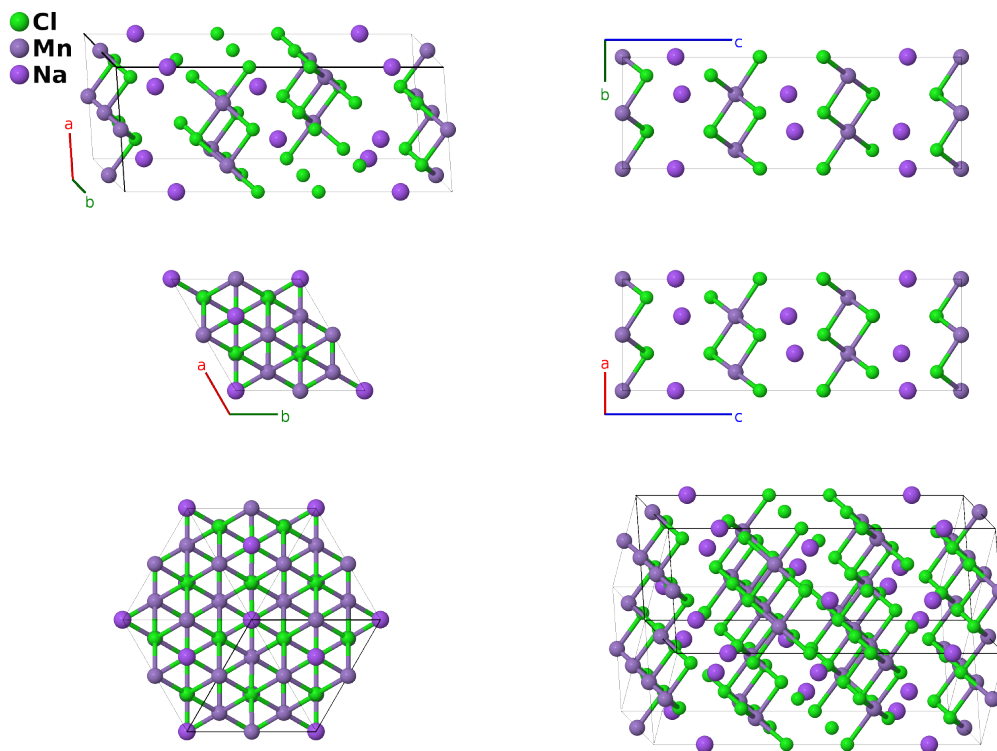


Na₂Mn₃Cl₈ Structure: A8B3C2_hR13_166_ch_e_c-001

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<https://aflow.org/p/799E>

https://aflow.org/p/A8B3C2_hR13_166_ch_e_c-001



Prototype	Cl ₈ Mn ₃ Na ₂
AFLOW prototype label	A8B3C2_hR13_166_ch_e_c-001
ICSD	1846
Pearson symbol	hR13
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A8B3C2_hR13_166_ch_e_c-001 --params=a, c/a, x₁, x₂, x₄, z₄</code>

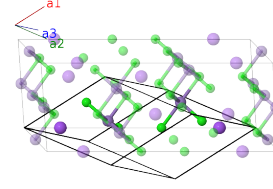
Other compounds with this structure

Ca₂Pt₃O₈, Na₂Cd₃Cl₈, Na₂Fe₃Cl₈, Na₂Mg₃Cl₈, α -Na₂Ti₃Cl₈

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(2c)	Cl I
\mathbf{B}_2	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-cx_1 \hat{\mathbf{z}}$	(2c)	Cl I
\mathbf{B}_3	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c)	Na I
\mathbf{B}_4	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c)	Na I
\mathbf{B}_5	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3e)	Mn I
\mathbf{B}_6	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3e)	Mn I
\mathbf{B}_7	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3e)	Mn I
\mathbf{B}_8	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	Cl II
\mathbf{B}_9	$= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	Cl II
\mathbf{B}_{10}	$= x_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	Cl II
\mathbf{B}_{11}	$= -z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	Cl II
\mathbf{B}_{12}	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	Cl II
\mathbf{B}_{13}	$= -x_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a(x_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	Cl II

References

- [1] C. J. J. van Loon and D. J. W. Ijdo, *The crystal structure of Na_6MnCl_8 and $\text{Na}_2\text{Mn}_3\text{Cl}_8$ and some isostructural compounds*, Acta Crystallogr. Sect. B **31**, 770–773 (1975), doi:10.1107/S0567740875003779.