β-Si_3N_4 (Nierite) Structure: A4B3_hP14_173_bc_c-001

This structure previously used the label(s) `A4B3_hP14_173_bc_c`. Calls to these addresses will be redirected here.

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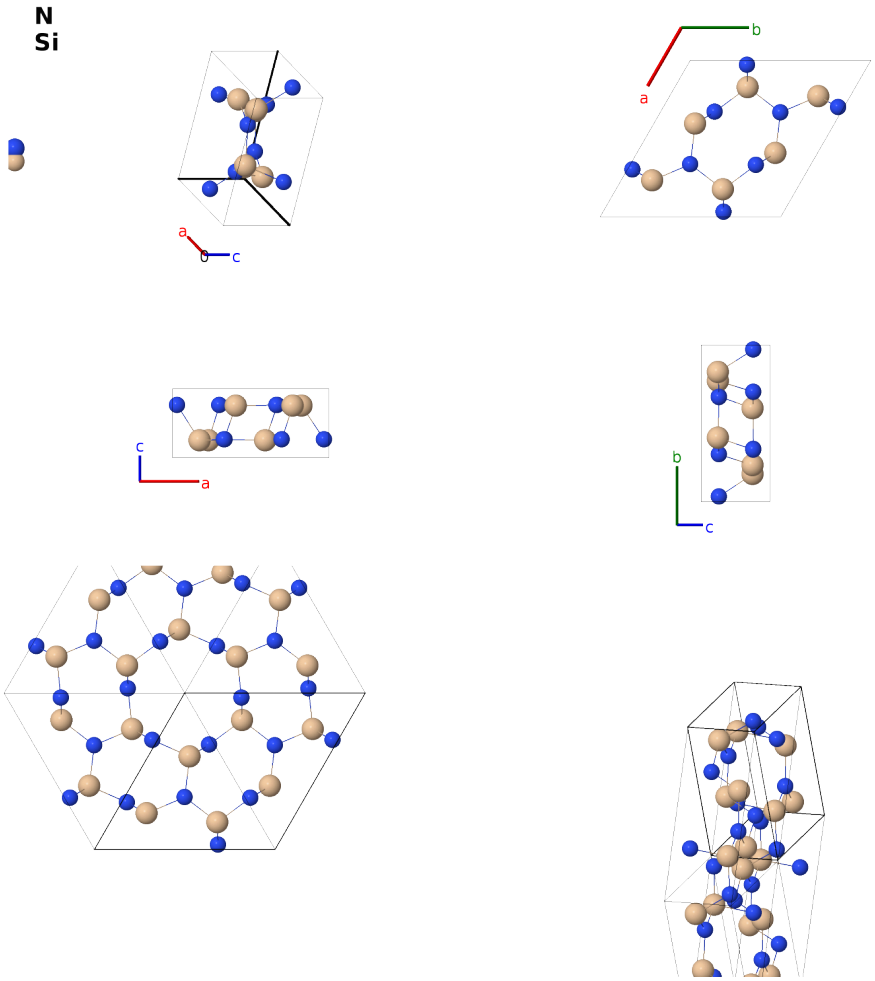
https://aflow.org/prototype-encyclopedia/Y4EE

https://aflow.org/prototype-encyclopedia/A4B3_hP14_173_bc_c-001



Prototype	N_4Si_3
AFLOW prototype label	A4B3_hP14_173_bc_c-001
Mineral name	nierite
ICSD	644690
CCDC	2138539

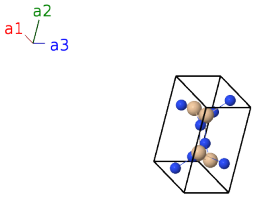
Pearson symbol	hP14
Space group number	173
Space group symbol	$P6_3$
AFLOW prototype command	`aflow --proto=A4B3_hP14_173_bc_c-001 --params=`$a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

Other compounds with this structure
Nb_3Te_4

- We have substantially revised this page. Originally, we used the reference (Forgeng, 1958), found in (Villars, 2013). This is duplicated by (Lartigue, 1985), referenced in (Villars, 2024). However neither of the quoted references actually have the atomic coordinates, with (Villars, 2024) stating "cell parameters determined and structure type assigned."
- (Grün, 1979) presents essentially the same structure with fully determined structure parameters, so we now use it as the reference.
- (Yang, 1995) places this structure in space group $P6_3/m$ #176. His structure is nearly indistinguishable from this one. The only difference is that the Yang *et al.* assign $z_1 = z_2 = z_3 = 1/4$, changing the space grop from polar $P6_3$ #173 to centrosymmetri $P6_3/m$ # 176. This involves moving the N II atom by 0.18Å and the Si I atom by 0.03Å, so the difference in the two structures is minimal.
- Si_3N_4 also exists as α-Si_3N_4.
- Space group $P6_3$ #173 is polar and so allows an arbitrary choice for the origin of the z-axis. We follow (Grün, 1979) and set $z_1 = 1/4$ for the N-I site.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2b)	N I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	N I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 + y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_2 - y_2)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6c)	N II
$\mathbf{B_4}$	=	$-y_2\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - 2y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6c)	N II
$\mathbf{B_5}$	=	$-(x_2 - y_2)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2 - y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6c)	N II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 + y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_2 - y_2)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	N II
$\mathbf{B_7}$	=	$y_2\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_2 + 2y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	N II
$\mathbf{B_8}$	=	$(x_2 - y_2)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_2 - y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	N II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	Si I

$$\mathbf{B_{10}} = -y_3\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_3 - 2y_3)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

$$\mathbf{B_{11}} = -(x_3 - y_3)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

$$\mathbf{B_{12}} = -x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

$$\mathbf{B_{13}} = y_3\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_3 + 2y_3)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

$$\mathbf{B_{14}} = (x_3 - y_3)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{Si I}$$

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