

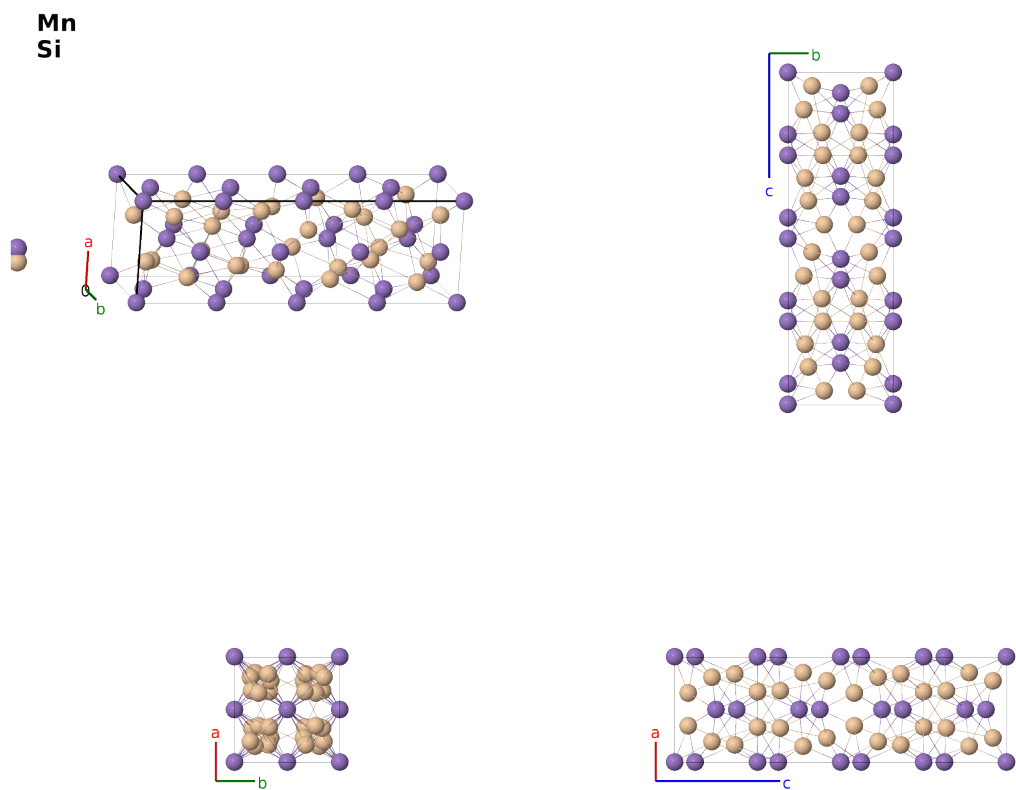
Mn₄Ge₇ Nowotny Chimney-Ladder Structure: A4B7_tP44_116_ach2i_e3j-001

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<https://aflow.org/prototype-encyclopedia/2NXF>

https://aflow.org/prototype-encyclopedia/A4B7_tP44_116_ach2i_e3j-001



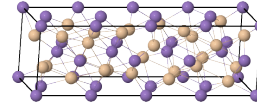
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ICSD	20323
CCDC	1598142
Pearson symbol	tP44
Space group number	116
Space group symbol	$P\bar{4}c2$

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- This 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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{25} =$	$x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Si II
$\mathbf{B}_{26} =$	$-x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Si II
$\mathbf{B}_{27} =$	$y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Si II
$\mathbf{B}_{28} =$	$-y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{33} =$	$x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Si III
$\mathbf{B}_{34} =$	$-x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Si III
$\mathbf{B}_{35} =$	$y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Si III
$\mathbf{B}_{36} =$	$-y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{40} =$	$-y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-ay_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8j)	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)	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)	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)	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)	Si IV

References

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- [2] O. G. Karpinskii and B. A. Evseev, *The crystal structure of the compound Mn_4Si_7* , *Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy* **5**, 525–529 (1969).
- [3] W. B. Pearson, *Phases with Nowotny chimney-ladder structures considered as ‘electron’ phases*, *Acta Crystallogr. Sect. B* **26**, 1044–1046 (1970), doi:10.1107/S0567740870003564.

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