$Ce_5Ga_7Rh_{12}$ Structure: A5B7C12_hR24_166_a2c_b3c_2h-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.

---

https://aflow.org/prototype-encyclopedia/TZ29

https://aflow.org/prototype-encyclopedia/A5B7C12_hR24_166_a2c_b3c_2h-001

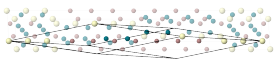
Prototype	$Ce_5Ga_7Rh_{12}$
AFLOW prototype label	A5B7C12_hR24_166_a2c_b3c_2h-001
ICSD	432161
CCDC	1791222
Pearson symbol	hR24
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A5B7C12_hR24_166_a2c_b3c_2h-001 --params=`$a, c/a, x_3, x_4, x_5, x_6, x_7, x_8, z_8, x_9, z_9$

Other compounds with this structure
$Nd_5Ga_7Rh_{12}$

- This is the ternary version of the Ce_5Co_{19} structure. We have arbitrarily chosen $Ce_5Ga_7Rh_{12}$ as the prototype.
- $Ce_4Ga_5Rh_9$ and $Ce_7Ga_{11}Rh_{18}$ are slightly gallium-enriched forms of this structure.

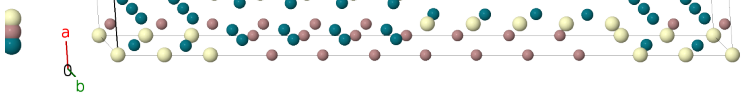
Rhombohedral primitive vectors

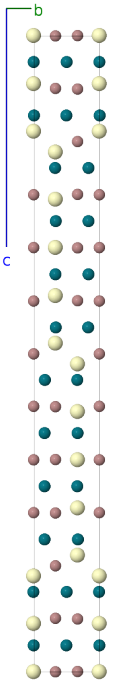
$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}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

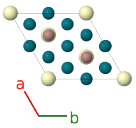


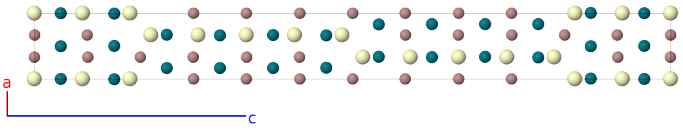
Basis vectors

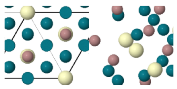
Ce
Ga
Rh











		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)	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 II
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$cx_6\,\hat{\mathbf{z}}$	(2c)	Ga III
$\mathbf{B_{10}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-cx_6\,\hat{\mathbf{z}}$	(2c)	Ga III
$\mathbf{B_{11}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$cx_7\,\hat{\mathbf{z}}$	(2c)	Ga IV
$\mathbf{B_{12}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$-cx_7\,\hat{\mathbf{z}}$	(2c)	Ga IV
$\mathbf{B_{13}}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - z_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_8 - z_8)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_8 + z_8)\,\hat{\mathbf{z}}$	(6h)	Rh I
$\mathbf{B_{14}}$	=	$z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_8 - z_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_8 - z_8)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_8 + z_8)\,\hat{\mathbf{z}}$	(6h)	Rh I
$\mathbf{B_{15}}$	=	$x_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_8 - z_8)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_8 + z_8)\,\hat{\mathbf{z}}$	(6h)	Rh I
$\mathbf{B_{16}}$	=	$-z_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - z_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_8 - z_8)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_8 + z_8)\,\hat{\mathbf{z}}$	(6h)	Rh I
$\mathbf{B_{17}}$	=	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_8 - z_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_8 - z_8)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_8 + z_8)\,\hat{\mathbf{z}}$	(6h)	Rh I
$\mathbf{B_{18}}$	=	$-x_8\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_8 - z_8)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_8 + z_8)\,\hat{\mathbf{z}}$	(6h)	Rh I
$\mathbf{B_{19}}$	=	$x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_9 - z_9)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_9 - z_9)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_9 + z_9)\,\hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B_{20}}$	=	$z_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + x_9\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_9 - z_9)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_9 - z_9)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_9 + z_9)\,\hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B_{21}}$	=	$x_9\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + x_9\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_9 - z_9)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_9 + z_9)\,\hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B_{22}}$	=	$-z_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - x_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_9 - z_9)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_9 - z_9)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_9 + z_9)\,\hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B_{23}}$	=	$-x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_9 - z_9)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_9 - z_9)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_9 + z_9)\,\hat{\mathbf{z}}$	(6h)	Rh II
$\mathbf{B_{24}}$	=	$-x_9\,\mathbf{a}_1 - z_9\,\mathbf{a}_2 - x_9\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_9 - z_9)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_9 + z_9)\,\hat{\mathbf{z}}$	(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.

Found in

[1] *Inorganic Crystal Structure Database*. Entry 432161 (Ce5Ga7Rh12).

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).