

Al₈C₃N₄ Structure:

A8B3C4_hR15_166_4c_ac_2c-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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

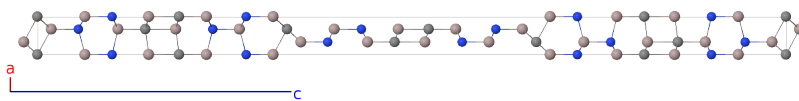
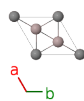
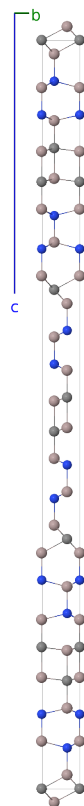
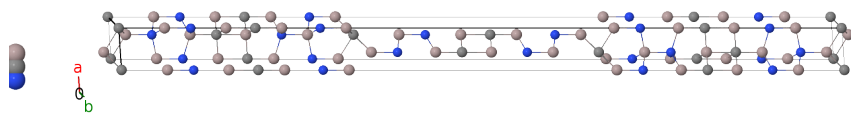
https://aflow.org/prototype-encyclopedia/A8B3C4_hR15_166_4c_ac_2c-001

Prototype	Al ₈ C ₃ N ₄
AFLOW prototype label	A8B3C4_hR15_166_4c_ac_2c-001
ICSD	41261
CCDC	1611051
Pearson symbol	hR15
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A8B3C4_hR15_166_4c_ac_2c-001</code> <code>--params=a, c/a, x₂, x₃, x₄, x₅, x₆, x₇, x₈</code>

- (Jeffrey, 1966) put this structure in space group $R\bar{3}m$ #166, but put one carbon atom at the (1a) Wyckoff position and 14 atoms on (2c) sites. This would put 29 atoms in the primitive cell, violating the claimed stoichiometry. In addition, as (Villars, 1999) points out, the atoms are much too close together, making the structure unphysical.
- We could make the assumption that the space group was actually $R3m$ #160. In that case the atoms are all on (1a) sites and the stoichiometry is correct, at the cost of losing the inversion symmetry from the $R\bar{3}m$ space group.
- (Daams, 1993) resolve this by replacing pairs of atoms (in the $R\bar{3}m$ setting) which are too close together by a single atom at the midpoint between them. This gives the proper symmetry and stoichiometry, and so we follow them here.
- ICSD entry #41261 is from (Jeffrey, 1966). ICSD entry #43861 is said to be from (Suzuki, 1993), but is better associated with (Daams, 1993).
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

Al
C
N





$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(1a) C I
$\mathbf{B}_2$	=	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$cx_2 \hat{\mathbf{z}}$	(2c) Al I
$\mathbf{B}_3$	=	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	=	$-cx_2 \hat{\mathbf{z}}$	(2c) Al I
$\mathbf{B}_4$	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$cx_3 \hat{\mathbf{z}}$	(2c) Al II
$\mathbf{B}_5$	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$-cx_3 \hat{\mathbf{z}}$	(2c) Al II
$\mathbf{B}_6$	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$cx_4 \hat{\mathbf{z}}$	(2c) Al III
$\mathbf{B}_7$	=	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	=	$-cx_4 \hat{\mathbf{z}}$	(2c) Al III
$\mathbf{B}_8$	=	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$cx_5 \hat{\mathbf{z}}$	(2c) Al IV
$\mathbf{B}_9$	=	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	=	$-cx_5 \hat{\mathbf{z}}$	(2c) Al IV
$\mathbf{B}_{10}$	=	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	=	$cx_6 \hat{\mathbf{z}}$	(2c) C II
$\mathbf{B}_{11}$	=	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - x_6 \mathbf{a}_3$	=	$-cx_6 \hat{\mathbf{z}}$	(2c) C II
$\mathbf{B}_{12}$	=	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$cx_7 \hat{\mathbf{z}}$	(2c) N I
$\mathbf{B}_{13}$	=	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	=	$-cx_7 \hat{\mathbf{z}}$	(2c) N I
$\mathbf{B}_{14}$	=	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	=	$cx_8 \hat{\mathbf{z}}$	(2c) N II
$\mathbf{B}_{15}$	=	$-x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - x_8 \mathbf{a}_3$	=	$-cx_8 \hat{\mathbf{z}}$	(2c) N II

References

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First cited in

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