Al_5C_3N ($E9_4$) Structure: A5B3C_hP18_186_2a3b_2ab_b-001

This structure originally had the label `A5B3C_hP18_186_2a3b_2ab_b`. Calls to that address will be redirected here.

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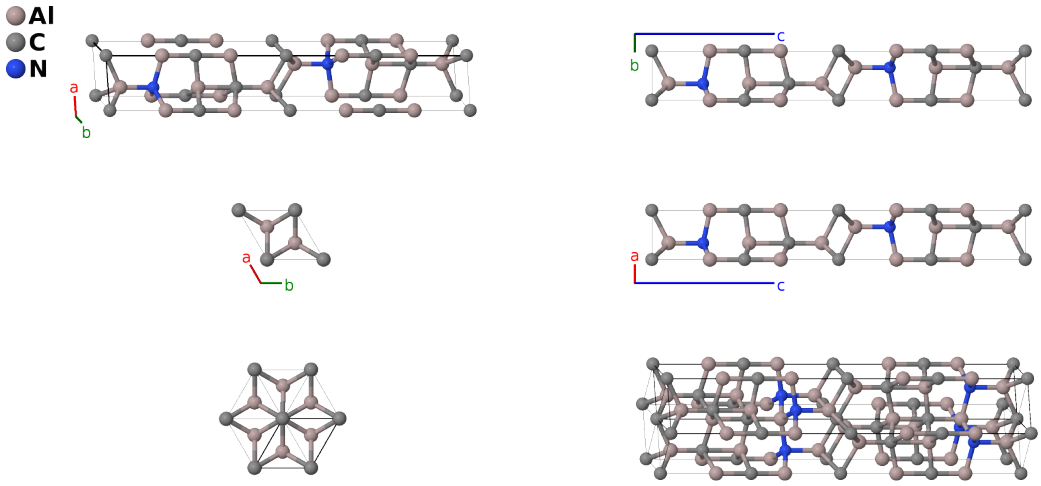
https://aflow.org/p/KHLK

https://aflow.org/p/A5B3C_hP18_186_2a3b_2ab_b-001



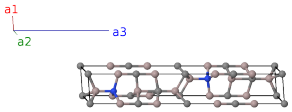
Prototype	Al_5C_3N
AFLOW prototype label	A5B3C_hP18_186_2a3b_2ab_b-001
***Strukturbericht* designation**	$E9_4$
ICSD	14398
Pearson symbol	hP18
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	`aflow --proto=A5B3C_hP18_186_2a3b_2ab_b-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, z_7, z_8, z_9$

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

[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.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.