

β -Si₃N₄ (Nierite) Structure: A4B3_hP14_176_ch_h-001

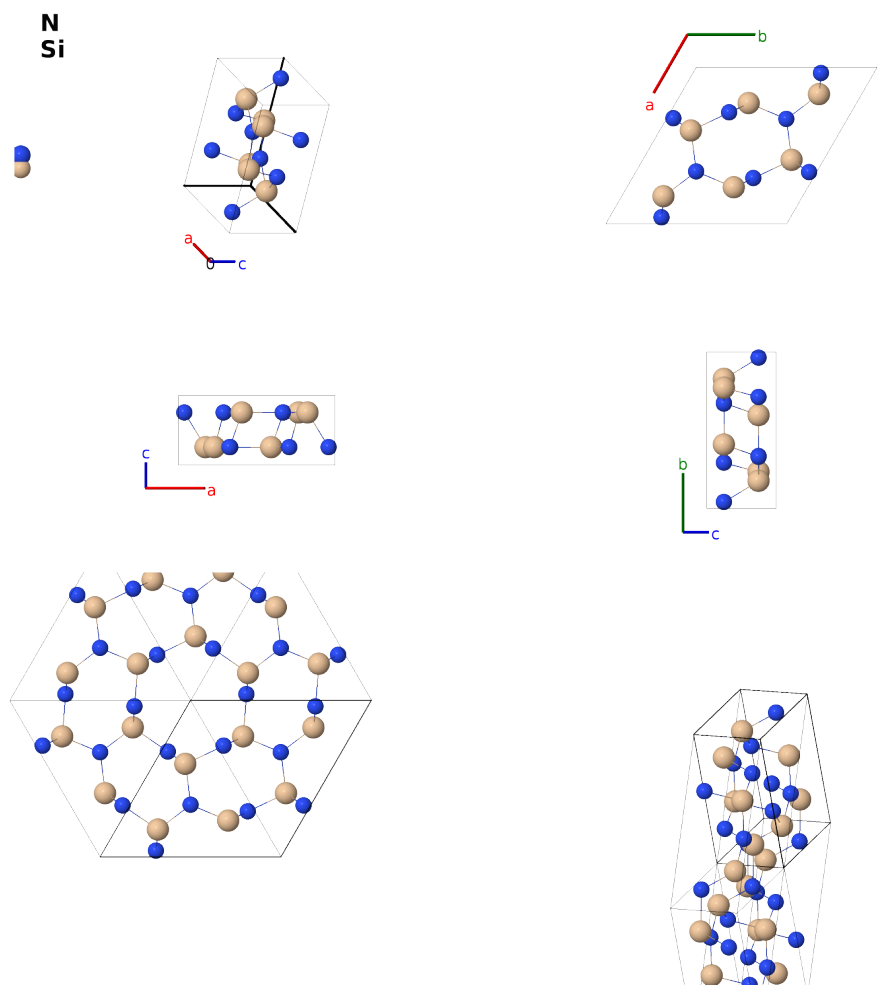
This structure previously used the label(s) **A4B3_hP14.176_ch.h**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A4B3_hP14_176_ch_h-001



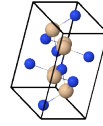
Prototype	N ₄ Si ₃
AFLOW prototype label	A4B3_hP14.176_ch_h-001
Mineral name	nierite
ICSD	79798
CCDC	1640033

Pearson symbol	hP14
Space group number	176
Space group symbol	$P6_3/m$
AFLOW prototype command	<code>aflow --proto=A4B3_hP14_176_ch_h-001</code> <code>--params=a, c/a, x₂, y₂, x₃, y₃</code>

- (Forgeng, 1958) and (Grun, 1979) place this structure in space group $P6_3$ #173. That structure is nearly indistinguishable from this one, as discussed on that page.
- Si_3N_4 also exists as $\alpha\text{-Si}_3\text{N}_4$.

Hexagonal primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	N I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	N I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_2 - y_2) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	N II
$\mathbf{B}_4$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	N II
$\mathbf{B}_5$	$= -(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	N II
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_2 - y_2) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	N II
$\mathbf{B}_7$	$= y_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_2 + 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	N II
$\mathbf{B}_8$	$= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	N II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Si I
$\mathbf{B}_{10}$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Si I
$\mathbf{B}_{11}$	$= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Si I
$\mathbf{B}_{12}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Si I
$\mathbf{B}_{13}$	$= y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Si I
$\mathbf{B}_{14}$	$= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Si I

References

- [1] P. Yang, H.-K. Fun, I. A. Rahman, and I. Saleh, *Two phase refinements of the structures of $\alpha\text{Si}_3\text{N}_4$ and $\beta\text{Si}_3\text{N}_4$ made from rice husk by Rietveld analysis*, Ceram. Int. **21**, 137–142 (1995), doi:10.1016/0272-8842(95)95885-L.
- [2] W. D. Forgeng and B. F. Decker, *Nitrides of silicon*, Trans. Am. Inst. Min. Met. Eng. **212**, 343–348 (1958).
- [3] R. Grün, *The crystal structure of $\beta\text{-Si}_3\text{N}_4$: structural and stability considerations between α - and $\beta\text{-Si}_3\text{N}_4$* , Acta Crystallogr. Sect. B **35**, 800–804 (1979), doi:10.1107/S0567740879004933.

Found in

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

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.