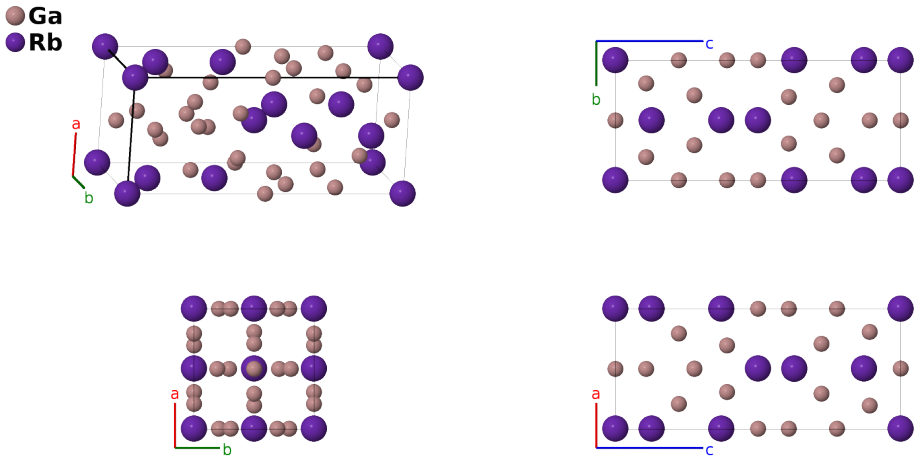
$RbGa_3$ Structure: A3B_tI24_119_a2i_bf-001

This structure originally had the label `A3B_tI24_119_b2i_af`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/6TQK

https://aflow.org/p/A3B_tI24_119_a2i_bf-001

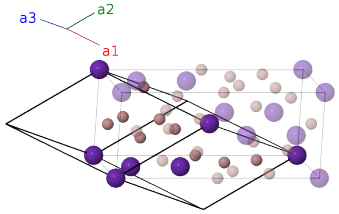


Prototype	Ga_3Rb
AFLOW prototype label	A3B_tI24_119_a2i_bf-001
ICSD	103943
Pearson symbol	tI24
Space group number	119
Space group symbol	$I\bar{4}m2$
AFLOW prototype command	`aflow --proto=A3B_tI24_119_a2i_bf-001 --params=`$a, c/a, z_3, x_4, z_4, x_5, z_5$

Other compounds with this structure
$CsGa_3$, KGa_3

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ga I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Rb I
$\mathbf{B_3}$	=	$\left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4f)	Rb II
$\mathbf{B_4}$	=	$-z_3\,\mathbf{a}_1 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_3\,\hat{\mathbf{z}}$	(4f)	Rb II
$\mathbf{B_5}$	=	$z_4\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(8i)	Ga II
$\mathbf{B_6}$	=	$z_4\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(8i)	Ga II
$\mathbf{B_7}$	=	$-(x_4 + z_4)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8i)	Ga II
$\mathbf{B_8}$	=	$(x_4 - z_4)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8i)	Ga II
$\mathbf{B_9}$	=	$z_5\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(8i)	Ga III
$\mathbf{B_{10}}$	=	$z_5\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(8i)	Ga III
$\mathbf{B_{11}}$	=	$-(x_5 + z_5)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8i)	Ga III
$\mathbf{B_{12}}$	=	$(x_5 - z_5)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8i)	Ga III

References

[1] R. G. Ling and C. Berlin, *Preparation and Crystal Structure Determination of the New Intermetallic Compound $RbGa_3$*, Z. Anorganische und Allgemeine Chemie **480**, 181–185 (1981), doi:10.1002/zaac.19814800923.

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OK, 1991), vol. III, chap. , p. 3545.