

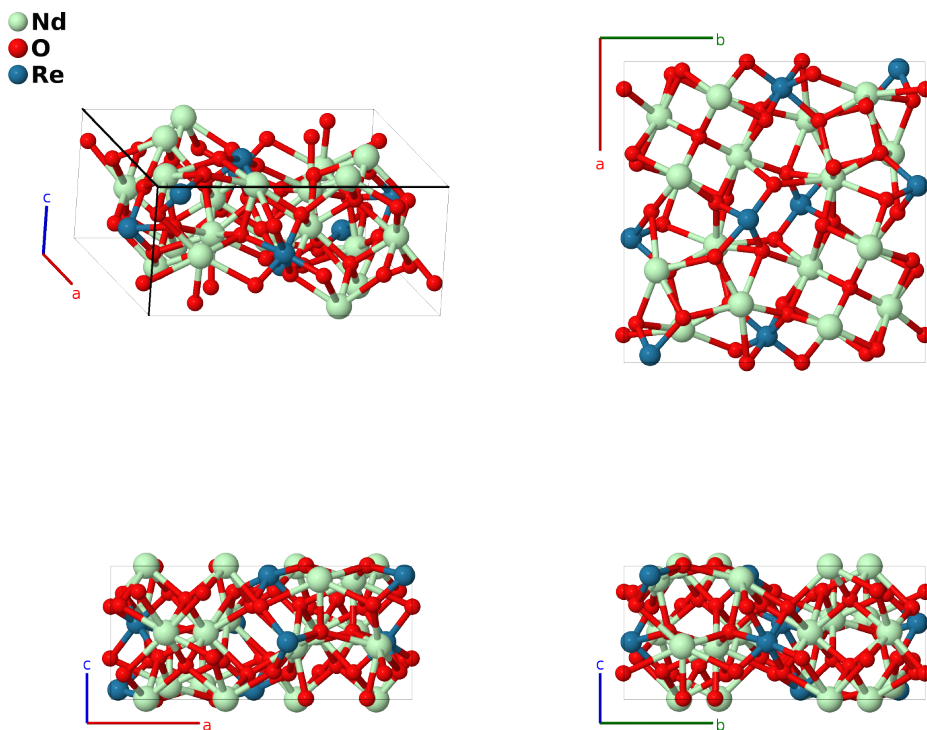
Nd₄Re₂O₁₁ Structure: A4B11C2_tP68_86_2g_ab5g_g-001

This structure originally had the label **A4B11C2_tP68_86_2g_ab5g_g**. Calls to that address will be redirected here.

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<https://aflow.org/p/8MQB>

https://aflow.org/p/A4B11C2_tP68_86_2g_ab5g_g-001

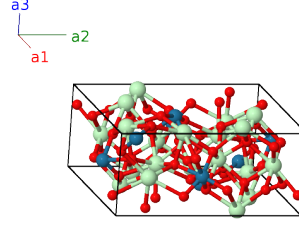


Prototype	Nd ₄ O ₁₁ Re ₂
AFLOW prototype label	A4B11C2_tP68_86_2g_ab5g_g-001
ICSD	15042
Pearson symbol	tP68
Space group number	86
Space group symbol	$P4_2/n$
AFLOW prototype command	<pre>aflow --proto=A4B11C2_tP68_86_2g_ab5g_g-001 --params=a, c/a, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10</pre>

- (Wilhelmi, 1970) has a misprint for the Wyckoff position of the Nd-II atom, although the nearest-neighbor distances are correct. (Downs, 2003) corrects the position to be consistent with those distances, and we use their value. The ICSD entry also includes this correction.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2a)	O I
\mathbf{B}_2	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2a)	O I
\mathbf{B}_3	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2b)	O II
\mathbf{B}_4	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2b)	O II
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	Nd I
\mathbf{B}_6	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	Nd I
\mathbf{B}_7	$= -y_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Nd I
\mathbf{B}_8	$= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Nd I
\mathbf{B}_9	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	Nd I
\mathbf{B}_{10}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	Nd I
\mathbf{B}_{11}	$= y_3 \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Nd I
\mathbf{B}_{12}	$= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Nd I
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	Nd II
\mathbf{B}_{14}	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	Nd II
\mathbf{B}_{15}	$= -y_4 \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Nd II
\mathbf{B}_{16}	$= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Nd II
\mathbf{B}_{17}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	Nd II
\mathbf{B}_{18}	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	Nd II
\mathbf{B}_{19}	$= y_4 \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Nd II
\mathbf{B}_{20}	$= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Nd II
\mathbf{B}_{21}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	O III

$$\begin{aligned}
\mathbf{B}_{54} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 + z_9 \mathbf{a}_3 &= -a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} &(8g) & \text{O VII} \\
\mathbf{B}_{55} &= -y_9 \mathbf{a}_1 + \left(x_9 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= -ay_9 \hat{\mathbf{x}} + a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) & \text{O VII} \\
\mathbf{B}_{56} &= \left(y_9 + \frac{1}{2}\right) \mathbf{a}_1 - x_9 \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) & \text{O VII} \\
\mathbf{B}_{57} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} &(8g) & \text{O VII} \\
\mathbf{B}_{58} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 - z_9 \mathbf{a}_3 &= a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} &(8g) & \text{O VII} \\
\mathbf{B}_{59} &= y_9 \mathbf{a}_1 - \left(x_9 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= ay_9 \hat{\mathbf{x}} - a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) & \text{O VII} \\
\mathbf{B}_{60} &= -\left(y_9 - \frac{1}{2}\right) \mathbf{a}_1 + x_9 \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) & \text{O VII} \\
\mathbf{B}_{61} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= ax_{10} \hat{\mathbf{x}} + ay_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} &(8g) & \text{Re I} \\
\mathbf{B}_{62} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= -a\left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} &(8g) & \text{Re I} \\
\mathbf{B}_{63} &= -y_{10} \mathbf{a}_1 + \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= -ay_{10} \hat{\mathbf{x}} + a\left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) & \text{Re I} \\
\mathbf{B}_{64} &= \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_1 - x_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) & \text{Re I} \\
\mathbf{B}_{65} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= -ax_{10} \hat{\mathbf{x}} - ay_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(8g) & \text{Re I} \\
\mathbf{B}_{66} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= a\left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(8g) & \text{Re I} \\
\mathbf{B}_{67} &= y_{10} \mathbf{a}_1 - \left(x_{10} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 &= ay_{10} \hat{\mathbf{x}} - a\left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) & \text{Re I} \\
\mathbf{B}_{68} &= -\left(y_{10} - \frac{1}{2}\right) \mathbf{a}_1 + x_{10} \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) & \text{Re I}
\end{aligned}$$

References

- [1] K.-A. Wilhelmi, E. Lagervall, and O. Muller, *On the Crystal Structure of Nd₄Re₂O₁₁*, Acta Chem. Scand. **24**, 3406–3408 (1970), doi:10.3891/acta.chem.scand.24-3409.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).