

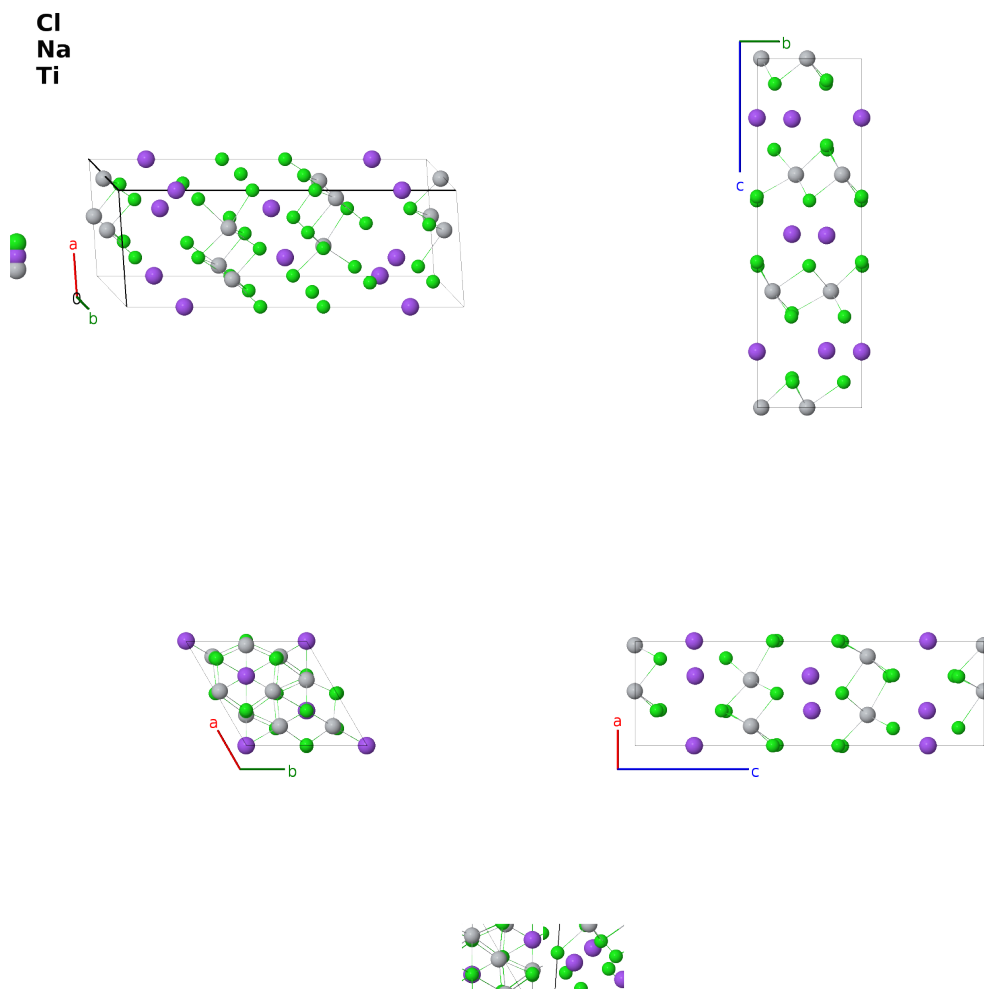
γ -Na₂Ti₃Cl₈ Structure: A8B2C3_hR13_160_2a2b_2a_b-001

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<https://aflow.org/prototype-encyclopedia/L333>

https://aflow.org/prototype-encyclopedia/A8B2C3_hR13_160_2a2b_2a_b-001



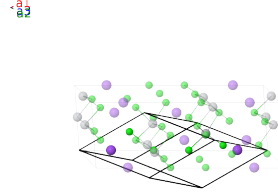
Prototype	Cl ₈ Na ₂ Ti ₃
AFLOW prototype label	A8B2C3_hR13_160_2a2b_2a_b-001
ICSD	259123
CCDC	1929785
Pearson symbol	hR13
Space group number	160
Space group symbol	<i>R</i> 3 <i>m</i>

AFLOW prototype command `aflow --proto=A8B2C3_hR13_160_2a2b_2a_b-001`
 `--params=a, c/a, x1, x2, x3, x4, x5, z5, x6, z6, x7, z7`

- Na₂Ti₃Cl₈ can be found in three different phases (Hänni, 2017):
 - γ -Na₂Ti₃Cl₈, below 210K (heating) or 190K (cooling) (this structure).
 - β -Na₂Ti₃Cl₈ is found between 190 and 210K when samples are cooled. It is in the $R\bar{3}m$ space group, but we have no atomic positions.
 - α -Na₂Ti₃Cl₈, above 190/210K, is in the Na₂Mn₃Cl₈ structure.
- (Hänni, 2017) give the lattice constants of γ -Na₂Ti₃Cl₈ at 2K, and the atomic positions at 1.6K.
- 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
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(1a)	Cl I
$\mathbf{B}_2$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(1a)	Cl II
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(1a)	Na I
$\mathbf{B}_4$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$cx_4 \hat{\mathbf{z}}$	(1a)	Na II
$\mathbf{B}_5$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(3b)	Cl III
$\mathbf{B}_6$	$= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(3b)	Cl III
$\mathbf{B}_7$	$= x_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(3b)	Cl III
$\mathbf{B}_8$	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(3b)	Cl IV
$\mathbf{B}_9$	$= z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(3b)	Cl IV
$\mathbf{B}_{10}$	$= x_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(3b)	Cl IV
$\mathbf{B}_{11}$	$= x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(3b)	Ti I
$\mathbf{B}_{12}$	$= z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(3b)	Ti I
$\mathbf{B}_{13}$	$= x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(3b)	Ti I

References

- [1] N. Hänni, M. Frontzek, J. Hauser, D. Cheptiakov, and K. Krämer, *Low Temperature Phases of $\text{Na}_2\text{Ti}_3\text{Cl}_8$ Revisited*, Z. Anorganische und Allgemeine Chemie **643**, 2063–2069 (2017), doi:10.1002/zaac.201700331.

First cited in

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