

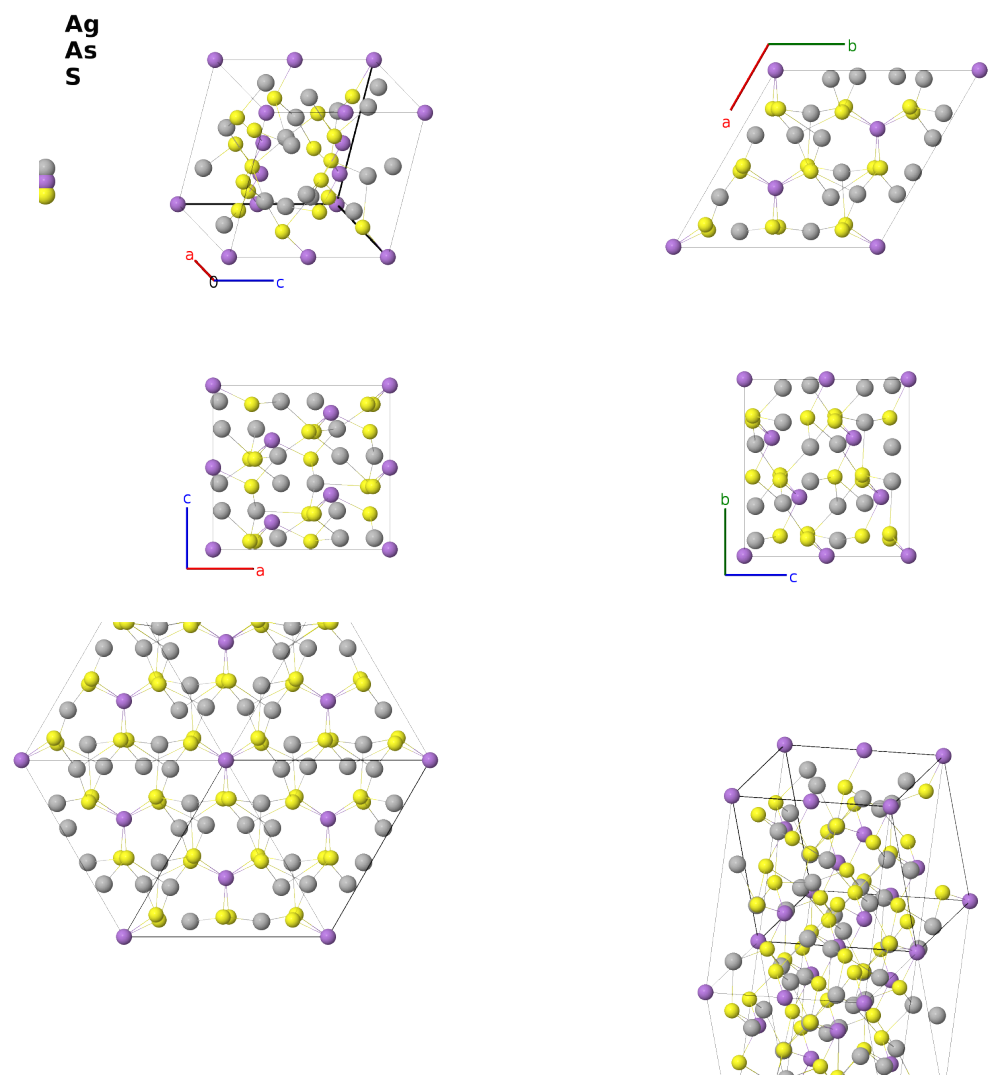
Proustite (Ag_3AsS_3) Structure: A3BC3_hR14_161_b_a_b-001

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

https://aflow.org/prototype-encyclopedia/A3BC3_hR14_161_b_a_b-001



Prototype	Ag_3AsS_3
AFLOW prototype label	A3BC3_hR14_161_b_a_b-001
Mineral name	proustite
ICSD	27841
CCDC	1603019

Pearson symbol	hR14
Space group number	161
Space group symbol	$R3c$
AFLOW prototype command	aflow --proto=A3BC3_hR14_161_b_a_b-001 --params= $a, c/a, x_1, x_2, y_2, z_2, x_3, y_3, z_3$

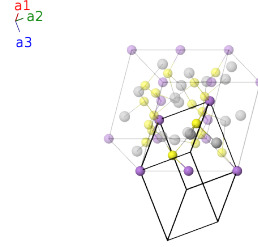
Other compounds with this structure

Ag_3AsSe_3 , Ag_3SbS_3 (pyrargyrite)

- Ag_3AsS_3 can also be found in the monoclinic xanthoconite structure. (Villars, 2018) shows phase diagrams with xanthoconite at 150°C and proustite at 350°C, but (Engel, 1968) state that “[xanthoconite] is obviously more unstable than proustite.”
- Space group $R3c$ #161 allows an arbitrary choice of the origin of the z -axis. Here we set $z_1 = 0$ for the arsenic atom.
- 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
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$cx_1 \hat{\mathbf{z}}$	(2a)	As I
$\mathbf{B}_2$	$(x_1 + \frac{1}{2}) \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 + (x_1 + \frac{1}{2}) \mathbf{a}_3$	=	$c(x_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	As I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2}a(x_2 - z_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_2 - 2y_2 + z_2) \hat{\mathbf{y}} + \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6b)	Ag I
$\mathbf{B}_4$	$z_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + y_2 \mathbf{a}_3$	=	$-\frac{1}{2}a(y_2 - z_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_2 - y_2 - z_2) \hat{\mathbf{y}} + \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6b)	Ag I
$\mathbf{B}_5$	$y_2 \mathbf{a}_1 + z_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$-\frac{1}{2}a(x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_2 + y_2 - 2z_2) \hat{\mathbf{y}} + \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6b)	Ag I
$\mathbf{B}_6$	$(z_2 + \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	=	$-\frac{1}{2}a(x_2 - z_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_2 - 2y_2 + z_2) \hat{\mathbf{y}} + \frac{1}{6}c(2x_2 + 2y_2 + 2z_2 + 3) \hat{\mathbf{z}}$	(6b)	Ag I
$\mathbf{B}_7$	$(y_2 + \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a(y_2 - z_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_2 - y_2 - z_2) \hat{\mathbf{y}} + \frac{1}{6}c(2x_2 + 2y_2 + 2z_2 + 3) \hat{\mathbf{z}}$	(6b)	Ag I
$\mathbf{B}_8$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + (z_2 + \frac{1}{2}) \mathbf{a}_2 + (y_2 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a(x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_2 + y_2 - 2z_2) \hat{\mathbf{y}} + \frac{1}{6}c(2x_2 + 2y_2 + 2z_2 + 3) \hat{\mathbf{z}}$	(6b)	Ag I
$\mathbf{B}_9$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6b)	S I

$$\begin{aligned}
\mathbf{B}_{10} &= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3 &= -\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}} &(6b) & \text{S I} \\
\mathbf{B}_{11} &= y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3 &= -\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}} &(6b) & \text{S I} \\
\mathbf{B}_{12} &= \left(z_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3 &= -\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{6}c(2x_3 + 2y_3 + 2z_3 + 3) \hat{\mathbf{z}} &(6b) & \text{S I} \\
\mathbf{B}_{13} &= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{6}c(2x_3 + 2y_3 + 2z_3 + 3) \hat{\mathbf{z}} &(6b) & \text{S I} \\
\mathbf{B}_{14} &= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{6}c(2x_3 + 2y_3 + 2z_3 + 3) \hat{\mathbf{z}} &(6b) & \text{S I}
\end{aligned}$$

References

- [1] D. Harker, *The Application of the Three-Dimensional Patterson Method and the Crystal Structures of Proustite, Ag_3AsS_3 , and Pyrargyrite, Ag_3SbS_3* , J. Chem. Phys. **4**, 381–390 (1936), doi:10.1063/1.1749863.
- [2] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. 1988 Schmid Fetzner R. (Silver-Arsenic-Sulfur). Copyright ©2006–2018 ASM International.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

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