ThMoB$_4$ Structure:
A4BC_oC24_65_gip_h_j-001

https://aflow.org/p/B95F

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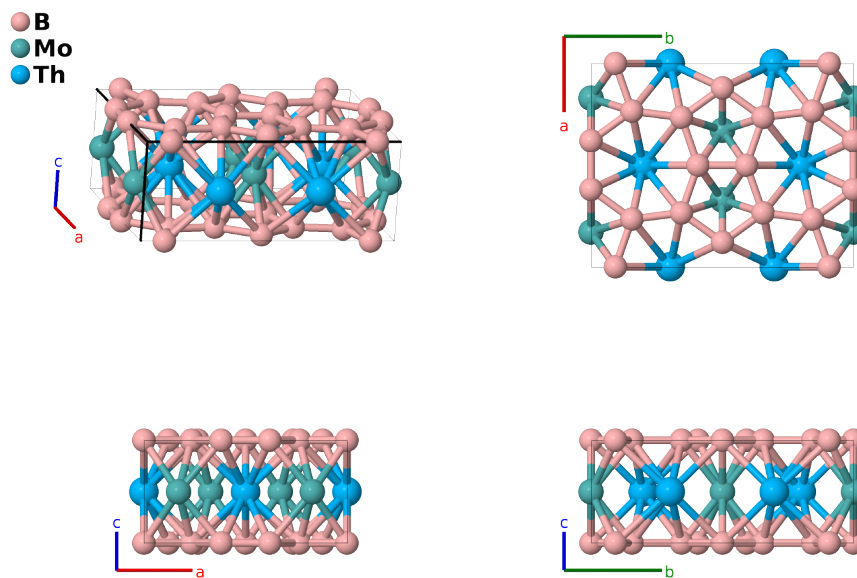
Prototype	B$_4$MoTh	
AFLOW prototype label	A4BC_oC24_65_gip_h_j-001	
ICSD	41819	
Pearson symbol	oC24	
Space group number	65	
Space group symbol	$Cmmm$	
AFLOW prototype command	aflow --proto=A4BC_oC24_65_gip_h_j-001	
	--params=$a, b/a, c/a, x_1, x_2, y_3, y_4, x_5, y_5$	

Other compounds with this structure

β-ErAlB$_4$, ThReB$_4$, ThVB$_4$, ThWB$_4$

Base-centered Orthorhombic primitive vectors
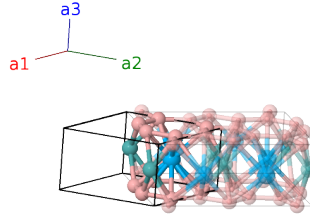
$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

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
$\mathbf{B_3}$	$=$	$x_2\,\mathbf{a_1} + x_2\,\mathbf{a_2} + \tfrac{1}{2}\,\mathbf{a_3}$	$=$	$ax_2\,\hat{\mathbf{x}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Mo I
$\mathbf{B_4}$	$=$	$-x_2\,\mathbf{a_1} - x_2\,\mathbf{a_2} + \tfrac{1}{2}\,\mathbf{a_3}$	$=$	$-ax_2\,\hat{\mathbf{x}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_7}$	$=$	$-y_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + \tfrac{1}{2}\,\mathbf{a_3}$	$=$	$by_4\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(4j)	Th I
$\mathbf{B_8}$	$=$	$y_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} + \tfrac{1}{2}\,\mathbf{a_3}$	$=$	$-by_4\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(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 ThMoB$_4$-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 ThMoB$_4$ type modification of ErAlB$_4$*, J. Appl. Phys. **103**, 07B730 (2008), doi:10.1063/1.2832855.