

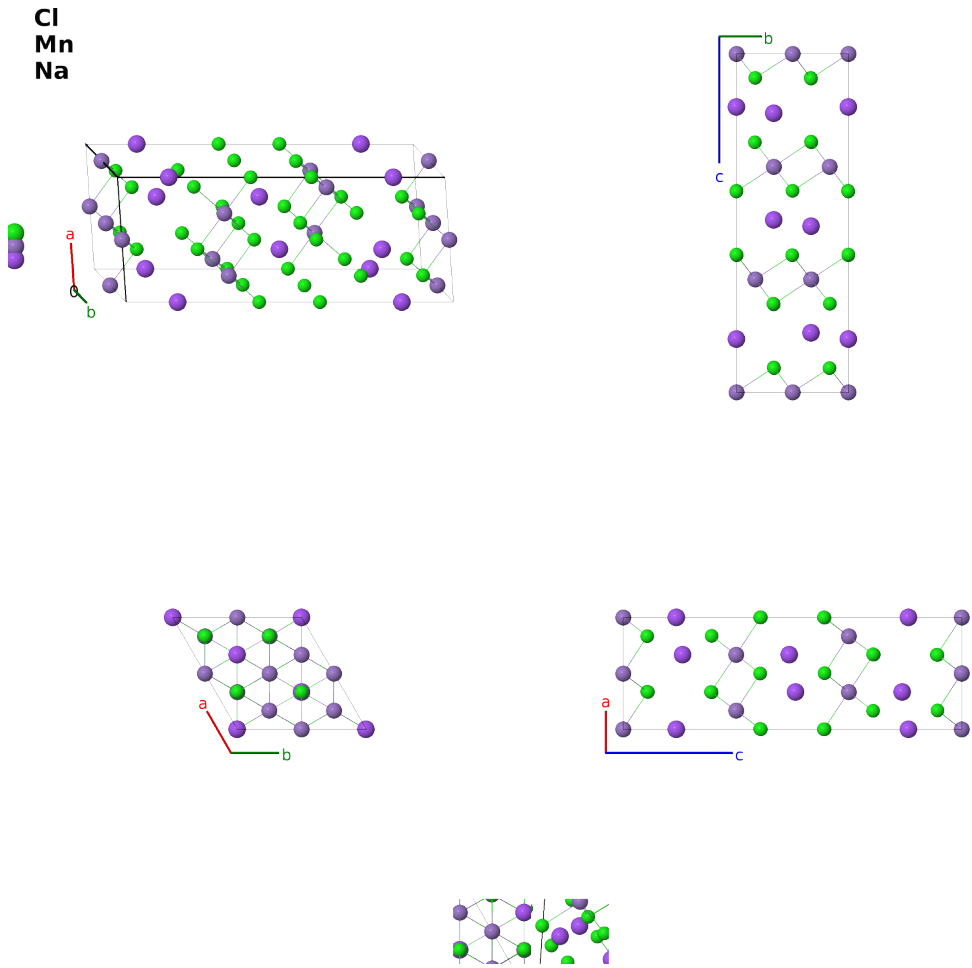
Na₂Mn₃Cl₈ Structure: A8B3C2_hR13_166_ch_e_c-001

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<https://aflow.org/prototype-encyclopedia/799E>

https://aflow.org/prototype-encyclopedia/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
CCDC	1591819
Pearson symbol	hR13
Space group number	166
Space group symbol	$R\bar{3}m$

AFLOW prototype command `aflow --proto=A8B3C2_hR13_166_ch_e_c-001`
 `--params=a,c/a,x1,x2,x4,z4`

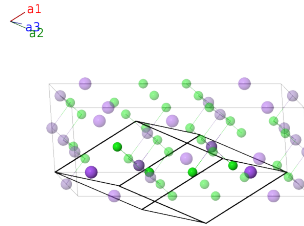
Other compounds with this structure

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 Na₆MnCl₈ and Na₂Mn₃Cl₈ and some isostructural compounds*, Acta Crystallogr. Sect. B **31**, 770–773 (1975), doi:10.1107/S0567740875003779.

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