Proustite (Ag_3AsS_3) Structure: A3BC3_hR14_161_b_a_b-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.

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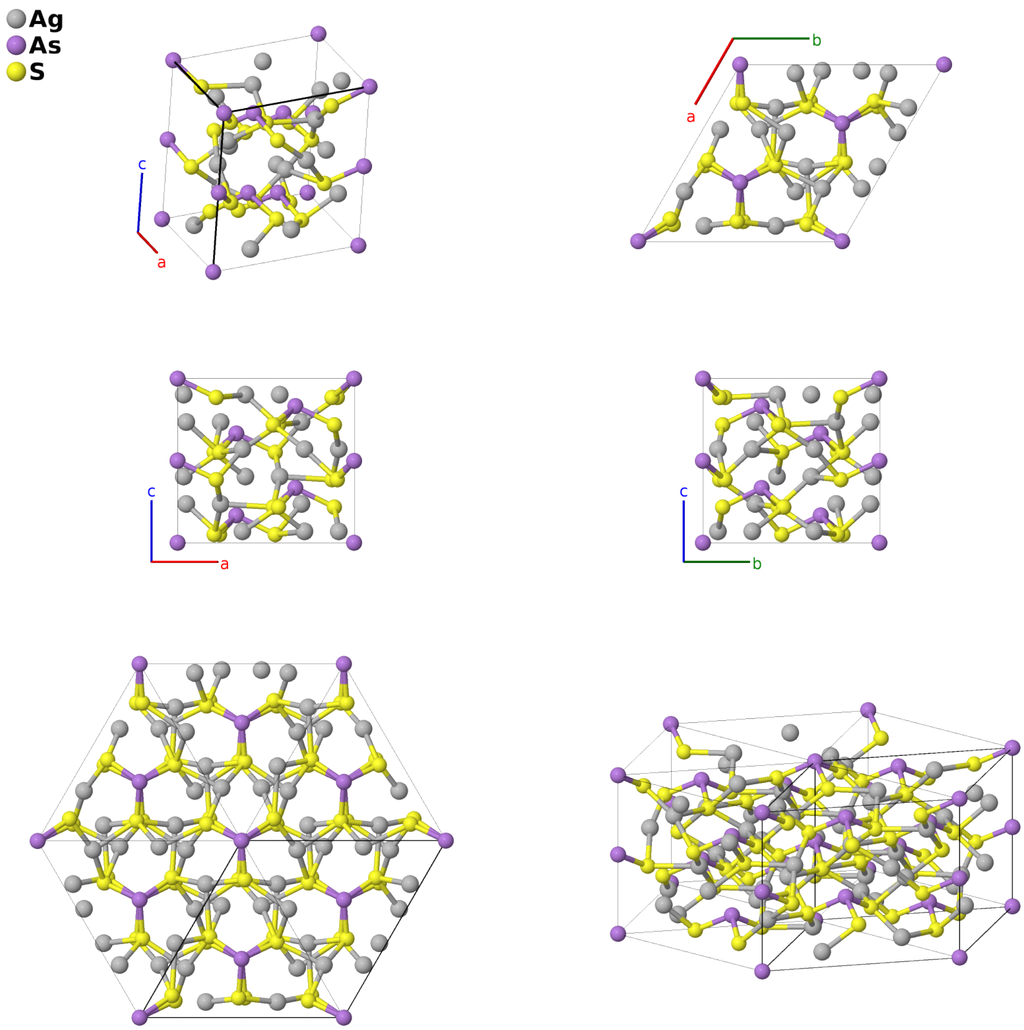
https://aflow.org/p/TXGA

https://aflow.org/p/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
Pearson symbol	hR14
Space group number	161
Space group symbol	$R3c$

AFLOW prototype command `aflow --proto=A3BC3_hR14_161_b_a_b-001`
`--params=`$a, c/a, x_1, x_2, y_2, z_2, x_3, y_3, z_3$

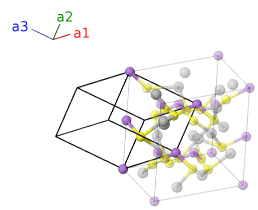
Other compounds with this structure

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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_2}$	$= \left(x_1+\frac{1}{2}\right)\mathbf{a_1} + \left(x_1+\frac{1}{2}\right)\mathbf{a_2} + \left(x_1+\frac{1}{2}\right)\mathbf{a_3}$	$= c\left(x_1+\frac{1}{2}\right)\hat{\mathbf{z}}$	(2a)	As I
$\mathbf{B_3}$	$= x_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$= \frac{1}{2}a\left(x_2-z_2\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_2-2y_2+z_2\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_2+y_2+z_2\right)\hat{\mathbf{z}}$	(6b)	Ag I
$\mathbf{B_4}$	$= z_2\,\mathbf{a_1} + x_2\,\mathbf{a_2} + y_2\,\mathbf{a_3}$	$= -\frac{1}{2}a\left(y_2-z_2\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_2-y_2-z_2\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_2+y_2+z_2\right)\hat{\mathbf{z}}$	(6b)	Ag I
$\mathbf{B_5}$	$= y_2\,\mathbf{a_1} + z_2\,\mathbf{a_2} + x_2\,\mathbf{a_3}$	$= -\frac{1}{2}a\left(x_2-y_2\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_2+y_2-2z_2\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_2+y_2+z_2\right)\hat{\mathbf{z}}$	(6b)	Ag I
$\mathbf{B_6}$	$= \left(z_2+\frac{1}{2}\right)\mathbf{a_1} + \left(y_2+\frac{1}{2}\right)\mathbf{a_2} + \left(x_2+\frac{1}{2}\right)\mathbf{a_3}$	$= -\frac{1}{2}a\left(x_2-z_2\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_2-2y_2+z_2\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_2+2y_2+2z_2+3\right)\hat{\mathbf{z}}$	(6b)	Ag I
$\mathbf{B_7}$	$= \left(y_2+\frac{1}{2}\right)\mathbf{a_1} + \left(x_2+\frac{1}{2}\right)\mathbf{a_2} + \left(z_2+\frac{1}{2}\right)\mathbf{a_3}$	$= \frac{1}{2}a\left(y_2-z_2\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_2-y_2-z_2\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_2+2y_2+2z_2+3\right)\hat{\mathbf{z}}$	(6b)	Ag I
$\mathbf{B_8}$	$= \left(x_2+\frac{1}{2}\right)\mathbf{a_1} + \left(z_2+\frac{1}{2}\right)\mathbf{a_2} + \left(y_2+\frac{1}{2}\right)\mathbf{a_3}$	$= \frac{1}{2}a\left(x_2-y_2\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_2+y_2-2z_2\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_2+2y_2+2z_2+3\right)\hat{\mathbf{z}}$	(6b)	Ag I
$\mathbf{B_9}$	$= x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$= \frac{1}{2}a\left(x_3-z_3\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_3-2y_3+z_3\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_3+y_3+z_3\right)\hat{\mathbf{z}}$	(6b)	S I
$\mathbf{B_{10}}$	$= z_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + y_3\,\mathbf{a_3}$	$= -\frac{1}{2}a\left(y_3-z_3\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_3-y_3-z_3\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_3+y_3+z_3\right)\hat{\mathbf{z}}$	(6b)	S I
$\mathbf{B_{11}}$	$= y_3\,\mathbf{a_1} + z_3\,\mathbf{a_2} + x_3\,\mathbf{a_3}$	$= -\frac{1}{2}a\left(x_3-y_3\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_3+y_3-2z_3\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_3+y_3+z_3\right)\hat{\mathbf{z}}$	(6b)	S I
$\mathbf{B_{12}}$	$= \left(z_3+\frac{1}{2}\right)\mathbf{a_1} + \left(y_3+\frac{1}{2}\right)\mathbf{a_2} + \left(x_3+\frac{1}{2}\right)\mathbf{a_3}$	$= -\frac{1}{2}a\left(x_3-z_3\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_3-2y_3+z_3\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_3+2y_3+2z_3+3\right)\hat{\mathbf{z}}$	(6b)	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)	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)	S I

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 Fetzer 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).