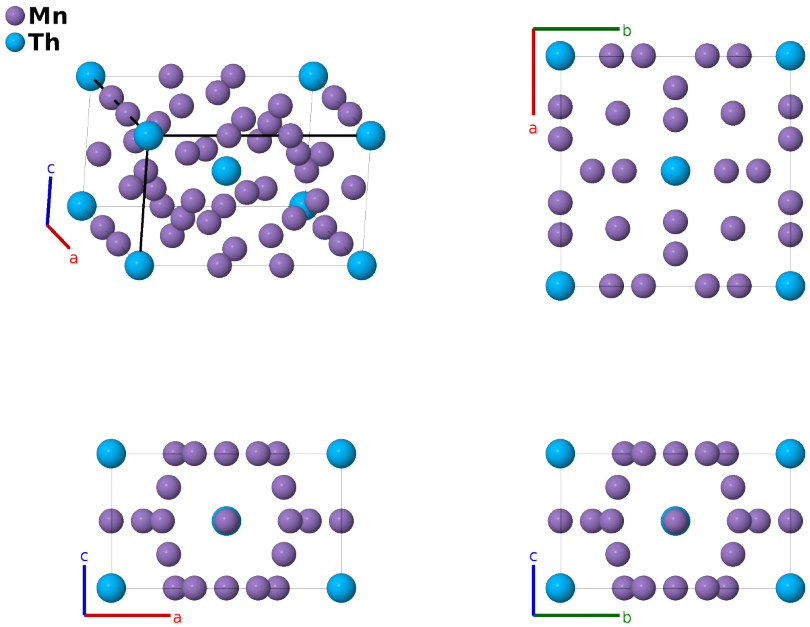
$Mn_{12}Th$ ($D2_b$) Structure: A12B_tI26_139_fij_a-001

This structure originally had the label `A12B_tI26_139_fij_a`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/AJGV

https://aflow.org/p/A12B_tI26_139_fij_a-001



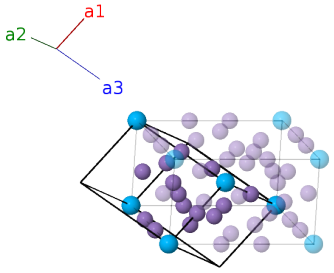
Prototype	$Mn_{12}Th$
AFLOW prototype label	A12B_tI26_139_fij_a-001
***Strukturbericht* designation**	$D2_b$
ICSD	104986
Pearson symbol	tI26
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A12B_tI26_139_fij_a-001 --params=`$a, c/a, x_3, x_4$

Other compounds with this structure

$Be_{12}Ag$, $Be_{12}Co$, $Be_{12}Cr$, $Be_{12}Fe$, $Be_{12}Mn$, $Be_{12}Mo$, $Be_{12}Nb$, $Be_{12}Pd$, $Be_{12}Pt$, $Be_{12}Th$, $Be_{12}Ti$, $Be_{12}V$, $Be_{12}W$, $Mg_{12}Ce$, $Mg_{12}Nd$, $Mg_{12}Pr$, $Mn_{12}Y$, Al_8Cr_4Er, Al_8Cu_4Ce, Al_8Mn_4Ce, Mn_8Fe_4, Fe_7Mn_5

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Th I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8f)	Mn I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - \frac{1}{4}c\,\hat{\mathbf{z}}$	(8f)	Mn I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8f)	Mn I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8f)	Mn I
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(8i)	Mn II
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(8i)	Mn II
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{y}}$	(8i)	Mn II
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{y}}$	(8i)	Mn II
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(8j)	Mn III
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(8j)	Mn III
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8j)	Mn III
$\mathbf{B_{13}}$	=	$-x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8j)	Mn III

References

[1] J. V. Florio, R. E. Rundle, and A. I. Snow, *Compounds of thorium with transition metals. I. The thorium-manganese system*, Acta Cryst. **5**, 449–457 (1952), doi:10.1107/S0365110X52001337.

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.