoms (Pd4 and Pd5), corresponding to the Rh3 atoms in structure (I). They change their positions considerably. However, the Pd4 atoms simply moves out of the way of the Ce2 atoms, *d*(Ce2—Pd4) = 2.903 (4) Å, while the Pd5 atoms pass into a new crystallographic position, *d*(Ce2—Pd5) = 3.339 (2) Å. These atom shifts in structure (II) cause, firstly, the change of crystal structure [space group *Fm*3*m*, *a* = 18.010 (2) Å], secondly, the decrease in Pd percentage and in

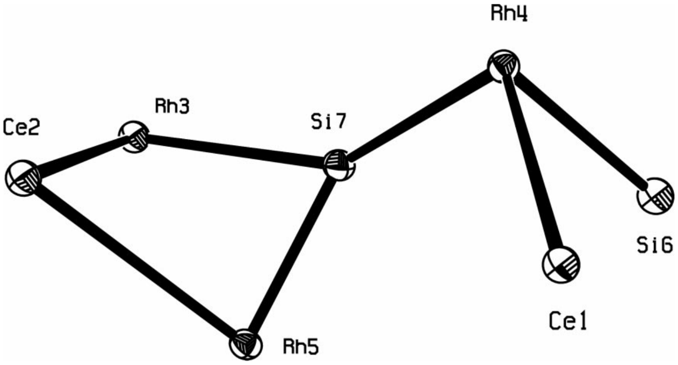

Figure 1
The asymmetric unit of the title compound with the atom numbering.

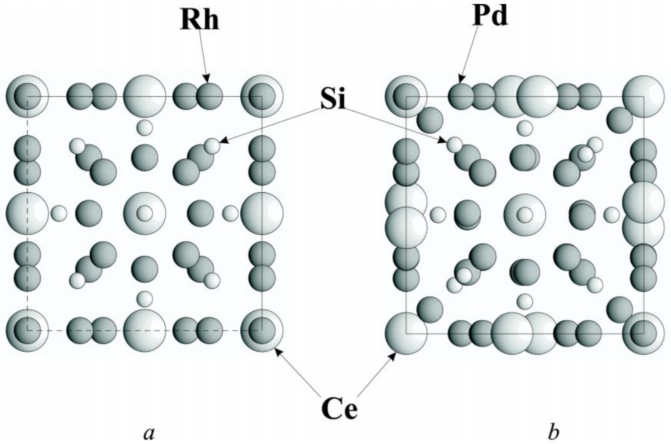

Figure 2
Projection onto the *xy* plane (*a*) of $Ce_2Rh_{15}Si_7$ unit cell and (*b*) of $Ce_4Pd_{29}Si_{14}$ 1/8 unit cell (x,y,z from 0 to $\frac{1}{2}$).

the number of atoms per unit cell. That is, D_x falls from 9.787 Mg m^{-3} in (I) to 9.186 Mg m^{-3} in (II).

Experimental

The title compound was prepared from pure elements (Ce 0.98, Rh 0.999, Si 0.99999) by arc-melting under an argon atmosphere. The sample was annealed in double quartz ampoules at 973 K for 600 h and quenched in cool water. The single crystal used for analysis was selected from the resultant alloy.

Crystal data

$Ce_2Rh_{15}Si_7$
$M_r = 2020.52$
Cubic, $Pm\bar{3}m$
$a = 8.818$ (1) Å
$V = 685.66$ (13) Å^3
$Z = 2$
$D_x = 9.787$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 13.1–17.7°$
$\mu = 24.57$ mm^{-1}
$T = 293$ (2) K
Prism, dark red
0.17 × 0.15 × 0.13 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{\rm min} = 0.034$, $T_{\rm max} = 0.098$
1756 measured reflections
358 independent reflections
251 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.131$
$\theta_{\rm max} = 34.9°$
$h = 0 \rightarrow 14$
$k = 0 \rightarrow 14$
$l = 0 \rightarrow 14$
3 standard reflections
frequency: 120 min
intensity decay: 2.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.148$
$S = 0.86$
358 reflections
22 parameters
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 4.22$ e Å^{-3}
$\Delta\rho_{\rm min} = -4.12$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0003 (2)

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *CAD*-4 *Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997).

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