

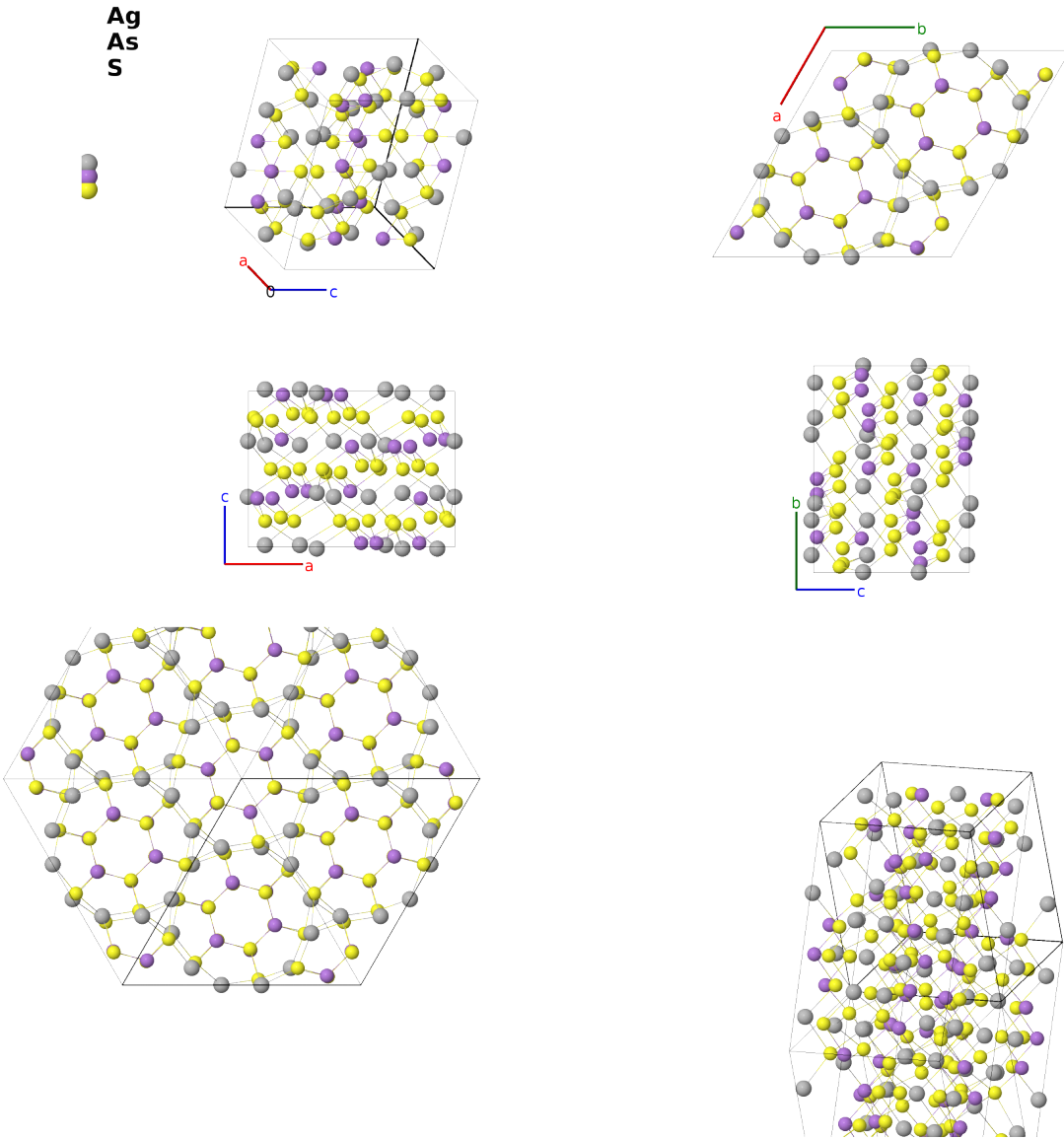
Trechmannite (AgAsS₂) Structure: ABC2_hR24_148_f_f_2f-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/3VWQ>

https://aflow.org/prototype-encyclopedia/ABC2_hR24_148_f_f_2f-001



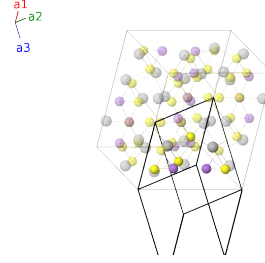
Prototype	AgAsS ₂
AFLOW prototype label	ABC2_hR24_148_f_f_2f-001
Mineral name	trechmannite

ICSD	18101
CCDC	1597658
Pearson symbol	hR24
Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	<code>aflow --proto=ABC2_hR24_148_f_f_2f-001</code> <code>--params=a, c/a, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄</code>

- AgAsS₂ also occurs as orthorhombic smithite.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \frac{1}{2}a(x_1 - z_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_1 - 2y_1 + z_1) \hat{\mathbf{y}} + \frac{1}{3}c(x_1 + y_1 + z_1) \hat{\mathbf{z}}$	(6f)	Ag I
$\mathbf{B}_2$	$z_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + y_1 \mathbf{a}_3$	$= -\frac{1}{2}a(y_1 - z_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_1 - y_1 - z_1) \hat{\mathbf{y}} + \frac{1}{3}c(x_1 + y_1 + z_1) \hat{\mathbf{z}}$	(6f)	Ag I
$\mathbf{B}_3$	$y_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$= -\frac{1}{2}a(x_1 - y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_1 + y_1 - 2z_1) \hat{\mathbf{y}} + \frac{1}{3}c(x_1 + y_1 + z_1) \hat{\mathbf{z}}$	(6f)	Ag I
$\mathbf{B}_4$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= -\frac{1}{2}a(x_1 - z_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_1 - 2y_1 + z_1) \hat{\mathbf{y}} - \frac{1}{3}c(x_1 + y_1 + z_1) \hat{\mathbf{z}}$	(6f)	Ag I
$\mathbf{B}_5$	$-z_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	$= \frac{1}{2}a(y_1 - z_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_1 - y_1 - z_1) \hat{\mathbf{y}} - \frac{1}{3}c(x_1 + y_1 + z_1) \hat{\mathbf{z}}$	(6f)	Ag I
$\mathbf{B}_6$	$-y_1 \mathbf{a}_1 - z_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$= \frac{1}{2}a(x_1 - y_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_1 + y_1 - 2z_1) \hat{\mathbf{y}} - \frac{1}{3}c(x_1 + y_1 + z_1) \hat{\mathbf{z}}$	(6f)	Ag I
$\mathbf{B}_7$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2}a(x_2 - z_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_2 - 2y_2 + z_2) \hat{\mathbf{y}} + \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6f)	As I
$\mathbf{B}_8$	$z_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + y_2 \mathbf{a}_3$	$= -\frac{1}{2}a(y_2 - z_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_2 - y_2 - z_2) \hat{\mathbf{y}} + \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6f)	As I
$\mathbf{B}_9$	$y_2 \mathbf{a}_1 + z_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$= -\frac{1}{2}a(x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_2 + y_2 - 2z_2) \hat{\mathbf{y}} + \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6f)	As I
$\mathbf{B}_{10}$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$= -\frac{1}{2}a(x_2 - z_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_2 - 2y_2 + z_2) \hat{\mathbf{y}} - \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6f)	As I
$\mathbf{B}_{11}$	$-z_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - y_2 \mathbf{a}_3$	$= \frac{1}{2}a(y_2 - z_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_2 - y_2 - z_2) \hat{\mathbf{y}} - \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6f)	As I

$\mathbf{B}_{12}$	$= -y_2 \mathbf{a}_1 - z_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_2 + y_2 - 2z_2) \hat{\mathbf{y}} - \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6f)	As I
$\mathbf{B}_{13}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B}_{14}$	$= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B}_{15}$	$= y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B}_{16}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B}_{17}$	$= -z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B}_{18}$	$= -y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	S I
$\mathbf{B}_{19}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	S II
$\mathbf{B}_{20}$	$= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	S II
$\mathbf{B}_{21}$	$= y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	S II
$\mathbf{B}_{22}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	S II
$\mathbf{B}_{23}$	$= -z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	S II
$\mathbf{B}_{24}$	$= -y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	S II

References

- [1] T. Matsumoto and W. Nowacki, *The crystal structure of trechmannite, AgAsS₂*, Z. Kristallogr. **129**, 163–177 (1969), doi:10.1524/zkri.1969.129.1-4.163.

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