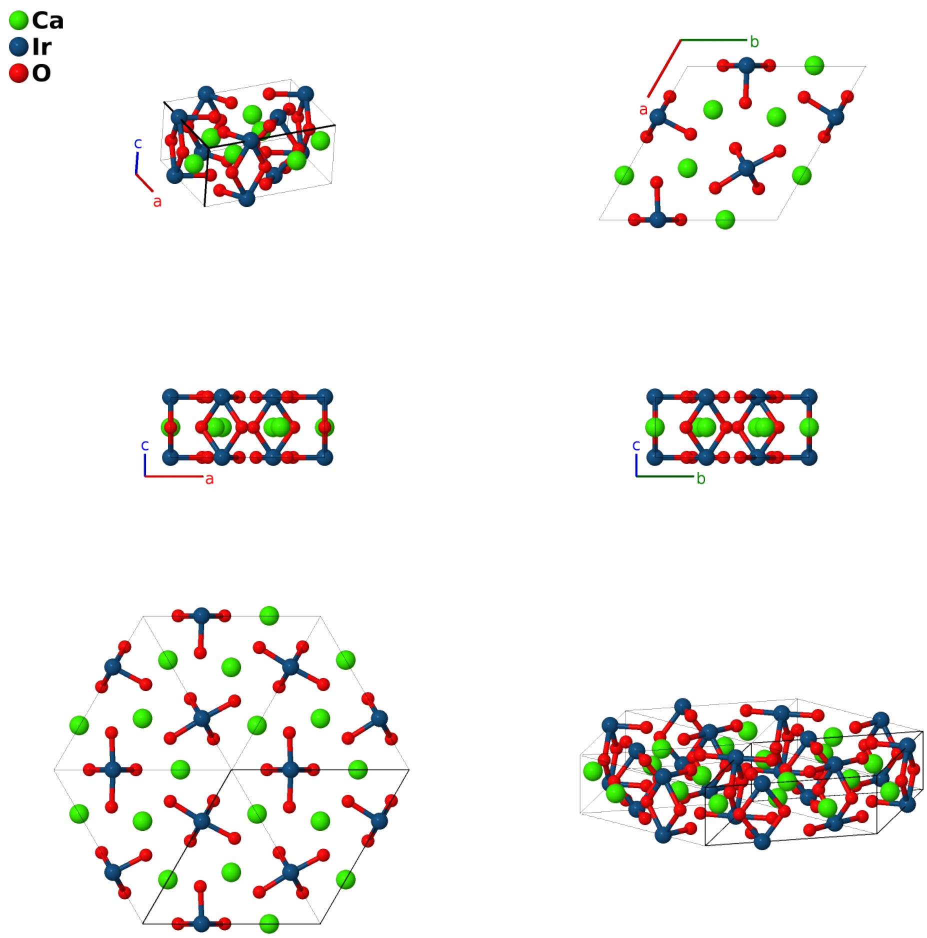
$Ca_5Ir_3O_{12}$ Structure: A5B3C12_hP20_189_dg_f_2gj-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

---

https://aflow.org/p/8TFL

https://aflow.org/p/A5B3C12_hP20_189_dg_f_2gj-001

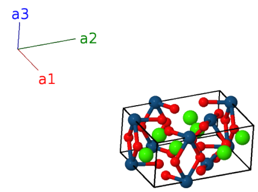


Prototype	$Ca_5Ir_3O_{12}$
AFLOW prototype label	A5B3C12_hP20_189_dg_f_2gj-001
ICSD	120112
Pearson symbol	hP20
Space group number	189
Space group symbol	$P\bar{6}2m$
AFLOW prototype command	`aflow --proto=A5B3C12_hP20_189_dg_f_2gj-001` `--params=`$a, c/a, x_2, x_3, x_4, x_5, x_6, y_6$

- The data for this structure was taken at 90K.
- There is no ICSD entry for (Wakeshima, 2003). We use the entry from (Cao, 2007), which the authors say is in agreement with the Wakeshima result.

Hexagonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(2d)	Ca I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(2d)	Ca I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1$	=	$\frac{1}{2}ax_2\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_2\,\mathbf{\hat{y}}$	(3f)	Ir I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_2$	=	$\frac{1}{2}ax_2\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_2\,\mathbf{\hat{y}}$	(3f)	Ir I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-ax_2\,\mathbf{\hat{x}}$	(3f)	Ir I
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_3\,\mathbf{\hat{y}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(3g)	Ca II
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_3\,\mathbf{\hat{y}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(3g)	Ca II
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(3g)	Ca II
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(3g)	O I
$\mathbf{B_{10}}$	=	$x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(3g)	O I
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(3g)	O I
$\mathbf{B_{12}}$	=	$x_5\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(3g)	O II
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(3g)	O II
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\mathbf{\hat{x}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(3g)	O II
$\mathbf{B_{15}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2$	=	$\frac{1}{2}a\left(x_6 + y_6\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}a\left(x_6 - y_6\right)\,\mathbf{\hat{y}}$	(6j)	O III
$\mathbf{B_{16}}$	=	$-y_6\,\mathbf{a}_1 + \left(x_6 - y_6\right)\,\mathbf{a}_2$	=	$\frac{1}{2}a\left(x_6 - 2y_6\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_6\,\mathbf{\hat{y}}$	(6j)	O III
$\mathbf{B_{17}}$	=	$-\left(x_6 - y_6\right)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2$	=	$-\frac{1}{2}a\left(2x_6 - y_6\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_6\,\mathbf{\hat{y}}$	(6j)	O III
$\mathbf{B_{18}}$	=	$y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2$	=	$\frac{1}{2}a\left(x_6 + y_6\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}a\left(x_6 - y_6\right)\,\mathbf{\hat{y}}$	(6j)	O III
$\mathbf{B_{19}}$	=	$\left(x_6 - y_6\right)\,\mathbf{a}_1 - y_6\,\mathbf{a}_2$	=	$\frac{1}{2}a\left(x_6 - 2y_6\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_6\,\mathbf{\hat{y}}$	(6j)	O III
$\mathbf{B_{20}}$	=	$-x_6\,\mathbf{a}_1 - \left(x_6 - y_6\right)\,\mathbf{a}_2$	=	$-\frac{1}{2}a\left(2x_6 - y_6\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_6\,\mathbf{\hat{y}}$	(6j)	O III

References

[1] M. Wakeshima, N. Taira, Y. Hinatsu, and Y. Ishiib, *Electrical and magnetic properties of pseudo-one-dimensional calcium iridium oxide $Ca_5Ir_3O_{12}$*, Solid State Commun. **125**, 311–315 (2003), doi:10.1016/S0038-1098(02)00823-2.

[2] G. Cao, V. Durairaj, S. Chikara, S. Parkin, and P. Schlottmann, *Partial antiferromagnetism in spin-chain $Sr_5Rh_4O_{12}$, $Ca_5Ir_3O_{12}$, and Ca4IrO6 single crystals*, Phys. Rev. B **75**, 075153 (2007), doi:10.1103/PhysRevB.75.134402.

Found in

[1] M. Charlebois, J.-B. Morée, K. Nakamura, Y. Nomura, T. Tadano, Y. Yoshimoto, Y. Yamaji, T. Hasegawa, K. Matsuhira, and M. Imada, Ab initio *Derivation of Low-Energy Hamiltonians for Systems with Strong Spin-Orbit Interaction and Its Application to* $Ca_5Ir_3O_{12}$, Phys. Rev. B **104**, 075153 (2021), doi:10.1103/PhysRevB.104.075153.