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# $Ce_2Ru_3Al_{15}$, an intermetallic compound of a new structure type

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**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(Al–Al) = 0.007 Å
$R$ factor = 0.029
$wR$ factor = 0.127
Data-to-parameter ratio = 15.2

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



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The title compound, dicerium triruthenium pentadecaaluminium, is a new intermetallic compound from the Al-rich region of the Ce–Ru–Al phase diagram. Two Ce atoms (6*g* and 2*a* sites of space group $P6_3/mcm$) are coordinated by 18 atoms, one Ru atom (12*i* site) and five Al atoms (12*k*, 12*i*, 12*j*, 12*j* and 12*k* sites) have 12 nearest neighbours each.

## Comment

During the systematic study of the ternary Ce–Ru–Al system, the existence of a new intermetallic compound $Ce_2Ru_3Al_{15}$ was established. Previously, the structure of only one ternary compound from this system has been determined, *viz*. $Ce_3Ru_4Al_{12}$ (Bukhan'ko *et al.*, 2004).

In the $Ce_2Ru_3Al_{15}$ structure, both crystallographically different Ce atoms are located in significantly distorted polyhedra formed by 18 atoms: Ce1[$Ru_4Al_{14}$] and Ce2[$Al_{18}$]. Around atom Ru3, ten Al atoms form a pentagonal antiprism

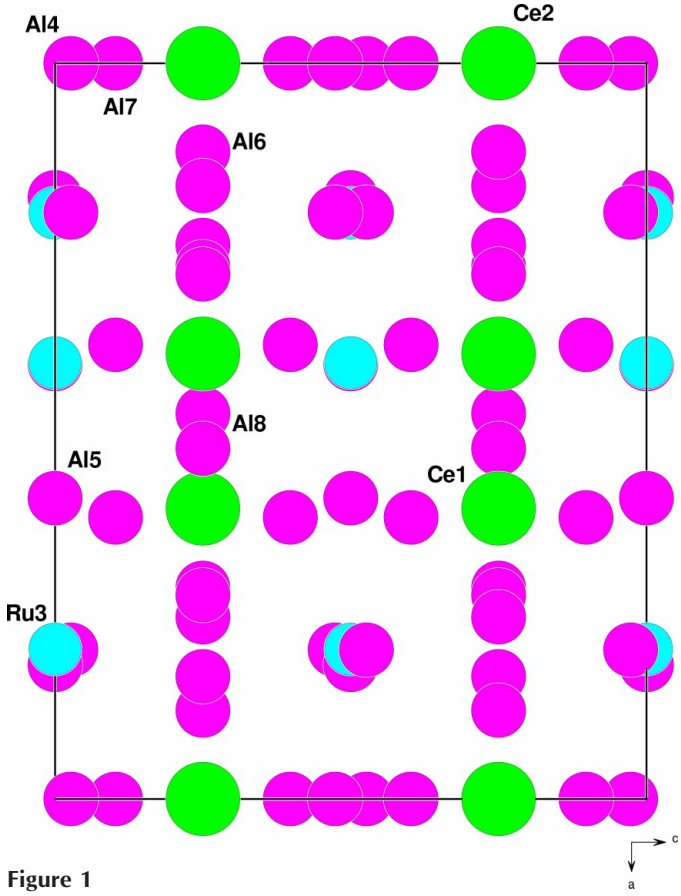


**Figure 1**
Projection of the unit-cell contents on to the $x0z$ plane, with Ce atoms shown as green circles, Ru atoms as blue circles and Si atoms as purple circles.

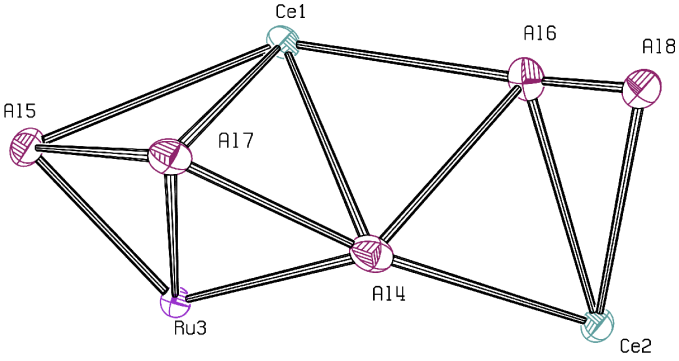


**Figure 2**
The asymmetric unit of the title compound, with atom labelling and displacement ellipsoids drawn at the 90% probability level.

capped by two Ce atoms on both basal faces. Five crystallographically independent Al atoms are surrounded by distorted pentagonal antiprisms with two additional atoms: Al4[$Ce_3Ru_2Al_7$], Al5[$Ce_2Ru_2Al_8$], Al6[$Ce_2Ru_2Al_8$], Al7[$Ce_1Ru_2Al_9$] and Al8[$Ce_2Ru_2Al_8$]. The Ru and Al atoms form a complex three-dimensional [$Ru_3Al_{15}$] network in which the Ce atoms are located (Fig. 1). Fig. 2 shows the asymmetric unit of the title compound.

## Experimental

$Ce_2Ru_3Al_{15}$ was prepared by arc melting of the elements (Ce 99.8, Ru 99.9, Al 99.99 wt% pure) under a high purity argon atmosphere on a water-cooled hearth. The arc-melted button with $Ce_{12}Ru_8Al_{80}$ composition was turned over and remelted to ensure its homogeneity. The weight loss was less than 1%. A single crystal was selected from the surface of the alloy obtained.

*Crystal data*

$Ce_2Ru_3Al_{15}$
$M_r$ = 988.15
Hexagonal, $P6_3/mcm$
$a$ = 13.122 (3) Å
$c$ = 9.0964 (18) Å
$V$ = 1356.4 (5) Å$^3$
$Z$ = 4
$D_x$ = 4.839 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 24 reflections
$\theta$ = 15.2–15.7°
$\mu$ = 10.78 mm$^{-1}$
$T$ = 293 (2) K
Prism, metallic light grey
0.12 × 0.03 × 0.02 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{min}$ = 0.750, $T_{max}$ = 0.806
2233 measured reflections
624 independent reflections
340 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.098
$\theta_{max}$ = 28.0°
$h = 0 \rightarrow 17$
$k = -17 \rightarrow 0$
$l = 0 \rightarrow 12$
1 standard reflection
frequency: 120 min
intensity decay: 0.2%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.127
$S$ = 0.74
624 reflections
41 parameters
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.05 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.57 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Ce1—Al6 | 3.145 (5) | Al4—Al8 | 2.639 (7) |
| Ce1—Al7 | 3.149 (5) | Al4—Al4$^{iv}$ | 2.703 (5) |
| Ce1—Al8$^{i}$ | 3.210 (5) | Al4—Al6 | 2.777 (5) |
| Ce1—Al8$^{ii}$ | 3.213 (5) | Al4—Al6$^{vi}$ | 2.881 (5) |
| Ce1—Al4$^{i}$ | 3.238 (5) | Al5—Al7$^{iii}$ | 2.724 (3) |
| Ce1—Al5$^{ii}$ | 3.371 (3) | Al5—Al8$^{ii}$ | 2.742 (5) |
| Ce2—Al6$^{iii}$ | 3.273 (5) | Al5—Al7$^{ii}$ | 2.931 (4) |
| Ce2—Al4$^{iii}$ | 3.346 (5) | Al5—Al5$^{vii}$ | 2.975 (9) |
| Ru3—Al5$^{iv}$ | 2.566 (4) | Al6—Al7$^{viii}$ | 2.696 (7) |
| Ru3—Al7$^{v}$ | 2.640 (2) | Al6—Al6$^{ix}$ | 2.730 (10) |
| Ru3—Al6 | 2.671 (3) | Al6—Al8$^{x}$ | 2.803 (6) |
| Ru3—Al4 | 2.688 (3) | Al7—Al7$^{xi}$ | 2.832 (8) |
| Ru3—Al8 | 2.693 (2) | Al8—Al8$^{xii}$ | 2.685 (9) |
| Ru3—Ce1$^{iv}$ | 3.4497 (7) | | |

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

The highest peak and the deepest hole in the final difference map are located 1.24 Å from Al4 and 1.94 Å from Al6, respectively.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1998) and *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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