

α -Na₂PrO₃ Structure: A2B3C_mC48_15_aef_3f_2e-001

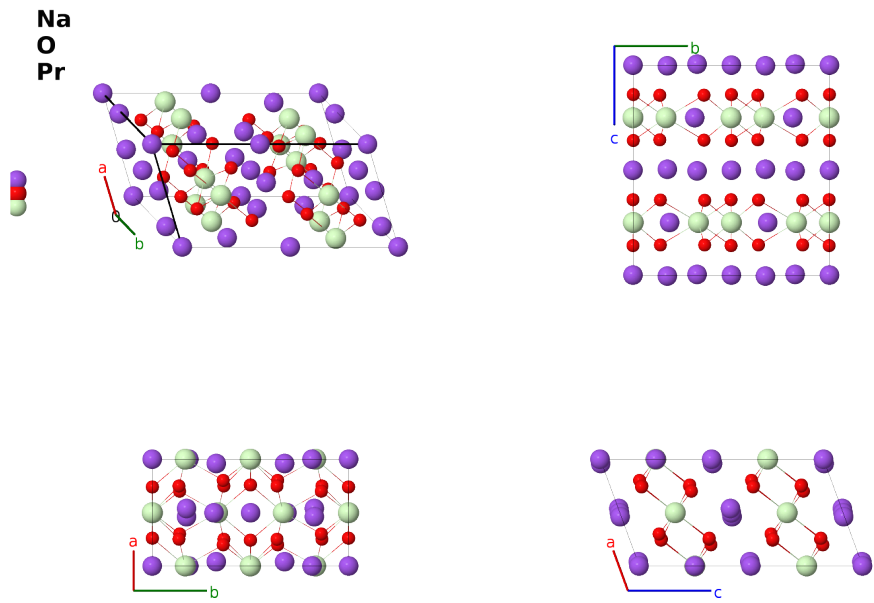
This structure previously used the label(s) **A2B3C_mC48_15_aef_3f_2e**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A2B3C_mC48_15_aef_3f_2e-001



Prototype	Na ₂ O ₃ Pr
AFLOW prototype label	A2B3C_mC48_15_aef_3f_2e-001
ICSD	154706
CCDC	1671329
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,y₂,y₃,y₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇,y₇,z₇,x₈,y₈,z₈</code>

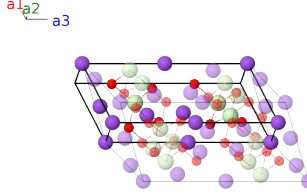
Other compounds with this structure

Li₂MnO₃, Li₂PbO₃, Li₂RuO₃, Li₂SnO₃, Li₂TiO₃, Na₂CeO₃, Na₂CrO₃, Na₂IrO₃, Na₂RuO₃, Na₂PdO₃, Na₂PrO₃, Na₂PtO₃, Na₂SnO₃, Na₂TbO₃, Na₂ZrO₃

- Na_2PrO_3 can be found in three forms (Okuma, 2024):
 - As monoclinic $\alpha\text{-Na}_2\text{PrO}_3$ (this structure),
 - As orthorhombic $\beta\text{-Na}_2\text{PrO}_3$, in the $\beta\text{-Na}_2\text{PtO}_3$ structure, or
 - As $\gamma\text{-Na}_2\text{PrO}_3$, in the rock salt ($B1$) structure, with the sodium and praseodymium mixed on the alkali site.
- (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, including the ICSD, use Li_2SnO_3 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

$$\begin{aligned}
\mathbf{B}_{16} &= \begin{pmatrix} (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \\ (z_6 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (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}} \end{pmatrix} & (8f) & \text{O I} \\
\mathbf{B}_{17} &= \begin{pmatrix} (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + \\ z_7 \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{O II} \\
\mathbf{B}_{18} &= \begin{pmatrix} -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - \\ (z_7 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(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}} \end{pmatrix} & (8f) & \text{O II} \\
\mathbf{B}_{19} &= \begin{pmatrix} -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - \\ z_7 \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{O II} \\
\mathbf{B}_{20} &= \begin{pmatrix} (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \\ (z_7 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (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}} \end{pmatrix} & (8f) & \text{O II} \\
\mathbf{B}_{21} &= \begin{pmatrix} (x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + \\ z_8 \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{O III} \\
\mathbf{B}_{22} &= \begin{pmatrix} -(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - \\ (z_8 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(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{pmatrix} & (8f) & \text{O III} \\
\mathbf{B}_{23} &= \begin{pmatrix} -(x_8 - y_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 - \\ z_8 \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{O III} \\
\mathbf{B}_{24} &= \begin{pmatrix} (x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + \\ (z_8 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (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{pmatrix} & (8f) & \text{O III}
\end{aligned}$$

References

- [1] Y. Hinatsu and Y. Doi, *Crystal structures and magnetic properties of alkali-metal lanthanide oxides $A_2\text{LnO}_3$ ($A = \text{Li}, \text{Na}; \text{Ln} = \text{Ce}, \text{Pr}, \text{Tb}$)*, J. Alloys Compd. **418**, 155–160 (2006), doi:10.1016/j.jallcom.2005.08.100.
- [2] R. Okuma, K. MacFarquharson, and R. Coldea, *Selective Synthesis and Crystal Chemistry of Candidate Rare-Earth Kitaev Materials: Honeycomb and Hyperhoneycomb Na_2PrO_3* , Inorganic Chemistry **63**, 15941–15950 (2024), doi:10.1021/acs.inorgchem.4c02294.

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