β-$ThCl_4$ Structure: A4B_tI20_141_h_a-001

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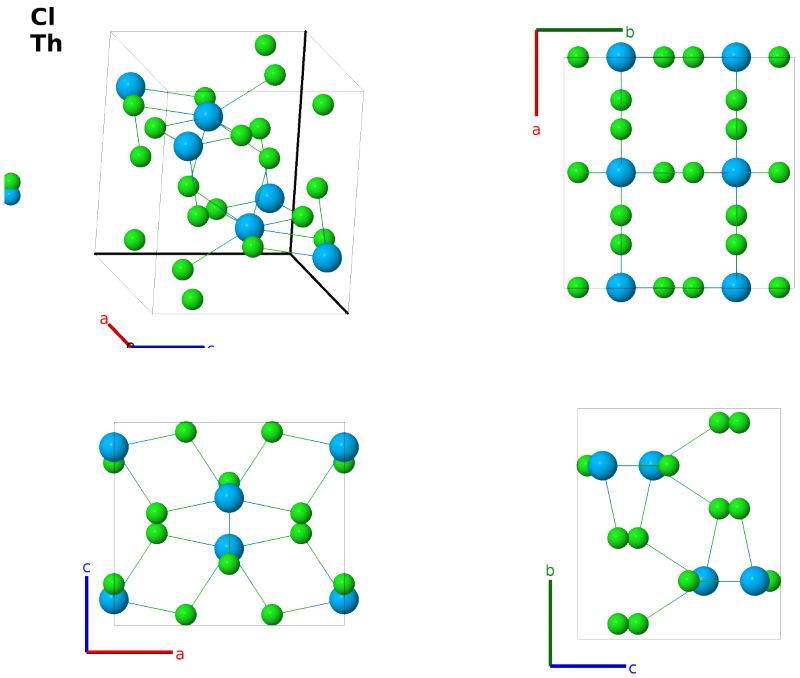
https://aflow.org/prototype-encyclopedia/NG21

https://aflow.org/prototype-encyclopedia/A4B_tI20_141_h_a-001

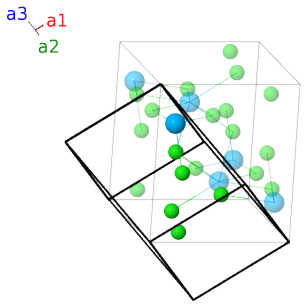


Prototype	Cl_4Th
AFLOW prototype label	A4B_tI20_141_h_a-001
ICSD	26197
CCDC	1601627
Pearson symbol	tI20
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=A4B_tI20_141_h_a-001 --params=`$a, c/a, y_2, z_2$

- β-$ThCl_4$ is stable above 405°C. Below that temperature it transforms into α-$ThCl_4$. (Mason, 1974)

Body-centered Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}\\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}\\ \mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}\end{aligned}$$



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
$\mathbf{B_4}$	=	$\left(-y_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16h)	Cl I
$\mathbf{B_5}$	=	$z_2\,\mathbf{a}_1 + \left(-y_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	Cl I
$\mathbf{B_6}$	=	$z_2\,\mathbf{a}_1 + (y_2 + z_2)\,\mathbf{a}_2 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	Cl I
$\mathbf{B_7}$	=	$\left(y_2 - z_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(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
$\mathbf{B_9}$	=	$-z_2\,\mathbf{a}_1 + \left(y_2 - z_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	Cl I
$\mathbf{B_{10}}$	=	$-z_2\,\mathbf{a}_1 - (y_2 + z_2)\,\mathbf{a}_2 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	Cl I

References

[1] K. Mucker, G. S. Smith, Q. Johnson, and R. E. Elson, *Refinement of the Crystal Structure of $ThCl_4$*, Acta Crystallogr. Sect. B **25**, 2362–2365 (1969), doi:10.1107/S056774086900570X.

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[1] J. T. Mason, M. C. Jha, and P. Chiotti, *Crystal Structures of the $ThCl_4$ Polymorphs*, J. Less-Common Met. **34**, 143–151 (1974), doi:10.1016/0022-5088(74)90224-0.

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