Trechmannite (AgAsS$_2$) Structure: ABC2_hR24_148_f_f_2f-001

https://aflow.org/p/3VWQ

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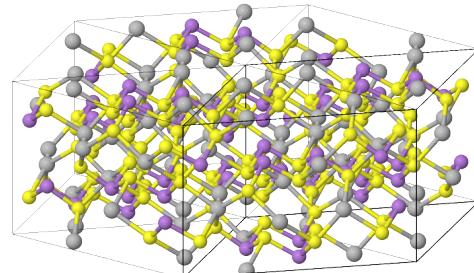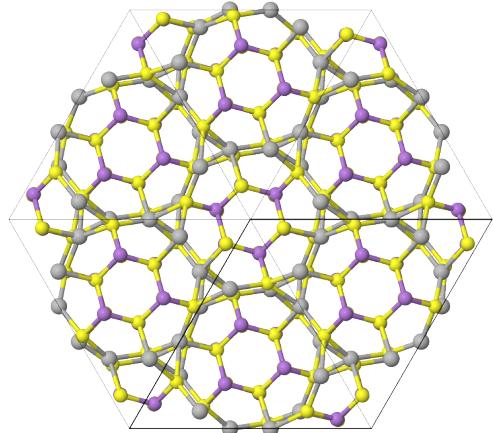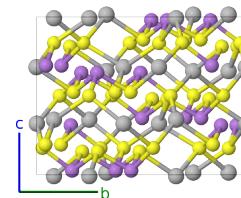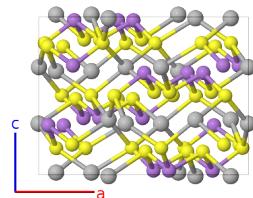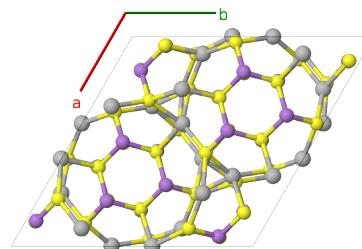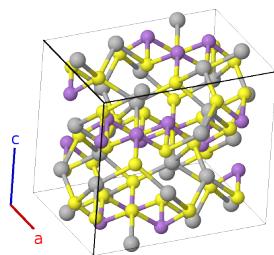
Prototype	AgAsS$_2$
AFLOW prototype label	ABC2_hR24_148_f_f_2f-001
Mineral name	trechmannite
ICSD	18101
Pearson symbol	hR24

		Space group number	148

Space group number   148

Space group symbol $R\bar{3}$

AFLOW prototype command   `aflow --proto=ABC2_hR24_148_f_f_2f-001`
                                  `--params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

- $AgAsS_2$ also occurs as orthorhombic smithite.

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$
\begin{aligned}
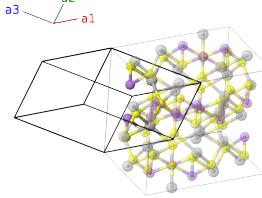\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}
$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_1} + y_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\left(x_1 - z_1\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_1 - 2y_1 + z_1\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_1 + y_1 + z_1\right)\hat{\mathbf{z}}$	(6f)	Ag I
$\mathbf{B_2}$	$=$	$z_1\,\mathbf{a_1} + x_1\,\mathbf{a_2} + y_1\,\mathbf{a_3}$	$=$	$-\frac{1}{2}a\left(y_1 - z_1\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_1 - y_1 - z_1\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_1 + y_1 + z_1\right)\hat{\mathbf{z}}$	(6f)	Ag I
$\mathbf{B_3}$	$=$	$y_1\,\mathbf{a_1} + z_1\,\mathbf{a_2} + x_1\,\mathbf{a_3}$	$=$	$-\frac{1}{2}a\left(x_1 - y_1\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_1 + y_1 - 2z_1\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_1 + y_1 + z_1\right)\hat{\mathbf{z}}$	(6f)	Ag I
$\mathbf{B_4}$	$=$	$-x_1\,\mathbf{a_1} - y_1\,\mathbf{a_2} - z_1\,\mathbf{a_3}$	$=$	$-\frac{1}{2}a\left(x_1 - z_1\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(x_1 - 2y_1 + z_1\right)\hat{\mathbf{y}} - \frac{1}{3}c\left(x_1 + y_1 + z_1\right)\hat{\mathbf{z}}$	(6f)	Ag I
$\mathbf{B_5}$	$=$	$-z_1\,\mathbf{a_1} - x_1\,\mathbf{a_2} - y_1\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\left(y_1 - z_1\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(2x_1 - y_1 - z_1\right)\hat{\mathbf{y}} - \frac{1}{3}c\left(x_1 + y_1 + z_1\right)\hat{\mathbf{z}}$	(6f)	Ag I
$\mathbf{B_6}$	$=$	$-y_1\,\mathbf{a_1} - z_1\,\mathbf{a_2} - x_1\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\left(x_1 - y_1\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(x_1 + y_1 - 2z_1\right)\hat{\mathbf{y}} - \frac{1}{3}c\left(x_1 + y_1 + z_1\right)\hat{\mathbf{z}}$	(6f)	Ag I
$\mathbf{B_7}$	$=$	$x_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\left(x_2 - z_2\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_2 - 2y_2 + z_2\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_2 + y_2 + z_2\right)\hat{\mathbf{z}}$	(6f)	As I
$\mathbf{B_8}$	$=$	$z_2\,\mathbf{a_1} + x_2\,\mathbf{a_2} + y_2\,\mathbf{a_3}$	$=$	$-\frac{1}{2}a\left(y_2 - z_2\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_2 - y_2 - z_2\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_2 + y_2 + z_2\right)\hat{\mathbf{z}}$	(6f)	As I
$\mathbf{B_9}$	$=$	$y_2\,\mathbf{a_1} + z_2\,\mathbf{a_2} + x_2\,\mathbf{a_3}$	$=$	$-\frac{1}{2}a\left(x_2 - y_2\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_2 + y_2 - 2z_2\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_2 + y_2 + z_2\right)\hat{\mathbf{z}}$	(6f)	As I
$\mathbf{B_{10}}$	$=$	$-x_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$-\frac{1}{2}a\left(x_2 - z_2\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(x_2 - 2y_2 + z_2\right)\hat{\mathbf{y}} - \frac{1}{3}c\left(x_2 + y_2 + z_2\right)\hat{\mathbf{z}}$	(6f)	As I
$\mathbf{B_{11}}$	$=$	$-z_2\,\mathbf{a_1} - x_2\,\mathbf{a_2} - y_2\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\left(y_2 - z_2\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(2x_2 - y_2 - z_2\right)\hat{\mathbf{y}} - \frac{1}{3}c\left(x_2 + y_2 + z_2\right)\hat{\mathbf{z}}$	(6f)	As I
$\mathbf{B_{12}}$	$=$	$-y_2\,\mathbf{a_1} - z_2\,\mathbf{a_2} - x_2\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\left(x_2 - y_2\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(x_2 + y_2 - 2z_2\right)\hat{\mathbf{y}} - \frac{1}{3}c\left(x_2 + y_2 + z_2\right)\hat{\mathbf{z}}$	(6f)	As I
$\mathbf{B_{13}}$	$=$	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\left(x_3 - z_3\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_3 - 2y_3 + z_3\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}}$	(6f)	S I

$$\mathbf{B_{14}} = z_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + y_3\,\mathbf{a_3} = -\tfrac{1}{2}a\left(y_3 - z_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_3 - y_3 - z_3\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{S I}$$

$$\mathbf{B_{15}} = y_3\,\mathbf{a_1} + z_3\,\mathbf{a_2} + x_3\,\mathbf{a_3} = -\tfrac{1}{2}a\left(x_3 - y_3\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_3 + y_3 - 2z_3\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{S I}$$

$$\mathbf{B_{16}} = -x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3} = -\tfrac{1}{2}a\left(x_3 - z_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_3 - 2y_3 + z_3\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{S I}$$

$$\mathbf{B_{17}} = -z_3\,\mathbf{a_1} - x_3\,\mathbf{a_2} - y_3\,\mathbf{a_3} = \tfrac{1}{2}a\left(y_3 - z_3\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(2x_3 - y_3 - z_3\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{S I}$$

$$\mathbf{B_{18}} = -y_3\,\mathbf{a_1} - z_3\,\mathbf{a_2} - x_3\,\mathbf{a_3} = \tfrac{1}{2}a\left(x_3 - y_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_3 + y_3 - 2z_3\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{S I}$$

$$\mathbf{B_{19}} = x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3} = \tfrac{1}{2}a\left(x_4 - z_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_4 - 2y_4 + z_4\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{S II}$$

$$\mathbf{B_{20}} = z_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + y_4\,\mathbf{a_3} = -\tfrac{1}{2}a\left(y_4 - z_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_4 - y_4 - z_4\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{S II}$$

$$\mathbf{B_{21}} = y_4\,\mathbf{a_1} + z_4\,\mathbf{a_2} + x_4\,\mathbf{a_3} = -\tfrac{1}{2}a\left(x_4 - y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_4 + y_4 - 2z_4\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{S II}$$

$$\mathbf{B_{22}} = -x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3} = -\tfrac{1}{2}a\left(x_4 - z_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_4 - 2y_4 + z_4\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{S II}$$

$$\mathbf{B_{23}} = -z_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} - y_4\,\mathbf{a_3} = \tfrac{1}{2}a\left(y_4 - z_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(2x_4 - y_4 - z_4\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{S II}$$

$$\mathbf{B_{24}} = -y_4\,\mathbf{a_1} - z_4\,\mathbf{a_2} - x_4\,\mathbf{a_3} = \tfrac{1}{2}a\left(x_4 - y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_4 + y_4 - 2z_4\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{S II}$$

References

[1] T. Matsumoto and W. Nowacki, *The crystal structure of trechmannite, AgAsS$_2$*, Z. Kristallogr. **129**, 163–177 (1969), doi:10.1524/zkri.1969.129.1-4.163.