TlF ($B24$) Structure (*Obsolete*): AB_oF8_69_a_b-001

This structure previously used the label(s) `AB_oF8_69_a_b`. Calls to these addresses will be redirected here.

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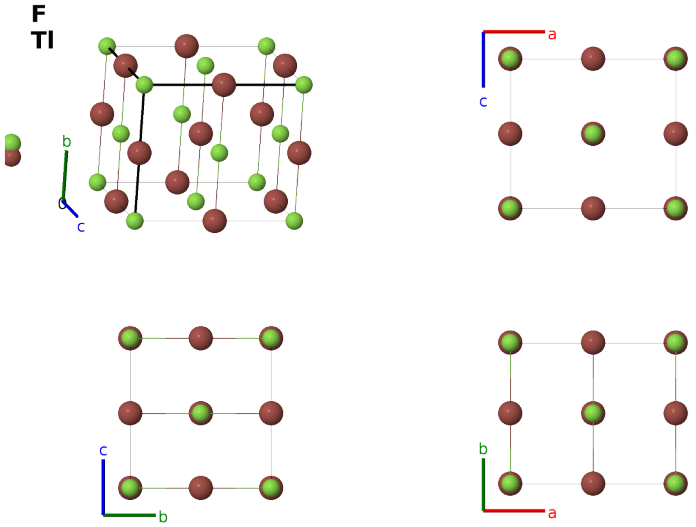
https://aflow.org/prototype-encyclopedia/XT4M

https://aflow.org/prototype-encyclopedia/AB_oF8_69_a_b-001

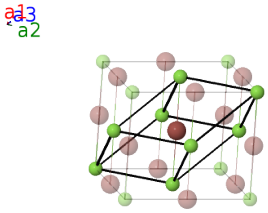


Prototype	FTl
AFLOW prototype label	AB_oF8_69_a_b-001
***Strukturbericht* designation**	$B24$
ICSD	30268
CCDC	1604636
Pearson symbol	oF8
Space group number	69
Space group symbol	$Fmmm$
AFLOW prototype command	`aflow --proto=AB_oF8_69_a_b-001 --params=`$a, b/a, c/a$

- Although this is the $B24$ structure defined in *Strukturbericht*, it is not the currently accepted structure for TlF. See (Berastegui, 2000) and the TlF-II page. The current structure is a slight distortion of rock salt ($B1$).

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	F I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4b)	Tl I

References

[1] J. A. A. Ketelaar, *Die Kristallstruktur des Thallofluorids*, Z. Kristallogr. **92**, 30–38 (1935), doi:10.1524/zkri.1935.92.1.30.

Found in

[1] P. Berastegui and S. Hull, *The Crystal Structures of Thallium(I) Fluoride*, Journal of Solid State Chemistry **150**, 266–275 (2000), doi:10.1006/jssc.1999.8587.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017