Mn$_3$Si$_2$Te$_6$ Structure:
A3B2C6_hP22_163_cf_e_i-001

https://aflow.org/p/ELB0

https://aflow.org/p/A3B2C6_hP22_163_cf_e_i-001
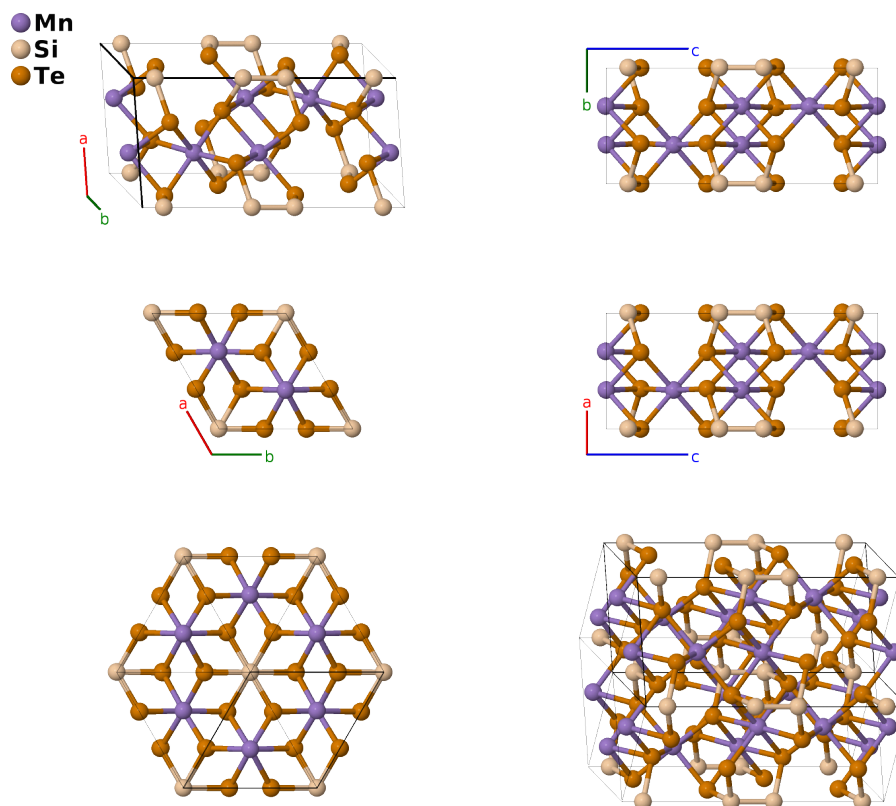
Prototype	Mn$_3$Si$_2$Te$_6$
AFLOW prototype label	A3B2C6_hP22_163_cf_e_i-001
ICSD	41021
Pearson symbol	hP22
Space group number	163
Space group symbol	$P\bar{3}1c$
AFLOW prototype command	aflow --proto=A3B2C6_hP22_163_cf_e_i-001 --params=$a, c/a, z_2, z_3, x_4, y_4, z_4$

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
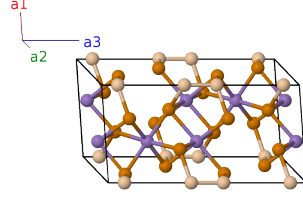
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Mn I
$\mathbf{B_2}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Mn I
$\mathbf{B_3}$	$=$	$z_2\,\mathbf{a_3}$	$=$	$cz_2\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_4}$	$=$	$-\left(z_2 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-c\left(z_2 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_5}$	$=$	$-z_2\,\mathbf{a_3}$	$=$	$-cz_2\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_6}$	$=$	$\left(z_2 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$c\left(z_2 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_7}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4f)	Mn II
$\mathbf{B_8}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} - \left(z_3 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	Mn II
$\mathbf{B_9}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4f)	Mn II
$\mathbf{B_{10}}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	Mn II
$\mathbf{B_{11}}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B_{12}}$	$=$	$-y_4\,\mathbf{a_1} + \left(x_4 - y_4\right)\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 - 2y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B_{13}}$	$=$	$-\left(x_4 - y_4\right)\mathbf{a_1} - x_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B_{14}}$	$=$	$-y_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B_{15}}$	$=$	$-\left(x_4 - y_4\right)\mathbf{a_1} + y_4\,\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(-x_4 + 2y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B_{16}}$	$=$	$x_4\,\mathbf{a_1} + \left(x_4 - y_4\right)\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B_{17}}$	$=$	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B_{18}}$	$=$	$y_4\,\mathbf{a_1} - \left(x_4 - y_4\right)\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(-x_4 + 2y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B_{19}}$	$=$	$\left(x_4 - y_4\right)\mathbf{a_1} + x_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B_{20}}$	$=$	$y_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B_{21}}$	$=$	$\left(x_4 - y_4\right)\mathbf{a_1} - y_4\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 - 2y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Te I
$\mathbf{B_{22}}$	$=$	$-x_4\,\mathbf{a_1} - \left(x_4 - y_4\right)\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(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.