α-Mn ($A12$) Structure: A_cI58_217_ac2g-001

This structure originally had the label `A_cI58_217_ac2g`. Calls to that address will be redirected here.

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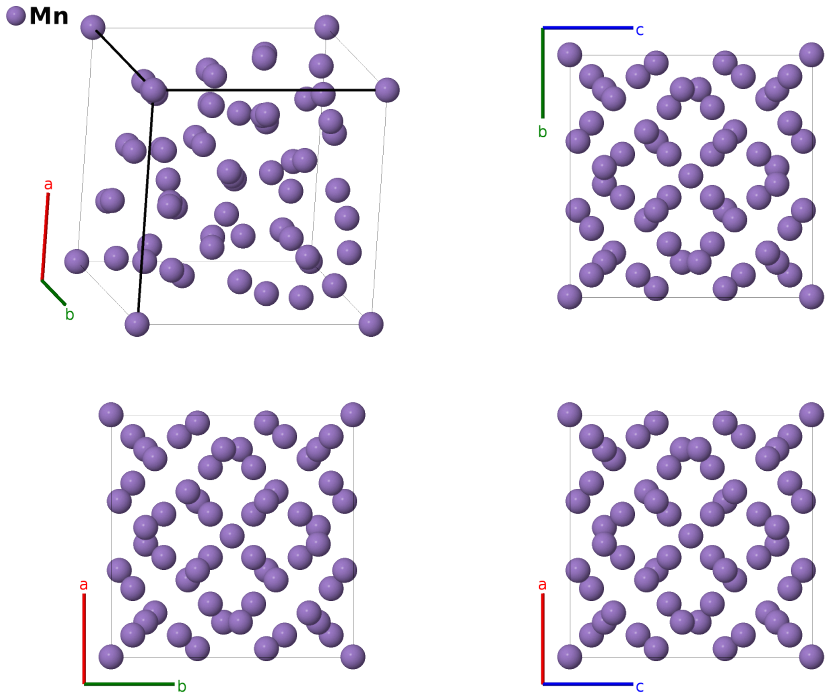
https://aflow.org/p/SV19

https://aflow.org/p/A_cI58_217_ac2g-001



Prototype Mn

AFLOW prototype label A_cI58_217_ac2g-001

***Strukturbericht* designation** $A12$

ICSD 42743

Pearson symbol cI58

Space group number 217

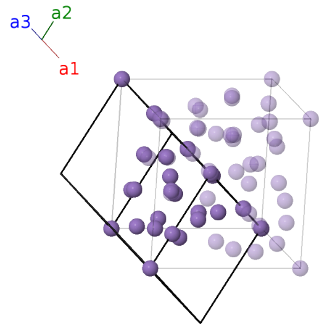
Space group symbol $I\bar{4}3m$

AFLOW prototype command `aflow --proto=A_cI58_217_ac2g-001`
`--params=`$a, x_2, x_3, z_3, x_4, z_4$

- This is the ground state structure of manganese. The high temperature structure, β-Mn ($A13$), is stable from 727-1095°C and metastable at room temperature (Donohue, 1982).
- $Mg_{17}Al_{12}$ is a binary form of this structure.

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Mn I
$\mathbf{B_2}$	=	$2x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	Mn II
$\mathbf{B_3}$	=	$-2x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	Mn II
$\mathbf{B_4}$	=	$-2x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	Mn II
$\mathbf{B_5}$	=	$-2x_2\,\mathbf{a}_1$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	Mn II
$\mathbf{B_6}$	=	$(x_3+z_3)\,\mathbf{a}_1 + (x_3+z_3)\,\mathbf{a}_2 + 2x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(24g)	Mn III
$\mathbf{B_7}$	=	$-(x_3-z_3)\,\mathbf{a}_1 - (x_3-z_3)\,\mathbf{a}_2 - 2x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(24g)	Mn III
$\mathbf{B_8}$	=	$(x_3-z_3)\,\mathbf{a}_1 - (x_3+z_3)\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(24g)	Mn III
$\mathbf{B_9}$	=	$-(x_3+z_3)\,\mathbf{a}_1 + (x_3-z_3)\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(24g)	Mn III
$\mathbf{B_{10}}$	=	$2x_3\,\mathbf{a}_1 + (x_3+z_3)\,\mathbf{a}_2 + (x_3+z_3)\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(24g)	Mn III
$\mathbf{B_{11}}$	=	$-2x_3\,\mathbf{a}_1 - (x_3-z_3)\,\mathbf{a}_2 - (x_3-z_3)\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24g)	Mn III
$\mathbf{B_{12}}$	=	$(x_3-z_3)\,\mathbf{a}_2 - (x_3+z_3)\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(24g)	Mn III
$\mathbf{B_{13}}$	=	$-(x_3+z_3)\,\mathbf{a}_2 + (x_3-z_3)\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24g)	Mn III
$\mathbf{B_{14}}$	=	$(x_3+z_3)\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + (x_3+z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(24g)	Mn III
$\mathbf{B_{15}}$	=	$-(x_3-z_3)\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_2 - (x_3-z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24g)	Mn III
$\mathbf{B_{16}}$	=	$-(x_3+z_3)\,\mathbf{a}_1 + (x_3-z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24g)	Mn III
$\mathbf{B_{17}}$	=	$(x_3-z_3)\,\mathbf{a}_1 - (x_3+z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(24g)	Mn III
$\mathbf{B_{18}}$	=	$(x_4+z_4)\,\mathbf{a}_1 + (x_4+z_4)\,\mathbf{a}_2 + 2x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(24g)	Mn IV
$\mathbf{B_{19}}$	=	$-(x_4-z_4)\,\mathbf{a}_1 - (x_4-z_4)\,\mathbf{a}_2 - 2x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(24g)	Mn IV
$\mathbf{B_{20}}$	=	$(x_4-z_4)\,\mathbf{a}_1 - (x_4+z_4)\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(24g)	Mn IV
$\mathbf{B_{21}}$	=	$-(x_4+z_4)\,\mathbf{a}_1 + (x_4-z_4)\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(24g)	Mn IV
$\mathbf{B_{22}}$	=	$2x_4\,\mathbf{a}_1 + (x_4+z_4)\,\mathbf{a}_2 + (x_4+z_4)\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(24g)	Mn IV

$\mathbf{B_{23}}$	=	$-2x_4\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - (x_4 - z_4)\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(24g)	Mn IV
$\mathbf{B_{24}}$	=	$(x_4 - z_4)\,\mathbf{a}_2 - (x_4 + z_4)\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(24g)	Mn IV
$\mathbf{B_{25}}$	=	$-(x_4 + z_4)\,\mathbf{a}_2 + (x_4 - z_4)\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(24g)	Mn IV
$\mathbf{B_{26}}$	=	$(x_4 + z_4)\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2 + (x_4 + z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(24g)	Mn IV
$\mathbf{B_{27}}$	=	$-(x_4 - z_4)\,\mathbf{a}_1 - 2x_4\,\mathbf{a}_2 - (x_4 - z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(24g)	Mn IV
$\mathbf{B_{28}}$	=	$-(x_4 + z_4)\,\mathbf{a}_1 + (x_4 - z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - az_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(24g)	Mn IV
$\mathbf{B_{29}}$	=	$(x_4 - z_4)\,\mathbf{a}_1 - (x_4 + z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - az_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(24g)	Mn IV

References

[1] J. A. Oberteuffer and J. A. Ibers, *A refinement of the atomic and thermal parameters of α-manganese from a single crystal*, Acta Crystallogr. Sect. B **26**, 1499–1504 (1970), doi:10.1107/S0567740870004399.

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