# Sb$_2$Tl$_7$ ($L2_2$) Structure: A2B7_cI54_229_e_afh-001
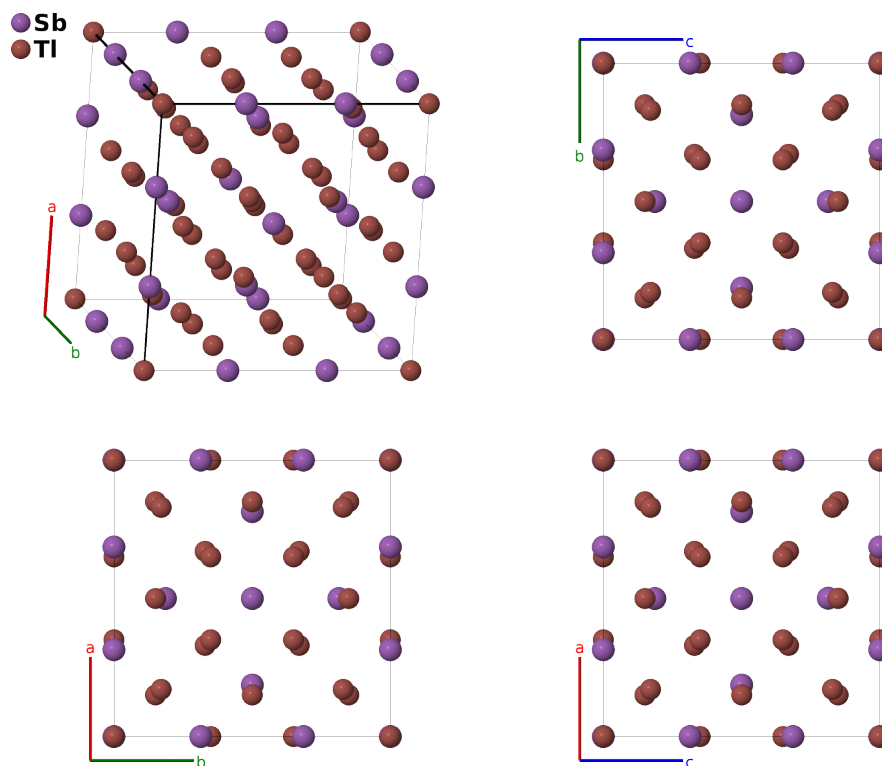
This structure originally had the label `A2B7_cI54_229_e_afh`. Calls to that address will be redirected here.

https://aflow.org/p/KM4R

https://aflow.org/p/A2B7_cI54_229_e_afh-001



| | |
|---|---|
| **Prototype** | Sb$_2$Tl$_7$ |
| **AFLOW prototype label** | A2B7_cI54_229_e_afh-001 |
| ***Strukturbericht* designation** | $L2_2$ |
| **ICSD** | 41816 |
| **Pearson symbol** | cI54 |
| **Space group number** | 229 |
| **Space group symbol** | $Im\overline{3}m$ |
| **AFLOW prototype command** | aflow --proto=A2B7_cI54_229_e_afh-001<br>    --params=$a, x_2, x_3, y_4$ |

**Body-centered Cubic primitive vectors**
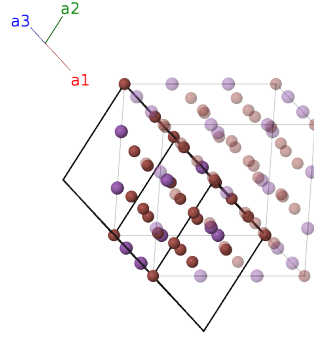
$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$$

$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}a\,\hat{\mathbf{z}}$$

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**Basis vectors**

| | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|
| $\mathbf{B_1}$ = | $0$ | = | $0$ | (2a) | Tl I |
| $\mathbf{B_2}$ = | $x_2\,\mathbf{a_2} + x_2\,\mathbf{a_3}$ | = | $ax_2\,\hat{\mathbf{x}}$ | (12e) | Sb I |
| $\mathbf{B_3}$ = | $-x_2\,\mathbf{a_2} - x_2\,\mathbf{a_3}$ | = | $-ax_2\,\hat{\mathbf{x}}$ | (12e) | Sb I |
| $\mathbf{B_4}$ = | $x_2\,\mathbf{a_1} + x_2\,\mathbf{a_3}$ | = | $ax_2\,\hat{\mathbf{y}}$ | (12e) | Sb I |
| $\mathbf{B_5}$ = | $-x_2\,\mathbf{a_1} - x_2\,\mathbf{a_3}$ | = | $-ax_2\,\hat{\mathbf{y}}$ | (12e) | Sb I |
| $\mathbf{B_6}$ = | $x_2\,\mathbf{a_1} + x_2\,\mathbf{a_2}$ | = | $ax_2\,\hat{\mathbf{z}}$ | (12e) | Sb I |
| $\mathbf{B_7}$ = | $-x_2\,\mathbf{a_1} - x_2\,\mathbf{a_2}$ | = | $-ax_2\,\hat{\mathbf{z}}$ | (12e) | Sb I |
| $\mathbf{B_8}$ = | $2x_3\,\mathbf{a_1} + 2x_3\,\mathbf{a_2} + 2x_3\,\mathbf{a_3}$ | = | $ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$ | (16f) | Tl II |
| $\mathbf{B_9}$ = | $-2x_3\,\mathbf{a_3}$ | = | $-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$ | (16f) | Tl II |
| $\mathbf{B_{10}}$ = | $-2x_3\,\mathbf{a_2}$ | = | $-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$ | (16f) | Tl II |
| $\mathbf{B_{11}}$ = | $-2x_3\,\mathbf{a_1}$ | = | $ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$ | (16f) | Tl II |
| $\mathbf{B_{12}}$ = | $2x_3\,\mathbf{a_3}$ | = | $ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$ | (16f) | Tl II |
| $\mathbf{B_{13}}$ = | $-2x_3\,\mathbf{a_1} - 2x_3\,\mathbf{a_2} - 2x_3\,\mathbf{a_3}$ | = | $-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$ | (16f) | Tl II |
| $\mathbf{B_{14}}$ = | $2x_3\,\mathbf{a_2}$ | = | $ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$ | (16f) | Tl II |
| $\mathbf{B_{15}}$ = | $2x_3\,\mathbf{a_1}$ | = | $-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$ | (16f) | Tl II |
| $\mathbf{B_{16}}$ = | $2y_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + y_4\,\mathbf{a_3}$ | = | $ay_4\,\hat{\mathbf{y}} + ay_4\,\hat{\mathbf{z}}$ | (24h) | Tl III |
| $\mathbf{B_{17}}$ = | $y_4\,\mathbf{a_2} - y_4\,\mathbf{a_3}$ | = | $-ay_4\,\hat{\mathbf{y}} + ay_4\,\hat{\mathbf{z}}$ | (24h) | Tl III |
| $\mathbf{B_{18}}$ = | $-y_4\,\mathbf{a_2} + y_4\,\mathbf{a_3}$ | = | $ay_4\,\hat{\mathbf{y}} - ay_4\,\hat{\mathbf{z}}$ | (24h) | Tl III |
| $\mathbf{B_{19}}$ = | $-2y_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - y_4\,\mathbf{a_3}$ | = | $-ay_4\,\hat{\mathbf{y}} - ay_4\,\hat{\mathbf{z}}$ | (24h) | Tl III |
| $\mathbf{B_{20}}$ = | $y_4\,\mathbf{a_1} + 2y_4\,\mathbf{a_2} + y_4\,\mathbf{a_3}$ | = | $ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}}$ | (24h) | Tl III |
| $\mathbf{B_{21}}$ = | $-y_4\,\mathbf{a_1} + y_4\,\mathbf{a_3}$ | = | $ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{z}}$ | (24h) | Tl III |
| $\mathbf{B_{22}}$ = | $y_4\,\mathbf{a_1} - y_4\,\mathbf{a_3}$ | = | $-ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}}$ | (24h) | Tl III |
| $\mathbf{B_{23}}$ = | $-y_4\,\mathbf{a_1} - 2y_4\,\mathbf{a_2} - y_4\,\mathbf{a_3}$ | = | $-ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{z}}$ | (24h) | Tl III |
| $\mathbf{B_{24}}$ = | $y_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + 2y_4\,\mathbf{a_3}$ | = | $ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$ | (24h) | Tl III |
| $\mathbf{B_{25}}$ = | $y_4\,\mathbf{a_1} - y_4\,\mathbf{a_2}$ | = | $-ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$ | (24h) | Tl III |
| $\mathbf{B_{26}}$ = | $-y_4\,\mathbf{a_1} + y_4\,\mathbf{a_2}$ | = | $ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$ | (24h) | Tl III |
| $\mathbf{B_{27}}$ = | $-y_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - 2y_4\,\mathbf{a_3}$ | = | $-ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$ | (24h) | Tl III |

## References

[1] R. Stokhuyzen, C. Chieh, and W. B. Pearson, *Crystal Structure of $Sb_2Tl_7$*, Can. J. Chem. **55**, 1120–1122 (1977), doi:10.1139/v77-157.

## Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.