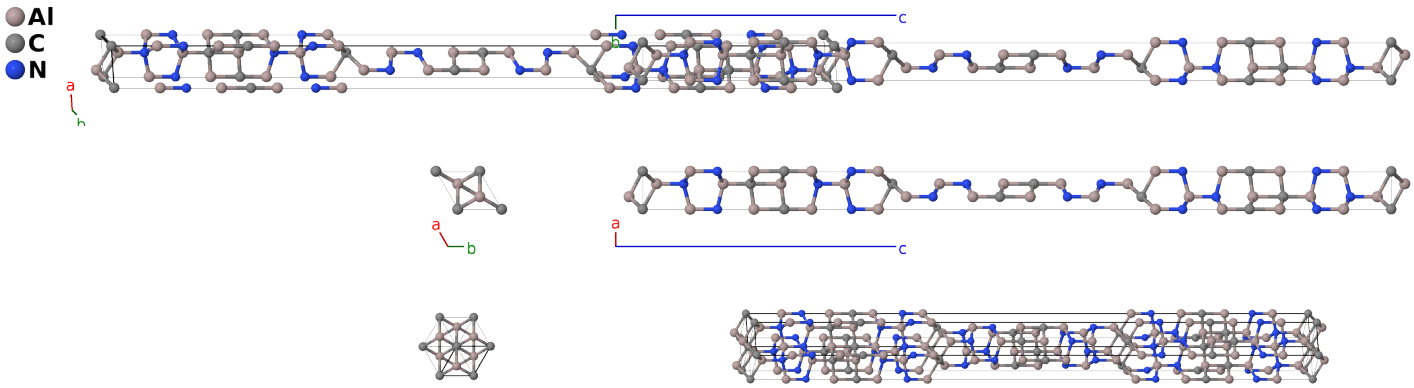
$Al_8C_3N_4$ Structure: A8B3C4_hR15_166_4c_ac_2c-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/HGYT

https://aflow.org/p/A8B3C4_hR15_166_4c_ac_2c-001

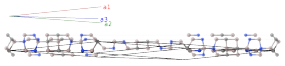


Prototype	$Al_8C_3N_4$
AFLOW prototype label	A8B3C4_hR15_166_4c_ac_2c-001
ICSD	43861, 41261
Pearson symbol	hR15
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A8B3C4_hR15_166_4c_ac_2c-001 --params=`$a, c/a, x_2, x_3, x_4, x_5, x_6, x_7, x_8$

- (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

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$



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

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

[2] J. L. C. Daams and P. Villars, *Atomic environment classification of the rhombohedral "intermetallic" structure types*, J. Alloys Compd. **197**, 243–269 (1993), doi:10.1016/0925-8388(93)90046-P.

[3] K. Suzuki, H. Morita, T. Kaneko, H. Yoshida, and H. Fujimori, *Crystal structure and magnetic properties of the compound FeN*, J. Alloys Compd. **201**, 11–16 (1993), doi:10.1016/0925-8388(93)90854-G.

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.