

Ce₄Ga₅Rh₉ Structure:

A4B5C9_hR18_166_2c_a2c_dh-001

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<https://aflow.org/prototype-encyclopedia/1911>

https://aflow.org/prototype-encyclopedia/A4B5C9_hR18_166_2c_a2c_dh-001

Prototype	Ce ₄ Ga ₅ Rh ₉
AFLOW prototype label	A4B5C9_hR18_166_2c_a2c_dh-001
ICSD	432164
CCDC	1791225
Pearson symbol	hR18
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A4B5C9_hR18_166_2c_a2c_dh-001</code> <code>--params=a, c/a, x₂, x₃, x₄, x₅, x₇, z₇</code>

Other compounds with this structure

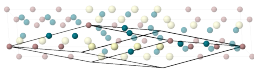
Gd₄Ga₅Rh₉

- This is a more compact version of Ce₅Ga₇Rh₁₂ and Ce₇Ga₁₁Rh₁₈.
- Aflow moves the Ga I atom from the published (1b) site to the origin (1a) site.

Rhombohedral primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$

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Basis vectors

Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
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$\mathbf{B}_1$	$=$	0	$=$	0	(1a)	Ga I
$\mathbf{B}_2$	$=$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c)	Ce I
$\mathbf{B}_3$	$=$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c)	Ce I
$\mathbf{B}_4$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(2c)	Ce II
$\mathbf{B}_5$	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-cx_3 \hat{\mathbf{z}}$	(2c)	Ce II
$\mathbf{B}_6$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$cx_4 \hat{\mathbf{z}}$	(2c)	Ga II
$\mathbf{B}_7$	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-cx_4 \hat{\mathbf{z}}$	(2c)	Ga II
$\mathbf{B}_8$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$cx_5 \hat{\mathbf{z}}$	(2c)	Ga III
$\mathbf{B}_9$	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-cx_5 \hat{\mathbf{z}}$	(2c)	Ga III
$\mathbf{B}_{10}$	$=$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	Rh I
$\mathbf{B}_{11}$	$=$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	Rh I
$\mathbf{B}_{12}$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	Rh I
$\mathbf{B}_{13}$	$=$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B}_{14}$	$=$	$z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B}_{15}$	$=$	$x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B}_{16}$	$=$	$-z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - z_7) \hat{\mathbf{y}} - \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B}_{17}$	$=$	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - z_7) \hat{\mathbf{y}} - \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B}_{18}$	$=$	$-x_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a(x_7 - z_7) \hat{\mathbf{y}} - \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(6h)	Rh II

References

- [1] S. Seidel, U. C. Rodewald, O. Janka, and R. Pöttgen, *Ternary gallides $RE_4Rh_9Ga_5$, $RE_5Rh_{12}Ga_7$ and $RE_7Rh_{18}Ga_{11}$ ($RE=Y, La-Nd, Sm, Gd, Tb$) – intergrowth structures with $MgCu_2$ and $CaCu_5$ related slabs*, Z. Krystallogr. **232**, 365–374 (2017), doi:10.1515/zkri-2016-2017.

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Ce
Ga
Rh

