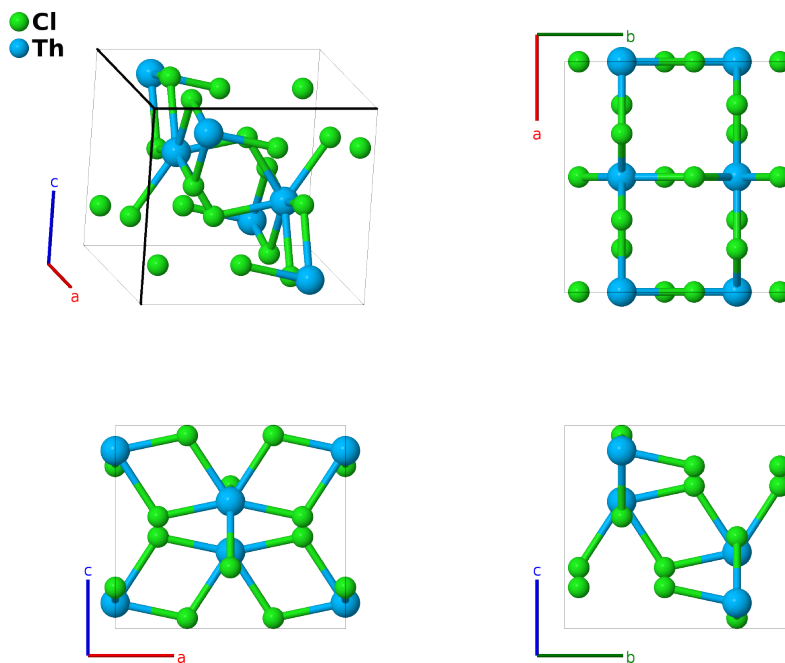


β -ThCl₄ Structure: A4B_tI20_141_h_a-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://afLOW.org/p/NG21>

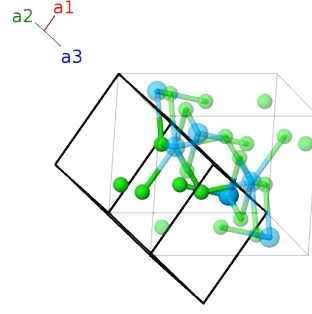
https://afLOW.org/p/A4B_tI20_141_h_a-001



Prototype	Cl ₄ Th
AFLOW prototype label	A4B_tI20_141_h_a-001
ICSD	26197
Pearson symbol	tI20
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	<code>afLOW --proto=A4B_tI20_141_h_a-001 --params=a, c/a, y₂, z₂</code>

- β -ThCl₄ is stable above 405°C. Below that temperature it transforms into α -ThCl₄. (Mason, 1974)

Body-centered Tetragonal primitive vectors



$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}\end{aligned}$$

Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{7}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{y}} + \frac{1}{8}c\hat{\mathbf{z}}$	(4a)	Th I
\mathbf{B}_2	$= \frac{1}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + \frac{3}{8}c\hat{\mathbf{z}}$	(4a)	Th I
\mathbf{B}_3	$= (y_2 + z_2)\mathbf{a}_1 + z_2\mathbf{a}_2 + y_2\mathbf{a}_3$	$=$	$ay_2\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(16h)	Cl I
\mathbf{B}_4	$= (-y_2 + z_2 + \frac{1}{2})\mathbf{a}_1 + z_2\mathbf{a}_2 - (y_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{2})\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(16h)	Cl I
\mathbf{B}_5	$= z_2\mathbf{a}_1 + (-y_2 + z_2 + \frac{1}{2})\mathbf{a}_2 - y_2\mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{4})\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + c(z_2 + \frac{1}{4})\hat{\mathbf{z}}$	(16h)	Cl I
\mathbf{B}_6	$= z_2\mathbf{a}_1 + (y_2 + z_2)\mathbf{a}_2 + (y_2 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(y_2 + \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + c(z_2 - \frac{1}{4})\hat{\mathbf{z}}$	(16h)	Cl I
\mathbf{B}_7	$= (y_2 - z_2 + \frac{1}{2})\mathbf{a}_1 - z_2\mathbf{a}_2 + (y_2 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(y_2 + \frac{1}{2})\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(16h)	Cl I
\mathbf{B}_8	$= -(y_2 + z_2)\mathbf{a}_1 - z_2\mathbf{a}_2 - y_2\mathbf{a}_3$	$=$	$-ay_2\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(16h)	Cl I
\mathbf{B}_9	$= -z_2\mathbf{a}_1 + (y_2 - z_2 + \frac{1}{2})\mathbf{a}_2 + y_2\mathbf{a}_3$	$=$	$a(y_2 + \frac{1}{4})\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} - c(z_2 - \frac{1}{4})\hat{\mathbf{z}}$	(16h)	Cl I
\mathbf{B}_{10}	$= -z_2\mathbf{a}_1 - (y_2 + z_2)\mathbf{a}_2 - (y_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - c(z_2 + \frac{1}{4})\hat{\mathbf{z}}$	(16h)	Cl I

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