

β -ThI₃ Structure: A3B_oC64_66_kl2m_acl-001

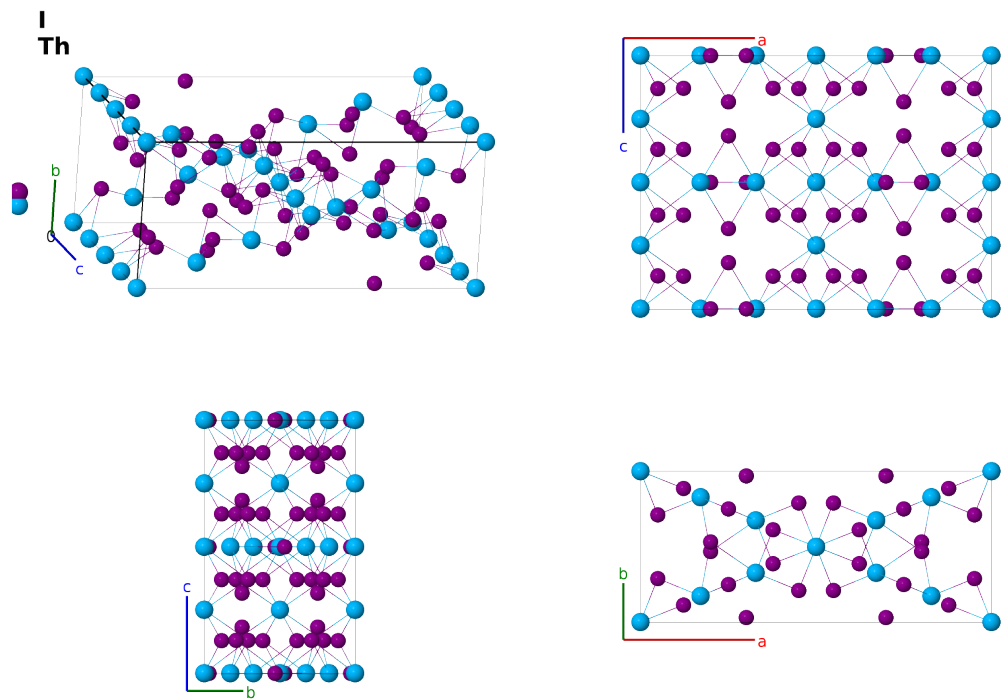
This structure previously used the label(s) **A3B_oC64_66_kl2m_bd1**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/7JBJ>

https://aflow.org/prototype-encyclopedia/A3B_oC64_66_kl2m_acl-001

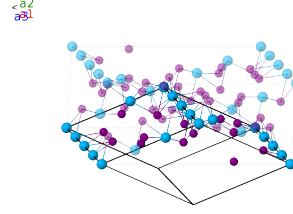


Prototype	I ₃ Th
AFLOW prototype label	A3B_oC64_66_kl2m_acl-001
ICSD	32681
CCDC	1606129
Pearson symbol	oC64
Space group number	66
Space group symbol	<i>Cccm</i>
AFLOW prototype command	<code>aflow --proto=A3B_oC64_66_kl2m_acl-001 --params=a,b/a,c/a,z₃,x₄,y₄,x₅,y₅,x₆,y₆,z₆,x₇,y₇,z₇</code>

- Our original entry (Hicks, 2019) reversed the a and b axis.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(4a)	Th I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(4a)	Th I
$\mathbf{B}_3$	$= 0$	$=$	0	(4c)	Th II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(4c)	Th II
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8k)	I I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8k)	I I
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8k)	I I
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8k)	I I
$\mathbf{B}_9$	$= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}}$	(8l)	I II
$\mathbf{B}_{10}$	$= -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}}$	(8l)	I II
$\mathbf{B}_{11}$	$= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8l)	I II
$\mathbf{B}_{12}$	$= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8l)	I II
$\mathbf{B}_{13}$	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}}$	(8l)	Th III
$\mathbf{B}_{14}$	$= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}}$	(8l)	Th III
$\mathbf{B}_{15}$	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8l)	Th III
$\mathbf{B}_{16}$	$= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8l)	Th III
$\mathbf{B}_{17}$	$= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(16m)	I III
$\mathbf{B}_{18}$	$= -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(16m)	I III
$\mathbf{B}_{19}$	$= -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(16m)	I III
$\mathbf{B}_{20}$	$= (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(16m)	I III
$\mathbf{B}_{21}$	$= -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(16m)	I III
$\mathbf{B}_{22}$	$= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(16m)	I III

$$\begin{aligned}
\mathbf{B}_{23} &= \begin{pmatrix} (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \\ (z_6 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2} \right) \hat{\mathbf{z}} & (16m) & \text{I III} \\
\mathbf{B}_{24} &= \begin{pmatrix} -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + \\ (z_6 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2} \right) \hat{\mathbf{z}} & (16m) & \text{I III} \\
\mathbf{B}_{25} &= \begin{pmatrix} (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + \\ z_7 \mathbf{a}_3 \end{pmatrix} = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16m) & \text{I IV} \\
\mathbf{B}_{26} &= \begin{pmatrix} -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 + \\ z_7 \mathbf{a}_3 \end{pmatrix} = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16m) & \text{I IV} \\
\mathbf{B}_{27} &= \begin{pmatrix} -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - \\ (z_7 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2} \right) \hat{\mathbf{z}} & (16m) & \text{I IV} \\
\mathbf{B}_{28} &= \begin{pmatrix} (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 - \\ (z_7 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2} \right) \hat{\mathbf{z}} & (16m) & \text{I IV} \\
\mathbf{B}_{29} &= \begin{pmatrix} -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - \\ z_7 \mathbf{a}_3 \end{pmatrix} = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16m) & \text{I IV} \\
\mathbf{B}_{30} &= \begin{pmatrix} (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 - \\ z_7 \mathbf{a}_3 \end{pmatrix} = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16m) & \text{I IV} \\
\mathbf{B}_{31} &= \begin{pmatrix} (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \\ (z_7 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2} \right) \hat{\mathbf{z}} & (16m) & \text{I IV} \\
\mathbf{B}_{32} &= \begin{pmatrix} -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 + \\ (z_7 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2} \right) \hat{\mathbf{z}} & (16m) & \text{I IV}
\end{aligned}$$

References

- [1] H. P. Beck and C. Strobel, *ThI₃, ein Janus unter den Verbindungen mit Metall-Metall-Wechselwirkungen*, Angew. Chem. Int. Ed. **94**, 558–559 (1982), doi:10.1002/ange.19820940731.

Found in

- [1] A. M. Fogg, J. S. O. Evens, and D. O'Hare, *Crystal structure of β -MNX ($M = \text{Zr, Hf}$; $X = \text{Cl, Br}$)*, Chem. Comm. **0**, 2269–2270 (1998), doi:10.1039/A806415F.

First cited in

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