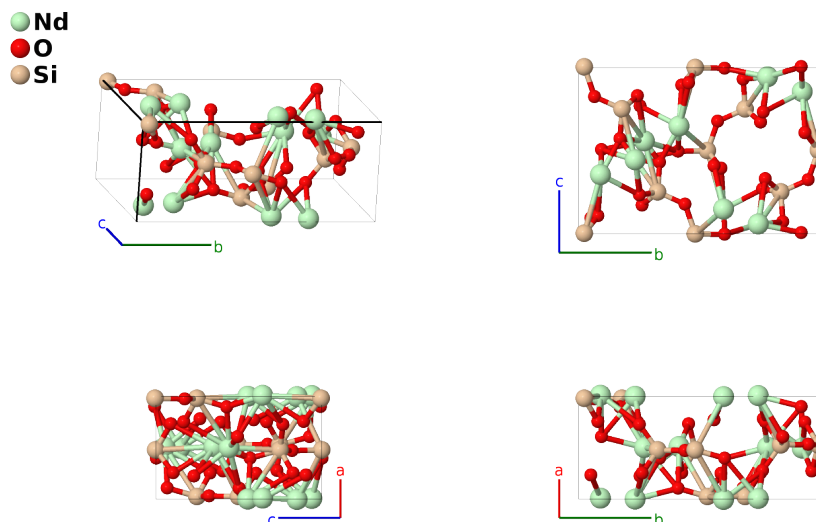


Nd₂Si₂O₇ Structure: A2B7C2_oP44_19_2a_7a_2a-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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

https://aflow.org/p/A2B7C2_oP44_19_2a_7a_2a-001



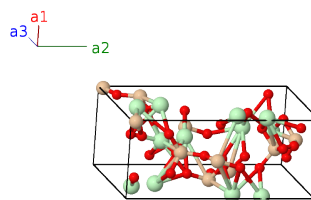
Prototype	Nd ₂ O ₇ Si ₂
AFLOW prototype label	A2B7C2_oP44_19_2a_7a_2a-001
ICSD	none
Pearson symbol	oP44
Space group number	19
Space group symbol	$P2_12_12_1$
AFLOW prototype command	aflow --proto=A2B7C2_oP44_19_2a_7a_2a-001 --params=a, b/a, c/a, x ₁ , y ₁ , z ₁ , x ₂ , y ₂ , z ₂ , x ₃ , y ₃ , z ₃ , x ₄ , y ₄ , z ₄ , x ₅ , y ₅ , z ₅ , x ₆ , y ₆ , z ₆ , x ₇ , y ₇ , z ₇ , x ₈ , y ₈ , z ₈ , x ₉ , y ₉ , z ₉ , x ₁₀ , y ₁₀ , z ₁₀ , x ₁₁ , y ₁₁ , z ₁₁

Other compounds with this structure

Ce₂Si₂O₇, Eu₂Si₂O₇, La₂Si₂O₇, Sm₂Si₂O₇

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	Nd I
\mathbf{B}_2	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 +$ $\left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Nd I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Nd I
\mathbf{B}_4	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4a)	Nd I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	Nd II
\mathbf{B}_6	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 +$ $\left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Nd II
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Nd II
\mathbf{B}_8	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4a)	Nd II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_{10}	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 +$ $\left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_{11}	$= -x_3 \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_{12}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{14}	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 +$ $\left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{15}	$= -x_4 \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{16}	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4a)	O III
\mathbf{B}_{18}	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - y_5 \mathbf{a}_2 +$ $\left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O III
\mathbf{B}_{19}	$= -x_5 \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O III
\mathbf{B}_{20}	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4a)	O III
\mathbf{B}_{21}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4a)	O IV
\mathbf{B}_{22}	$= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 - y_6 \mathbf{a}_2 +$ $\left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O IV
\mathbf{B}_{23}	$= -x_6 \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(z_6 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O IV
\mathbf{B}_{24}	$= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4a)	O IV
\mathbf{B}_{25}	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4a)	O V
\mathbf{B}_{26}	$= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 - y_7 \mathbf{a}_2 +$ $\left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O V
\mathbf{B}_{27}	$= -x_7 \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(z_7 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O V

$$\begin{aligned}
\mathbf{B}_{28} &= (x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3 = a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{29} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{30} &= -(x_8 - \frac{1}{2}) \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = -a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{31} &= -x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 = -ax_8 \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{32} &= (x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3 = a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{33} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (4a) & \text{O VII} \\
\mathbf{B}_{34} &= -(x_9 - \frac{1}{2}) \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 = -a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O VII} \\
\mathbf{B}_{35} &= -x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3 = -ax_9 \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O VII} \\
\mathbf{B}_{36} &= (x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3 = a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (4a) & \text{O VII} \\
\mathbf{B}_{37} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (4a) & \text{Si I} \\
\mathbf{B}_{38} &= -(x_{10} - \frac{1}{2}) \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{Si I} \\
\mathbf{B}_{39} &= -x_{10} \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3 = -ax_{10} \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{Si I} \\
\mathbf{B}_{40} &= (x_{10} + \frac{1}{2}) \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3 = a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (4a) & \text{Si I} \\
\mathbf{B}_{41} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (4a) & \text{Si II} \\
\mathbf{B}_{42} &= -(x_{11} - \frac{1}{2}) \mathbf{a}_1 - y_{11} \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{Si II} \\
\mathbf{B}_{43} &= -x_{11} \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 - (z_{11} - \frac{1}{2}) \mathbf{a}_3 = -ax_{11} \hat{\mathbf{x}} + b(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{Si II} \\
\mathbf{B}_{44} &= (x_{11} + \frac{1}{2}) \mathbf{a}_1 - (y_{11} - \frac{1}{2}) \mathbf{a}_2 - z_{11} \mathbf{a}_3 = a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{11} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (4a) & \text{Si II}
\end{aligned}$$

References

- [1] Y. I. Smolin and Y. F. Shepelev, *Crystal Structure of Neodymium Pyrosilicate*, J. Struc. Chem. **12**, 425–430 (1971), doi:10.1007/BF00744629.