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$CeRu_2Al_{10}$ with the $YbFe_2Al_{10}$ structure type

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(l–Al) = 0.003 Å
R factor = 0.043
wR factor = 0.123
Data-to-parameter ratio = 17.1

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

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The structure of cerium diruthenium decaaluminium, $CeRu_2Al_{10}$, is characterized by seven crystallographic sites in space group *Cmcm*, *viz.* Ce in 4*c*, Ru in 8*a*, two Al atoms in 8*g*, two Al atoms in 8*f* and one Al atom in 8*e*. The structure can be interpreted as a stacking of alternating columns running along [001], each formed by only one type of Ru cuboid with composition $RuAl_6$ or $CeRuAl_4$.

Comment

There are only limited data available on the formation of ternary cerium ruthenium aluminides and their crystal structures. In recent studies, the structures of two compounds were determined from single-crystal X-ray diffraction, namely $Ce_3Ru_4Al_{12}$ (Bukhan'ko *et al.*, 2004) with the $Nd_3Ru_4Al_{12}$ structure type (Gladyshevskii *et al.*, 1993) and $Ce_2Ru_3Al_{15}$ with a new structure type (Tursina *et al.*, 2004). $CeRu_2Al_{10}$ was first synthesized by Thiede *et al.* (1998) and, on the basis of the analysis of X-ray powder diffraction data, was assumed to be isotypic to the $YbFe_2Al_{10}$ structure (Niemann & Jeitschko, 1995).

In the title compound, the three-dimensional network of Ru atoms hypothetically divides the structure into equal cuboids of dimension $a/2 \times b/2 \times c/2$, with Ru atoms in the vertices of the cuboids. Ce and Al atoms occupy these cuboids in two ways, giving the composition $RuAl_6$ for the first type of cuboid (Fig. 1*a*) and $CeRuAl_4$ for the second type of cuboid (Fig. 1*b*). The structure can be described as the stacking of alternating columns running along [001], each formed by only one type of cuboid (Fig. 2).

The Ce atom is surrounded by four Ru and 16 Al atoms at distances of 3.188 (3)–3.6660 (13) Å, which results in a distorted hexagonal prism with eight additional atoms capping

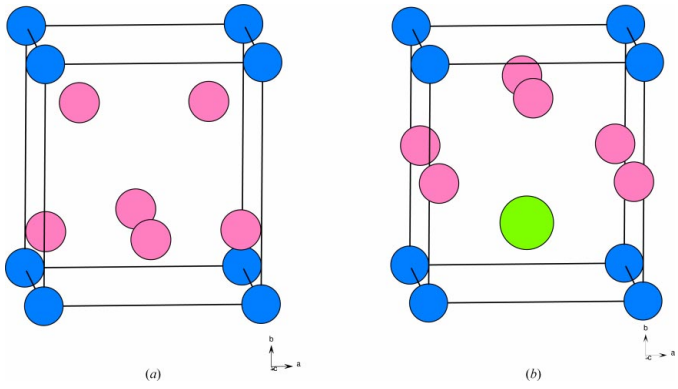

Figure 1
Views of (*a*) an $RuAl_6$ cuboid and (*b*) a $CeRuAl_4$ cuboid, with Ce atoms shown as green circles, Ru atoms as blue circles and Al atoms as pink circles.

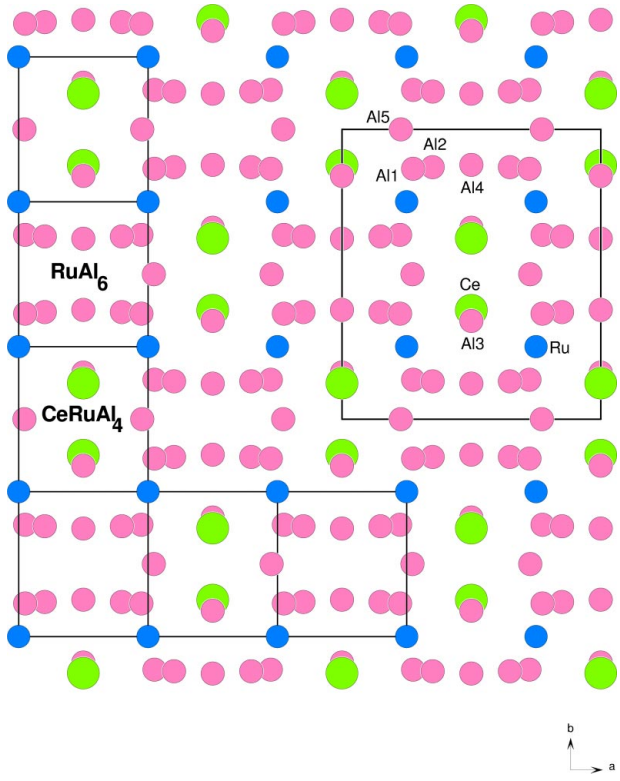

Figure 2
Projection of the structure along the *c* axis. Ru cuboids $RuAl_6$ and $CeRuAl_4$, as well as the unit cell, are outlined.

all faces of the prism $Ce[Ru_4Al_{16}]$. The Ru atom in $CeRu_2Al_{10}$, as well as in $Ce_2Ru_3Al_{15}$, has a distorted icosahedral coordination, $Ru[Ce_2Al_{10}]$, with Ru—Al interatomic distances ranging from 2.5786 (6) to 2.7640 (14) Å. The Ce—Ru distances are 3.4884 (4) Å. Whereas the coordination polyhedra of the Al atoms in $Ce_2Ru_3Al_{15}$ could be also regarded as distorted icosahedra, in $CeRu_2Al_{10}$ the polyhedra around the Al atoms are irregular. Distorted pentagonal antiprisms around atoms Al1 ($Al[CeRu_2Al_8]$) and Al4 ($Al[CeRu_2Al_8]$) are capped on one basal face, while antiprisms around atoms Al2 ($Al[CeRu_2Al_9]$), Al3 ($Al[Ce_2Ru_2Al_8]$) and Al5 ($Al[Ce_2Ru_2Al_8]$) are capped on both basal faces. The analysis of the interatomic distances in the isotypic compound UFe_2Al_{10} (Noël *et al.*, 2004) leads to the same coordination numbers for the Al atoms. However, for the prototype compound $YbFe_2Al_{10}$, greater coordination numbers of the Al atoms were reported. Here it was considered that the interatomic contacts significantly exceed the sum of the metallic radii.

Fig. 3 shows the asymmetric unit of the title compound.

Experimental

The title compound was prepared by arc-melting of the constituent elements (all with nominal purities equal to or greater than 99.8%) with the composition $Ce_{8.9}Ru_{13.3}Al_{77.8}$. The weight loss was less than 1%. The melted button was subsequently sealed in an evacuated silica tube and annealed at 1170 K for one week. A single crystal was isolated from the annealed sample by mechanical fragmentation.

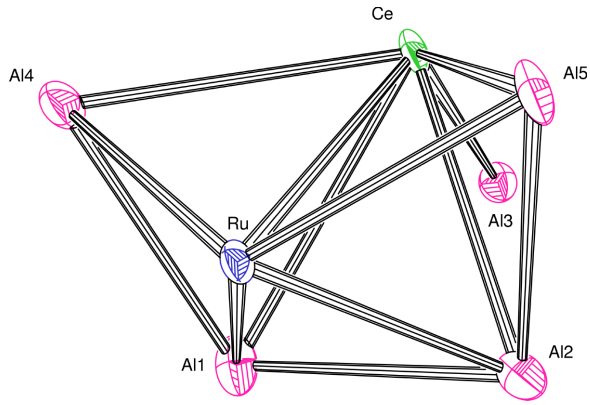

Figure 3
The asymmetric unit of the title compound, with the atomic labelling scheme and with displacement ellipsoids drawn at the 90% probability level.

Crystal data

$CeRu_2Al_{10}$
M_r = 612.06
Orthorhombic, *Cmcm*
a = 9.1272 (16) Å
b = 10.282 (2) Å
c = 9.1902 (14) Å
V = 862.5 (3) Å^3
Z = 4
D_x = 4.714 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 18.1–27.8°
μ = 9.59 mm^{-1}
T = 293 (2) K
Prism, metallic light grey
0.15 × 0.10 × 0.03 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.321, T_{max} = 0.746
769 measured reflections
703 independent reflections
661 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 29.9°
$h = -12 \rightarrow 0$
$k = -14 \rightarrow 1$
$l = 0 \rightarrow 12$
1 standard reflection
frequency: 120 min
intensity decay: 0.6%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.123
S = 1.10
703 reflections
41 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0963P)^2 + 3.3337P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.0001$
$\Delta\rho_{max}$ = 3.91 e Å^{-3}
$\Delta\rho_{min}$ = −4.50 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0127 (10)

Table 1
Selected geometric parameters (Å).

Al1—Ru	2.5902 (12)	Al3—Ru^{iv}	2.6290 (13)
Al1—Al2	2.665 (4)	Al3—Al3	2.737 (5)
Al1—Al5^{i}	2.7237 (15)	Al3—Al5^{v}	2.812 (3)
Al1—Al4	2.755 (3)	Al3—Ce^{vi}	3.230 (2)
Al1—Al2	2.823 (3)	Al3—Ce	3.249 (3)
Al1—Al3^{ii}	2.872 (3)	Al4—Ru^{vii}	2.6715 (12)
Al1—Ce	3.212 (3)	Al4—Al4^{viii}	2.686 (5)
Al2—Al2^{iii}	2.722 (5)	Al4—Al5	2.826 (3)
Al2—Ru^{i}	2.7640 (14)	Al4—Ce	3.188 (3)
Al2—Al3^{ii}	2.888 (3)	Al5—Ru	2.5786 (6)
Al2—Al5	2.888 (2)	Al5—Ce^{ix}	3.349 (2)
Al2—Ce	3.203 (3)	Ru—Ce	3.4884 (4)
Al3—Al4	2.627 (3)		

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

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 0.90 and 0.81 Å, respectively, from the Ce atom.

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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References

Brandenburg, K. (1998). *DIAMOND*. Version 2.1b. Crystal Impact GbR, Bonn, Germany.
Bukhan'ko, N. G., Tursina, A. I., Malyshev, S. V., Gribanov, A. V., Seropegin, Yu. D. & Bodak, O. I. (2004). *J. Alloys Compd.* **367**, 149–151.
Enraf–Nonius (1994). *CAD-4 EXPRESS*. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Gelato, L. M. & Parthé, E. (1987). *J. Appl. Cryst.* **20**, 139–143.
Gladyshevskii, R. E., Strusievicz, O. R., Cenzual, K. & Parthé, E. (1993). *Acta Cryst.* B**49**, 474–478.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Niemann, S. & Jeitschko, W. (1995). *Z. Kristallogr.* **210**, 338–341.
Noël, H., Gonçalves, A. P. & Waerenborgh, J. C. (2004). *Intermetallics*, **12**, 189–194.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta. Cryst.* A**24**, 351.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Thiede, V. M. T., Ebel, T. & Jeitschko, W. (1998). *J. Mater. Chem.* **8**, 125–130.
Tursina, A. I., Nesterenko, S. N., Murashova, E. V., Chernyshev, I. V., Noël, H. & Seropegin, Y. D. (2004). *Acta Cryst.* E**60**, i145–i146.