$Yb_6Ir_5Ga_7$ Structure: A7B5C6_hP36_193_bj_dg_k-001

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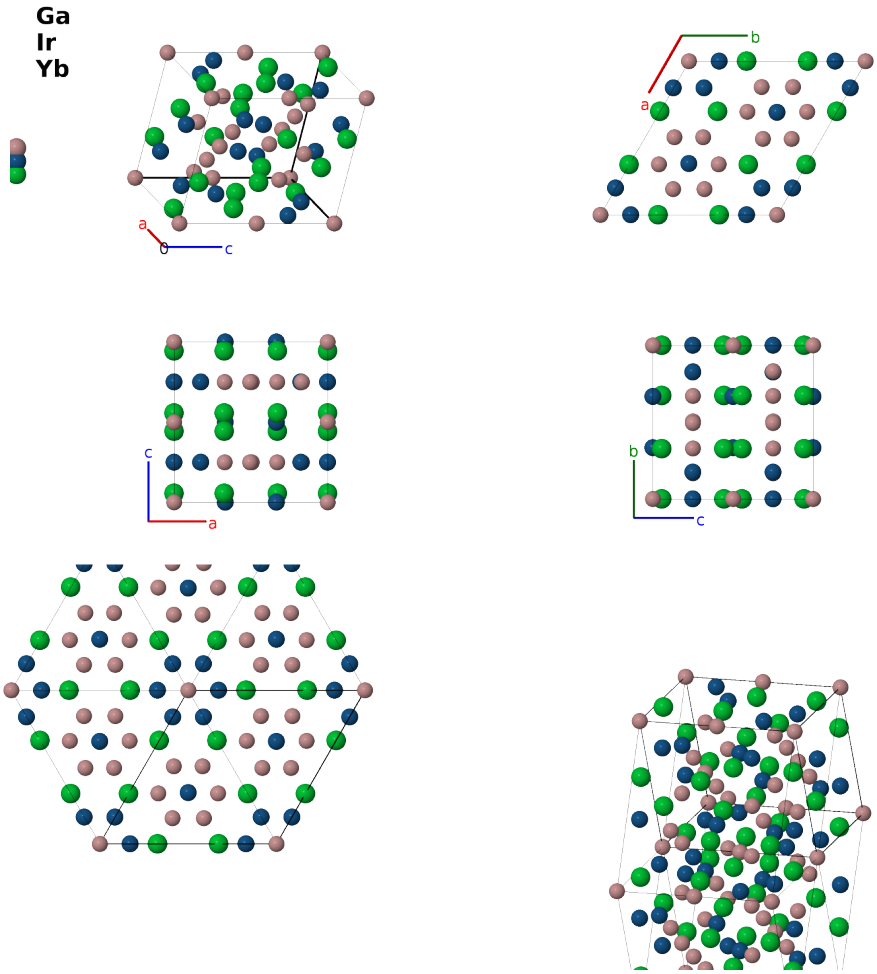
https://aflow.org/prototype-encyclopedia/CV59

https://aflow.org/prototype-encyclopedia/A7B5C6_hP36_193_bj_dg_k-001



Prototype	$Ga_7Ir_5Yb_6$
AFLOW prototype label	A7B5C6_hP36_193_bj_dg_k-001
ICSD	432187
CCDC	1791247
Pearson symbol	hP36
Space group number	193
Space group symbol	$P6_3/mcm$

AFLOW prototype command `aflow --proto=A7B5C6_hP36_193_bj_dg_k-001 --params=`$a, c/a, x_3, x_4, y_4, x_5, z_5$

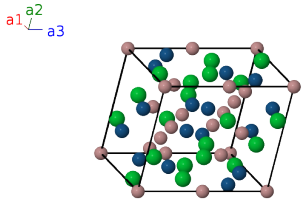
Other compounds with this structure

$Ho_6Ru_5Al_7$, $Sc_6Ir_5Al_7$, $Sc_6Ir_5Ga_7$

- (Seidel, 2017) call this a variant of the $MgZn_2$ hexagonal Laves structure ($C14$).
- The ICSD considers VCoSi as the prototype for this structure, but VCoSi and many other compounds with this structure have substantial disorder on all Wyckoff positions. The structures listed here are the only ordered ones in the ICSD. We arbitrarily chose $Yb_6Ir_5Ga_7$ as our prototype.

Hexagonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2b)	Ga I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Ga I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(4d)	Ir I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4d)	Ir I
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(4d)	Ir I
$\mathbf{B_6}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4d)	Ir I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	Ir II
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	Ir II
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	Ir II
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	Ir II
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	Ir II
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	Ir II
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(12j)	Ga II
$\mathbf{B_{14}}$	=	$-y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(12j)	Ga II
$\mathbf{B_{15}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(12j)	Ga II
$\mathbf{B_{16}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(12j)	Ga II
$\mathbf{B_{17}}$	=	$y_4\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_4 + 2y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(12j)	Ga II
$\mathbf{B_{18}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(12j)	Ga II
$\mathbf{B_{19}}$	=	$y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(12j)	Ga II
$\mathbf{B_{20}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(12j)	Ga II
$\mathbf{B_{21}}$	=	$-x_4\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(12j)	Ga II

$\mathbf{B_{22}}$	$=$	$-y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_4 + y_4)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\;\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(12j)	Ga II
$\mathbf{B_{23}}$	$=$	$-\,(x_4 - y_4)\;\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_4 + 2y_4)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(12j)	Ga II
$\mathbf{B_{24}}$	$=$	$x_4\,\mathbf{a}_1 + (x_4 - y_4)\;\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_4 - y_4)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(12j)	Ga II
$\mathbf{B_{25}}$	$=$	$x_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_3$	$=$	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12k)	Yb I
$\mathbf{B_{26}}$	$=$	$x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	$=$	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12k)	Yb I
$\mathbf{B_{27}}$	$=$	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(12k)	Yb I
$\mathbf{B_{28}}$	$=$	$-x_5\,\mathbf{a}_1 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Yb I
$\mathbf{B_{29}}$	$=$	$-x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Yb I
$\mathbf{B_{30}}$	$=$	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Yb I
$\mathbf{B_{31}}$	$=$	$x_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Yb I
$\mathbf{B_{32}}$	$=$	$x_5\,\mathbf{a}_1 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Yb I
$\mathbf{B_{33}}$	$=$	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Yb I
$\mathbf{B_{34}}$	$=$	$-x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	$=$	$-\frac{1}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12k)	Yb I
$\mathbf{B_{35}}$	$=$	$-x_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_3$	$=$	$-\frac{1}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12k)	Yb I
$\mathbf{B_{36}}$	$=$	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$	(12k)	Yb I

References

[1] S. Seidel and R. Pöttgen, *$Yb_6Ir_5Ga_7$ - A $MgZn_2$ Superstructure*, Z. Anorganische und Allgemeine Chemie **643**, 261–265 (2017), doi:10.1002/zaac.201600422.

Found in

[1] *Inorganic Crystal Structure Database*. Entry 432187 (Ga7Ir5Yb6).

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