

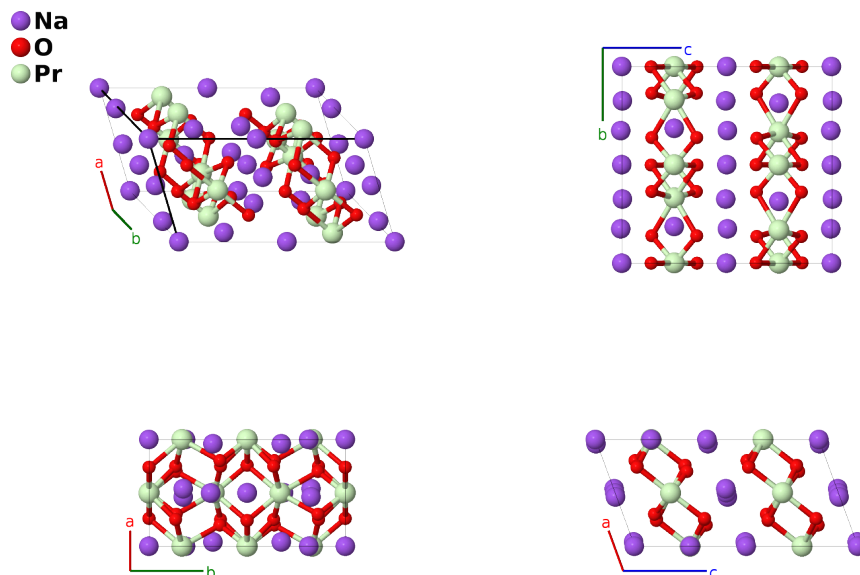
# Na<sub>2</sub>PrO<sub>3</sub> Structure: A2B3C\_mC48\_15\_aef\_3f\_2e-001

This structure originally had the label `A2B3C_mC48_15_aef_3f_2e`. Calls to that address will be redirected here.

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<https://aflow.org/p/NFQU>

[https://aflow.org/p/A2B3C\\_mC48\\_15\\_aef\\_3f\\_2e-001](https://aflow.org/p/A2B3C_mC48_15_aef_3f_2e-001)



Prototype	Na <sub>2</sub> O <sub>3</sub> Pr
AFLOW prototype label	A2B3C_mC48_15_aef_3f_2e-001
ICSD	154706
Pearson symbol	mC48
Space group number	15
Space group symbol	<i>C</i> 2/ <i>c</i>
AFLOW prototype command	<code>aflow --proto=A2B3C_mC48_15_aef_3f_2e-001</code> <code>--params=a, b/a, c/a, β, y<sub>2</sub>, y<sub>3</sub>, y<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub></code>

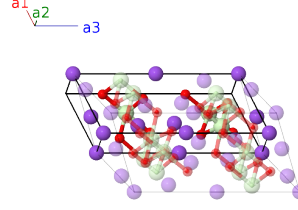
## Other compounds with this structure

Li<sub>2</sub>SnO<sub>3</sub>, Na<sub>2</sub>CrO<sub>3</sub>, Na<sub>2</sub>TbO<sub>3</sub>

- (Hinatsu, 2006) found that the site we have labeled Na-II is actually 2/3 sodium and 1/3 praseodymium, statistically distributed, while the site we label Pr-I is 1/3 sodium and 2/3 praseodymium.
- Some authors use Li<sub>2</sub>SnO<sub>3</sub> as the prototype for this structure.

## Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$0$	$=$	$0$	(4a)	Na I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B}_3$	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B}_4$	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B}_5$	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Pr I
$\mathbf{B}_6$	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Pr I
$\mathbf{B}_7$	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Pr II
$\mathbf{B}_8$	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Pr II
$\mathbf{B}_9$	$(x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(8f)	Na III
$\mathbf{B}_{10}$	$-(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Na III
$\mathbf{B}_{11}$	$-(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(8f)	Na III
$\mathbf{B}_{12}$	$(x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Na III
$\mathbf{B}_{13}$	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B}_{14}$	$-(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_6 + c(z_6 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B}_{15}$	$-(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B}_{16}$	$(x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B}_{17}$	$(x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{18}$	$-(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_7 + c(z_7 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{19}$	$-(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{20}$	$(x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	O II

$$\mathbf{B}_{21} = \begin{matrix} (x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + \\ z_8 \mathbf{a}_3 \end{matrix} = (ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}} \quad (8f) \quad \text{O III}$$

$$\mathbf{B}_{22} = \begin{matrix} -(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - \\ (z_8 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} -(ax_8 + c(z_8 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - \\ c(z_8 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (8f) \quad \text{O III}$$

$$\mathbf{B}_{23} = \begin{matrix} -(x_8 - y_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 - \\ z_8 \mathbf{a}_3 \end{matrix} = -(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}} \quad (8f) \quad \text{O III}$$

$$\mathbf{B}_{24} = \begin{matrix} (x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + \\ (z_8 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} (ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + \\ c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (8f) \quad \text{O III}$$

## References

- [1] Y. Hinatsu and Y. Doi, *Crystal structures and magnetic properties of alkali-metal lanthanide oxides  $A_2LnO_3$  ( $A = Li, Na; Ln = Ce, Pr, Tb$ )*, J. Alloys Compd. **418**, 155–160 (2006), doi:10.1016/j.jallcom.2005.08.100.