

Al₉Mn₃Si (*E9_c*) Structure: A9B3C_hP26_194_hk_h_a-001

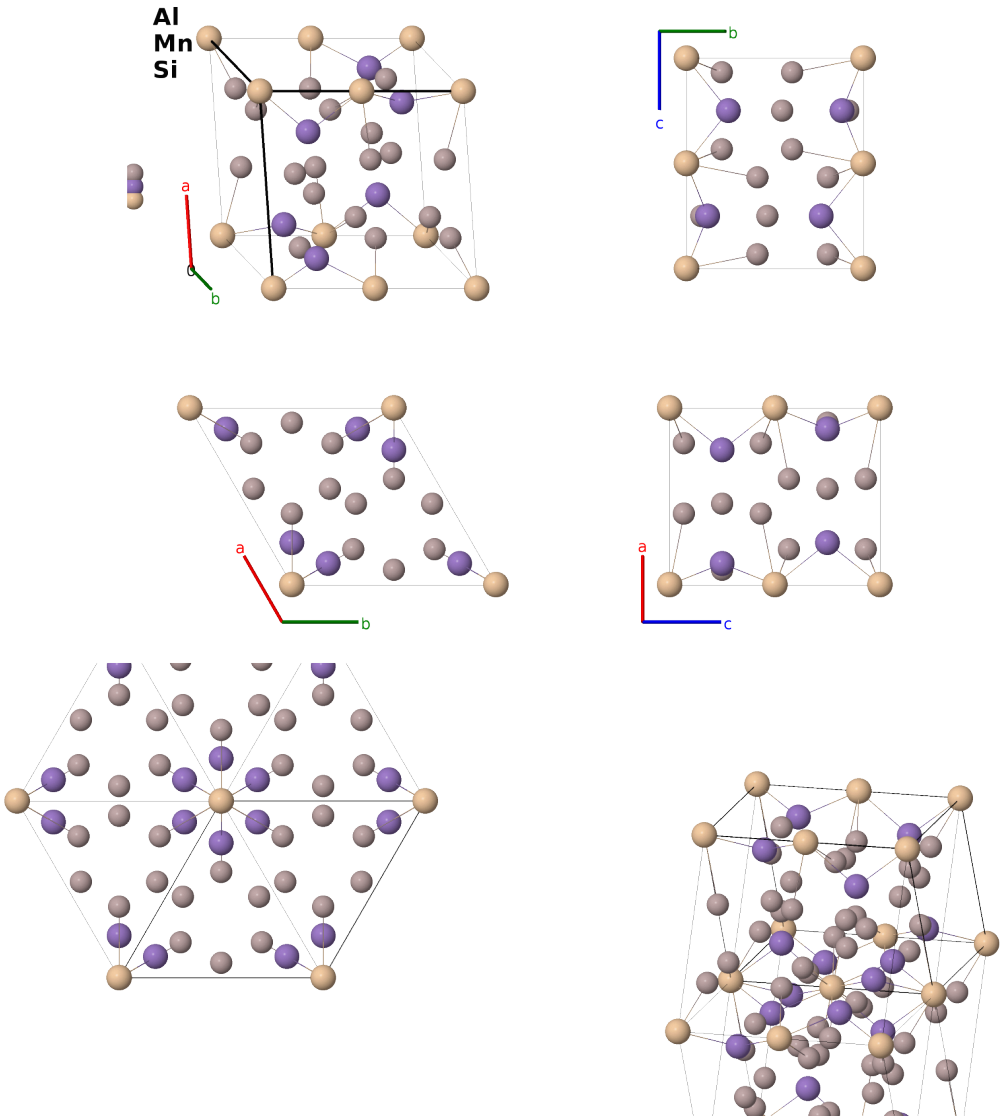
This structure previously used the label(s) **A9B3C_hP26_194_hk_h_a**. Calls to these addresses will be redirected here.

Cite this page as:

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- 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.

<https://aflow.org/prototype-encyclopedia/KM59>

https://aflow.org/prototype-encyclopedia/A9B3C_hP26_194_hk_h_a-001



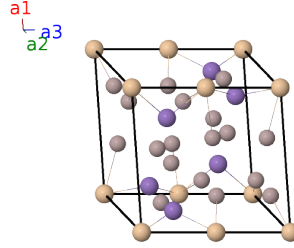
Prototype	Al ₉ Mn ₃ Si
AFLOW prototype label	A9B3C_hP26_194_hk_h_a-001
Strukturbericht designation	<i>E9_c</i>

ICSD	76249
CCDC	1636861
Pearson symbol	hP26
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=A9B3C_hP26_194_hk_h_a-001</code> <code>--params=a, c/a, x₂, x₃, x₄, z₄</code>

- The previous version of this page (Hicks, 2019) used scattered sources for the input data. We have now updated this page using the complete data from (Robinson, 1952).
- This structure is also referred to as $\beta(\text{AlMnSi})$.

Hexagonal primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(2a)	Si I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(2a)	Si I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_4$	$-2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_5$	$x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_6$	$-x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_7$	$2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_8$	$-x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\sqrt{3}ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Al I
$\mathbf{B}_9$	$x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Mn I
$\mathbf{B}_{10}$	$-2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Mn I
$\mathbf{B}_{11}$	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Mn I
$\mathbf{B}_{12}$	$-x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Mn I
$\mathbf{B}_{13}$	$2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Mn I
$\mathbf{B}_{14}$	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\sqrt{3}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Mn I
$\mathbf{B}_{15}$	$x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12k)	Al II
$\mathbf{B}_{16}$	$-2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12k)	Al II

$$\begin{aligned}
\mathbf{B}_{17} &= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= -\sqrt{3}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} &(12k) &\text{Al II} \\
\mathbf{B}_{18} &= -x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 &= -\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\text{Al II} \\
\mathbf{B}_{19} &= 2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\text{Al II} \\
\mathbf{B}_{20} &= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 &= \sqrt{3}ax_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\text{Al II} \\
\mathbf{B}_{21} &= 2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(12k) &\text{Al II} \\
\mathbf{B}_{22} &= -x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(12k) &\text{Al II} \\
\mathbf{B}_{23} &= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \sqrt{3}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(12k) &\text{Al II} \\
\mathbf{B}_{24} &= -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 &= -\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\text{Al II} \\
\mathbf{B}_{25} &= x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 &= \frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\text{Al II} \\
\mathbf{B}_{26} &= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 &= -\sqrt{3}ax_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\text{Al II}
\end{aligned}$$

References

- [1] K. Robinson, *The Structure of $\beta(\text{AlMnSi}) - \text{Mn}_3\text{SiAl}_9$* , Acta Cryst. **5**, 397–403 (1952), doi:10.1107/S0365110X52001246.

Found in

- [1] G. T. de Laissardière, *Interplay between electronic structure and medium-range atomic order in hexagonal $\beta\text{-Al}_9\text{Mn}_3\text{Si}$ and $\psi\text{-Al}_40\text{Mn}_3$ crystals*, Phys. Rev. B **68**, 045117 (2003), doi:10.1103/PhysRevB.68.045117.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043