$Ti_3Al_2N_2$ Structure: A2B4C5_hP22_186_ab_4b_a4b-001

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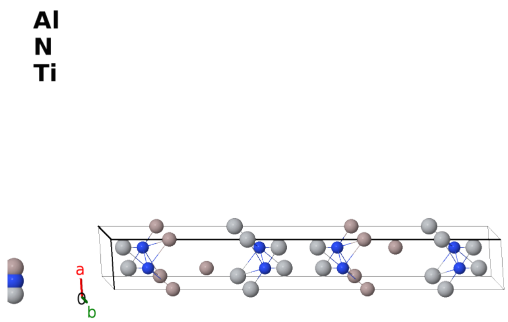
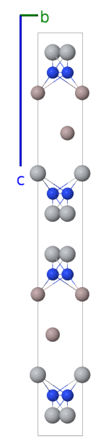
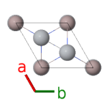
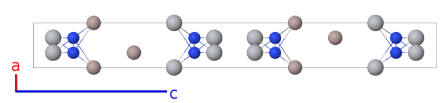
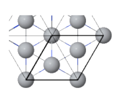
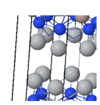












Prototype $Al_2N_2Ti_2$

AFLOW prototype label A2B4C5_hP22_186_ab_4b_a4b-001

ICSD 52643

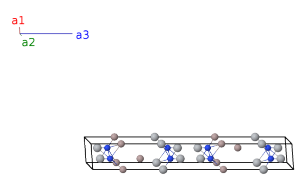
CCDC 1617377

Pearson symbol	hP22
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	`aflow --proto=A2B4C5_hP22_186_ab_4b_a4b-001` `--params=`$a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, z_7, z_8, z_9, z_{10}, z_{11}$

- This compound may exist at temperatures near 1573K, where this data was taken, however (Lee, 1997) reexamined the Al-N-Ti system and did not find any evidence of this phase, though they did find a $Ti_3Al_{1-x}N_2$ structure.
- (Schuster, 1984) placed this system in the trigonal space group $P31c$ #159. The (2a) and (2b) Wyckoff positions for space group #159 are identical to those in the hexagonal space group $P6_3mc$ #186, so we follow (Cenzual, 1991, ICSD 71097) and place this in the higher symmetry space group.
- The origin of the z-axis in space group $P6_3mc$ is arbitrary. We use the origin specified by (Schuster, 1984).
- Most of the Wyckoff positions in this structure are only partially occupied:
  - Sites Al-I and Ti-I are fully occupied.
  - Sites Ni-I, Ni-II, Ti-II, and Ti-III are 90% occupied.
  - Sites Ni-III, Ni-IV, Ti-IV, and Ti-V are 10% occupied.
- This explains the short Ti-N bond lengths shown in the figure – for any given Ti-N pair, only one of the two atoms is actually present.

Hexagonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(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)	Ti I
$\mathbf{B_4}$	=	$\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Ti I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(2b)	Al II
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Al II
$\mathbf{B_7}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(2b)	N I
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	N I
$\mathbf{B_9}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(2b)	N II

$\mathbf{B_{10}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(2b)	N II
$\mathbf{B_{11}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + cz_6\,\mathbf{\hat{z}}$	(2b)	N III
$\mathbf{B_{12}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + c\left(z_6 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(2b)	N III
$\mathbf{B_{13}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + cz_7\,\mathbf{\hat{z}}$	(2b)	N IV
$\mathbf{B_{14}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + c\left(z_7 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(2b)	N IV
$\mathbf{B_{15}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + cz_8\,\mathbf{\hat{z}}$	(2b)	Ti II
$\mathbf{B_{16}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + c\left(z_8 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(2b)	Ti II
$\mathbf{B_{17}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + cz_9\,\mathbf{\hat{z}}$	(2b)	Ti III
$\mathbf{B_{18}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + c\left(z_9 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(2b)	Ti III
$\mathbf{B_{19}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + cz_{10}\,\mathbf{\hat{z}}$	(2b)	Ti IV
$\mathbf{B_{20}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + c\left(z_{10} + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(2b)	Ti IV
$\mathbf{B_{21}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + cz_{11}\,\mathbf{\hat{z}}$	(2b)	Ti V
$\mathbf{B_{22}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(2b)	Ti V

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