

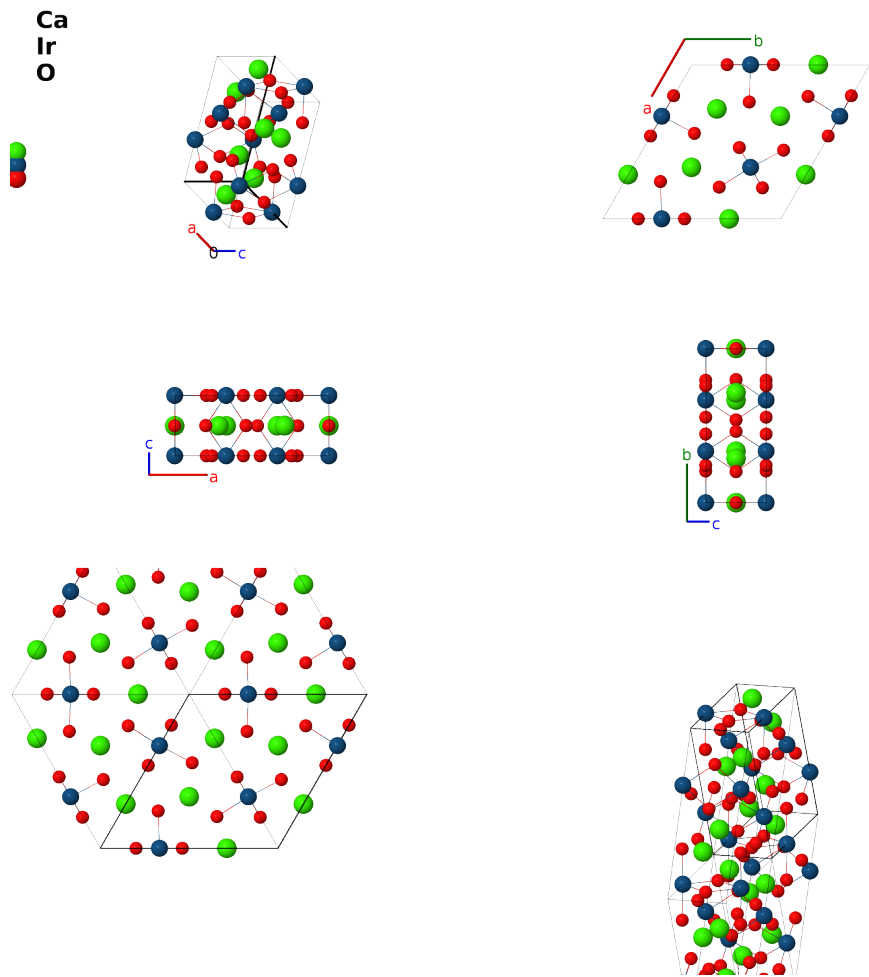
Ca₅Ir₃O₁₂ Structure: A5B3C12_hP20_189_dg_f_2gj-001

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<https://aflow.org/prototype-encyclopedia/8TFL>

https://aflow.org/prototype-encyclopedia/A5B3C12_hP20_189_dg_f_2gj-001



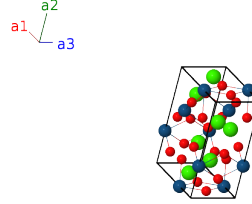
Prototype	Ca ₅ Ir ₃ O ₁₂
AFLOW prototype label	A5B3C12_hP20_189_dg_f_2gj-001
ICSD	120112
CCDC	2135004
Pearson symbol	hP20
Space group number	189
Space group symbol	$P\bar{6}2m$

AFLOW prototype command `aflow --proto=A5B3C12_hP20_189_dg_f_2gj-001`
 `--params=a, c/a, x2, x3, x4, x5, x6, y6`

- 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

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates		Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$		(2d)	Ca I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$		(2d)	Ca I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1$	$=$	$\frac{1}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}}$		(3f)	Ir I
$\mathbf{B}_4$	$= x_2 \mathbf{a}_2$	$=$	$\frac{1}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}}$		(3f)	Ir I
$\mathbf{B}_5$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}}$		(3f)	Ir I
$\mathbf{B}_6$	$= x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$		(3g)	Ca II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$		(3g)	Ca II
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$		(3g)	Ca II
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$		(3g)	O I
$\mathbf{B}_{10}$	$= x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$		(3g)	O I
$\mathbf{B}_{11}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$		(3g)	O I
$\mathbf{B}_{12}$	$= x_5 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$		(3g)	O II
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$		(3g)	O II
$\mathbf{B}_{14}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$		(3g)	O II
$\mathbf{B}_{15}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_6 - y_6) \hat{\mathbf{y}}$		(6j)	O III
$\mathbf{B}_{16}$	$= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}}$		(6j)	O III
$\mathbf{B}_{17}$	$= -(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}}$		(6j)	O III
$\mathbf{B}_{18}$	$= y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_6 + y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_6 - y_6) \hat{\mathbf{y}}$		(6j)	O III
$\mathbf{B}_{19}$	$= (x_6 - y_6) \mathbf{a}_1 - y_6 \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_6 - 2y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}}$		(6j)	O III
$\mathbf{B}_{20}$	$= -x_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2$	$=$	$-\frac{1}{2}a (2x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}}$		(6j)	O III

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Found in

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