

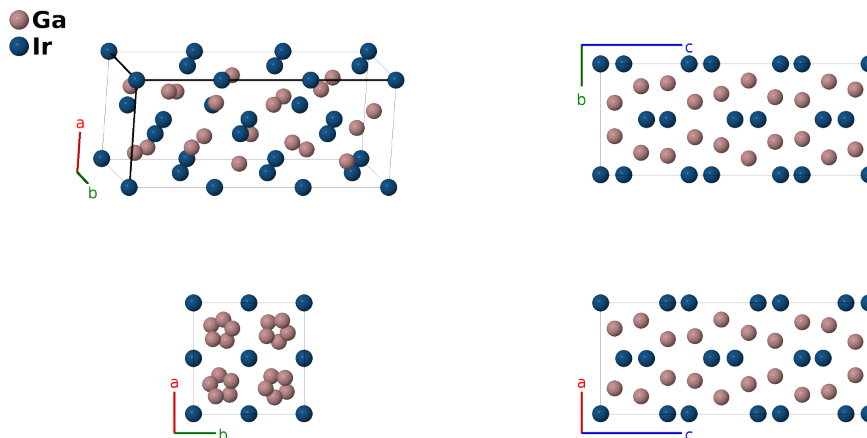
Ir₃Ga₅ Structure: A5B3_tP32_118_f2i_aceh-001

This structure originally had the label A5B3_tP32_118_g2i_aceh. Calls to that address will be redirected here.

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<https://afLOW.org/p/DCPJ>

https://afLOW.org/p/A5B3_tP32_118_f2i_aceh-001

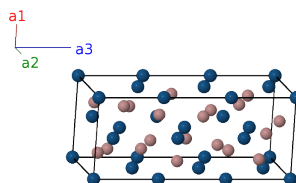


Prototype	Ga ₅ Ir ₃
AFLOW prototype label	A5B3_tP32_118_f2i_aceh-001
ICSD	103761
Pearson symbol	tP32
Space group number	118
Space group symbol	$P\bar{4}n2$
AFLOW prototype command	afLOW --proto=A5B3_tP32_118_f2i_aceh-001 --params=a, c/a, z ₃ , x ₄ , z ₅ , x ₆ , y ₆ , z ₆ , x ₇ , y ₇ , z ₇

- In our original publication (Hicks, 2019) the iridium atoms on the (2d) site were inadvertently placed on the (3c) site.

Simple Tetragonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{x} \\ \mathbf{a}_2 &= a \hat{y} \\ \mathbf{a}_3 &= c \hat{z} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= 0$	$=$	0	(2a)	Ir I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Ir I
\mathbf{B}_3	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2c)	Ir II
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2c)	Ir II
\mathbf{B}_5	$= z_3 \mathbf{a}_3$	$=$	$cz_3 \hat{\mathbf{z}}$	(4e)	Ir III
\mathbf{B}_6	$= -z_3 \mathbf{a}_3$	$=$	$-cz_3 \hat{\mathbf{z}}$	(4e)	Ir III
\mathbf{B}_7	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Ir III
\mathbf{B}_8	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Ir III
\mathbf{B}_9	$= x_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4f)	Ga I
\mathbf{B}_{10}	$= -x_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4f)	Ga I
\mathbf{B}_{11}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4f)	Ga I
\mathbf{B}_{12}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4f)	Ga I
\mathbf{B}_{13}	$= \frac{1}{2} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4h)	Ir IV
\mathbf{B}_{14}	$= \frac{1}{2} \mathbf{a}_1 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_5 \hat{\mathbf{z}}$	(4h)	Ir IV
\mathbf{B}_{15}	$= \frac{1}{2} \mathbf{a}_1 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Ir IV
\mathbf{B}_{16}	$= \frac{1}{2} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - c (z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Ir IV
\mathbf{B}_{17}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8i)	Ga II
\mathbf{B}_{18}	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8i)	Ga II
\mathbf{B}_{19}	$= y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8i)	Ga II
\mathbf{B}_{20}	$= -y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8i)	Ga II
\mathbf{B}_{21}	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_6 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	Ga II
\mathbf{B}_{22}	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_6 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_6 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	Ga II
\mathbf{B}_{23}	$= (y_6 + \frac{1}{2}) \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_6 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_6 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	Ga II
\mathbf{B}_{24}	$= -(y_6 - \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_6 - \frac{1}{2}) \hat{\mathbf{x}} - a (x_6 - \frac{1}{2}) \hat{\mathbf{y}} - c (z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	Ga II
\mathbf{B}_{25}	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8i)	Ga III
\mathbf{B}_{26}	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8i)	Ga III
\mathbf{B}_{27}	$= y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8i)	Ga III
\mathbf{B}_{28}	$= -y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8i)	Ga III
\mathbf{B}_{29}	$= (x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_7 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_7 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	Ga III
\mathbf{B}_{30}	$= -(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_7 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_7 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	Ga III
\mathbf{B}_{31}	$= (y_7 + \frac{1}{2}) \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_7 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_7 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	Ga III
\mathbf{B}_{32}	$= -(y_7 - \frac{1}{2}) \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_7 - \frac{1}{2}) \hat{\mathbf{x}} - a (x_7 - \frac{1}{2}) \hat{\mathbf{y}} - c (z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	Ga III

References

- [1] H. Völlenkle, A. Wittmann, and H. Nowotny, *Die Kristallstrukturen von $Rh_{10}Ga_{17}$ und Ir_3Ga_5* , *Monatsh. Chem.* **98**, 176–183 (1967), doi:10.1007/BF00901115.
- [2] 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–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.