

β -Mn (A13) Structure: A_cP20_213_cd-001

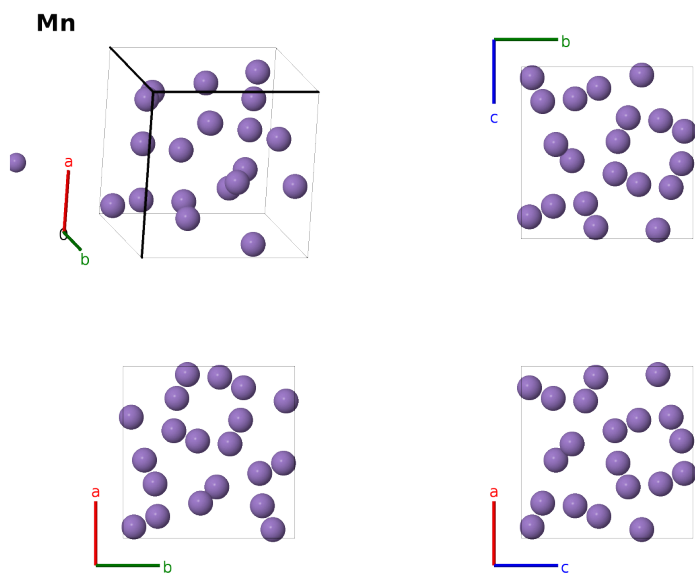
This structure previously used the label(s) **A.cP20_213_cd**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/4VEQ>

https://aflow.org/prototype-encyclopedia/A_cP20_213_cd-001



Prototype	Mn
AFLOW prototype label	A_cP20_213_cd-001
<i>Strukturbericht</i> designation	A13
ICSD	41775
CCDC	1611528
Pearson symbol	cP20
Space group number	213
Space group symbol	$P4_132$
AFLOW prototype command	<code>aflow --proto=A_cP20_213_cd-001 --params=a, x_1, y_2</code>

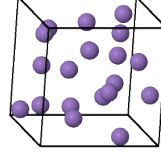
- This is the high temperature form of manganese, stable in the range 727-1095°C and metastable at room temperature (Donohue, 1982). The ground state is α -Mn (A12).

- This structure may also be found in the enantiomorphic space group $P4_332$ #212.

Simple Cubic primitive vectors

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

$\mathbf{a}_1$
 $\mathbf{a}_2$
 $\mathbf{a}_3$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} + a x_1 \hat{\mathbf{y}} + a x_1 \hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 +$ $\left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - a x_1 \hat{\mathbf{y}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Mn I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - a x_1 \hat{\mathbf{z}}$	(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
$\mathbf{B}_9$	$= \frac{1}{8} \mathbf{a}_1 + y_2 \mathbf{a}_2 + \left(y_2 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$\frac{1}{8} a \hat{\mathbf{x}} + a y_2 \hat{\mathbf{y}} + a \left(y_2 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(12d)	Mn II
$\mathbf{B}_{10}$	$= \frac{3}{8} \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(y_2 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$\frac{3}{8} a \hat{\mathbf{x}} - a y_2 \hat{\mathbf{y}} + a \left(y_2 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{13}$	$= \left(y_2 + \frac{1}{4}\right) \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + y_2 \mathbf{a}_3$	$=$	$a \left(y_2 + \frac{1}{4}\right) \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} + a y_2 \hat{\mathbf{z}}$	(12d)	Mn II
$\mathbf{B}_{14}$	$= \left(y_2 + \frac{3}{4}\right) \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 - y_2 \mathbf{a}_3$	$=$	$a \left(y_2 + \frac{3}{4}\right) \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} - a y_2 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{17}$	$= y_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{4}\right) \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3$	$=$	$a y_2 \hat{\mathbf{x}} + a \left(y_2 + \frac{1}{4}\right) \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}}$	(12d)	Mn II
$\mathbf{B}_{18}$	$= -y_2 \mathbf{a}_1 + \left(y_2 + \frac{3}{4}\right) \mathbf{a}_2 + \frac{3}{8} \mathbf{a}_3$	$=$	$-a y_2 \hat{\mathbf{x}} + a \left(y_2 + \frac{3}{4}\right) \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}}$	(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 Wiley & Sons edition.

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