$TlAlF_4$ ($H0_8$) Structure: AB4C_tP6_123_b_eg_c-001

This structure previously used the label(s) `AB4C_tP6_123_d_eh_a`. Calls to these addresses will be redirected here.

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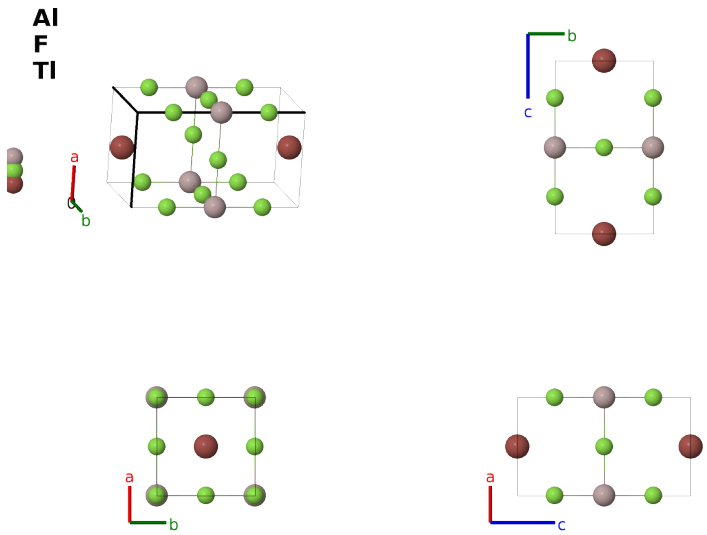
https://aflow.org/prototype-encyclopedia/416G

https://aflow.org/prototype-encyclopedia/AB4C_tP6_123_b_eg_c-001



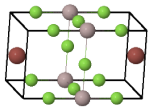
Prototype	AlF_4Tl
AFLOW prototype label	AB4C_tP6_123_b_eg_c-001
***Strukturbericht* designation**	$H0_8$
ICSD	25615
CCDC	1601265
Pearson symbol	tP6
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=AB4C_tP6_123_b_eg_c-001 --params=`$a, c/a, z_4$

Other compounds with this structure

β-$RbFeF_4$, $CsFeF_4$, $KAlF_4$, $RbAlF_4$

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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 $TlAlF_4$ und Tl_2AlF_5*, Z. Anorganische und Allgemeine Chemie **235**, 139–147 (1937), doi:10.1002/zaac.19372350119.

Found in

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

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