

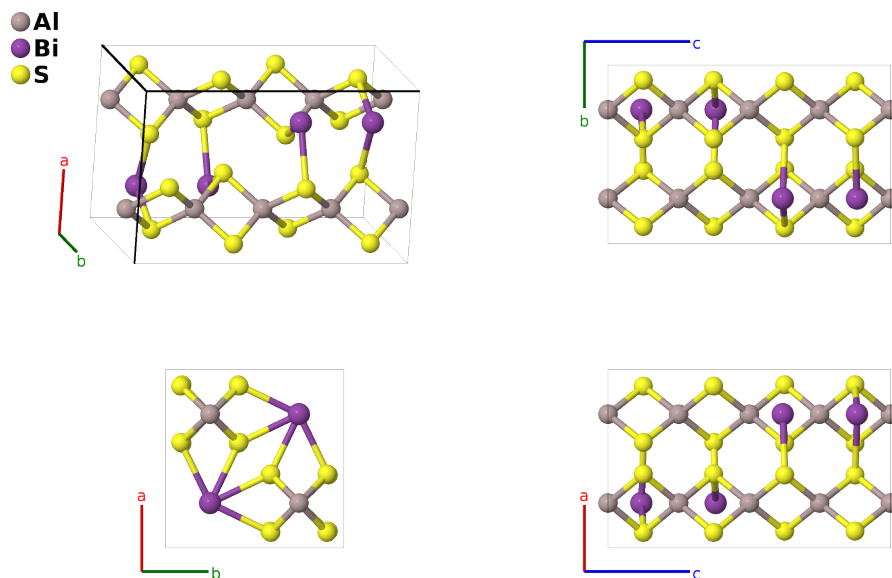
BiAl₂S₄ Structure: A2BC4_tP28_126_cd_e_k-001

This structure originally had the label A2BC4_tP28_126_cd_e_k. Calls to that address will be redirected here.

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<https://aflow.org/p/4WPC>

https://aflow.org/p/A2BC4_tP28_126_cd_e_k-001



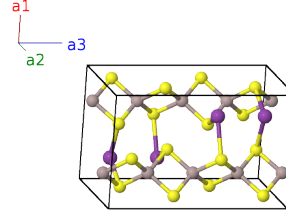
Prototype	Al ₂ BiS ₄
AFLOW prototype label	A2BC4_tP28_126_cd_e_k-001
ICSD	408439
Pearson symbol	tP28
Space group number	126
Space group symbol	<i>P4/nnc</i>
AFLOW prototype command	<code>aflow --proto=A2BC4_tP28_126_cd_e_k-001 --params=a, c/a, z₃, x₄, y₄, z₄</code>

Other compounds with this structure

BiAl₂Se₄, BiGa₂S₄, BiGa₂Se₄, Bi(Al, Ga)₂S₄, Bi(Al, Ga)₂Se₄

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Al I
\mathbf{B}_2	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Al I
\mathbf{B}_3	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Al I
\mathbf{B}_4	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Al I
\mathbf{B}_5	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(4d)	Al II
\mathbf{B}_6	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(4d)	Al II
\mathbf{B}_7	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4d)	Al II
\mathbf{B}_8	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4d)	Al II
\mathbf{B}_9	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4e)	Bi I
\mathbf{B}_{10}	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Bi I
\mathbf{B}_{11}	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4e)	Bi I
\mathbf{B}_{12}	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Bi I
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16k)	S I
\mathbf{B}_{14}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16k)	S I
\mathbf{B}_{15}	$= -(y_4 - \frac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16k)	S I
\mathbf{B}_{16}	$= y_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16k)	S I
\mathbf{B}_{17}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	S I
\mathbf{B}_{18}	$= x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	S I
\mathbf{B}_{19}	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	S I
\mathbf{B}_{20}	$= -(y_4 - \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	S I
\mathbf{B}_{21}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16k)	S I
\mathbf{B}_{22}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16k)	S I
\mathbf{B}_{23}	$= (y_4 + \frac{1}{2}) \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16k)	S I
\mathbf{B}_{24}	$= -y_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16k)	S I
\mathbf{B}_{25}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	S I
\mathbf{B}_{26}	$= -x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	S I
\mathbf{B}_{27}	$= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	S I

$$\mathbf{B}_{28} = \begin{pmatrix} (y_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a (y_4 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}} \quad (16k) \quad \text{S I}$$

References

- [1] H. Kalpen, W. Höhle, M. Somer, U. Schwarz, K. Peters, H. G. von Schnering, and R. Blachnik, *Bismut(II)-chalkogenometallate(III) Bi₂M₄X₈, Verbindungen mit Bi₂-Hanteln (M=Al, Ga; X=S, Se)*, *Z. Anorganische und Allgemeine Chemie* **624**, 1137–1147 (1998), doi:10.1002/(SICI)1521-3749(199807)624:7<1137::AID-ZAAC1137>3.0.CO;2-B.

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- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.