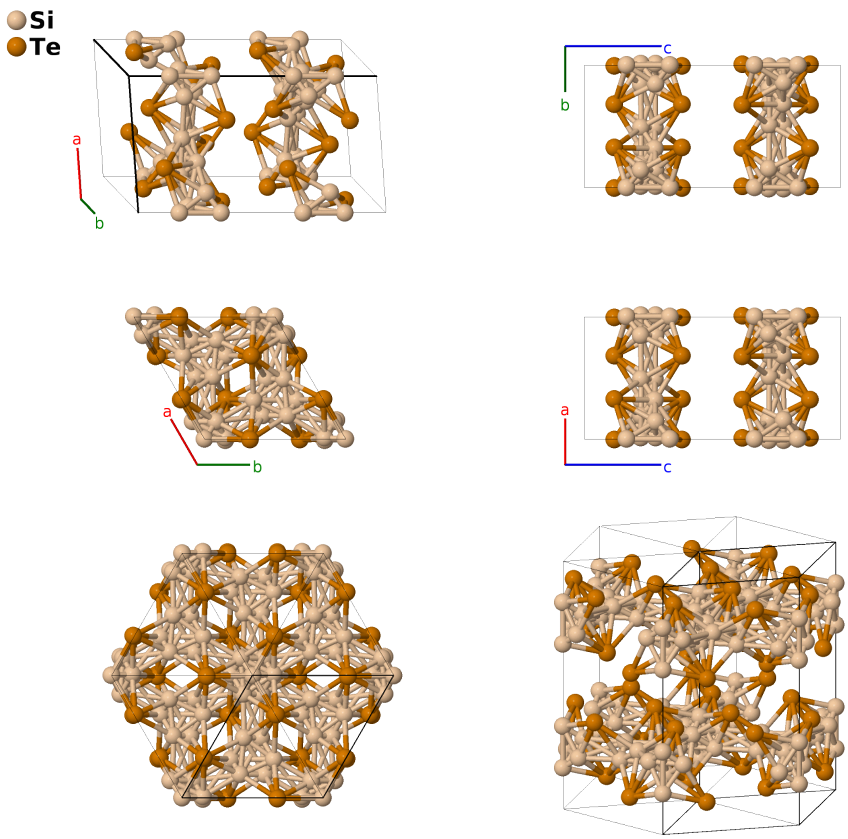
Si_2Te_3 Structure: A7B3_hP40_163_e2i_i-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

---

https://aflow.org/p/MVBJ

https://aflow.org/p/A7B3_hP40_163_e2i_i-001

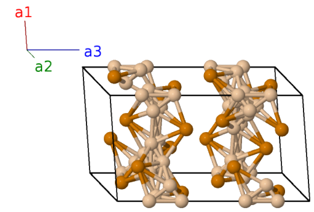


Prototype	Si_2Te_3
AFLOW prototype label	A7B3_hP40_163_e2i_i-001
ICSD	30071
Pearson symbol	hP40
Space group number	163
Space group symbol	$P\bar{3}1c$
AFLOW prototype command	`aflow --proto=A7B3_hP40_163_e2i_i-001` `--params=`$a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

- 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

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(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
$\mathbf{B_3}$	=	$-z_1\,\mathbf{a}_3$	=	$-cz_1\,\hat{\mathbf{z}}$	(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
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1+y_2\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_2+y_2\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\left(x_2-y_2\right)\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B_6}$	=	$-y_2\,\mathbf{a}_1+\left(x_2-y_2\right)\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_2-2y_2\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B_7}$	=	$-\left(x_2-y_2\right)\,\mathbf{a}_1-x_2\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_2-y_2\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B_8}$	=	$-y_2\,\mathbf{a}_1-x_2\,\mathbf{a}_2-\left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_2+y_2\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\left(x_2-y_2\right)\,\hat{\mathbf{y}}-c\left(z_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B_9}$	=	$-\left(x_2-y_2\right)\,\mathbf{a}_1+y_2\,\mathbf{a}_2-\left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_2+2y_2\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}-c\left(z_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B_{10}}$	=	$x_2\,\mathbf{a}_1+\left(x_2-y_2\right)\,\mathbf{a}_2-\left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_2-y_2\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}}-c\left(z_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B_{11}}$	=	$-x_2\,\mathbf{a}_1-y_2\,\mathbf{a}_2-z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_2+y_2\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\left(x_2-y_2\right)\,\hat{\mathbf{y}}-cz_2\,\hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B_{12}}$	=	$y_2\,\mathbf{a}_1-\left(x_2-y_2\right)\,\mathbf{a}_2-z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_2+2y_2\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}-cz_2\,\hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B_{13}}$	=	$\left(x_2-y_2\right)\,\mathbf{a}_1+x_2\,\mathbf{a}_2-z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_2-y_2\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}}-cz_2\,\hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B_{14}}$	=	$y_2\,\mathbf{a}_1+x_2\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_2+y_2\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\left(x_2-y_2\right)\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B_{15}}$	=	$\left(x_2-y_2\right)\,\mathbf{a}_1-y_2\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_2-2y_2\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B_{16}}$	=	$-x_2\,\mathbf{a}_1-\left(x_2-y_2\right)\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_2-y_2\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Si II
$\mathbf{B_{17}}$	=	$x_3\,\mathbf{a}_1+y_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3+y_3\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\left(x_3-y_3\right)\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(12i)	Si III
$\mathbf{B_{18}}$	=	$-y_3\,\mathbf{a}_1+\left(x_3-y_3\right)\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3-2y_3\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(12i)	Si III
$\mathbf{B_{19}}$	=	$-\left(x_3-y_3\right)\,\mathbf{a}_1-x_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_3-y_3\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(12i)	Si III
$\mathbf{B_{20}}$	=	$-y_3\,\mathbf{a}_1-x_3\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_3+y_3\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\left(x_3-y_3\right)\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Si III
$\mathbf{B_{21}}$	=	$-\left(x_3-y_3\right)\,\mathbf{a}_1+y_3\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_3+2y_3\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Si III
$\mathbf{B_{22}}$	=	$x_3\,\mathbf{a}_1+\left(x_3-y_3\right)\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_3-y_3\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	Si III
$\mathbf{B_{23}}$	=	$-x_3\,\mathbf{a}_1-y_3\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_3+y_3\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\left(x_3-y_3\right)\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(12i)	Si III
$\mathbf{B_{24}}$	=	$y_3\,\mathbf{a}_1-\left(x_3-y_3\right)\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_3+2y_3\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(12i)	Si III
$\mathbf{B_{25}}$	=	$\left(x_3-y_3\right)\,\mathbf{a}_1+x_3\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_3-y_3\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(12i)	Si III

$\mathbf{B_{26}}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3 + y_3\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}a\left(x_3 - y_3\right)\,\mathbf{\hat{y}} + c\left(z_3 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	Si III
$\mathbf{B_{27}}$	=	$\left(x_3 - y_3\right)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3 - 2y_3\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_3\,\mathbf{\hat{y}} + c\left(z_3 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	Si III
$\mathbf{B_{28}}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - y_3\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_3 - y_3\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_3\,\mathbf{\hat{y}} + c\left(z_3 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	Si III
$\mathbf{B_{29}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 + y_4\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(12i)	Te I
$\mathbf{B_{30}}$	=	$-y_4\,\mathbf{a}_1 + \left(x_4 - y_4\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 - 2y_4\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(12i)	Te I
$\mathbf{B_{31}}$	=	$-\left(x_4 - y_4\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_4 - y_4\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_4\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(12i)	Te I
$\mathbf{B_{32}}$	=	$-y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_4 + y_4\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	Te I
$\mathbf{B_{33}}$	=	$-\left(x_4 - y_4\right)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_4 + 2y_4\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	Te I
$\mathbf{B_{34}}$	=	$x_4\,\mathbf{a}_1 + \left(x_4 - y_4\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_4 - y_4\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_4\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	Te I
$\mathbf{B_{35}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_4 + y_4\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(12i)	Te I
$\mathbf{B_{36}}$	=	$y_4\,\mathbf{a}_1 - \left(x_4 - y_4\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_4 + 2y_4\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(12i)	Te I
$\mathbf{B_{37}}$	=	$\left(x_4 - y_4\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_4 - y_4\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_4\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(12i)	Te I
$\mathbf{B_{38}}$	=	$y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 + y_4\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	Te I
$\mathbf{B_{39}}$	=	$\left(x_4 - y_4\right)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 - 2y_4\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	Te I
$\mathbf{B_{40}}$	=	$-x_4\,\mathbf{a}_1 - \left(x_4 - y_4\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_4 - y_4\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_4\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	Te I

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.