

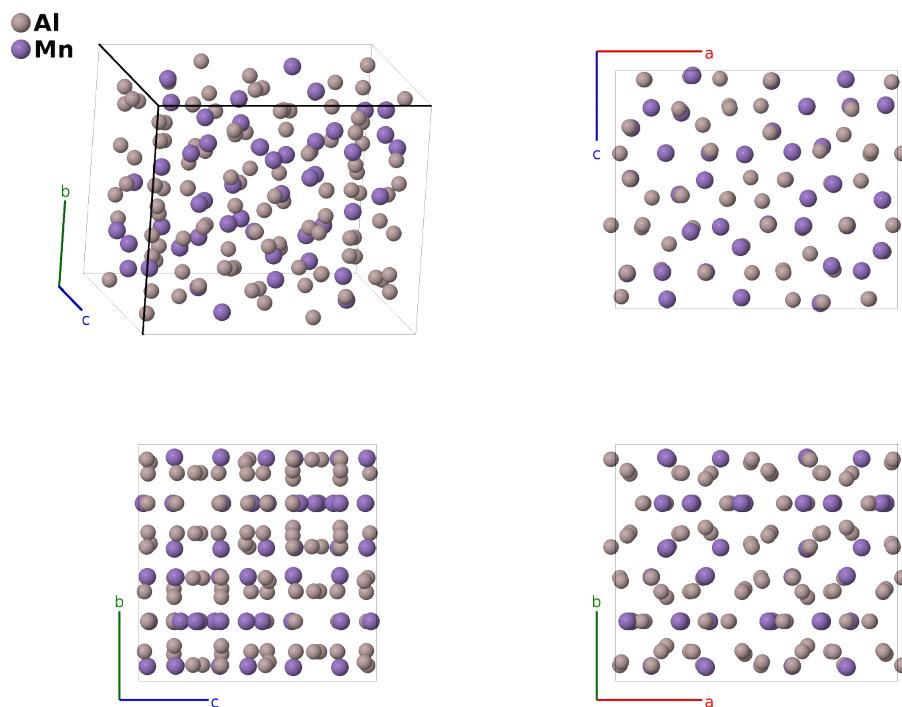
Al₃Mn Structure:

A9B4_oP156_62_5c11d_6c3d-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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

https://aflow.org/p/A9B4_oP156_62_5c11d_6c3d-001



Prototype	Al ₃ Mn
AFLOW prototype label	A9B4_oP156_62_5c11d_6c3d-001
ICSD	105512
Pearson symbol	oP156
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<pre>aflow --proto=A9B4_oP156_62_5c11d_6c3d-001 --params=a, b/a, c/a, x1, z1, x2, z2, x3, z3, x4, z4, x5, z5, x6, z6, x7, z7, x8, z8, x9, z9, x10, z10, x11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17, z17, x18, y18, z18, x19, y19, z19, x20, y20, z20, x21, y21, z21, x22, y22, z22, x23, y23, z23, x24, y24, z24, x25, y25, z25</pre>

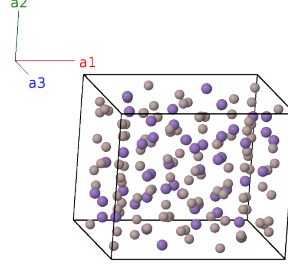
- While all sites are fully occupied, there is some mixing of aluminum and manganese atoms:
 - The Mn-V site is 70% Mn and 30% Al,
 - The Mn-VI site is 80% Mn and 20% Al,

- The Al-VI site is 10% Mn and 90% Al,
- The Mn-VIII site is 50% Mn and 50% Al, and
- The Mn-IX site is 60% Mn and 40% Al.

- This gives a final composition of $\text{Al}_{2.94}\text{Mn}$.

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	Al I
\mathbf{B}_2	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Al I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	Al I
\mathbf{B}_4	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Al I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	Al II
\mathbf{B}_6	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Al II
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	Al II
\mathbf{B}_8	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Al II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Al III
\mathbf{B}_{10}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Al III
\mathbf{B}_{11}	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	Al III
\mathbf{B}_{12}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Al III
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	Al IV
\mathbf{B}_{14}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Al IV
\mathbf{B}_{15}	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	Al IV
\mathbf{B}_{16}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Al IV
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	Al V
\mathbf{B}_{18}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Al V
\mathbf{B}_{19}	$= -x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4c)	Al V
\mathbf{B}_{20}	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Al V
\mathbf{B}_{21}	$= x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	Mn I

$$\begin{aligned}
\mathbf{B}_{144} &= \begin{pmatrix} (x_{24} + \frac{1}{2}) \mathbf{a}_1 - (y_{24} - \frac{1}{2}) \mathbf{a}_2 - \\ (z_{24} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a(x_{24} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{24} - \frac{1}{2}) \hat{\mathbf{y}} - \\ c(z_{24} - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (8d) & \text{Mn VIII} \\
\mathbf{B}_{145} &= -x_{24} \mathbf{a}_1 - y_{24} \mathbf{a}_2 - z_{24} \mathbf{a}_3 = -ax_{24} \hat{\mathbf{x}} - by_{24} \hat{\mathbf{y}} - cz_{24} \hat{\mathbf{z}} & (8d) & \text{Mn VIII} \\
\mathbf{B}_{146} &= \begin{pmatrix} (x_{24} + \frac{1}{2}) \mathbf{a}_1 + y_{24} \mathbf{a}_2 - \\ (z_{24} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a(x_{24} + \frac{1}{2}) \hat{\mathbf{x}} + by_{24} \hat{\mathbf{y}} - c(z_{24} - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (8d) & \text{Mn VIII} \\
\mathbf{B}_{147} &= x_{24} \mathbf{a}_1 - (y_{24} - \frac{1}{2}) \mathbf{a}_2 + z_{24} \mathbf{a}_3 = ax_{24} \hat{\mathbf{x}} - b(y_{24} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{24} \hat{\mathbf{z}} & (8d) & \text{Mn VIII} \\
\mathbf{B}_{148} &= -\begin{pmatrix} (x_{24} - \frac{1}{2}) \mathbf{a}_1 + (y_{24} + \frac{1}{2}) \mathbf{a}_2 + \\ (z_{24} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(x_{24} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{24} + \frac{1}{2}) \hat{\mathbf{y}} + \\ & c(z_{24} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Mn VIII} \\
\mathbf{B}_{149} &= x_{25} \mathbf{a}_1 + y_{25} \mathbf{a}_2 + z_{25} \mathbf{a}_3 = ax_{25} \hat{\mathbf{x}} + by_{25} \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} & (8d) & \text{Mn IX} \\
\mathbf{B}_{150} &= -\begin{pmatrix} (x_{25} - \frac{1}{2}) \mathbf{a}_1 - y_{25} \mathbf{a}_2 + \\ (z_{25} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(x_{25} - \frac{1}{2}) \hat{\mathbf{x}} - by_{25} \hat{\mathbf{y}} + c(z_{25} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Mn IX} \\
\mathbf{B}_{151} &= -x_{25} \mathbf{a}_1 + (y_{25} + \frac{1}{2}) \mathbf{a}_2 - z_{25} \mathbf{a}_3 = -ax_{25} \hat{\mathbf{x}} + b(y_{25} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{25} \hat{\mathbf{z}} & (8d) & \text{Mn IX} \\
\mathbf{B}_{152} &= \begin{pmatrix} (x_{25} + \frac{1}{2}) \mathbf{a}_1 - (y_{25} - \frac{1}{2}) \mathbf{a}_2 - \\ (z_{25} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a(x_{25} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{25} - \frac{1}{2}) \hat{\mathbf{y}} - \\ c(z_{25} - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (8d) & \text{Mn IX} \\
\mathbf{B}_{153} &= -x_{25} \mathbf{a}_1 - y_{25} \mathbf{a}_2 - z_{25} \mathbf{a}_3 = -ax_{25} \hat{\mathbf{x}} - by_{25} \hat{\mathbf{y}} - cz_{25} \hat{\mathbf{z}} & (8d) & \text{Mn IX} \\
\mathbf{B}_{154} &= \begin{pmatrix} (x_{25} + \frac{1}{2}) \mathbf{a}_1 + y_{25} \mathbf{a}_2 - \\ (z_{25} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a(x_{25} + \frac{1}{2}) \hat{\mathbf{x}} + by_{25} \hat{\mathbf{y}} - c(z_{25} - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (8d) & \text{Mn IX} \\
\mathbf{B}_{155} &= x_{25} \mathbf{a}_1 - (y_{25} - \frac{1}{2}) \mathbf{a}_2 + z_{25} \mathbf{a}_3 = ax_{25} \hat{\mathbf{x}} - b(y_{25} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} & (8d) & \text{Mn IX} \\
\mathbf{B}_{156} &= -\begin{pmatrix} (x_{25} - \frac{1}{2}) \mathbf{a}_1 + (y_{25} + \frac{1}{2}) \mathbf{a}_2 + \\ (z_{25} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(x_{25} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{25} + \frac{1}{2}) \hat{\mathbf{y}} + \\ & c(z_{25} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Mn IX}
\end{aligned}$$

References

- [1] K. Hiraga, M. Kaneko, Y. Matsuo, and S. Hashimoto, *The structure of Al_3Mn : Close relationship to decagonal quasicrystals*, *Phil. Mag. B* **67**, 193–205 (1993), doi:10.1080/13642819308207867.