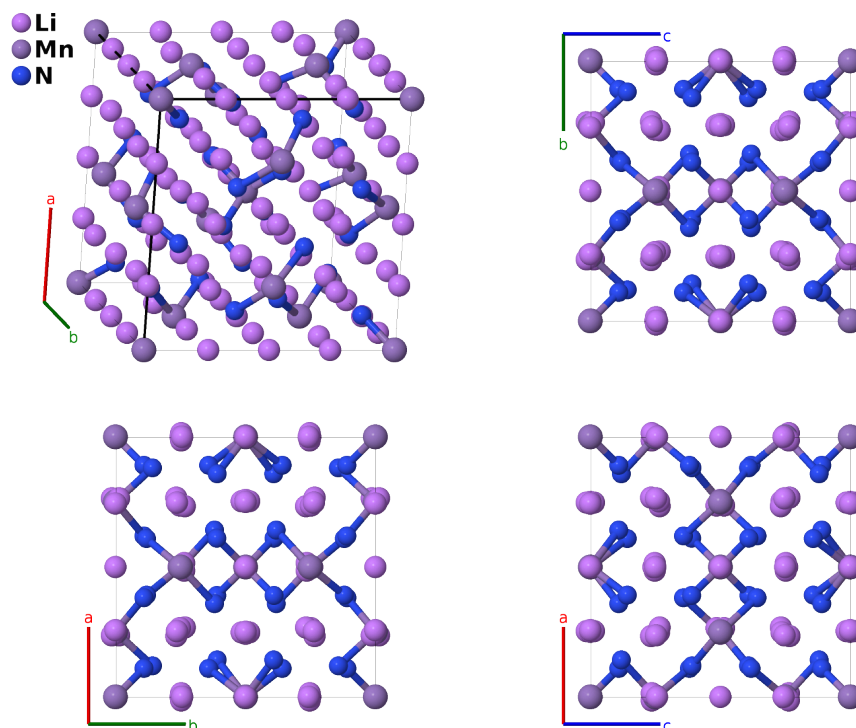


# Li<sub>7</sub>MnN<sub>4</sub> Structure: A7BC4\_cP96\_218\_bcefi\_ad\_ei-001

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<https://aflow.org/p/HJWV>

[https://aflow.org/p/A7BC4\\_cP96\\_218\\_bcefi\\_ad\\_ei-001](https://aflow.org/p/A7BC4_cP96_218_bcefi_ad_ei-001)



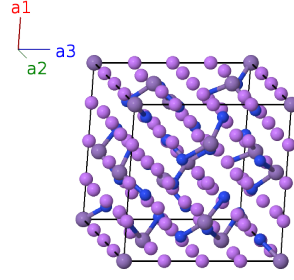
Prototype	Li <sub>7</sub> MnN <sub>4</sub>
AFLOW prototype label	A7BC4_cP96_218_bcefi_ad_ei-001
ICSD	154076
Pearson symbol	cP96
Space group number	218
Space group symbol	$P\bar{4}3n$
AFLOW prototype command	<code>aflow --proto=A7BC4_cP96_218_bcefi_ad_ei-001 --params=a, x<sub>5</sub>, x<sub>6</sub>, x<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub>, x<sub>9</sub>, y<sub>9</sub>, z<sub>9</sub></code>

## Other compounds with this structure

Li<sub>7</sub>PN<sub>4</sub>, Li<sub>7</sub>VN<sub>4</sub>

## Simple Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	$0$	(2a)	Mn I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(2a)	Mn I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6b)	Li I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6b)	Li I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6b)	Li I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(6b)	Li I
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(6b)	Li I
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{z}}$	(6b)	Li I
$\mathbf{B}_9$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6c)	Li II
$\mathbf{B}_{10}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6c)	Li II
$\mathbf{B}_{11}$	$= \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6c)	Li II
$\mathbf{B}_{12}$	$= \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6c)	Li II
$\mathbf{B}_{13}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6c)	Li II
$\mathbf{B}_{14}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6c)	Li II
$\mathbf{B}_{15}$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6d)	Mn II
$\mathbf{B}_{16}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6d)	Mn II
$\mathbf{B}_{17}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(6d)	Mn II
$\mathbf{B}_{18}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(6d)	Mn II
$\mathbf{B}_{19}$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6d)	Mn II
$\mathbf{B}_{20}$	$= \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6d)	Mn II
$\mathbf{B}_{21}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(8e)	Li III
$\mathbf{B}_{22}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(8e)	Li III
$\mathbf{B}_{23}$	$= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(8e)	Li III
$\mathbf{B}_{24}$	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(8e)	Li III
$\mathbf{B}_{25}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Li III
$\mathbf{B}_{26}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Li III
$\mathbf{B}_{27}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Li III





$$\begin{aligned}
\mathbf{B}_{91} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_2 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24i) & \text{N II} \\
\mathbf{B}_{92} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_2 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24i) & \text{N II} \\
\mathbf{B}_{93} &= \left(z_9 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_9 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(z_9 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24i) & \text{N II} \\
\mathbf{B}_{94} &= \left(z_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_9 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(z_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24i) & \text{N II} \\
\mathbf{B}_{95} &= -\left(z_9 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_9 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24i) & \text{N II} \\
\mathbf{B}_{96} &= -\left(z_9 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_9 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24i) & \text{N II}
\end{aligned}$$

## References

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