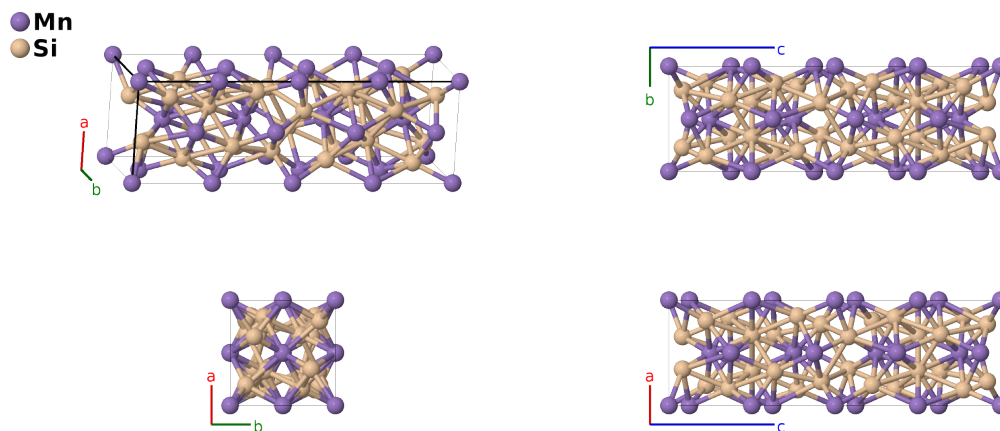


Mn₄Ge₇ Nowotny Chimney-Ladder Structure: A4B7_tP44_116_ach2i_e3j-001

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<https://afLOW.org/p/2NXF>

https://afLOW.org/p/A4B7_tP44_116_ach2i_e3j-001

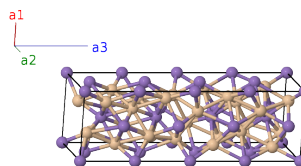


Prototype	Mn ₄ Si ₇
AFLOW prototype label	A4B7_tP44_116_ach2i_e3j-001
ICSD	20323
Pearson symbol	tP44
Space group number	116
Space group symbol	$P\bar{4}c2$
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- This is an example of a “Nowotny chimney-ladder structure” (Pearson, 1970), T_nX_m, where “T” is a transition metal, “X” is a row III or IV metal (or semiconductor), and $1.25 \leq m/n < 2$. The transition metal atoms are arranged similarly to the atoms in the β-Sn (A5).

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} c \hat{\mathbf{z}}$	(2a)	Mn I
\mathbf{B}_2	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} c \hat{\mathbf{z}}$	(2a)	Mn I
\mathbf{B}_3	$= 0$	$=$	0	(2c)	Mn II
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2c)	Mn II
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4e)	Si I
\mathbf{B}_6	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4e)	Si I
\mathbf{B}_7	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4e)	Si I
\mathbf{B}_8	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4e)	Si I
\mathbf{B}_9	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4h)	Mn III
\mathbf{B}_{10}	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4h)	Mn III
\mathbf{B}_{11}	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Mn III
\mathbf{B}_{12}	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c (z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Mn III
\mathbf{B}_{13}	$= \frac{1}{2} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4i)	Mn IV
\mathbf{B}_{14}	$= \frac{1}{2} \mathbf{a}_1 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_5 \hat{\mathbf{z}}$	(4i)	Mn IV
\mathbf{B}_{15}	$= \frac{1}{2} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4i)	Mn IV
\mathbf{B}_{16}	$= \frac{1}{2} \mathbf{a}_1 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - c (z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4i)	Mn IV
\mathbf{B}_{17}	$= \frac{1}{2} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4i)	Mn V
\mathbf{B}_{18}	$= \frac{1}{2} \mathbf{a}_1 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_6 \hat{\mathbf{z}}$	(4i)	Mn V
\mathbf{B}_{19}	$= \frac{1}{2} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4i)	Mn V
\mathbf{B}_{20}	$= \frac{1}{2} \mathbf{a}_1 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - c (z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(4i)	Mn V
\mathbf{B}_{21}	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8j)	Si II
\mathbf{B}_{22}	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8j)	Si II
\mathbf{B}_{23}	$= y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8j)	Si II
\mathbf{B}_{24}	$= -y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8j)	Si II
\mathbf{B}_{25}	$= x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Si II
\mathbf{B}_{26}	$= -x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Si II
\mathbf{B}_{27}	$= y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - c (z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Si II
\mathbf{B}_{28}	$= -y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - c (z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Si II
\mathbf{B}_{29}	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8j)	Si III
\mathbf{B}_{30}	$= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8j)	Si III
\mathbf{B}_{31}	$= y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8j)	Si III
\mathbf{B}_{32}	$= -y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8j)	Si III
\mathbf{B}_{33}	$= x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + c (z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Si III
\mathbf{B}_{34}	$= -x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + c (z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Si III
\mathbf{B}_{35}	$= y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - c (z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Si III
\mathbf{B}_{36}	$= -y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - c (z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Si III
\mathbf{B}_{37}	$= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8j)	Si IV
\mathbf{B}_{38}	$= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8j)	Si IV
\mathbf{B}_{39}	$= y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$ay_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8j)	Si IV

$$\begin{aligned}
\mathbf{B}_{40} &= -y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 &= -ay_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (8j) & \text{Si IV} \\
\mathbf{B}_{41} &= x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8j) & \text{Si IV} \\
\mathbf{B}_{42} &= -x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8j) & \text{Si IV} \\
\mathbf{B}_{43} &= y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= ay_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8j) & \text{Si IV} \\
\mathbf{B}_{44} &= -y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= -ay_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8j) & \text{Si IV}
\end{aligned}$$

References

- [1] O. G. Karpinskii and B. A. Evseev, *Crystal Structure of the Compound Mn₄Si₇*, in *Chemical Bonds in Solids*, edited by N. N. Sirota (Consultants Bureau, New York – London, 1972), vol. 4, pp. 3–7. Proceedings of the International Symposium on Chemical Bonds in Semiconducting Crystals, Minsk, USSR, 1967.
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