$Al_6C_3N_2$ Structure: A6B3C2_hR11_166_3c_ac_c-001

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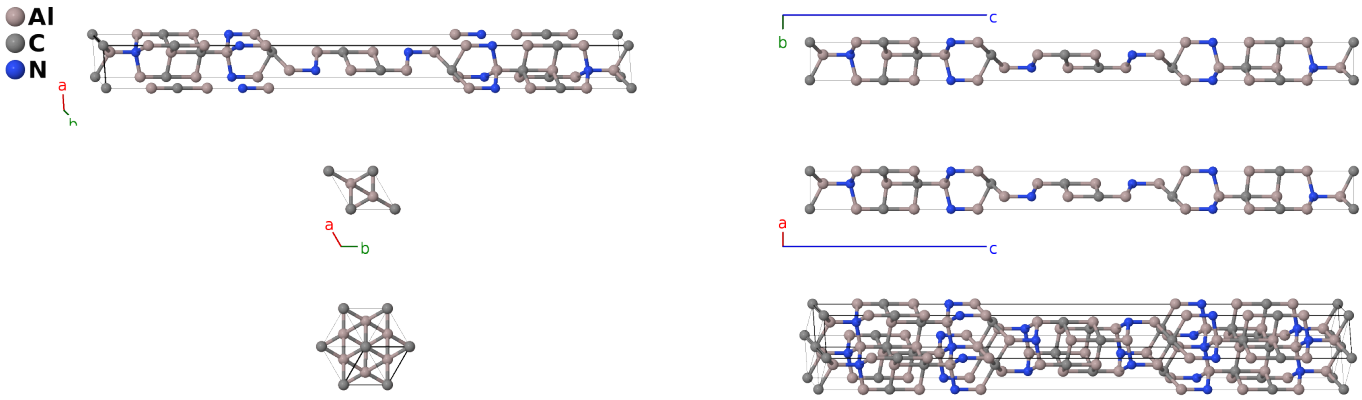
https://aflow.org/p/T8T4

https://aflow.org/p/A6B3C2_hR11_166_3c_ac_c-001

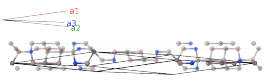


Prototype	$Al_6C_3N_2$
AFLOW prototype label	A6B3C2_hR11_166_3c_ac_c-001
ICSD	654993, 41260
Pearson symbol	hR11
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A6B3C2_hR11_166_3c_ac_c-001 --params=`$a, c/a, x_2, x_3, x_4, x_5, x_6$

- The structure presented by (Jeffrey, 1966) has problems similar to those of $Al_8C_3N_4$. See that page for a discussion of our resolution of the problems.
- The ICSD is rather confused about this compound. The entry associated with (Jeffrey, 1996), #41260, has the original structure. Entry #654993 gives a structure quite similar to ours, but it is attributed to (Suzuki, 1993), a paper concerning the structure of iron nitride. It is better associated with (Daams, 1993). We list both ICSDs, but consider #654993 the correct structure.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

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



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)	C II
$\mathbf{B_9}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-cx_5\,\hat{\mathbf{z}}$	(2c)	C II
$\mathbf{B_{10}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$cx_6\,\hat{\mathbf{z}}$	(2c)	N I
$\mathbf{B_{11}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-cx_6\,\hat{\mathbf{z}}$	(2c)	N I

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] 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.

[3] 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.

Found in

[1] P. Villars, *Pearson's Handbook* (ASM International, Materials Park OH, 1999), vol. 1, chap. Compound Table, pp. 296–297, desk edition edn.