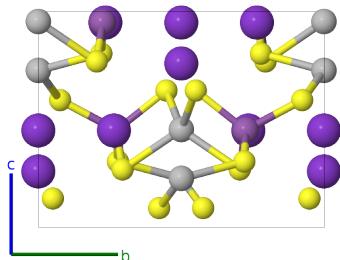
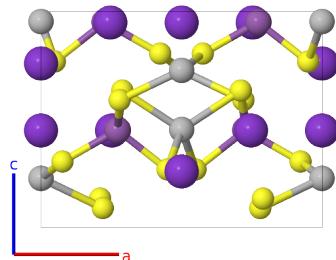
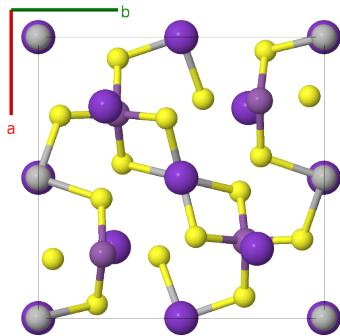
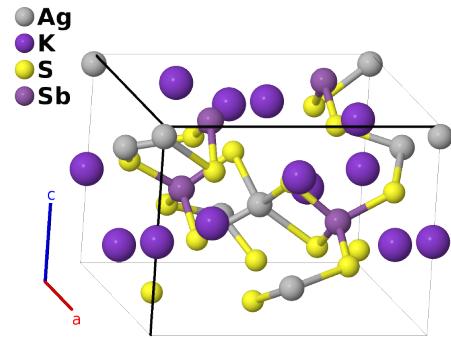


K₂AgSbS₄ Structure: AB2C4D_oP32_34_ab_abc_4c_c-001

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.

<https://aflow.org/p/Z6KJ>

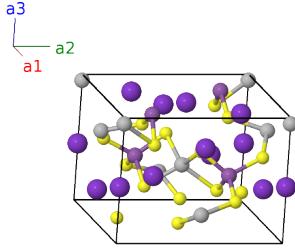
https://aflow.org/p/AB2C4D_oP32_34_ab_abc_4c_c-001



Prototype	AgK ₂ S ₄ Sb
AFLOW prototype label	AB2C4D_oP32_34_ab_abc_4c_c-001
ICSD	82144
Pearson symbol	oP32
Space group number	34
Space group symbol	<i>Pnn2</i>
AFLOW prototype command	<pre>aflow --proto=AB2C4D_oP32_34_ab_abc_4c_c-001 --params=a, b/a, c/a, z1, z2, z3, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10</pre>

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$z_1 \mathbf{a}_3$	$cz_1 \hat{\mathbf{z}}$	(2a)	Ag I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Ag I
\mathbf{B}_3	$z_2 \mathbf{a}_3$	$cz_2 \hat{\mathbf{z}}$	(2a)	K I
\mathbf{B}_4	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	K I
\mathbf{B}_5	$\frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$\frac{1}{2}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2b)	Ag II
\mathbf{B}_6	$\frac{1}{2} \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$\frac{1}{2}a \hat{\mathbf{x}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Ag II
\mathbf{B}_7	$\frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$\frac{1}{2}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2b)	K II
\mathbf{B}_8	$\frac{1}{2} \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$\frac{1}{2}a \hat{\mathbf{x}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	K II
\mathbf{B}_9	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	K III
\mathbf{B}_{10}	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	K III
\mathbf{B}_{11}	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	K III
\mathbf{B}_{12}	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	K III
\mathbf{B}_{13}	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	S I
\mathbf{B}_{14}	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	S I
\mathbf{B}_{15}	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	S I
\mathbf{B}_{16}	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	S I
\mathbf{B}_{17}	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4c)	S II
\mathbf{B}_{18}	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4c)	S II
\mathbf{B}_{19}	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	S II
\mathbf{B}_{20}	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	S II
\mathbf{B}_{21}	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4c)	S III
\mathbf{B}_{22}	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4c)	S III
\mathbf{B}_{23}	$(x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	S III
\mathbf{B}_{24}	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	S III

B₂₅	=	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4c)	S IV
B₂₆	=	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4c)	S IV
B₂₇	=	$(x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	=	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	S IV
B₂₈	=	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	S IV
B₂₉	=	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(4c)	Sb I
B₃₀	=	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$-ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(4c)	Sb I
B₃₁	=	$(x_{10} + \frac{1}{2}) \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	=	$a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Sb I
B₃₂	=	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Sb I

References

- [1] G. L. Schimek, W. T. Pennington, P. T. Wood, and J. W. Kolis, *Supercritical Ammonia Synthesis and Characterization of Four New Alkali Metal Silver Antimony Sulfides: MAg₂SbS₄ and M₂AgSbS₄ (M= K, Rb)*, J. Solid State Chem. **123**, 277–284 (1996), doi:10.1006/jssc.1996.0179.

Found in

- [1] A. Jain, S. Ping, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Materials **1**, 011002 (2013), doi:10.1063/1.4812323.