

MnF₂ Structure:

A2B_tP12_111_2n_bce-001

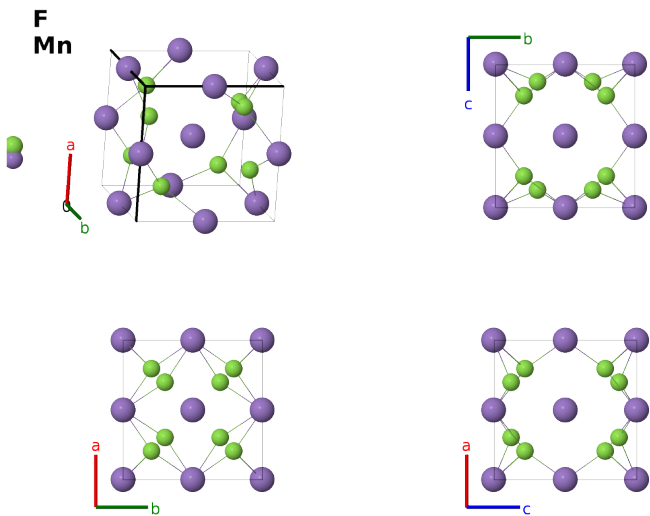
This structure previously used the label(s) **A2B_tP12_111_2n_adf**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A2B_tP12_111_2n_bce-001

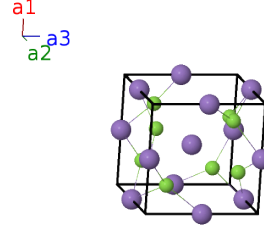


Prototype	F ₂ Mn
AFLOW prototype label	A2B_tP12_111_2n_bce-001
ICSD	12167
CCDC	1595411
Pearson symbol	tP12
Space group number	111
Space group symbol	$P\bar{4}2m$
AFLOW prototype command	<pre>aflow --proto=A2B_tP12_111_2n_bce-001 --params=a,c/a,x₄,z₄,x₅,z₅</pre>

- This is the high pressure phase of MnF₂, with data taken at 200°C and 35 kbar. At standard temperature and pressure MnF₂ is in the rutile (*C4*) structure.
- (Yagi, 1979) consistently refers to space group $P\bar{4}2m$ as “#113,” but it is actually #111, and the Wyckoff positions are consistent with $P\bar{4}2m$ #111.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(1b)	Mn I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(1c)	Mn II
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	(2e)	Mn III
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{y}}$	(2e)	Mn III
$\mathbf{B}_5$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4n)	F I
$\mathbf{B}_6$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4n)	F I
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4n)	F I
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4n)	F I
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4n)	F II
$\mathbf{B}_{10}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4n)	F II
$\mathbf{B}_{11}$	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4n)	F II
$\mathbf{B}_{12}$	$= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4n)	F II

References

- [1] T. Yagi, *Polymorphism in MnF_2 (rutile type) at high pressures*, J. Geophys. Res. **84**, 1113–1115 (1979), doi:10.1029/JB084iB03p01113.

Found in

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

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D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043