Y_2Rh_3Ga Structure: AB3C2_hR6_166_a_d_c-001

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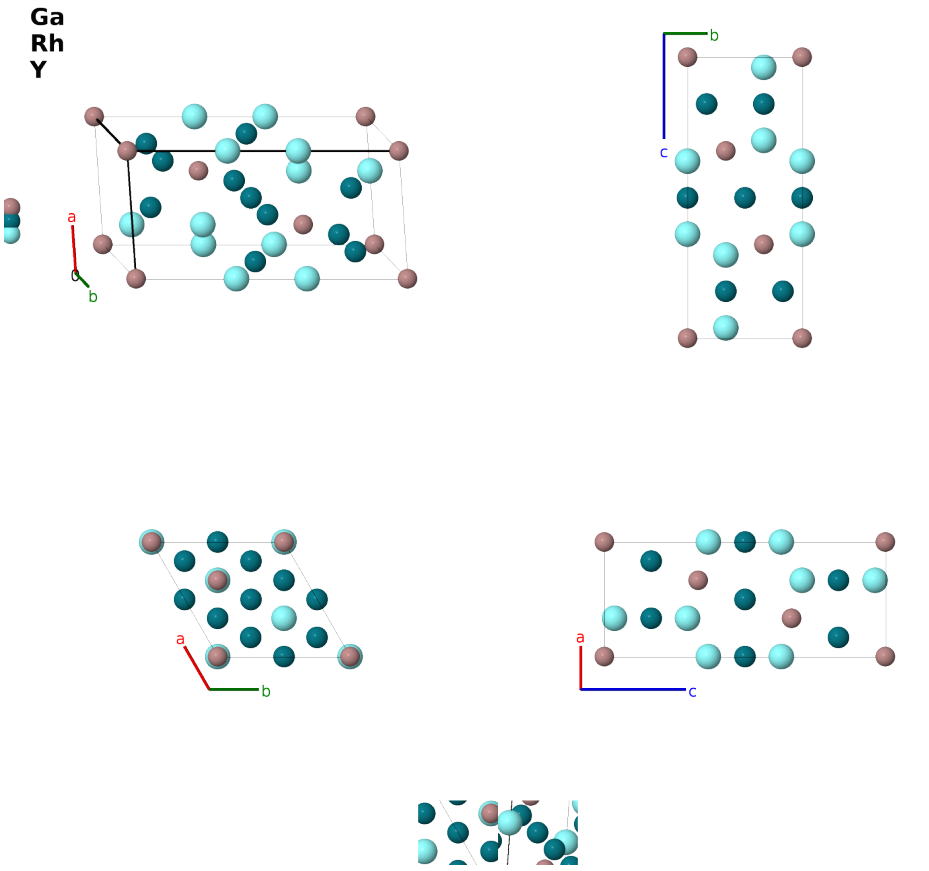
https://aflow.org/prototype-encyclopedia/NAW4

https://aflow.org/prototype-encyclopedia/AB3C2_hR6_166_a_d_c-001



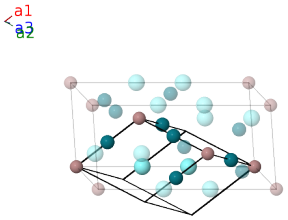
Prototype	$GaRh_3Y_2$
AFLOW prototype label	AB3C2_hR6_166_a_d_c-001
ICSD	432339
CCDC	1791359
Pearson symbol	hR6
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=AB3C2_hR6_166_a_d_c-001 --params=`$a, c/a, x_2$

Other compounds with this structure
Ce_2Rh_3Ga, Dy_2Rh_3Ga, Er_2Rh_3Ga, Gd_2Rh_3Ga, Ho_2Rh_3Ga, La_2Rh_3Ga, Nd_2Rh_3Ga, Pr_2Rh_3Ga, Sm_2Rh_3Ga, Tb_2Rh_3Ga

- (Seidel, 2017) call this a rhombohedral Laves phase, a ternary varient of the $MgZn_2$ hexagonal Laves phase ($C14$).

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

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	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)	Y 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)	Y I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Rh I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Rh I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Rh I

References

[1] S. Seidel, O. Janka, C. Benndorf, B. Mausolf, F. Haarmann, H. Eckert, L. Heletta, and R. Pöttgen, *Ternary rhombohedral Laves phases RE_2Rh_3Ga (RE=Y, La–Nd, Sm, Gd–Er)*, Z. Naturforsch. B **72**, 289–303 (2017), doi:10.1515/znb-2016-0265.

Found in

[1] *Inorganic Crystal Structure Database*. Entry 432339 (Y2Rh3Ga).

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