

ThMoB₄ Structure:

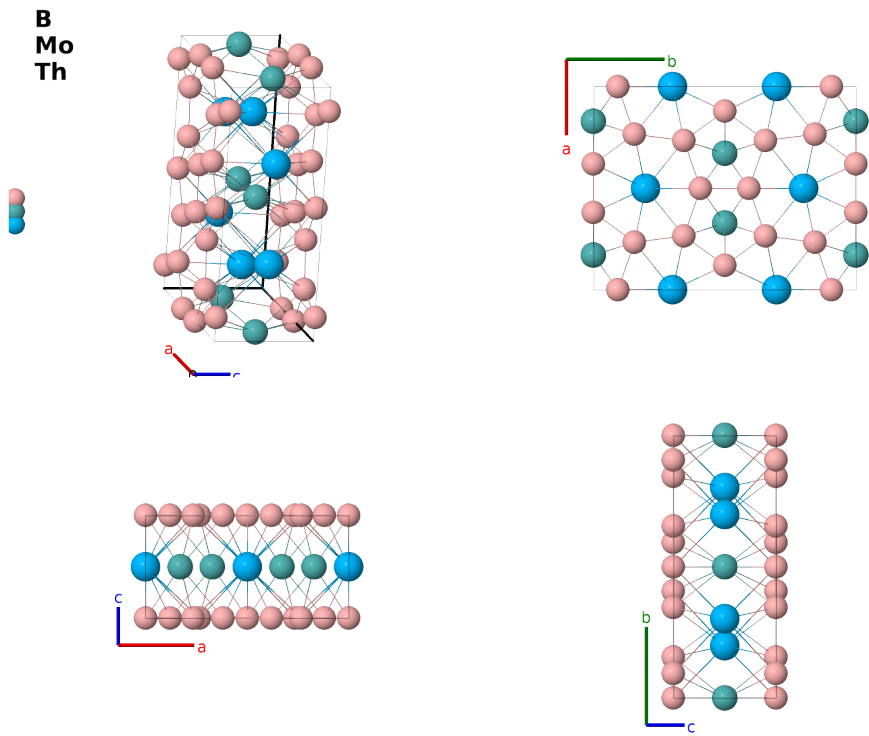
A4BC_oC24_65_gip_h_j-001

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<https://aflow.org/prototype-encyclopedia/B95F>

https://aflow.org/prototype-encyclopedia/A4BC_oC24_65_gip_h_j-001



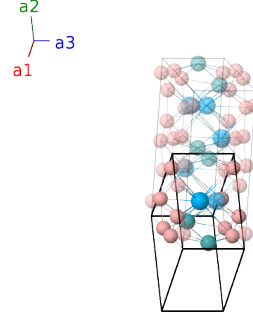
Prototype	B ₄ MoTh
AFLOW prototype label	A4BC_oC24_65_gip_h_j-001
ICSD	41819
CCDC	1611570
Pearson symbol	oC24
Space group number	65
Space group symbol	Cmmm
AFLOW prototype command	<code>aflow --proto=A4BC_oC24_65_gip_h_j-001</code> <code>--params=a, b/a, c/a, x₁, x₂, y₃, y₄, x₅, y₅</code>

Other compounds with this structure

β -ErAlB₄, ThReB₄, ThVB₄, ThWB₄

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
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}}$	(4g)	B I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}}$	(4g)	B I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	Mo I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	Mo I
$\mathbf{B}_5$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$by_3 \hat{\mathbf{y}}$	(4i)	B II
$\mathbf{B}_6$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-by_3 \hat{\mathbf{y}}$	(4i)	B II
$\mathbf{B}_7$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4j)	Th I
$\mathbf{B}_8$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4j)	Th I
$\mathbf{B}_9$	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}}$	(8p)	B III
$\mathbf{B}_{10}$	$= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}}$	(8p)	B III
$\mathbf{B}_{11}$	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}}$	(8p)	B III
$\mathbf{B}_{12}$	$= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}}$	(8p)	B III

References

- [1] P. Rogl and H. Howotny, *Ternäre Komplexboride mit ThMoB₄-Typ.*, Monat. Chemie **105**, 1082–1098 (1974), doi:10.1007/BF00910277.

Found in

- [1] T. Mori, R. Cardoso-Gil, A. Leithe-Jasper, W. Schnelle, H. Borrmann, and Y. Grin, *Synthesis and magnetic properties of the ThMoB₄ type modification of ErAlB₄*, J. Appl. Phys. **103**, 07B730 (2008), doi:10.1063/1.2832855.

First cited in

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