Al_4C_3 ($D7_1$) Structure: A4B3_hR7_166_2c_ac-001

This structure originally had the label `A4B3_hR7_166_2c_ac`. Calls to that address will be redirected here.

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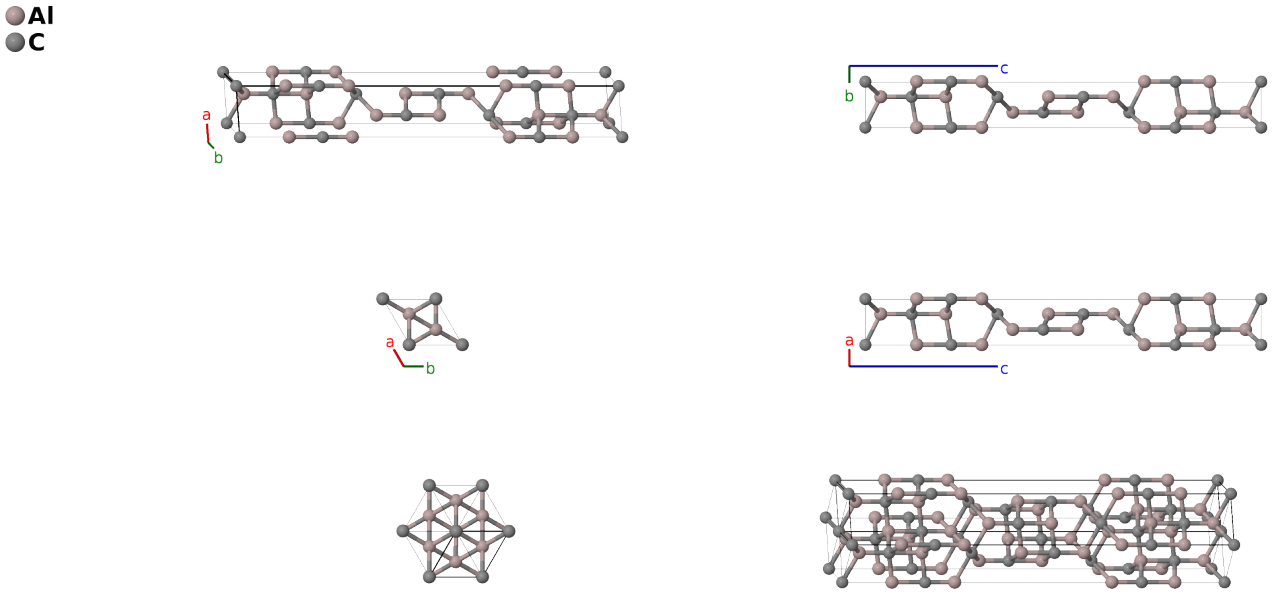
https://aflow.org/p/YAHB

https://aflow.org/p/A4B3_hR7_166_2c_ac-001



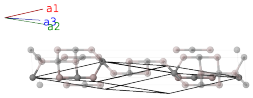
Prototype	Al_4C_3
AFLOW prototype label	A4B3_hR7_166_2c_ac-001
***Strukturbericht* designation**	$D7_1$
ICSD	66751
Pearson symbol	hR7
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A4B3_hR7_166_2c_ac-001 --params=`$a, c/a, x_2, x_3, x_4$

Other compounds with this structure
Th_3N_4

- Al_4C_3 ($D7_1$) and Bi_4Te_3 have the same AFLOW prototype label, A4B3_hR7_166_2c_ac. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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)	C II
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	C II

References

[1] T. M. Gesing and W. Jeitschko, *The Crystal Structure and Chemical Properties of $U_2Al_3C_4$ and Structure Refinement of Al_4C_3*, Z. Naturforsch. B **50**, 196–200 (1995), doi:10.1515/znb-1995-0206.