

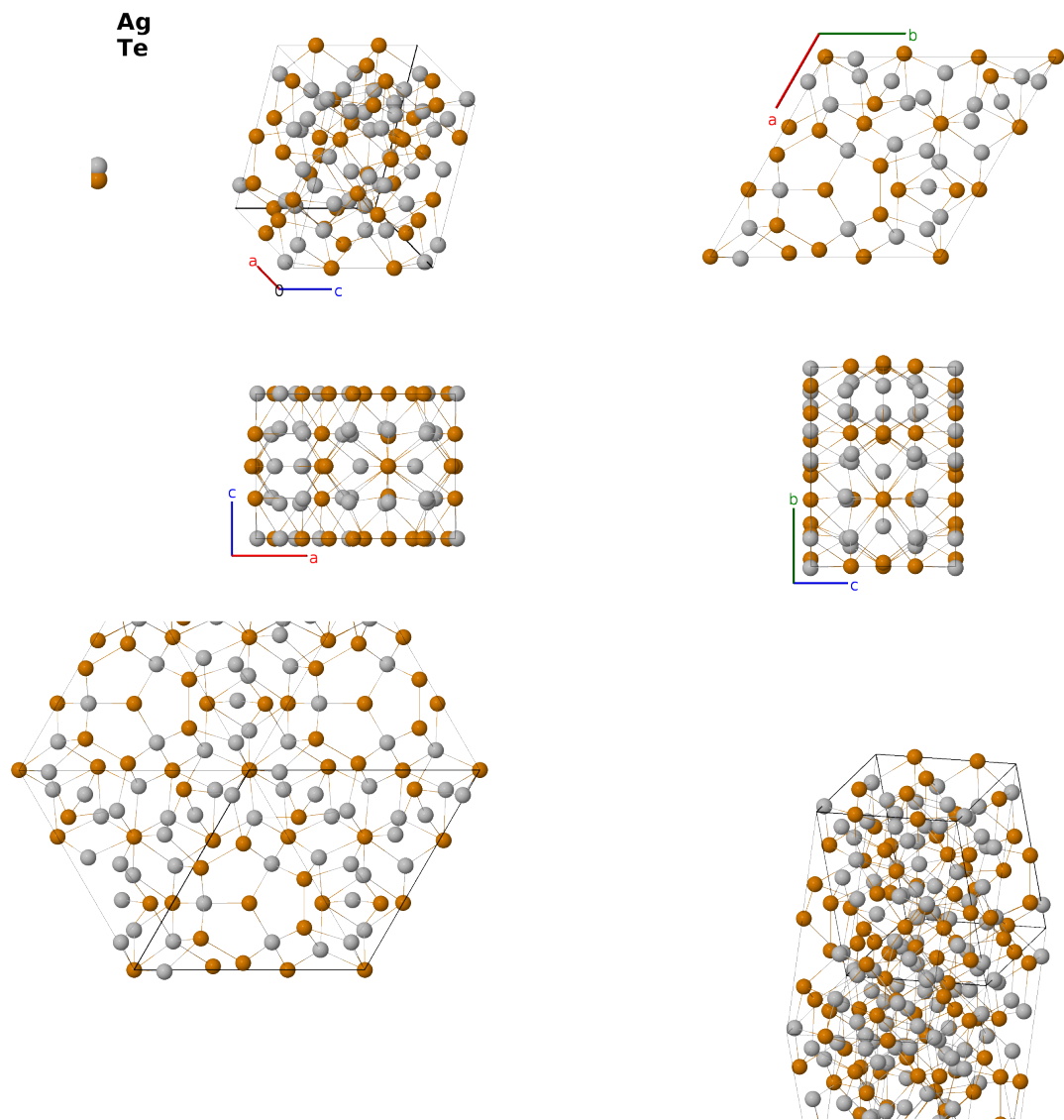
Stützite ($\text{Ag}_{5-x}\text{Te}_3$) Structure: A12B7_hP57_174_2j2k4l_ghi3j2k-001

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<https://aflow.org/prototype-encyclopedia/T2R2>

https://aflow.org/prototype-encyclopedia/A12B7_hP57_174_2j2k4l_ghi3j2k-001

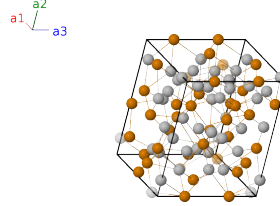


Prototype	$\text{Ag}_{5-x}\text{Te}_3$
AFLOW prototype label	A12B7_hP57_174_2j2k4l_ghi3j2k-001
Mineral name	stützite
ICSD	263525

CCDC	1930360
Pearson symbol	hP57
Space group number	174
Space group symbol	$P\bar{6}$
AFLOW prototype command	aflow --proto=A12B7_hP57_174_2j2k4l_ghi3j2k-001 --params= $a, c/a, z_1, z_2, z_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, x_8, y_8, x_9, y_9, x_{10}, y_{10}, x_{11}, y_{11}, x_{12}, y_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}$

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
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2g)	Te I
$\mathbf{B}_2$	$= -z_1 \mathbf{a}_3$	$=$	$-c z_1 \hat{\mathbf{z}}$	(2g)	Te I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(2h)	Te II
$\mathbf{B}_4$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(2h)	Te II
$\mathbf{B}_5$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(2i)	Te III
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(2i)	Te III
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}}$	(3j)	Ag I
$\mathbf{B}_8$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_4 \hat{\mathbf{y}}$	(3j)	Ag I
$\mathbf{B}_9$	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_4 \hat{\mathbf{y}}$	(3j)	Ag I
$\mathbf{B}_{10}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}}$	(3j)	Ag II
$\mathbf{B}_{11}$	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}}$	(3j)	Ag II
$\mathbf{B}_{12}$	$= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_5 \hat{\mathbf{y}}$	(3j)	Ag II
$\mathbf{B}_{13}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_6 - y_6) \hat{\mathbf{y}}$	(3j)	Te IV
$\mathbf{B}_{14}$	$= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}}$	(3j)	Te IV
$\mathbf{B}_{15}$	$= -(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_6 \hat{\mathbf{y}}$	(3j)	Te IV
$\mathbf{B}_{16}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_7 - y_7) \hat{\mathbf{y}}$	(3j)	Te V
$\mathbf{B}_{17}$	$= -y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_7 - 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_7 \hat{\mathbf{y}}$	(3j)	Te V
$\mathbf{B}_{18}$	$= -(x_7 - y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_7 \hat{\mathbf{y}}$	(3j)	Te V
$\mathbf{B}_{19}$	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_8 + y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_8 - y_8) \hat{\mathbf{y}}$	(3j)	Te VI
$\mathbf{B}_{20}$	$= -y_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_8 - 2y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_8 \hat{\mathbf{y}}$	(3j)	Te VI
$\mathbf{B}_{21}$	$= -(x_8 - y_8) \mathbf{a}_1 - x_8 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (2x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_8 \hat{\mathbf{y}}$	(3j)	Te VI
$\mathbf{B}_{22}$	$= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_9 + y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_9 - y_9) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3k)	Ag III

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