

ZnSb₂O₄ Structure:

A4B2C_tP28_135_gh_h_d-001

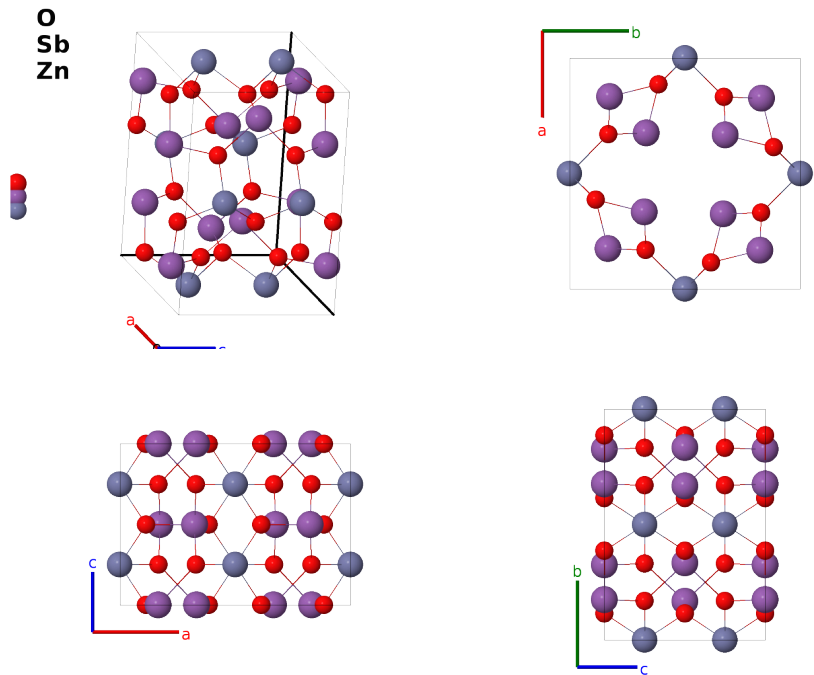
This structure previously used the label(s) **A4B2C.tP28_135_gh_h.d**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/20MM>

https://aflow.org/prototype-encyclopedia/A4B2C_tP28_135_gh_h_d-001



Prototype	O ₄ Sb ₂ Zn
AFLOW prototype label	A4B2C_tP28_135_gh_h_d-001
ICSD	647391
CCDC	1762754
Pearson symbol	tP28
Space group number	135
Space group symbol	$P4_2/mbc$
AFLOW prototype command	<pre>aflow --proto=A4B2C_tP28_135_gh_h_d-001 --params=a, c/a, x₂, x₃, y₃, x₄, y₄</pre>

Other compounds with this structure

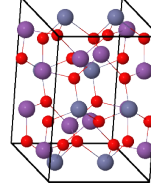
CoSb₂O₄, CuAs₂O₄, FeSb₂O₄ (schafarzikite), MgSb₂O₄, MnSb₂O₄, NiAs₂O₄, NiSb₂O₄, SnPb₂O₄, TiSn₂O₄

- The ICSD assigns these structures to the Pb_3O_4 -T prototype. We moved the tenary compounds over to this structure.

Simple Tetragonal primitive vectors

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

a₁^{a2}
a₃



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	Zn I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	Zn I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	Zn I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	Zn I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_7$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_9$	$= -x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_{10}$	$= x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_{11}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_{12}$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_{13}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B}_{14}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B}_{15}$	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B}_{16}$	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B}_{17}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B}_{18}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B}_{19}$	$= (y_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B}_{20}$	$= -(y_3 - \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B}_{21}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}}$	(8h)	Sb I
$\mathbf{B}_{22}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}}$	(8h)	Sb I
$\mathbf{B}_{23}$	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	Sb I
$\mathbf{B}_{24}$	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	Sb I
$\mathbf{B}_{25}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	Sb I
$\mathbf{B}_{26}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	Sb I

$$\begin{aligned} \mathbf{B}_{27} &= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = a \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (8h) & \text{Sb I} \\ \mathbf{B}_{28} &= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (8h) & \text{Sb I} \end{aligned}$$

References

- [1] S. Ståhl, *The crystal structure of ZnSb_2O_4 and isomorphous compounds*, Ark. Kem. Mineral. Geol. **17B**, 1–7 (1943).

Found in

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

First cited in

- D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043