$Ce_7Ga_{11}Rh_{18}$ Structure: A7B11C18_hR36_166_a3c_b5c_3h-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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https://aflow.org/prototype-encyclopedia/830S

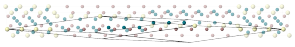
https://aflow.org/prototype-encyclopedia/A7B11C18_hR36_166_a3c_b5c_3h-001

Prototype	$Ce_7Ga_{11}Rh_{18}$
AFLOW prototype label	A7B11C18_hR36_166_a3c_b5c_3h-001
ICSD	432163
CCDC	1791224
Pearson symbol	hR36
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A7B11C18_hR36_166_a3c_b5c_3h-001 --params=`$a, c/a, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, z_{11}, x_{12}, z_{12}, x_{13}, z_{13}$

- This is a stretched out version of the $Ce_4Ga_5Rh_9$ and $Ce_5Ga_7Rh_{12}$ structures.

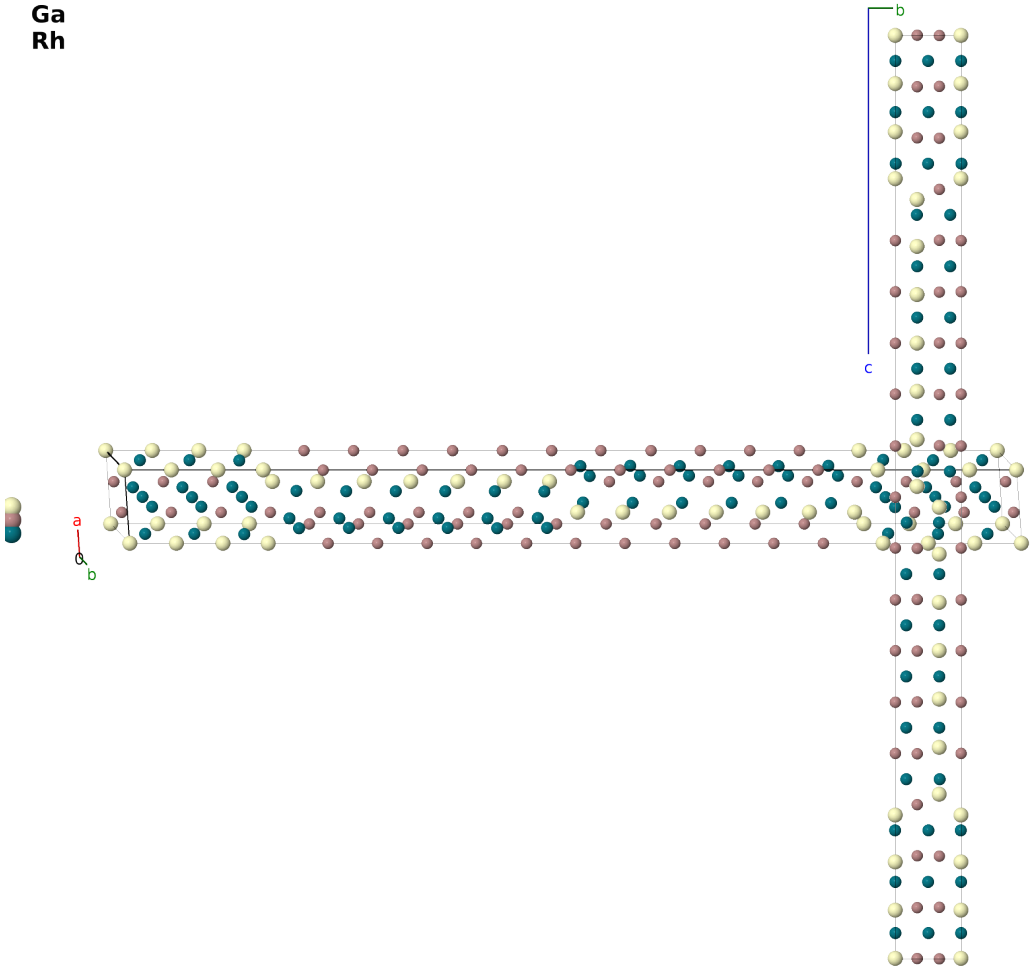
Rhombohedral primitive vectors

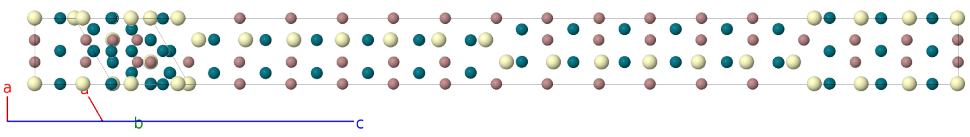
$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

Ce
Ga
Rh





		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Ce I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Ga I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Ce II
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Ce II
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	Ce III
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	Ce III
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$cx_5\,\hat{\mathbf{z}}$	(2c)	Ce IV
$\mathbf{B_8}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-cx_5\,\hat{\mathbf{z}}$	(2c)	Ce IV
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$cx_6\,\hat{\mathbf{z}}$	(2c)	Ga II
$\mathbf{B_{10}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-cx_6\,\hat{\mathbf{z}}$	(2c)	Ga II
$\mathbf{B_{11}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$cx_7\,\hat{\mathbf{z}}$	(2c)	Ga III
$\mathbf{B_{12}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$-cx_7\,\hat{\mathbf{z}}$	(2c)	Ga III
$\mathbf{B_{13}}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$cx_8\,\hat{\mathbf{z}}$	(2c)	Ga IV
$\mathbf{B_{14}}$	=	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$-cx_8\,\hat{\mathbf{z}}$	(2c)	Ga IV
$\mathbf{B_{15}}$	=	$x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + x_9\,\mathbf{a}_3$	=	$cx_9\,\hat{\mathbf{z}}$	(2c)	Ga V
$\mathbf{B_{16}}$	=	$-x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - x_9\,\mathbf{a}_3$	=	$-cx_9\,\hat{\mathbf{z}}$	(2c)	Ga V
$\mathbf{B_{17}}$	=	$x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + x_{10}\,\mathbf{a}_3$	=	$cx_{10}\,\hat{\mathbf{z}}$	(2c)	Ga VI
$\mathbf{B_{18}}$	=	$-x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 - x_{10}\,\mathbf{a}_3$	=	$-cx_{10}\,\hat{\mathbf{z}}$	(2c)	Ga VI
$\mathbf{B_{19}}$	=	$x_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{11} - z_{11})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_{11} - z_{11})\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_{11} + z_{11})\,\hat{\mathbf{z}}$	(6h)	Rh I
$\mathbf{B_{20}}$	=	$z_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + x_{11}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_{11} - z_{11})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_{11} - z_{11})\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_{11} + z_{11})\,\hat{\mathbf{z}}$	(6h)	Rh I
$\mathbf{B_{21}}$	=	$x_{11}\,\mathbf{a}_1 + z_{11}\,\mathbf{a}_2 + x_{11}\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_{11} - z_{11})\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_{11} + z_{11})\,\hat{\mathbf{z}}$	(6h)	Rh I
$\mathbf{B_{22}}$	=	$-z_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 - x_{11}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{11} - z_{11})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_{11} - z_{11})\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_{11} + z_{11})\,\hat{\mathbf{z}}$	(6h)	Rh I
$\mathbf{B_{23}}$	=	$-x_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_{11} - z_{11})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_{11} - z_{11})\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_{11} + z_{11})\,\hat{\mathbf{z}}$	(6h)	Rh I
$\mathbf{B_{24}}$	=	$-x_{11}\,\mathbf{a}_1 - z_{11}\,\mathbf{a}_2 - x_{11}\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_{11} - z_{11})\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_{11} + z_{11})\,\hat{\mathbf{z}}$	(6h)	Rh I
$\mathbf{B_{25}}$	=	$x_{12}\,\mathbf{a}_1 + x_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{12} - z_{12})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_{12} - z_{12})\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_{12} + z_{12})\,\hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B_{26}}$	=	$z_{12}\,\mathbf{a}_1 + x_{12}\,\mathbf{a}_2 + x_{12}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_{12} - z_{12})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_{12} - z_{12})\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_{12} + z_{12})\,\hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B_{27}}$	=	$x_{12}\,\mathbf{a}_1 + z_{12}\,\mathbf{a}_2 + x_{12}\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_{12} - z_{12})\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_{12} + z_{12})\,\hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B_{28}}$	=	$-z_{12}\,\mathbf{a}_1 - x_{12}\,\mathbf{a}_2 - x_{12}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{12} - z_{12})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_{12} - z_{12})\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_{12} + z_{12})\,\hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B_{29}}$	=	$-x_{12}\,\mathbf{a}_1 - x_{12}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_{12} - z_{12})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_{12} - z_{12})\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_{12} + z_{12})\,\hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B_{30}}$	=	$-x_{12}\,\mathbf{a}_1 - z_{12}\,\mathbf{a}_2 - x_{12}\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_{12} - z_{12})\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_{12} + z_{12})\,\hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B_{31}}$	=	$x_{13}\,\mathbf{a}_1 + x_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{13} - z_{13})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_{13} - z_{13})\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_{13} + z_{13})\,\hat{\mathbf{z}}$	(6h)	Rh III
$\mathbf{B_{32}}$	=	$z_{13}\,\mathbf{a}_1 + x_{13}\,\mathbf{a}_2 + x_{13}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_{13} - z_{13})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_{13} - z_{13})\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_{13} + z_{13})\,\hat{\mathbf{z}}$	(6h)	Rh III

$\mathbf{B_{33}}$	=	$x_{13}\,\mathbf{a}_1 + z_{13}\,\mathbf{a}_2 + x_{13}\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_{13} - z_{13})\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_{13} + z_{13})\;\hat{\mathbf{z}}$	(6h)	Rh III
$\mathbf{B_{34}}$	=	$-z_{13}\,\mathbf{a}_1 - x_{13}\,\mathbf{a}_2 - x_{13}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{13} - z_{13})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_{13} - z_{13})\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_{13} + z_{13})\;\hat{\mathbf{z}}$	(6h)	Rh III
$\mathbf{B_{35}}$	=	$-x_{13}\,\mathbf{a}_1 - x_{13}\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_{13} - z_{13})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_{13} - z_{13})\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_{13} + z_{13})\;\hat{\mathbf{z}}$	(6h)	Rh III
$\mathbf{B_{36}}$	=	$-x_{13}\,\mathbf{a}_1 - z_{13}\,\mathbf{a}_2 - x_{13}\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_{13} - z_{13})\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_{13} + z_{13})\;\hat{\mathbf{z}}$	(6h)	Rh III

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.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5.* Submitted to Computational Materials Science (2026).