

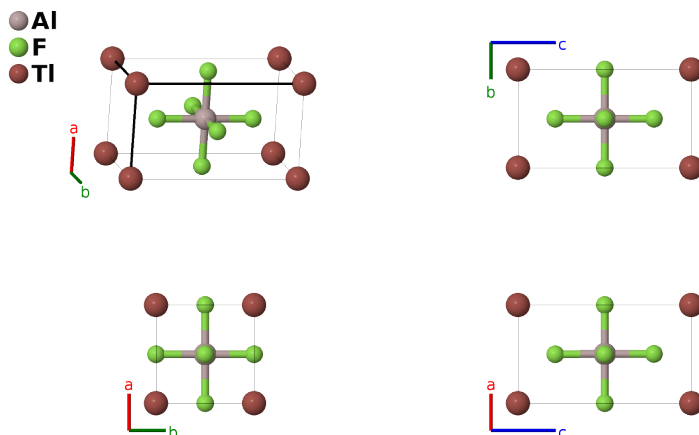
TlAlF₄ (*H*0₈) Structure: AB4C_tP6_123_b_eg_c-001

This structure originally had the label AB4C_tP6_123_d_eh_a. Calls to that address will be redirected here.

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<https://aflow.org/p/416G>

https://aflow.org/p/AB4C_tP6_123_b_eg_c-001



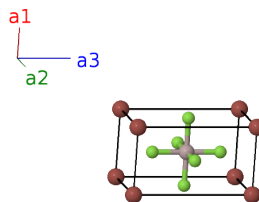
Prototype	AlF ₄ Tl
AFLOW prototype label	AB4C_tP6_123_b_eg_c-001
<i>Strukturbericht</i> designation	<i>H</i> 0 ₈
ICSD	25615
Pearson symbol	tP6
Space group number	123
Space group symbol	<i>P</i> 4/ <i>mmm</i>
AFLOW prototype command	<code>aflow --proto=AB4C_tP6_123_b_eg_c-001 --params=a, c/a, z₄</code>

Other compounds with this structure

β -RbFeF₄, CsFeF₄, KAlF₄, RbAlF₄

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(1b) Al I
\mathbf{B}_2	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(1c) Tl I
\mathbf{B}_3	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2e) F I
\mathbf{B}_4	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2e) F I
\mathbf{B}_5	$=$	$z_4 \mathbf{a}_3$	$=$	$cz_4 \hat{\mathbf{z}}$	(2g) F II
\mathbf{B}_6	$=$	$-z_4 \mathbf{a}_3$	$=$	$-cz_4 \hat{\mathbf{z}}$	(2g) F II

References

- [1] C. Brosset, *Herstellung und Kristallbau der Verbindungen TlAlF₄ und Tl₂AlF₅*, Z. Anorganische und Allgemeine Chemie **235**, 139–147 (1937), doi:10.1002/zaac.19372350119.

Found in

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