$Al_7C_3N_3$ Structure: A7B3C3_hP26_186_3a4b_2ab_a2b-001

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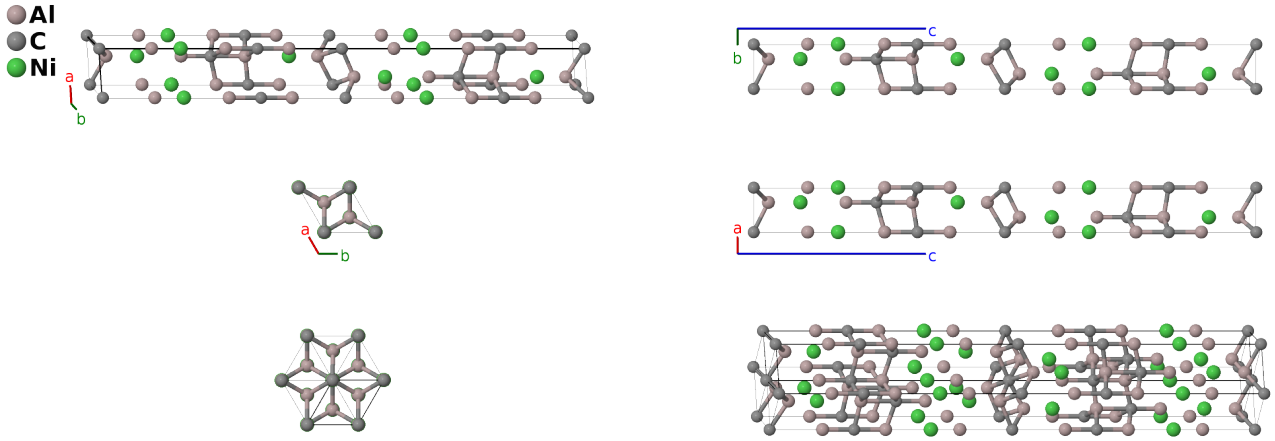


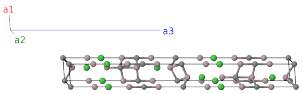
Prototype	$Al_7C_3N_3$
AFLOW prototype label	A7B3C3_hP26_186_3a4b_2ab_a2b-001
ICSD	14400
Pearson symbol	hP26
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	`aflow --proto=A7B3C3_hP26_186_3a4b_2ab_a2b-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, z_7, z_8, z_9, z_{10}, z_{11}, z_{12}, z_{13}$

Other compounds with this structure
$(Al_{7-x}Si_x)(O_yC_zN_{6-y-z})$

- (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

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	Al II
$\mathbf{B_4}$	=	$\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Al II
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2a)	Al III
$\mathbf{B_6}$	=	$\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Al III
$\mathbf{B_7}$	=	$z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B_8}$	=	$\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B_9}$	=	$z_5\,\mathbf{a}_3$	=	$cz_5\,\hat{\mathbf{z}}$	(2a)	C II
$\mathbf{B_{10}}$	=	$\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	C II
$\mathbf{B_{11}}$	=	$z_6\,\mathbf{a}_3$	=	$cz_6\,\hat{\mathbf{z}}$	(2a)	Ni I
$\mathbf{B_{12}}$	=	$\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{14}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{16}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{18}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{20}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_{10}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_{10}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{22}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_{11}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_{11}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{24}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_{12}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_{12}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{26}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_{13}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_{13}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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.

Found in

[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.