

AlN₃Ti₄ Structure: AB3C4_hP16_194_c_af_ef-001

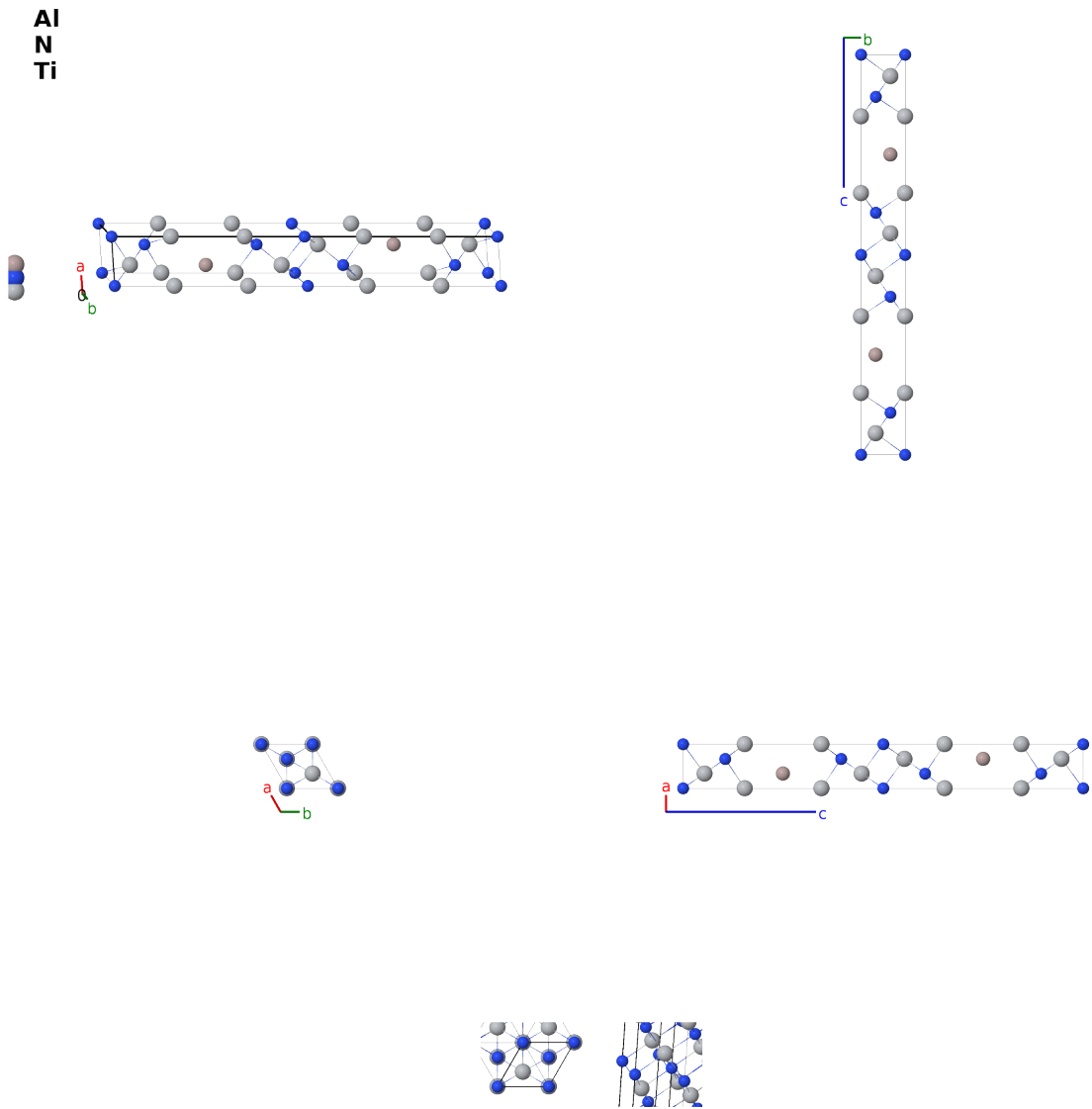
This structure previously used the label(s) **AB3C4_hP16_194_c_af_ef**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/53FU>

https://aflow.org/prototype-encyclopedia/AB3C4_hP16_194_c_af_ef-001



Prototype	AlN ₃ Ti ₄
AFLOW prototype label	AB3C4_hP16_194_c_af_ef-001
ICSD	190338

CCDC	1699276
Pearson symbol	hP16
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	aflow --proto=AB3C4_hP16_194_c_af_ef-001 --params= $a, c/a, z_3, z_4, z_5$

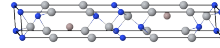
Other compounds with this structure

CaAl₃Ti₄, CsYb₃Se₄

- This is a so-called MAX phase. For more information, see (Radovic, 2013).
- The nitrogen (2a) site is only occupied 86% of the time.
- We use the data from (Barsoum, 2000) taken at 298K. This is a slight shift from our previous report (Mehl, 2017).

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
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	N I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(2a)	N I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Al I
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Al I
$\mathbf{B}_5$	$= z_3 \mathbf{a}_3$	$=$	$cz_3 \hat{\mathbf{z}}$	(4e)	Ti I
$\mathbf{B}_6$	$= (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Ti I
$\mathbf{B}_7$	$= -z_3 \mathbf{a}_3$	$=$	$-cz_3 \hat{\mathbf{z}}$	(4e)	Ti I
$\mathbf{B}_8$	$= -(z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Ti I
$\mathbf{B}_9$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4f)	N II
$\mathbf{B}_{10}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	N II
$\mathbf{B}_{11}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4f)	N II
$\mathbf{B}_{12}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	N II
$\mathbf{B}_{13}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4f)	Ti II
$\mathbf{B}_{14}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Ti II

$$\mathbf{B}_{15} = \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_5 \mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} \quad (4f) \quad \text{Ti II}$$

$$\mathbf{B}_{16} = \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}} \quad (4f) \quad \text{Ti II}$$

References

- [1] M. W. Barsoum, C. J. Rawn, T. El-Raghy, A. T. Procopio, W. D. Porter, H. Wang, and C. R. Hubbard, *Thermal Properties of Ti_4AlN_3* , J. Appl. Phys. **87**, 8407–8414 (2000), doi:10.1063/1.373555.
- [2] M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.

Found in

- [1] M. Radovic and M. W. Barsoum, *MAX phases: Bridging the gap between metals and ceramics*, Am. Ceram. Soc. Bull. **92**, 20–27 (2013).

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