# $TlZn_2Sb_2$ Structure: A2BC2_tI20_79_c_2a_c-001

This structure originally had the label `A2BC2_tI20_79_c_2a_c`. Calls to that address will be redirected here.

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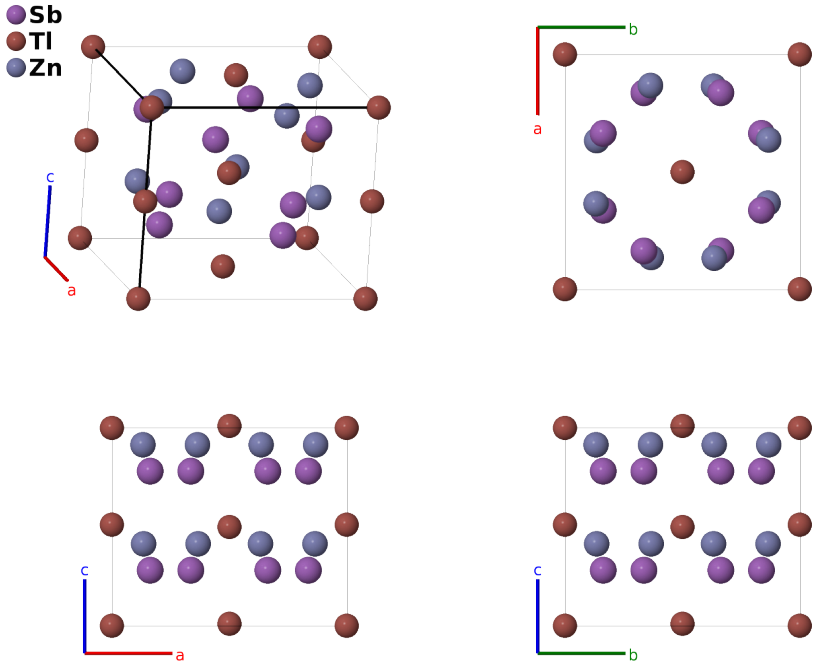
https://aflow.org/p/T892

https://aflow.org/p/A2BC2_tI20_79_c_2a_c-001




| | |
|---|---|
| **Prototype** | $Sb_2TlZn_2$ |
| **AFLOW prototype label** | A2BC2_tI20_79_c_2a_c-001 |
| **ICSD** | 76499 |
| **Pearson symbol** | tI20 |
| **Space group number** | 79 |
| **Space group symbol** | $I4$ |
| **AFLOW prototype command** | `aflow --proto=A2BC2_tI20_79_c_2a_c-001 --params=`$a, c/a, z_1, z_2, x_3, y_3, z_3, x_4, y_4, z_4$ |

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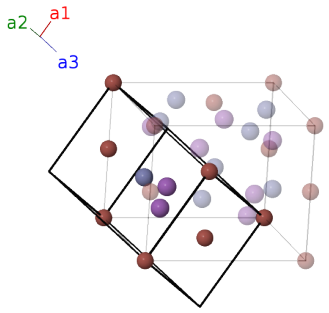
- Space group $I4$ #79 allows us to make an arbitrary choice for the origin of the $z$-axes, which we used to move the Tl-I atom to the origin. Our original version of this structure (Hicks, 2019) did not do this correctly. We now present the correct structure.

## Body-centered Tetragonal primitive vectors

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




## 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, *$TlZn_2Sb_2$ Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.