

# $\alpha$ -ThCl<sub>4</sub> Structure: A4B\_tI20\_88\_f\_a-001

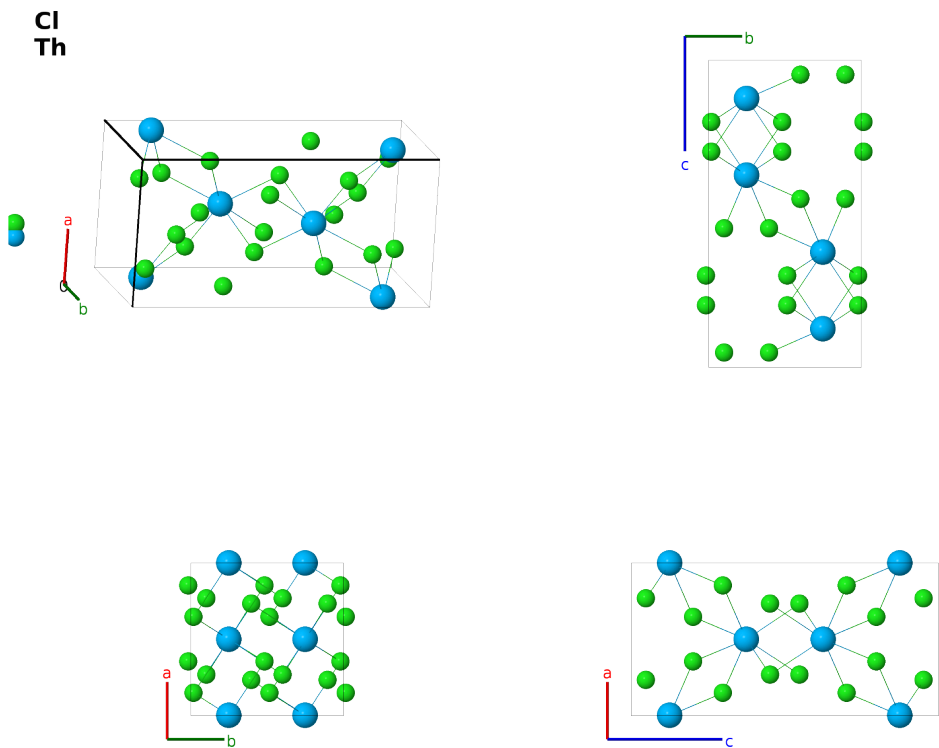
This structure previously used the label(s) **A4B\_tI20\_88\_f\_a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/5VT7>

[https://aflow.org/prototype-encyclopedia/A4B\\_tI20\\_88\\_f\\_a-001](https://aflow.org/prototype-encyclopedia/A4B_tI20_88_f_a-001)



|                         |                                                                                                                 |
|-------------------------|-----------------------------------------------------------------------------------------------------------------|
| Prototype               | Cl <sub>4</sub> Th                                                                                              |
| AFLOW prototype label   | A4B_tI20_88_f_a-001                                                                                             |
| ICSD                    | 6055                                                                                                            |
| CCDC                    | 1593571                                                                                                         |
| Pearson symbol          | tI20                                                                                                            |
| Space group number      | 88                                                                                                              |
| Space group symbol      | $I4_1/a$                                                                                                        |
| AFLOW prototype command | <code>aflow --proto=A4B_tI20_88_f_a-001<br/>--params=a, c/a, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub></code> |

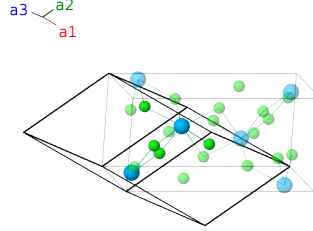
## Other compounds with this structure

ThBr<sub>4</sub>

- $\alpha$ -ThCl<sub>4</sub> is stable below 405°C. Above that temperature it transforms into  $\beta$ -ThCl<sub>4</sub>. (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 |
|-------------------|-----------------------------------------------------------------------------------------------------------------------------|-----|-----------------------------------------------------------------------------------------------------------------------|--|------------------|-----------|
| $\mathbf{B}_1$    | $= \frac{3}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$                                             | $=$ | $\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{8}c\hat{\mathbf{z}}$                                                         |  | (4a)             | Th I      |
| $\mathbf{B}_2$    | $= \frac{5}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$                                             | $=$ | $\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{3}{8}c\hat{\mathbf{z}}$                          |  | (4a)             | Th I      |
| $\mathbf{B}_3$    | $= (y_2 + z_2)\mathbf{a}_1 + (x_2 + z_2)\mathbf{a}_2 + (x_2 + y_2)\mathbf{a}_3$                                             | $=$ | $ax_2\hat{\mathbf{x}} + ay_2\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$                                                  |  | (16f)            | Cl I      |
| $\mathbf{B}_4$    | $= (-y_2 + z_2 + \frac{1}{2})\mathbf{a}_1 - (x_2 - z_2)\mathbf{a}_2 - (x_2 + y_2 - \frac{1}{2})\mathbf{a}_3$                | $=$ | $-ax_2\hat{\mathbf{x}} - a(y_2 - \frac{1}{2})\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$                                 |  | (16f)            | Cl I      |
| $\mathbf{B}_5$    | $= (x_2 + z_2 + \frac{1}{2})\mathbf{a}_1 - (y_2 - z_2)\mathbf{a}_2 + (x_2 - y_2)\mathbf{a}_3$                               | $=$ | $-a(y_2 + \frac{1}{4})\hat{\mathbf{x}} + a(x_2 + \frac{1}{4})\hat{\mathbf{y}} + c(z_2 + \frac{1}{4})\hat{\mathbf{z}}$ |  | (16f)            | Cl I      |
| $\mathbf{B}_6$    | $= (-x_2 + z_2 + \frac{1}{2})\mathbf{a}_1 + (y_2 + z_2 + \frac{1}{2})\mathbf{a}_2 + (-x_2 + y_2 + \frac{1}{2})\mathbf{a}_3$ | $=$ | $a(y_2 + \frac{1}{4})\hat{\mathbf{x}} - a(x_2 - \frac{1}{4})\hat{\mathbf{y}} + c(z_2 + \frac{1}{4})\hat{\mathbf{z}}$  |  | (16f)            | Cl I      |
| $\mathbf{B}_7$    | $= -(y_2 + z_2)\mathbf{a}_1 - (x_2 + z_2)\mathbf{a}_2 - (x_2 + y_2)\mathbf{a}_3$                                            | $=$ | $-ax_2\hat{\mathbf{x}} - ay_2\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$                                                 |  | (16f)            | Cl I      |
| $\mathbf{B}_8$    | $= (y_2 - z_2 + \frac{1}{2})\mathbf{a}_1 + (x_2 - z_2)\mathbf{a}_2 + (x_2 + y_2 + \frac{1}{2})\mathbf{a}_3$                 | $=$ | $ax_2\hat{\mathbf{x}} + a(y_2 + \frac{1}{2})\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$                                  |  | (16f)            | Cl I      |
| $\mathbf{B}_9$    | $= -(x_2 + z_2 - \frac{1}{2})\mathbf{a}_1 + (y_2 - z_2)\mathbf{a}_2 - (x_2 - y_2)\mathbf{a}_3$                              | $=$ | $a(y_2 - \frac{1}{4})\hat{\mathbf{x}} - a(x_2 - \frac{1}{4})\hat{\mathbf{y}} - c(z_2 - \frac{1}{4})\hat{\mathbf{z}}$  |  | (16f)            | Cl I      |
| $\mathbf{B}_{10}$ | $= (x_2 - z_2 + \frac{1}{2})\mathbf{a}_1 - (y_2 + z_2 - \frac{1}{2})\mathbf{a}_2 + (x_2 - y_2 + \frac{1}{2})\mathbf{a}_3$   | $=$ | $-a(y_2 - \frac{1}{4})\hat{\mathbf{x}} + a(x_2 + \frac{1}{4})\hat{\mathbf{y}} - c(z_2 - \frac{1}{4})\hat{\mathbf{z}}$ |  | (16f)            | Cl I      |

## References

- [1] J. T. Mason, M. C. Jha, and P. Chiotti, *Crystal Structures of the ThCl<sub>4</sub> Polymorphs*, J. Less-Common Met. **34**, 143–151 (1974), doi:10.1016/0022-5088(74)90224-0.

**Found in**

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

**First cited in**

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