

MnF_{1-x}(OH)_x Structure: A2BC2_oP10_34_c_a_c-001

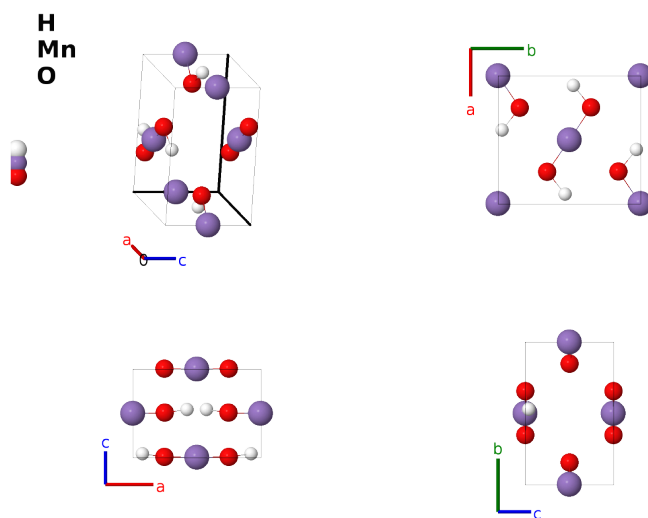
This structure previously used the label(s) **A2BC2_oP10_34_c_a_c**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/5413>

https://aflow.org/prototype-encyclopedia/A2BC2_oP10_34_c_a_c-001



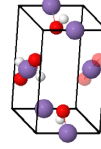
Prototype	$F_{1-x}H_xMnO_x$
AFLOW prototype label	A2BC2_oP10_34_c_a_c-001
Pearson symbol	oP10
Space group number	34
Space group symbol	$Pnn2$
AFLOW prototype command	<pre>aflow --proto=A2BC2_oP10_34_c_a_c-001 --params=a,b/a,c/a,z1,x2,y2,z2,x3,y3,z3</pre>

- We use the data (Yahia, 2013) give for $x = 0.399$. That is, for and (4c) (F/OH) site, 60% of the time the (4c) F site are occupied and 40% of the time (4c) H and O sites are occupied. Here we show the positions of the oxygen and hydrogen atoms.
- Space group $Pnn2$ #34 allows an arbitrary choice of the origin of the z -coordinate. Here we use this to put the manganese atom at the origin, setting $z_1 = 0$.

Simple Orthorhombic primitive vectors



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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Mn I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Mn I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B}_5$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B}_6$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_2 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_9$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{10}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_3 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I

References

- [1] H. B. Yahia, M. Shikano, H. Kobayashi, M. Avdeev, S. Liu, and C. D. Ling, *Synthesis and characterization of the crystal structure and magnetic properties of the hydroxyfluoride $\text{MnF}_{2-x}(\text{OH})_x$ ($x \approx 0.8$)*, Phys. Chem. Chem. Phys. **15**, 13061–13069 (2013), doi:10.1039/C3CP50740H.

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