Al_5C_3N ($E9_4$) Structure: A5B3C_hP18_186_2a3b_2ab_b-001

This structure previously used the label(s) `A5B3C_hP18_186_2a3b_2ab_b`. Calls to these addresses will be redirected here.

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. Oses, 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.

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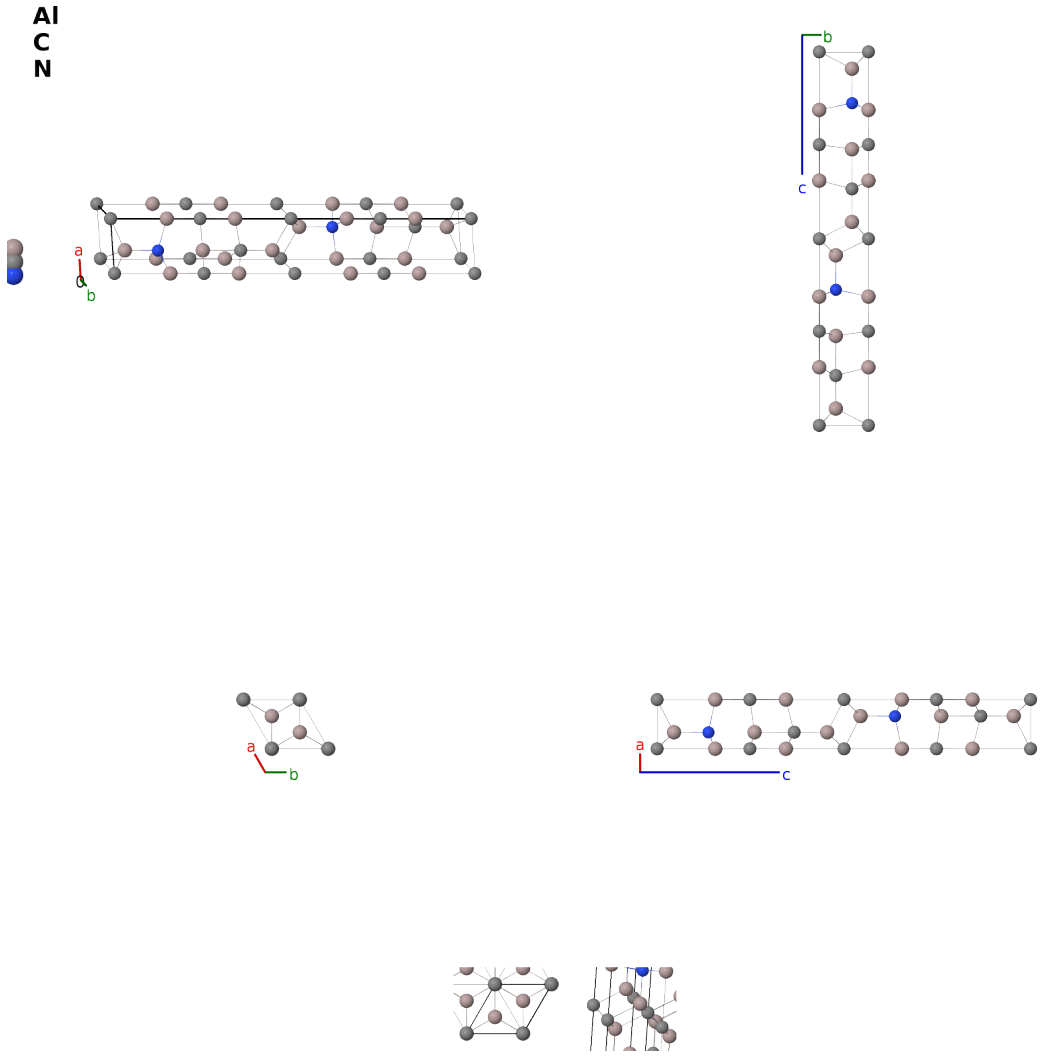
https://aflow.org/prototype-encyclopedia/KHLK

https://aflow.org/prototype-encyclopedia/A5B3C_hP18_186_2a3b_2ab_b-001



Prototype	Al_5C_3N
AFLOW prototype label	A5B3C_hP18_186_2a3b_2ab_b-001
***Strukturbericht* designation**	$E9_4$
ICSD	14398

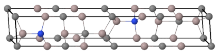
CCDC	1595782
Pearson symbol	hP18
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	`aflow --proto=A5B3C_hP18_186_2a3b_2ab_b-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, z_7, z_8, z_9$

Other compounds with this structure
$U_2Al_3C_4$

- Space group $P6_3mc$ #186 allows for an arbitary placement of the origin of the z-axis. We set this by taking $z_3 = 0$ for the C-I atom.

Hexagonal primitive vectors

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



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)	Al II
$\mathbf{B_4}$	=	$\left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Al II
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B_6}$	=	$\left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B_7}$	=	$z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(2a)	C II
$\mathbf{B_8}$	=	$\left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	C II
$\mathbf{B_9}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(2b)	Al III
$\mathbf{B_{10}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Al III
$\mathbf{B_{11}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(2b)	Al IV
$\mathbf{B_{12}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Al IV
$\mathbf{B_{13}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(2b)	Al V
$\mathbf{B_{14}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Al V
$\mathbf{B_{15}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(2b)	C III
$\mathbf{B_{16}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	C III

$\mathbf{B_{17}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(2b)	N I
$\mathbf{B_{18}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	N I

References

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First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017