

γ -Li₂IrO₃ Structure:

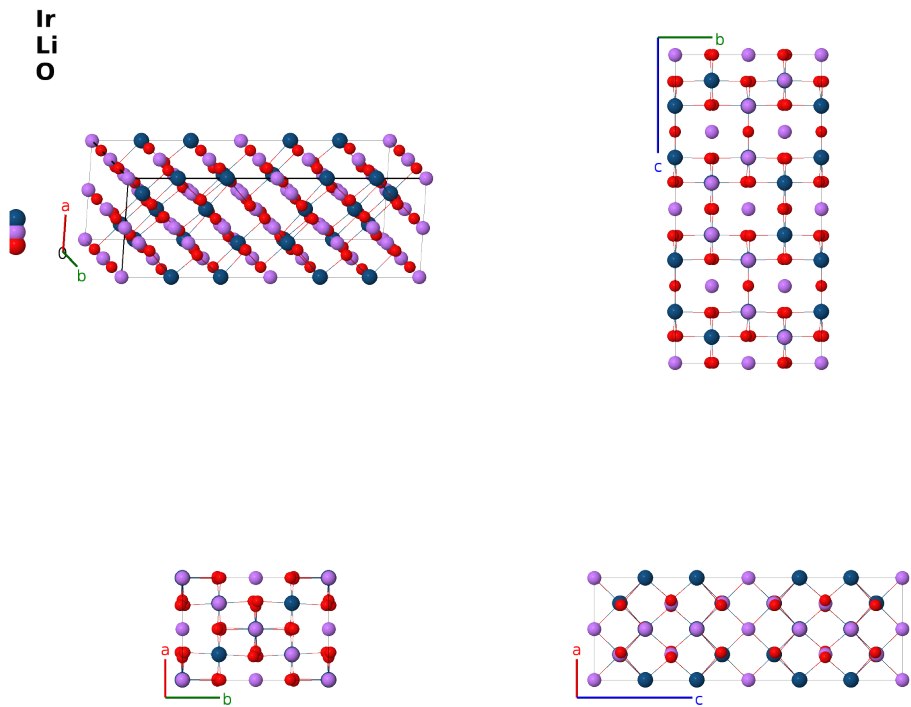
AB2C3_oC96_66_ik_cdj2k_gl2m-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/9VYY>

https://aflow.org/prototype-encyclopedia/AB2C3_oC96_66_ik_cdj2k_gl2m-001



Prototype	IrLi ₂ O ₃
AFLOW prototype label	AB2C3_oC96_66_ik_cdj2k_gl2m-001
Pearson symbol	oC96
Space group number	66
Space group symbol	<i>Cccm</i>
AFLOW prototype command	<code>aflow --proto=AB2C3_oC96_66_ik_cdj2k_gl2m-001</code> <code>--params=a, b/a, c/a, x₃, z₄, z₅, z₆, z₇, z₈, x₉, y₉, x₁₀, y₁₀, z₁₀, x₁₁, y₁₁, z₁₁</code>

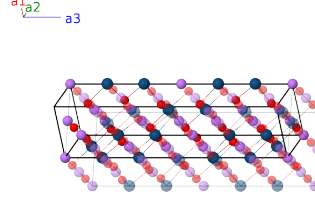
- Li₂IrO₃ can be found in three structures (Choi, 2020):
 - α -Li₂IrO₃, which is isostructural with Na₂PrO₃,

- β -Li₂IrO₃, which is isostructural with β -Na₂PtO₃, and
- the current structure, γ -Li₂IrO₃.

- 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

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



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
$\mathbf{B}_{10}$	$-(z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	Ir I
$\mathbf{B}_{11}$	$-z_4 \mathbf{a}_3$	$=$	$-cz_4 \hat{\mathbf{z}}$	(8i)	Ir I
$\mathbf{B}_{12}$	$(z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{16}$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{18}$	$\frac{1}{2} \mathbf{a}_1 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{20}$	$\frac{1}{2} \mathbf{a}_1 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{22}$	$\frac{1}{2} \mathbf{a}_1 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{24}$	$\frac{1}{2} \mathbf{a}_1 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{26} =$	$\frac{1}{2} \mathbf{a}_1 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - \frac{1}{4} b \hat{\mathbf{y}} - c (z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{28} =$	$\frac{1}{2} \mathbf{a}_1 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - \frac{1}{4} b \hat{\mathbf{y}} + c (z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{35} =$	$-(x_{10} + y_{10}) \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - c (z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(16m)	O III
$\mathbf{B}_{36} =$	$(x_{10} + y_{10}) \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - c (z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{39} =$	$(x_{10} + y_{10}) \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c (z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(16m)	O III
$\mathbf{B}_{40} =$	$-(x_{10} + y_{10}) \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + c (z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{43} =$	$-(x_{11} + y_{11}) \mathbf{a}_1 - (x_{11} - y_{11}) \mathbf{a}_2 - (z_{11} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - c (z_{11} - \frac{1}{2}) \hat{\mathbf{z}}$	(16m)	O IV
$\mathbf{B}_{44} =$	$(x_{11} + y_{11}) \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 - (z_{11} - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - c (z_{11} - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{47} =$	$(x_{11} + y_{11}) \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + c (z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(16m)	O IV
$\mathbf{B}_{48} =$	$-(x_{11} + y_{11}) \mathbf{a}_1 - (x_{11} - y_{11}) \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + c (z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(16m)	O IV

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- [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 -Li₂IrO₃ investigated by high-pressure Raman scattering*, Phys. Rev. B **101**, 054120 (2020), doi:10.1103/PhysRevB.101.054102.

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