Li_2MnO_3 Structure: A2BC3_mC24_12_acg_h_ij-002

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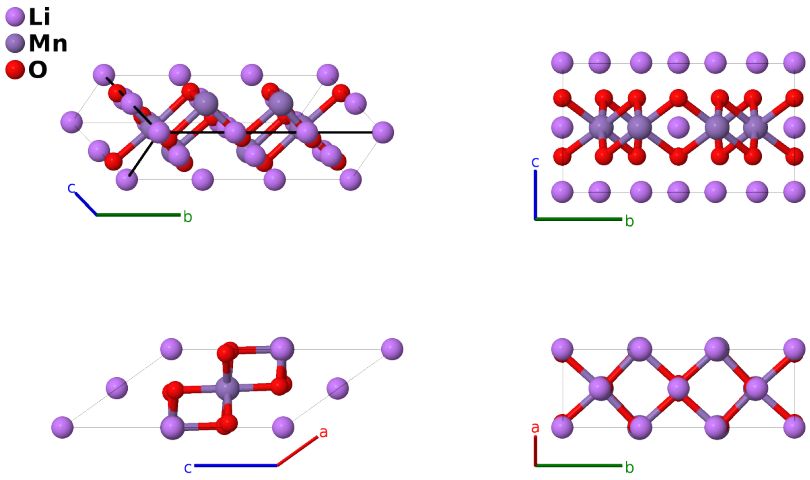
https://aflow.org/p/R3L4

https://aflow.org/p/A2BC3_mC24_12_acg_h_ij-002



Prototype	Li_2MnO_3
AFLOW prototype label	A2BC3_mC24_12_acg_h_ij-002
ICSD	202639
Pearson symbol	mC24
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A2BC3_mC24_12_acg_h_ij-002 --params=`$a, b/a, c/a, \beta, y_3, y_4, x_5, z_5, x_6, y_6, z_6$

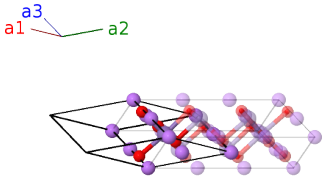
Other compounds with this structure

Li_2IrO_3, Li_2PtO_3, Na_2IrO_3

- 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



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.