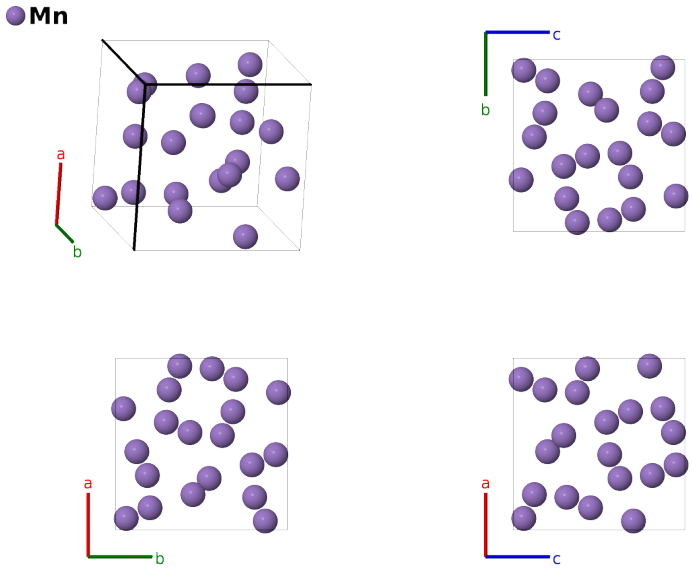
β-Mn ($A13$) Structure: A_cP20_213_cd-001

This structure originally had the label `A_cP20_213_cd`. 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/4VEQ

https://aflow.org/p/A_cP20_213_cd-001

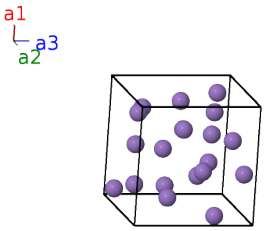


Prototype	Mn
AFLOW prototype label	A_cP20_213_cd-001
***Strukturbericht* designation**	$A13$
ICSD	41775
Pearson symbol	cP20
Space group number	213
Space group symbol	$P4_132$
AFLOW prototype command	`aflow --proto=A_cP20_213_cd-001 --params=`a, x_1, y_2

- This is the high temperature form of manganese, stable in the range 727-1095°C and metastable at room temperature (Donohue, 1982). The ground state is α-Mn ($A12$).
- This structure may also be found in the enantiomorphic space group $P4_332$ #212.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B_5}$	=	$\left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B_6}$	=	$-\left(x_1 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{3}{4}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{3}{4}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{3}{4}\right)\,\hat{\mathbf{y}} - a\left(x_1 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B_7}$	=	$\left(x_1 + \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_1 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B_8}$	=	$-\left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B_9}$	=	$\frac{1}{8}\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} + a\left(y_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(12d)	Mn II
$\mathbf{B_{10}}$	=	$\frac{3}{8}\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} + a\left(y_2 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(12d)	Mn II
$\mathbf{B_{11}}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(12d)	Mn II
$\mathbf{B_{12}}$	=	$\frac{5}{8}\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{5}{8}a\,\hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_2 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(12d)	Mn II
$\mathbf{B_{13}}$	=	$\left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}}$	(12d)	Mn II
$\mathbf{B_{14}}$	=	$\left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}}$	(12d)	Mn II
$\mathbf{B_{15}}$	=	$-\left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Mn II
$\mathbf{B_{16}}$	=	$-\left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{5}{8}a\,\hat{\mathbf{y}} - a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Mn II
$\mathbf{B_{17}}$	=	$y_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + a\left(y_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(12d)	Mn II
$\mathbf{B_{18}}$	=	$-y_2\,\mathbf{a}_1 + \left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + a\left(y_2 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(12d)	Mn II
$\mathbf{B_{19}}$	=	$\left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{7}{8}a\,\hat{\mathbf{z}}$	(12d)	Mn II
$\mathbf{B_{20}}$	=	$-\left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_2 - \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{5}{8}a\,\hat{\mathbf{z}}$	(12d)	Mn II

References

[1] C. B. Shoemaker, D. P. Shoemaker, T. E. Hopkins, and S. Yindepti, *Refinement of the structure of β-manganese and of a related phase in the Mn-Ni-Si system*, Acta Crystallogr. Sect. B **34**, 3573–3576 (1978), doi:10.1107/S0567740878011620.

[2] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, Malabar, Florida, 1982). Reprint of the 1974 John Wilely & Sons edition.