γ-$Na_2Ti_3Cl_8$ Structure: A8B2C3_hR13_160_2a2b_2a_b-001

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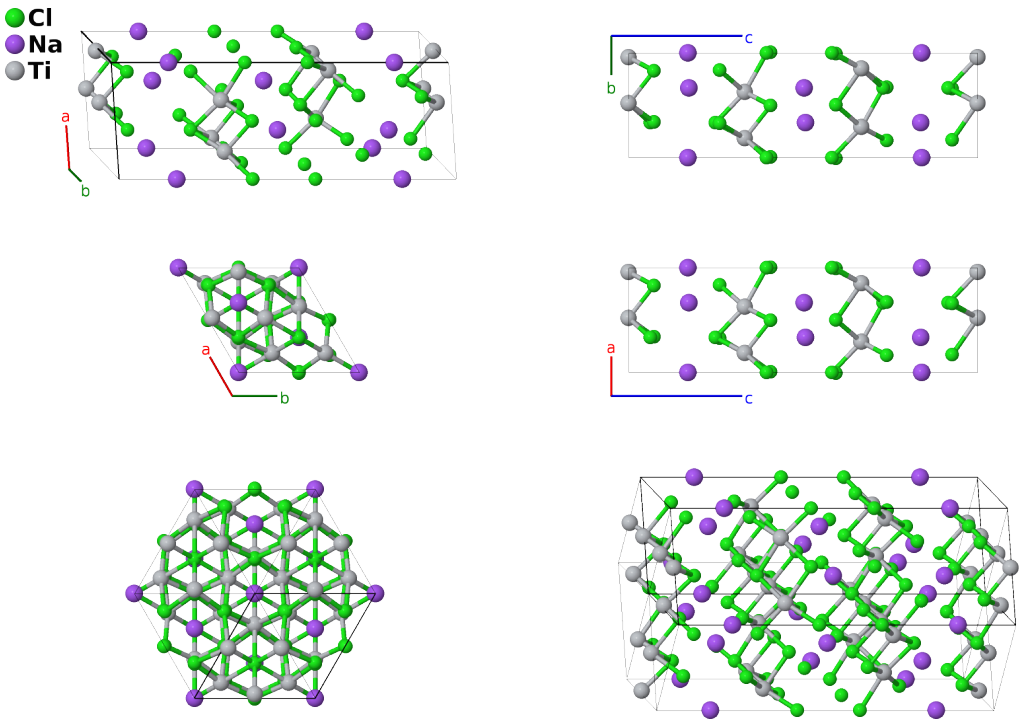
https://aflow.org/p/L333

https://aflow.org/p/A8B2C3_hR13_160_2a2b_2a_b-001



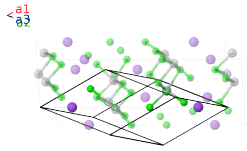
Prototype	$Cl_8Na_2Ti_3$
AFLOW prototype label	A8B2C3_hR13_160_2a2b_2a_b-001
ICSD	259123
Pearson symbol	hR13
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=A8B2C3_hR13_160_2a2b_2a_b-001 --params=`$a, c/a, x_1, x_2, x_3, x_4, x_5, z_5, x_6, z_6, x_7, z_7$

- $Na_2Ti_3Cl_8$ can be found in three different phases (Hänni, 2017):
  - γ-$Na_2Ti_3Cl_8$, below 210K (heating) or 190K (cooling) (this structure).
  - β-$Na_2Ti_3Cl_8$ 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-$Na_2Ti_3Cl_8$, above 190/210K, is in the $Na_2Mn_3Cl_8$ structure.

- (Hänni, 2017) give the lattice constants of γ-$Na_2Ti_3Cl_8$ at 2K, and the atomic positions at 1.6K.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



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 $Na_2Ti_3Cl_8$ Revisited*, Z. Anorganische und Allgemeine Chemie **643**, 2063–2069 (2017), doi:10.1002/zaac.201700331.