# $K3_3$ ($Tl_2AlF_5$) Structure: AB5C2_oC32_20_a_2abc_c-001

This structure previously used the label(s) `AB5C2_oC32_20_b_a2bc_c`. Calls to these addresses will be redirected here.

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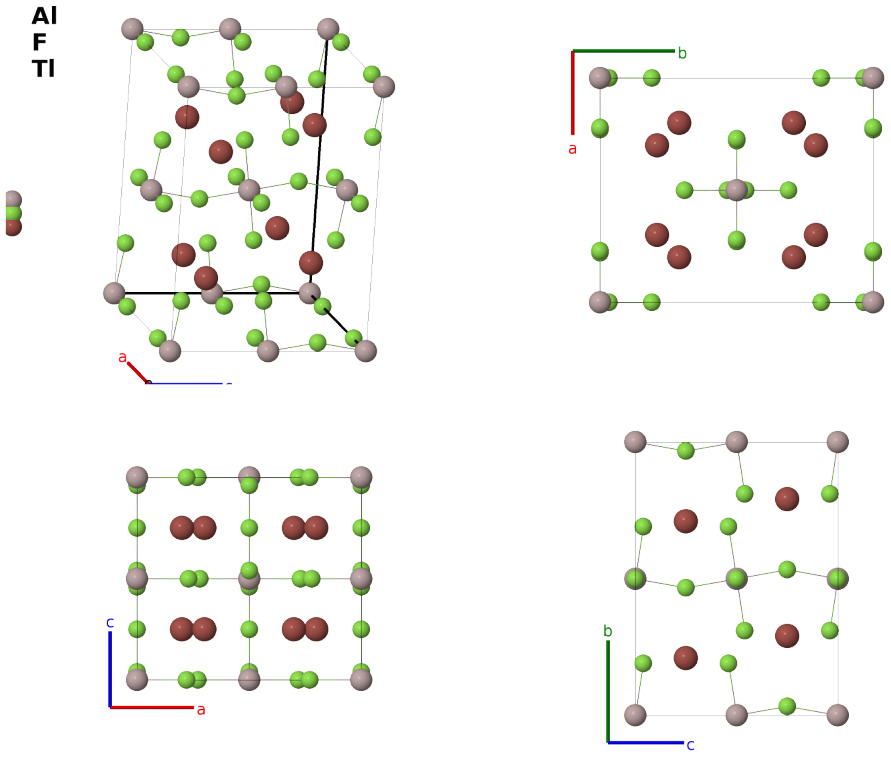
https://aflow.org/prototype-encyclopedia/XBH3

https://aflow.org/prototype-encyclopedia/AB5C2_oC32_20_a_2abc_c-001

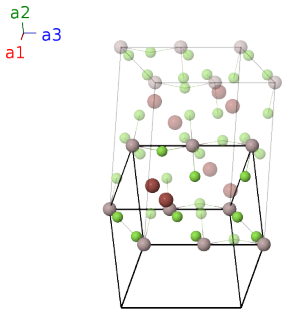



| | |
|---|---|
| **Prototype** | $AlF_5Tl_2$ |
| **AFLOW prototype label** | AB5C2_oC32_20_a_2abc_c-001 |
| ***Strukturbericht* designation** | $K3_3$ |
| **ICSD** | 25616 |
| **CCDC** | 1601266 |
| **Pearson symbol** | oC32 |
| **Space group number** | 20 |
| **Space group symbol** | $C222_1$ |
| **AFLOW prototype command** | `aflow --proto=AB5C2_oC32_20_a_2abc_c-001 --params=`$a, b/a, c/a, x_1, x_2, x_3, y_4, x_5, y_5, z_5, x_6, y_6, z_6$ |

- There are several problems with this structure:
- First, (Brosset, 1937) gives coordinates $y_3 = -y_2$, which gives the structure an inversion site and makes the space group $Cmcm$ #63. We have adjusted the coordinates of the third atom slightly to avoid this.
- Second, (Molinier, 1993) makes the argument that the structure observed by Brosset is actually $Tl_2AlF_5{\cdot}H_2O$.
- A refined version of this structure in space group $Cmcm$ was found by (Brosset, 1942).

**Base-centered Orthorhombic primitive vectors**

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$




**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$ | = | $ax_1\,\hat{\mathbf{x}}$ | (4a) | Al I |
| $\mathbf{B_2}$ | = | $-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-ax_1\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4a) | Al I |
| $\mathbf{B_3}$ | = | $x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$ | = | $ax_2\,\hat{\mathbf{x}}$ | (4a) | F I |
| $\mathbf{B_4}$ | = | $-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4a) | F I |
| $\mathbf{B_5}$ | = | $x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$ | = | $ax_3\,\hat{\mathbf{x}}$ | (4a) | F II |
| $\mathbf{B_6}$ | = | $-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4a) | F II |
| $\mathbf{B_7}$ | = | $-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4b) | F III |
| $\mathbf{B_8}$ | = | $y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $-by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (4b) | F III |
| $\mathbf{B_9}$ | = | $(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$ | = | $ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (8c) | F IV |
| $\mathbf{B_{10}}$ | = | $-(x_5 - y_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8c) | F IV |
| $\mathbf{B_{11}}$ | = | $-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8c) | F IV |
| $\mathbf{B_{12}}$ | = | $(x_5 + y_5)\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$ | = | $ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$ | (8c) | F IV |
| $\mathbf{B_{13}}$ | = | $(x_6 - y_6)\,\mathbf{a}_1 + (x_6 + y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8c) | Tl I |
| $\mathbf{B_{14}}$ | = | $-(x_6 - y_6)\,\mathbf{a}_1 - (x_6 + y_6)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8c) | Tl I |
| $\mathbf{B_{15}}$ | = | $-(x_6 + y_6)\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8c) | Tl I |
| $\mathbf{B_{16}}$ | = | $(x_6 + y_6)\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$ | = | $ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (8c) | Tl I |

## References


[1] C. Brosset, *Herstellung und Kristallbau der Verbindungen $TlAlF_4$ und $Tl_2AlF_5$*, Z. Anorganische und Allgemeine Chemie **235**, 139–147 (1937), doi:10.1002/zaac.19372350119.

[2] M. Molinier and W. Massa, *Refinement of the structure of $Tl_2AlF_5 \cdot H_2O$*, Acta Crystallogr. Sect. C **49**, 782–784 (1993), doi:10.1107/S010827019201148X.

[3] C. Brosset, *Electrochemical and X-ray investigations of complex aluminium fluorides*, Ph.D. thesis, University of Stockholm (1942).


## Found in


[1] A. Pabst, *A Structural Classification of Fluoaluminates*, Am. Mineral. **35**, 149–165 (1950).


## First cited in


D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.