

Li₂MnO₃ Structure:

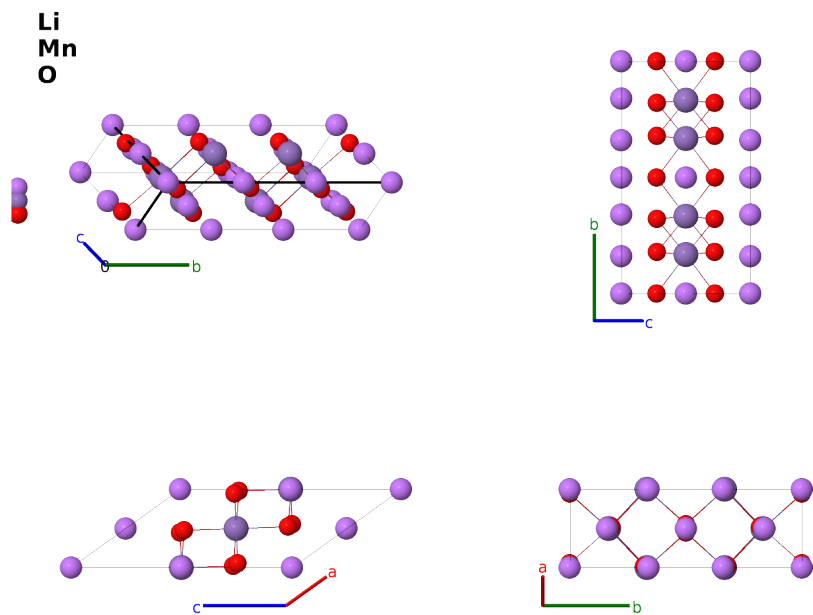
A2BC3_mC24_12_acg_h_ij-002

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<https://aflow.org/prototype-encyclopedia/R3L4>

https://aflow.org/prototype-encyclopedia/A2BC3_mC24_12_acg_h_ij-002



Prototype	Li ₂ MnO ₃
AFLOW prototype label	A2BC3_mC24_12_acg_h_ij-002
ICSD	202639
CCDC	1707205
Pearson symbol	mC24
Space group number	12
Space group symbol	<i>C</i> 2/ <i>m</i>
AFLOW prototype command	<code>aflow --proto=A2BC3_mC24_12_acg_h_ij-002</code> <code>--params=a, b/a, c/a, β, y₃, y₄, x₅, z₅, x₆, y₆, z₆</code>

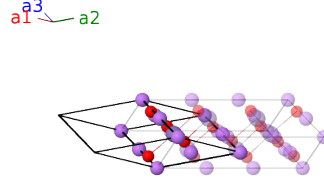
Other compounds with this structure

Li₂IrO₃, Li₂PtO₃, Na₂IrO₃

- This seems to be the consensus structure for these compounds. Others place them in space group $C2/c$ #15, possibly with a doubled unit cell.

Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(2a)	Li I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(2c)	Li II
$\mathbf{B}_3$	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$by_3 \hat{\mathbf{y}}$	(4g)	Li III
$\mathbf{B}_4$	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-by_3 \hat{\mathbf{y}}$	(4g)	Li III
$\mathbf{B}_5$	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	Mn I
$\mathbf{B}_6$	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	Mn I
$\mathbf{B}_7$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	O I
$\mathbf{B}_8$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	O I
$\mathbf{B}_9$	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(8j)	O II
$\mathbf{B}_{10}$	$-(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(8j)	O II
$\mathbf{B}_{11}$	$-(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(8j)	O II
$\mathbf{B}_{12}$	$(x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(8j)	O II

References

- [1] P. Strobel and B. Lambert-Andron, *Crystallographic and Magnetic Structure of Li_2MnO_3* , J. Solid State Chem. **75**, 90–98 (1988), doi:10.1016/0022-4596(88)90305-2.

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