

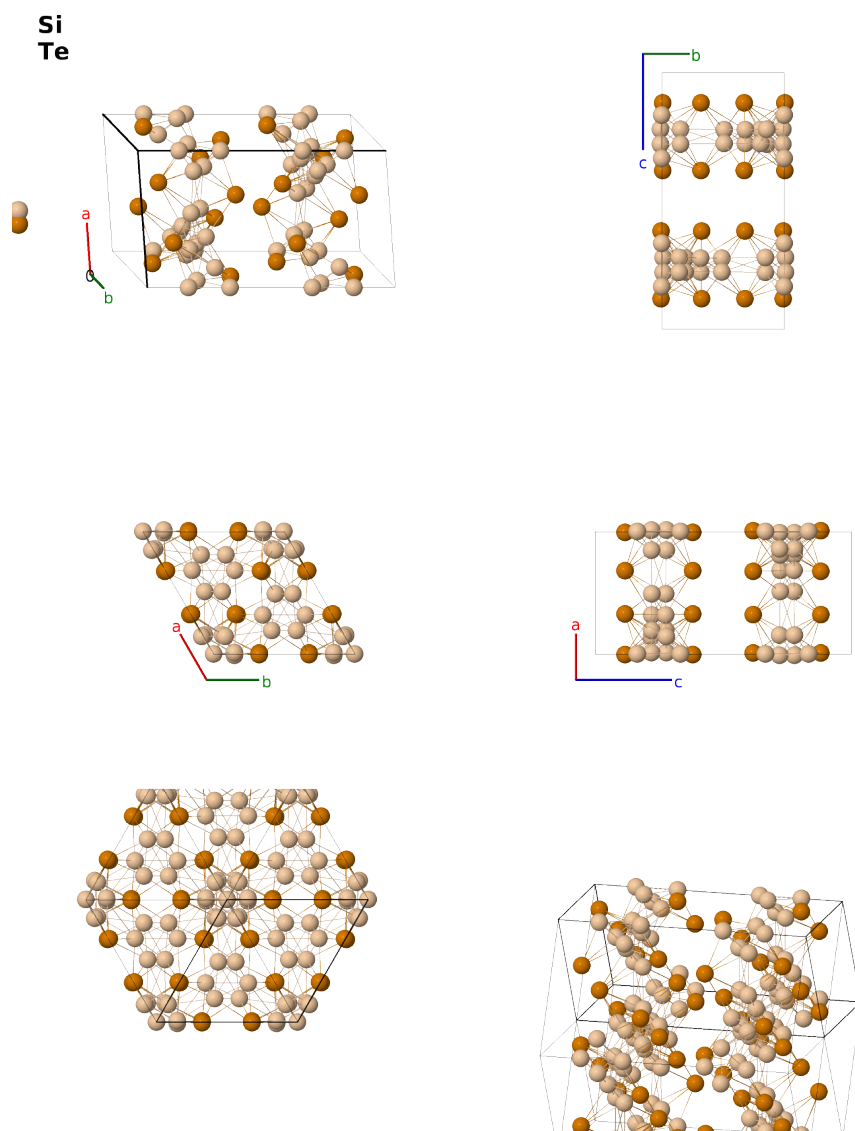
Si₂Te₃ Structure: A7B3_hP40_163_e2i_i-001

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

https://aflow.org/prototype-encyclopedia/A7B3_hP40_163_e2i_i-001



Prototype

Si₂Te₃

AFLOW prototype label

A7B3_hP40_163_e2i_i-001

ICSD

30071

CCDC

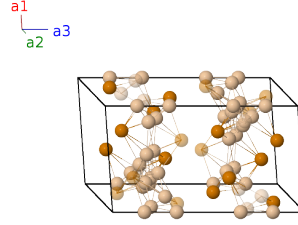
1604529

Pearson symbol	hP40
Space group number	163
Space group symbol	$P\bar{3}1c$
AFLOW prototype command	aflow --proto=A7B3_hP40_163_e2i_i-001 --params= $a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

- All of the silicon sites are only partially occupied: Si-I (4c) is 47% filled, Si-II (12i) 18%, and Si-III (12i) 33%.

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
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B}_2$	$= -\left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B}_3$	$= -z_1 \mathbf{a}_3$	$=$	$-c z_1 \hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B}_4$	$= \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_2 - y_2) \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B}_6$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B}_7$	$= -(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B}_8$	$= -y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_2 - y_2) \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B}_9$	$= -(x_2 - y_2) \mathbf{a}_1 + y_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_2 + 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B}_{10}$	$= x_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B}_{11}$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_2 - y_2) \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B}_{12}$	$= y_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_2 + 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_2 \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B}_{13}$	$= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_2 \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B}_{14}$	$= y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_2 - y_2) \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B}_{15}$	$= (x_2 - y_2) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_2 - 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B}_{16}$	$= -x_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B}_{17}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(12i)	Si III

$$\begin{aligned}
\mathbf{B}_{18} &= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3 = \frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}} & (12i) & \text{Si III} \\
\mathbf{B}_{19} &= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 = -\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}} & (12i) & \text{Si III} \\
\mathbf{B}_{20} &= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{Si III} \\
\mathbf{B}_{21} &= -(x_3 - y_3) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{Si III} \\
\mathbf{B}_{22} &= x_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{Si III} \\
\mathbf{B}_{23} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 = -\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} & (12i) & \text{Si III} \\
\mathbf{B}_{24} &= y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3 = \frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} & (12i) & \text{Si III} \\
\mathbf{B}_{25} &= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 = \frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} & (12i) & \text{Si III} \\
\mathbf{B}_{26} &= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{Si III} \\
\mathbf{B}_{27} &= (x_3 - y_3) \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{Si III} \\
\mathbf{B}_{28} &= -x_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{Si III} \\
\mathbf{B}_{29} &= 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) & \text{Te I} \\
\mathbf{B}_{30} &= -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) & \text{Te I} \\
\mathbf{B}_{31} &= -(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) & \text{Te I} \\
\mathbf{B}_{32} &= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \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(z_4 - \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{Te I} \\
\mathbf{B}_{33} &= -(x_4 - y_4) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{Te I} \\
\mathbf{B}_{34} &= x_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{Te I} \\
\mathbf{B}_{35} &= -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) & \text{Te I} \\
\mathbf{B}_{36} &= 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) & \text{Te I} \\
\mathbf{B}_{37} &= (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) & \text{Te I} \\
\mathbf{B}_{38} &= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \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(z_4 + \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{Te I} \\
\mathbf{B}_{39} &= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{Te I} \\
\mathbf{B}_{40} &= -x_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}} & (12i) & \text{Te I}
\end{aligned}$$

References

- [1] K. Ploog, W. Stetter, A. Nowitzki, and E. Schönherr, *Crystal growth and structure determination of silicon telluride Si_2Te_3* , Mater. Res. Bull. **11**, 1147–1154 (1976), doi:10.1016/0025-5408(76)90014-3.

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