

TlF-II Structure:

AB_oP8_57_d_d-001

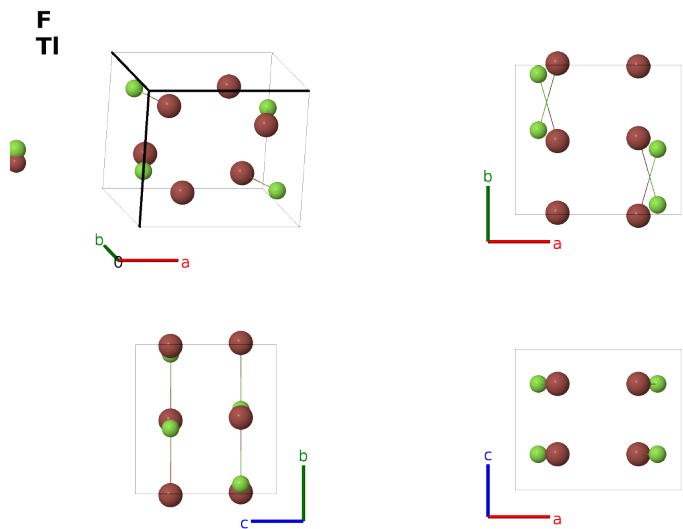
This structure previously used the label(s) **AB_oP8_57_d.d**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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.

<https://aflow.org/prototype-encyclopedia/E914>

https://aflow.org/prototype-encyclopedia/AB_oP8_57_d_d-001



Prototype	FTl
AFLOW prototype label	AB_oP8_57_d_d-001
ICSD	90992
CCDC	1650562
Pearson symbol	oP8
Space group number	57
Space group symbol	<i>Pbcm</i>
AFLOW prototype command	<code>aflow --proto=AB_oP8_57_d_d-001 --params=a, b/a, c/a, x₁, y₁, x₂, y₂</code>

Other compounds with this structure

PbO (massicot)

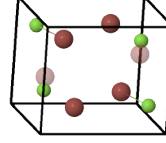
- This is the true low-temperature ground state of TlF. Like the depreciated *B24* structure, it is a distortion of the rock salt (B1) structure.

- At higher temperatures TlF transforms into TlF-I, which is isostructural with litharge (tetragonal PbO, $B10$).

Simple Orthorhombic primitive vectors

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

$\mathbf{a}_1$
 $\mathbf{a}_2$
 $\mathbf{a}_3$



Basis vectors

	Lattice coordinates		Cartesian coordinates		Wyckoff position	Atom type
B₁	=	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	F I
B₂	=	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	F I
B₃	=	$-x_1 \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	F I
B₄	=	$x_1 \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	F I
B₅	=	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	Tl I
B₆	=	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	Tl I
B₇	=	$-x_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	Tl I
B₈	=	$x_2 \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	Tl I

References

- [1] P. Berastegui and S. Hull, *The Crystal Structures of Thallium(I) Fluoride*, J. Solid State Chem. **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