Mn_2B ($D1_f$) Structure: AB2_oF48_70_e_ef-001

This structure originally had the label `AB2_oF48_70_f_fg`. Calls to that address will be redirected here.

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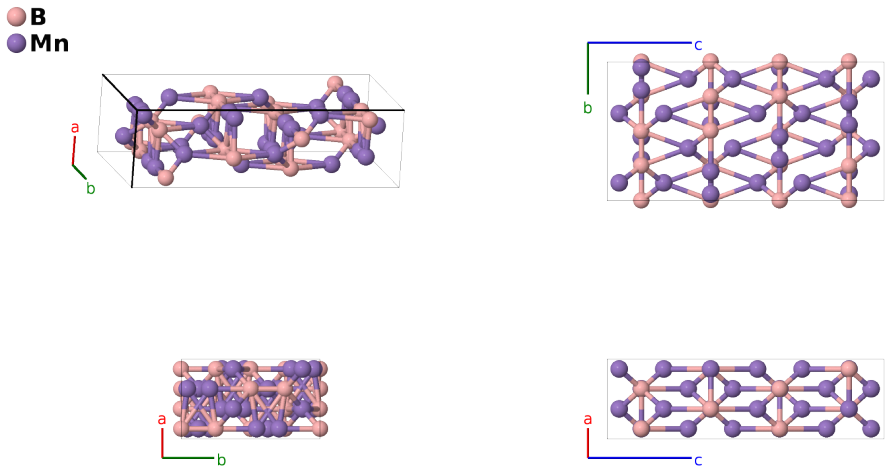
https://aflow.org/p/RZ74

https://aflow.org/p/AB2_oF48_70_e_ef-001



Prototype	BMn_2
AFLOW prototype label	AB2_oF48_70_e_ef-001
***Strukturbericht* designation**	$D1_f$
ICSD	86398
Pearson symbol	oF48
Space group number	70
Space group symbol	$Fddd$
AFLOW prototype command	`aflow --proto=AB2_oF48_70_e_ef-001 --params=`$a, b/a, c/a, x_1, x_2, y_3$

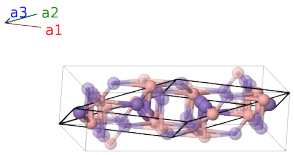
Other compounds with this structure
Cr_2B

- Early works, *e.g.* (Pearson, 1958), referred to this structure as Mn_4B, with the same space group and Wyckoff positions. The stoichiometry was fixed by assuming that the (16e) boron positions were only half-occupied. The (Tergenius, 1981) refinement of the structure showed that the (16e) sites were totally filled, fixing the stoichiometry to Mn_2B. A similar reanalysis showed that the similar structure known as Cr_4B also had composition Cr_2B.
- Tergenius gives the atomic positions using the first setting of space group $Fddd$ #70. We have translated this into the second setting, where the origin is on an inversion site. As a part of this process the primitive axes were also rotated compared to Tergenius.

- Mn_2B ($D1_f$) and $CuMg_2$ (C_b) have the same AFLOW prototype label, AB2_oF48_70_e_ef. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-\left(x_1-\frac{1}{4}\right)\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	B I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_1 - \left(x_1-\frac{1}{4}\right)\mathbf{a}_2 - \left(x_1-\frac{1}{4}\right)\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{4}\right)\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	B I
$\mathbf{B_3}$	=	$\left(x_1+\frac{3}{4}\right)\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	B I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 + \left(x_1+\frac{3}{4}\right)\mathbf{a}_2 + \left(x_1+\frac{3}{4}\right)\mathbf{a}_3$	=	$a\left(x_1+\frac{3}{4}\right)\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	B I
$\mathbf{B_5}$	=	$-\left(x_2-\frac{1}{4}\right)\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Mn I
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_1 - \left(x_2-\frac{1}{4}\right)\mathbf{a}_2 - \left(x_2-\frac{1}{4}\right)\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{4}\right)\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Mn I
$\mathbf{B_7}$	=	$\left(x_2+\frac{3}{4}\right)\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Mn I
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2+\frac{3}{4}\right)\mathbf{a}_2 + \left(x_2+\frac{3}{4}\right)\mathbf{a}_3$	=	$a\left(x_2+\frac{3}{4}\right)\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Mn I
$\mathbf{B_9}$	=	$y_3\,\mathbf{a}_1 - \left(y_3-\frac{1}{4}\right)\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Mn II
$\mathbf{B_{10}}$	=	$-\left(y_3-\frac{1}{4}\right)\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(y_3-\frac{1}{4}\right)\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{4}\right)\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Mn II
$\mathbf{B_{11}}$	=	$-y_3\,\mathbf{a}_1 + \left(y_3+\frac{3}{4}\right)\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	Mn II
$\mathbf{B_{12}}$	=	$\left(y_3+\frac{3}{4}\right)\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(y_3+\frac{3}{4}\right)\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + b\left(y_3+\frac{3}{4}\right)\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	Mn II

References

[1] L.-E. Tergenius, *Refinement of the crystal structure of orthorhombic Mn_2B (formerly denoted Mn_4B)*, J. Less-Common Met. **82**, 335–340 (1981), doi:10.1016/0022-5088(81)90236-8.

[2] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, no. N.R.C. No. 4303 in International Series of Monographs on Metal Physics and Physical Metallurgy (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfort, 1958), 1964 reprint with corrections edn.