

TlZn₂Sb₂ Structure:

A2BC2_tI20_79_c_2a_c-001

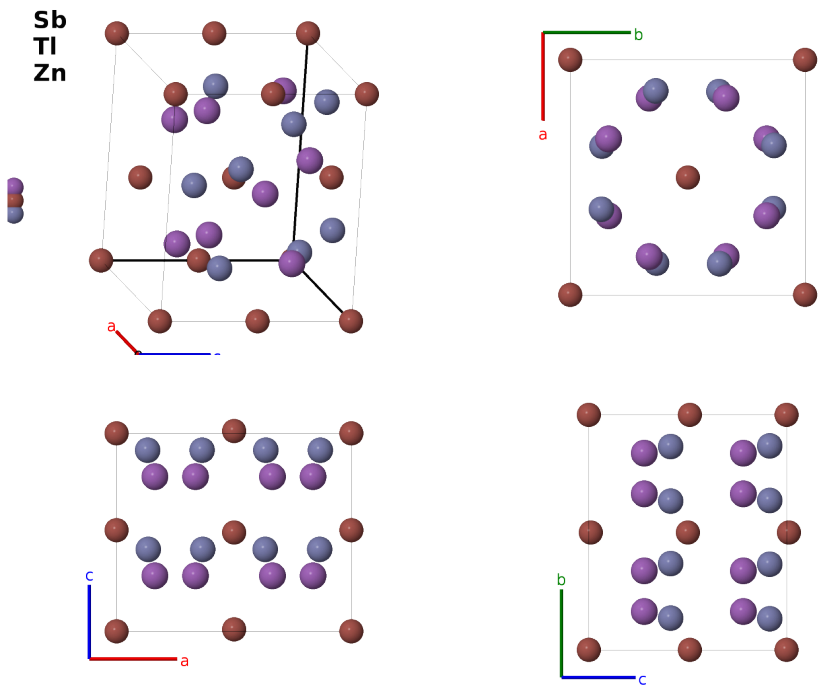
This structure previously used the label(s) **A2BC2.tI20_79.c_2a.c**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/T892>

https://aflow.org/prototype-encyclopedia/A2BC2_tI20_79_c_2a_c-001

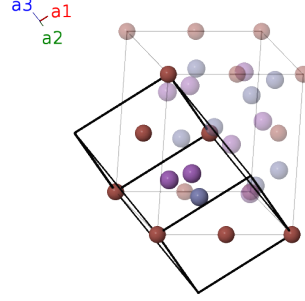


Prototype	Sb ₂ TlZn ₂
AFLOW prototype label	A2BC2_tI20_79_c_2a_c-001
ICSD	76499
CCDC	1637081
Pearson symbol	tI20
Space group number	79
Space group symbol	I4
AFLOW prototype command	<code>aflow --proto=A2BC2_tI20_79_c_2a_c-001</code> <code>--params=a, c/a, z₁, z₂, x₃, y₃, z₃, x₄, y₄, z₄</code>

- Space group *I4* #79 allows us to make an arbitrary choice for the origin of the z -axes, which we used to move the Tl-I atom to the origin. Our original version of this structure (Hicks, 2019) did not do this correctly. We now present the correct structure.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2$	$=$	$cz_1 \hat{\mathbf{z}}$	(2a)	Tl I
$\mathbf{B}_2$	$= z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2$	$=$	$cz_2 \hat{\mathbf{z}}$	(2a)	Tl II
$\mathbf{B}_3$	$= (y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	Sb I
$\mathbf{B}_4$	$= -(y_3 - z_3) \mathbf{a}_1 - (x_3 - z_3) \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	Sb I
$\mathbf{B}_5$	$= (x_3 + z_3) \mathbf{a}_1 - (y_3 - z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	Sb I
$\mathbf{B}_6$	$= -(x_3 - z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	Sb I
$\mathbf{B}_7$	$= (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8c)	Zn I
$\mathbf{B}_8$	$= -(y_4 - z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8c)	Zn I
$\mathbf{B}_9$	$= (x_4 + z_4) \mathbf{a}_1 - (y_4 - z_4) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8c)	Zn I
$\mathbf{B}_{10}$	$= -(x_4 - z_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8c)	Zn I

References

- [1] A. Czybulka, B. Krenkel, and H.-U. Schuster, *Ternäre zintl-Verbindungen mit thallium als elektronendonator*, J. Less-Common Met. **137**, 311–322 (1988), doi:10.1016/0022-5088(88)90096-3.
- [2] 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–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

Found in

- [1] P. Villars, *TlZn₂Sb₂ Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.

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