γ-Li_2IrO_3 Structure: AB2C3_oC96_66_ik_cdj2k_gl2m-001

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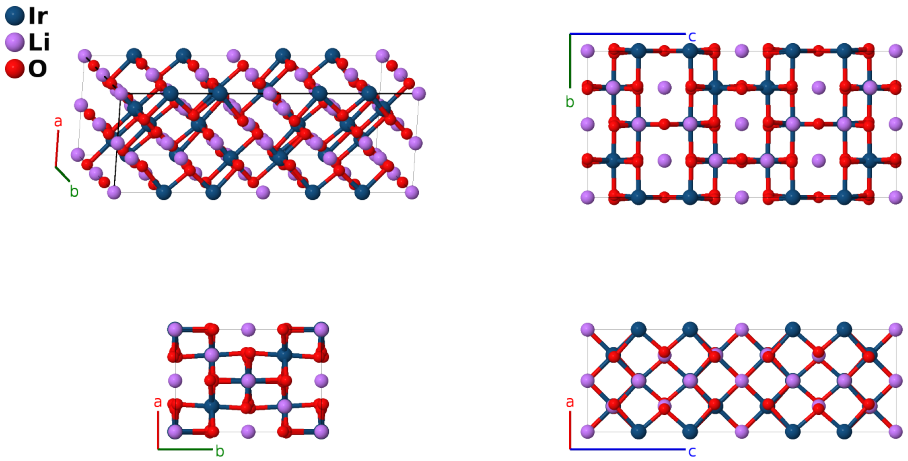
https://aflow.org/p/9VYY

https://aflow.org/p/AB2C3_oC96_66_ik_cdj2k_gl2m-001

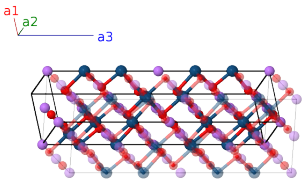


Prototype	$IrLi_2O_3$
AFLOW prototype label	AB2C3_oC96_66_ik_cdj2k_gl2m-001
ICSD	none
Pearson symbol	oC96
Space group number	66
Space group symbol	$Cccm$
AFLOW prototype command	`aflow --proto=AB2C3_oC96_66_ik_cdj2k_gl2m-001 --params=`$a, b/a, c/a, x_3, z_4, z_5, z_6, z_7, z_8, x_9, y_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

- Li_2IrO_3 can be found in three structures (Choi, 2020):
  - α-Li_2IrO_3, which is isostructural with Li_2SnO_3,
  - β-Li_2IrO_3, which is isostructural with β-Na_2PtO_3, and
  - the current structure, γ-Li_2IrO_3.
- There is no ICSD entry for (Modic, 2014), but they do provide their own CIF as part of their supplementary material.

Base-centered Orthorhombic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4c)	Li I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	Li I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4d)	Li II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4d)	Li II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_9}$	=	$z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(8i)	Ir I
$\mathbf{B_{10}}$	=	$-\left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8i)	Ir I
$\mathbf{B_{11}}$	=	$-z_4\,\mathbf{a}_3$	=	$-cz_4\,\hat{\mathbf{z}}$	(8i)	Ir I
$\mathbf{B_{12}}$	=	$\left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8i)	Ir I
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(8j)	Li III
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8j)	Li III
$\mathbf{B_{15}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$	(8j)	Li III
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8j)	Li III
$\mathbf{B_{17}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8k)	Ir II
$\mathbf{B_{18}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8k)	Ir II
$\mathbf{B_{19}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8k)	Ir II
$\mathbf{B_{20}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8k)	Ir II
$\mathbf{B_{21}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8k)	Li IV
$\mathbf{B_{22}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8k)	Li IV
$\mathbf{B_{23}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8k)	Li IV
$\mathbf{B_{24}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8k)	Li IV
$\mathbf{B_{25}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8k)	Li V
$\mathbf{B_{26}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8k)	Li V
$\mathbf{B_{27}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8k)	Li V
$\mathbf{B_{28}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8k)	Li V
$\mathbf{B_{29}}$	=	$(x_9 - y_9)\,\mathbf{a}_1 + (x_9 + y_9)\,\mathbf{a}_2$	=	$ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}}$	(8l)	O II
$\mathbf{B_{30}}$	=	$-(x_9 - y_9)\,\mathbf{a}_1 - (x_9 + y_9)\,\mathbf{a}_2$	=	$-ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}}$	(8l)	O II
$\mathbf{B_{31}}$	=	$-(x_9 + y_9)\,\mathbf{a}_1 - (x_9 - y_9)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8l)	O II

$\mathbf{B_{32}}$	=	$(x_9+y_9)\ \mathbf{a}_1+(x_9-y_9)\ \mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8l)	O II
$\mathbf{B_{33}}$	=	$(x_{10}-y_{10})\ \mathbf{a}_1+$ $(x_{10}+y_{10})\ \mathbf{a}_2+z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(16m)	O III
$\mathbf{B_{34}}$	=	$-(x_{10}-y_{10})\ \mathbf{a}_1-$ $(x_{10}+y_{10})\ \mathbf{a}_2+z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(16m)	O III
$\mathbf{B_{35}}$	=	$-(x_{10}+y_{10})\ \mathbf{a}_1-$ $(x_{10}-y_{10})\ \mathbf{a}_2-\left(z_{10}-\frac{1}{2}\right)\ \mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}-c\left(z_{10}-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16m)	O III
$\mathbf{B_{36}}$	=	$(x_{10}+y_{10})\ \mathbf{a}_1+$ $(x_{10}-y_{10})\ \mathbf{a}_2-\left(z_{10}-\frac{1}{2}\right)\ \mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}-c\left(z_{10}-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16m)	O III
$\mathbf{B_{37}}$	=	$-(x_{10}-y_{10})\ \mathbf{a}_1-$ $(x_{10}+y_{10})\ \mathbf{a}_2-z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}}$	(16m)	O III
$\mathbf{B_{38}}$	=	$(x_{10}-y_{10})\ \mathbf{a}_1+$ $(x_{10}+y_{10})\ \mathbf{a}_2-z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}}$	(16m)	O III
$\mathbf{B_{39}}$	=	$(x_{10}+y_{10})\ \mathbf{a}_1+$ $(x_{10}-y_{10})\ \mathbf{a}_2+\left(z_{10}+\frac{1}{2}\right)\ \mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}+c\left(z_{10}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16m)	O III
$\mathbf{B_{40}}$	=	$-(x_{10}+y_{10})\ \mathbf{a}_1-$ $(x_{10}-y_{10})\ \mathbf{a}_2+\left(z_{10}+\frac{1}{2}\right)\ \mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+c\left(z_{10}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16m)	O III
$\mathbf{B_{41}}$	=	$(x_{11}-y_{11})\ \mathbf{a}_1+$ $(x_{11}+y_{11})\ \mathbf{a}_2+z_{11}\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}}$	(16m)	O IV
$\mathbf{B_{42}}$	=	$-(x_{11}-y_{11})\ \mathbf{a}_1-$ $(x_{11}+y_{11})\ \mathbf{a}_2+z_{11}\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}}$	(16m)	O IV
$\mathbf{B_{43}}$	=	$-(x_{11}+y_{11})\ \mathbf{a}_1-$ $(x_{11}-y_{11})\ \mathbf{a}_2-\left(z_{11}-\frac{1}{2}\right)\ \mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}-c\left(z_{11}-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16m)	O IV
$\mathbf{B_{44}}$	=	$(x_{11}+y_{11})\ \mathbf{a}_1+$ $(x_{11}-y_{11})\ \mathbf{a}_2-\left(z_{11}-\frac{1}{2}\right)\ \mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}-c\left(z_{11}-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16m)	O IV
$\mathbf{B_{45}}$	=	$-(x_{11}-y_{11})\ \mathbf{a}_1-$ $(x_{11}+y_{11})\ \mathbf{a}_2-z_{11}\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}-cz_{11}\,\hat{\mathbf{z}}$	(16m)	O IV
$\mathbf{B_{46}}$	=	$(x_{11}-y_{11})\ \mathbf{a}_1+$ $(x_{11}+y_{11})\ \mathbf{a}_2-z_{11}\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}-cz_{11}\,\hat{\mathbf{z}}$	(16m)	O IV
$\mathbf{B_{47}}$	=	$(x_{11}+y_{11})\ \mathbf{a}_1+$ $(x_{11}-y_{11})\ \mathbf{a}_2+\left(z_{11}+\frac{1}{2}\right)\ \mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}+c\left(z_{11}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16m)	O IV
$\mathbf{B_{48}}$	=	$-(x_{11}+y_{11})\ \mathbf{a}_1-$ $(x_{11}-y_{11})\ \mathbf{a}_2+\left(z_{11}+\frac{1}{2}\right)\ \mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}+c\left(z_{11}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16m)	O IV

References

[1] K. A. Modic, T. E. Smidt, I. Kimchi, N. P. Breznay, A. Biffin, S. Choi, R. D. Johnson, R. Coldea, P. Watkins-Curry, G. T. McCandless, J. Y. Chan, F. Gandara, Z. Islam, A. Vishwanath, A. Shekhter, R. D. McDonald, and J. G. Analytis, *Realization of a three-dimensional spin–anisotropic harmonic honeycomb iridate*, Nature Comm. **5**, 4203 (2014), doi:10.1038/ncomms5203.

Found in

[1] S. Choi, H.-S. Kim, H.-H. Kim, A. Krajewska, G. Kim, M. Minola, T. Takayama, H. Takagi, K. Haule, D. Vanderbilt, and B. Keimer, *Lattice dynamics and structural transition of the hyperhoneycomb iridate β-Li_2IrO_3 investigated by high-pressure Raman scattering*, Phys. Rev. B **101**, 054120 (2020), doi:10.1103/PhysRevB.101.054102.