

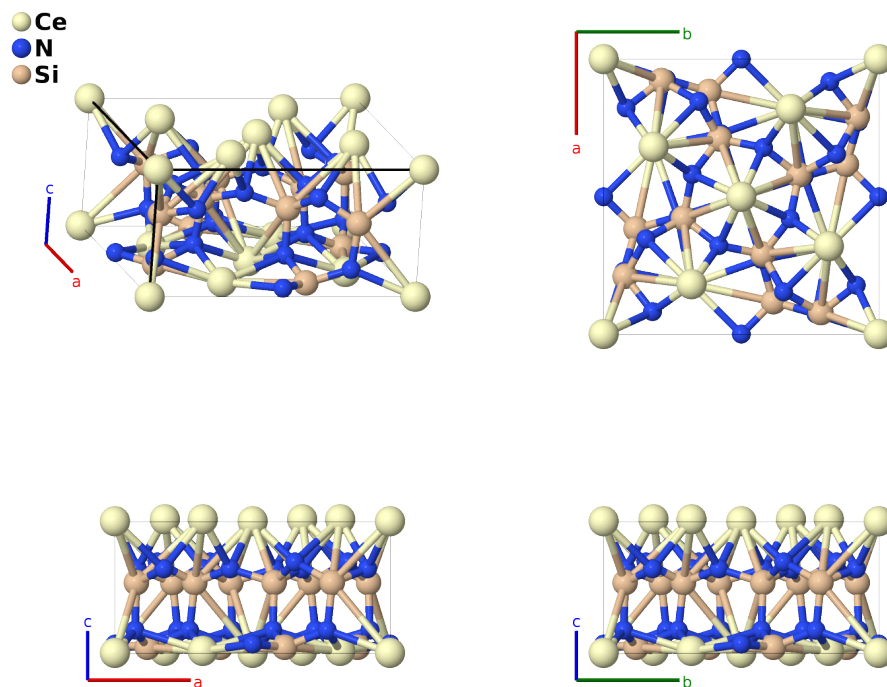
# Ce<sub>3</sub>Si<sub>6</sub>N<sub>11</sub> Structure: A3B11C6\_tP40\_100\_ac\_bc2d\_cd-001

This structure originally had the label A3B11C6\_tP40\_100\_ac\_bc2d\_cd. Calls to that address will be redirected here.

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<https://aflow.org/p/LZ7C>

[https://aflow.org/p/A3B11C6\\_tP40\\_100\\_ac\\_bc2d\\_cd-001](https://aflow.org/p/A3B11C6_tP40_100_ac_bc2d_cd-001)



Prototype	Ce <sub>3</sub> N <sub>11</sub> Si <sub>6</sub>
AFLOW prototype label	A3B11C6_tP40_100_ac_bc2d_cd-001
ICSD	401679
Pearson symbol	tP40
Space group number	100
Space group symbol	<i>P4bm</i>
AFLOW prototype command	<pre>aflow --proto=A3B11C6_tP40_100_ac_bc2d_cd-001 --params=a, c/a, z1, z2, x3, z3, x4, z4, x5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8</pre>

## Other compounds with this structure

La<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>, Nd<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>, Pr<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>, Sm<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>

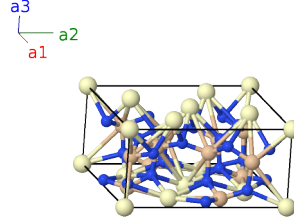
- (Woiike, 1995) does not have in ICSD listing for Ce<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>, so we use the one from (Schlieper, 1995).

- Some sites use  $\text{Sm}_3\text{Si}_6\text{N}_{11}$  as the prototype for this structure.

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### Simple Tetragonal primitive vectors

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




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### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Ce I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(2a)	Ce I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + c z_2 \hat{\mathbf{z}}$	(2b)	N I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(2b)	N I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + a (x_3 + \frac{1}{2}) \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4c)	Ce II
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - a (x_3 - \frac{1}{2}) \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4c)	Ce II
$\mathbf{B}_7$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4c)	Ce II
$\mathbf{B}_8$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4c)	Ce II
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4c)	N II
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4c)	N II
$\mathbf{B}_{11}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4c)	N II
$\mathbf{B}_{12}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4c)	N II
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + a (x_5 + \frac{1}{2}) \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B}_{14}$	$= -x_5 \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} - a (x_5 - \frac{1}{2}) \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B}_{15}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a (x_5 - \frac{1}{2}) \hat{\mathbf{x}} + a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B}_{16}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a (x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B}_{17}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a x_6 \hat{\mathbf{x}} + a y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8d)	N III
$\mathbf{B}_{18}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a x_6 \hat{\mathbf{x}} - a y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8d)	N III
$\mathbf{B}_{19}$	$= -y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a y_6 \hat{\mathbf{x}} + a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8d)	N III
$\mathbf{B}_{20}$	$= y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a y_6 \hat{\mathbf{x}} - a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8d)	N III
$\mathbf{B}_{21}$	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a (x_6 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8d)	N III
$\mathbf{B}_{22}$	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a (x_6 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_6 + \frac{1}{2}) \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8d)	N III
$\mathbf{B}_{23}$	$= -(y_6 - \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a (y_6 - \frac{1}{2}) \hat{\mathbf{x}} - a (x_6 - \frac{1}{2}) \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8d)	N III
$\mathbf{B}_{24}$	$= (y_6 + \frac{1}{2}) \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a (y_6 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_6 + \frac{1}{2}) \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8d)	N III
$\mathbf{B}_{25}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$a x_7 \hat{\mathbf{x}} + a y_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(8d)	N IV
$\mathbf{B}_{26}$	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a x_7 \hat{\mathbf{x}} - a y_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(8d)	N IV

$$\begin{aligned}
\mathbf{B}_{27} &= -y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= & -ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8d) & \text{N IV} \\
\mathbf{B}_{28} &= y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= & ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8d) & \text{N IV} \\
\mathbf{B}_{29} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= & a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8d) & \text{N IV} \\
\mathbf{B}_{30} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= & -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8d) & \text{N IV} \\
\mathbf{B}_{31} &= -\left(y_7 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= & -a \left(y_7 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8d) & \text{N IV} \\
\mathbf{B}_{32} &= \left(y_7 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_7 + \frac{1}{2}\right) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= & a \left(y_7 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8d) & \text{N IV} \\
\mathbf{B}_{33} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= & ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8d) & \text{Si II} \\
\mathbf{B}_{34} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= & -ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8d) & \text{Si II} \\
\mathbf{B}_{35} &= -y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= & -ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8d) & \text{Si II} \\
\mathbf{B}_{36} &= y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= & ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8d) & \text{Si II} \\
\mathbf{B}_{37} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= & a \left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8d) & \text{Si II} \\
\mathbf{B}_{38} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= & -a \left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8d) & \text{Si II} \\
\mathbf{B}_{39} &= -\left(y_8 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_8 - \frac{1}{2}\right) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= & -a \left(y_8 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8d) & \text{Si II} \\
\mathbf{B}_{40} &= \left(y_8 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_8 + \frac{1}{2}\right) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= & a \left(y_8 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8d) & \text{Si II}
\end{aligned}$$

## References

- [1] M. Woike and W. Jeitschko, *Preparation and Crystal Structure of the Nitridosilicates  $\text{Ln}_3\text{Si}_6\text{N}_{11}$  ( $\text{Ln} = \text{La}, \text{Ce}, \text{Pr}, \text{Nd}, \text{Sm}$ ) and  $\text{LnSi}_3\text{N}_5$  ( $\text{Ln} = \text{Ce}, \text{Pr}, \text{Nd}$ )*, Inorg. Chem. **34**, 5105–5108 (1995), doi:10.1021/ic00125a005.
- [2] T. Schlieper and W. Schnick, *Nitrido-silicate. III. Hochtemperatur-Synthese, Kristallstruktur und magnetische Eigenschaften von  $\text{Ce}_3[\text{Si}_6\text{N}_{11}]$* , Z. Anorganische und Allgemeine Chemie **621**, 1535–1538 (1995), doi:10.1002/zaac.19956210917.

## Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.