

Al₇C₃N₃ Structure:

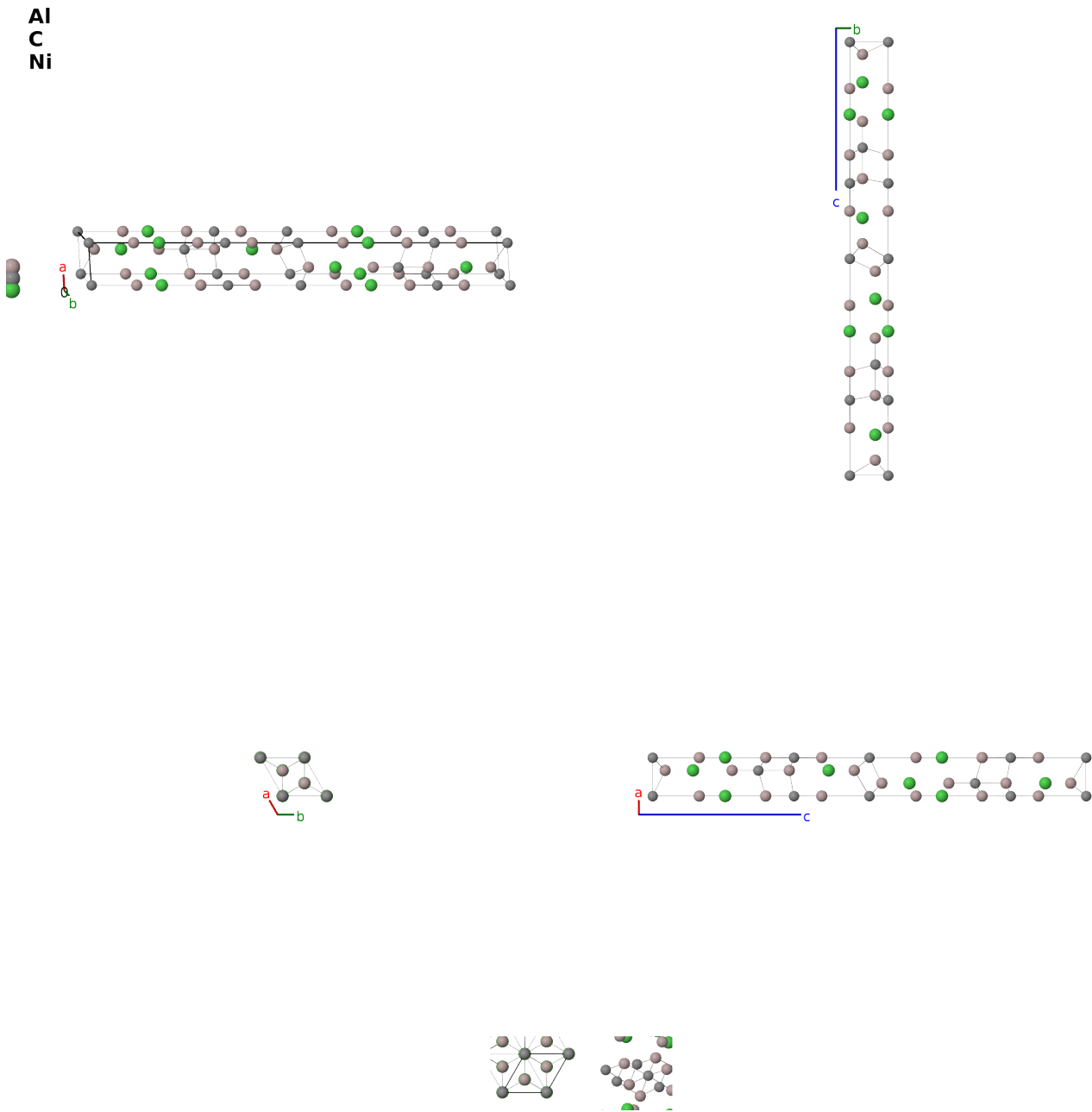
A7B3C3_hP26_186_3a4b_2ab_a2b-001

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

https://aflow.org/prototype-encyclopedia/A7B3C3_hP26_186_3a4b_2ab_a2b-001



Prototype

Al₇C₃N₃

AFLOW prototype label	A7B3C3_hP26_186_3a4b_2ab_a2b-001
ICSD	14400
CCDC	1595784
Pearson symbol	hP26
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	aflow --proto=A7B3C3_hP26_186_3a4b_2ab_a2b-001 --params= $a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, z_7, z_8, z_9, z_{10}, z_{11}, z_{12}, z_{13}$

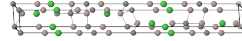
Other compounds with this structure

$(\text{Al}_{7-x}\text{Si}_x)(\text{O}_y\text{C}_z\text{N}_{6-y-z})$

- (Jeffrey, 1963) place the structure in space group $P6_3mc$ #186, but give the structure in a pseudo-hexagonal cell in space group $Cmc2_1$ #36. With the help of FINDSYM we converted this to the hexagonal structure.
- (Jeffrey, 1966) uses the $P6_3mc$ space group exclusively, and we list the ICSD entry associated with that paper.

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
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B}_2$	$= (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B}_3$	$= z_2 \mathbf{a}_3$	$=$	$c z_2 \hat{\mathbf{z}}$	(2a)	Al II
$\mathbf{B}_4$	$= (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al II
$\mathbf{B}_5$	$= z_3 \mathbf{a}_3$	$=$	$c z_3 \hat{\mathbf{z}}$	(2a)	Al III
$\mathbf{B}_6$	$= (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al III
$\mathbf{B}_7$	$= z_4 \mathbf{a}_3$	$=$	$c z_4 \hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B}_8$	$= (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B}_9$	$= z_5 \mathbf{a}_3$	$=$	$c z_5 \hat{\mathbf{z}}$	(2a)	C II
$\mathbf{B}_{10}$	$= (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	C II
$\mathbf{B}_{11}$	$= z_6 \mathbf{a}_3$	$=$	$c z_6 \hat{\mathbf{z}}$	(2a)	Ni I
$\mathbf{B}_{12}$	$= (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Ni I

$\mathbf{B}_{13} =$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(2b)	Al IV
$\mathbf{B}_{14} =$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Al IV
$\mathbf{B}_{15} =$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(2b)	Al V
$\mathbf{B}_{16} =$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Al V
$\mathbf{B}_{17} =$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(2b)	Al VI
$\mathbf{B}_{18} =$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Al VI
$\mathbf{B}_{19} =$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(2b)	Al VII
$\mathbf{B}_{20} =$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Al VII
$\mathbf{B}_{21} =$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(2b)	C III
$\mathbf{B}_{22} =$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	C III
$\mathbf{B}_{23} =$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	(2b)	Ni II
$\mathbf{B}_{24} =$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_{12} + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Ni II
$\mathbf{B}_{25} =$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$	(2b)	Ni III
$\mathbf{B}_{26} =$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_{13} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Ni III

References

- [1] G. A. Jeffrey and V. Y. Wu, *The structures of the aluminum carbonitrides*, Acta Cryst. **16**, 559–566 (1963), doi:10.1107/S0365110X63001468.
- [2] G. A. Jeffrey and V. Y. Wu, *The structure of the aluminum carbonitrides. II*, Acta Cryst. **20**, 538–547 (1966), doi:10.1107/S0365110X66001208.

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- [1] D. Urushihara, M. Kaga, T. Asaka, H. Nakano, and K. Fukuda, *Synthesis and structural characterization of $Al_7C_3N_3$ -homeotypic aluminum silicon oxycarbonitride, $(Al_{7-x}Si_x)(O_yC_zN_{6-y-z})$ ($x \sim 1.2$, $y \sim 1.0$ and $z \sim 3.5$)*, J. Solid State Chem. **184**, 2278–2284 (2011), doi:10.1016/j.jssc.2011.06.030.

First cited in

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