

Mn₃Si₂Te₆ Structure:

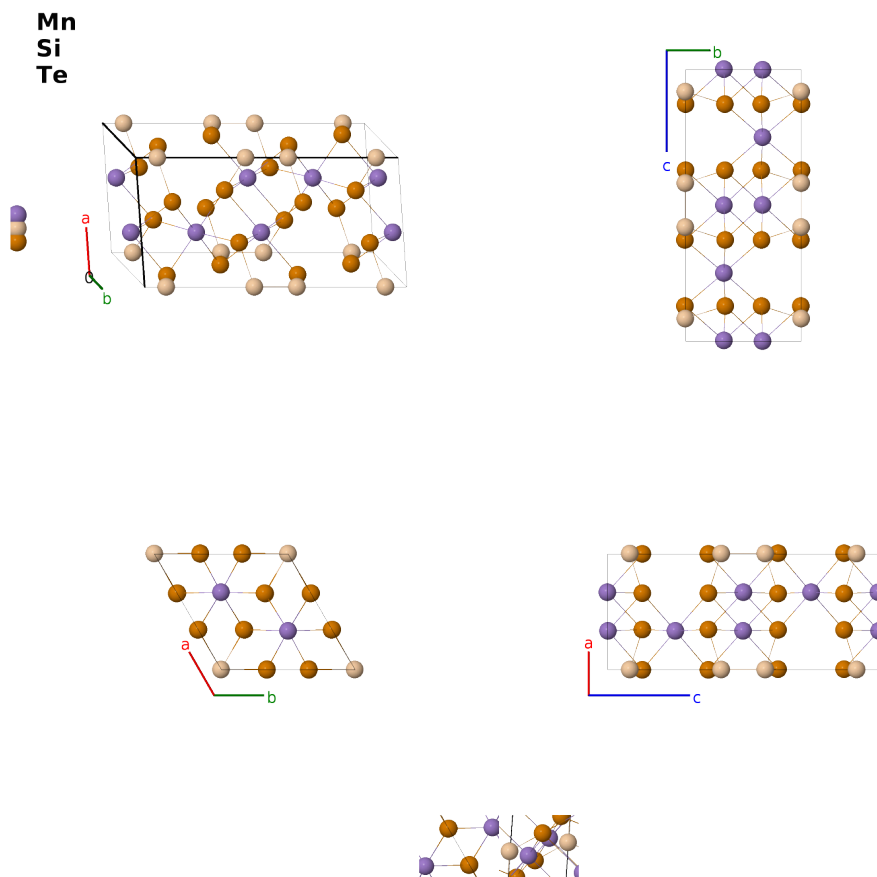
A3B2C6_hP22_163_cf_e_i-001

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<https://aflow.org/prototype-encyclopedia/ELB0>

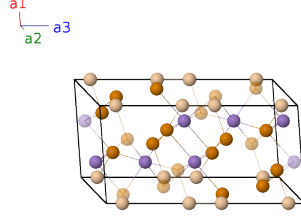
https://aflow.org/prototype-encyclopedia/A3B2C6_hP22_163_cf_e_i-001



Prototype	Mn ₃ Si ₂ Te ₆
AFLOW prototype label	A3B2C6_hP22_163_cf_e_i-001
ICSD	41021
CCDC	1610827
Pearson symbol	hP22
Space group number	163
Space group symbol	$P\bar{3}1c$
AFLOW prototype command	<code>aflow --proto=A3B2C6_hP22_163_cf_e_i-001 --params=a, c/a, z₂, z₃, x₄, y₄, z₄</code>

Trigonal (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
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Mn I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Mn I
$\mathbf{B}_3$	$= z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B}_4$	$= -\left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B}_5$	$= -z_2 \mathbf{a}_3$	$=$	$-cz_2 \hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B}_6$	$= \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B}_7$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4f)	Mn II
$\mathbf{B}_8$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4f)	Mn II
$\mathbf{B}_9$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4f)	Mn II
$\mathbf{B}_{10}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4f)	Mn II
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B}_{12}$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B}_{13}$	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B}_{14}$	$= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B}_{15}$	$= -(x_4 - y_4) \mathbf{a}_1 + y_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B}_{16}$	$= x_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B}_{17}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B}_{18}$	$= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B}_{19}$	$= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B}_{20}$	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B}_{21}$	$= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B}_{22}$	$= -x_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	Te I

References

- [1] H. Vincent, D. Leroux, D. Bijaoui, R. Rimet, and C. Schlenker, *Crystal Structure of $Mn_3Si_2Te_6$* , J. Solid State Chem. **63**, 349–352 (1986), doi:10.1016/0022-4596(86)90190-8.

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