$Li_2Mn_3O_7$ Structure: ABC2_hR4_166_a_b_c-011

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, 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.

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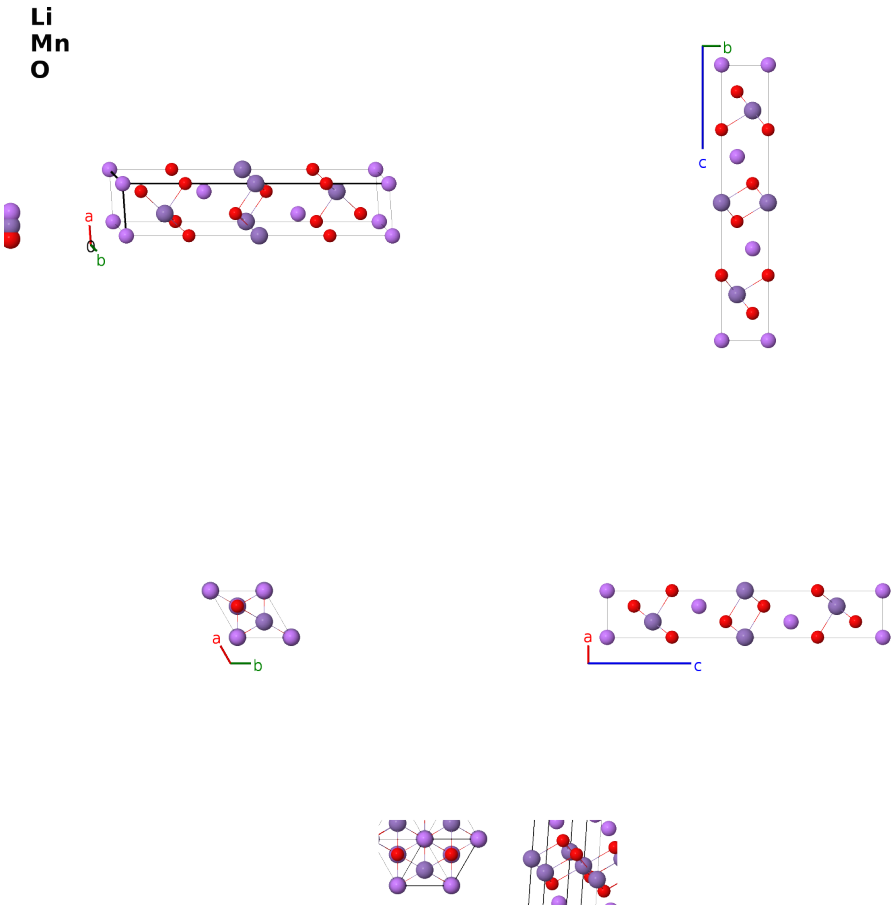
https://aflow.org/prototype-encyclopedia/FWBA

https://aflow.org/prototype-encyclopedia/ABC2_hR4_166_a_b_c-011

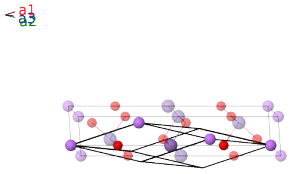


Prototype	$Li_2Mn_3O_7$
AFLOW prototype label	ABC2_hR4_166_a_b_c-011
ICSD	92859
CCDC	1652340
Pearson symbol	hR4
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=ABC2_hR4_166_a_b_c-011 --params=`$a, c/a, x_3$

- The given stoichiometry is approximate, the lithium site is only 48% occupied and the manganese site 89%, so the true stoichiometry is $Li_{1.62}Mn_3O_{6.74}$.
- (Raekelboom, 2001) label Li as being on the (3a) site and Mn on the (3b) site, but give the coordinates for (1b) and (1a) respectively. The ICSD uses the coordinates, not the labels, and we follow them.
- However, the AFLOW Label standard shifts the origin of the z-axis by 1/2 c, putting the lithium and manganese atoms on the (1a) and (1b) site and shifting z_3 from 0.2646 to 0.7646.
- The ICSD assigns this to the $NaFeO_2$ structure type, but we feel the vacancies warrant putting it into its own AFLOW prototype.
- α-$NaFeO_2$, rhombohedral delafossite, $CuFeO_2$, caswellsilverite ($F5_1$), $LiNiO_2$ and $Li_2Mn_3O_7$ have the same prototype label, ABC2_hR4_166_a_b_c. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Li I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Mn I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	O I

References

[1] E. A. Raekelboom, A. L. Hector, J. Owen, G. Vitins, and M. T. Weller, *Syntheses, Structures, and Preliminary Electrochemistry of the Layered Lithium and Sodium Manganese(IV) Oxides, $A_2Mn_3O_7$*, Chem. of Mater. **13**, 4618–4623 (2001), doi:10.1021/cm011105j.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5.* Submitted to Computational Materials Science (2026).