

WAl₅ Structure:

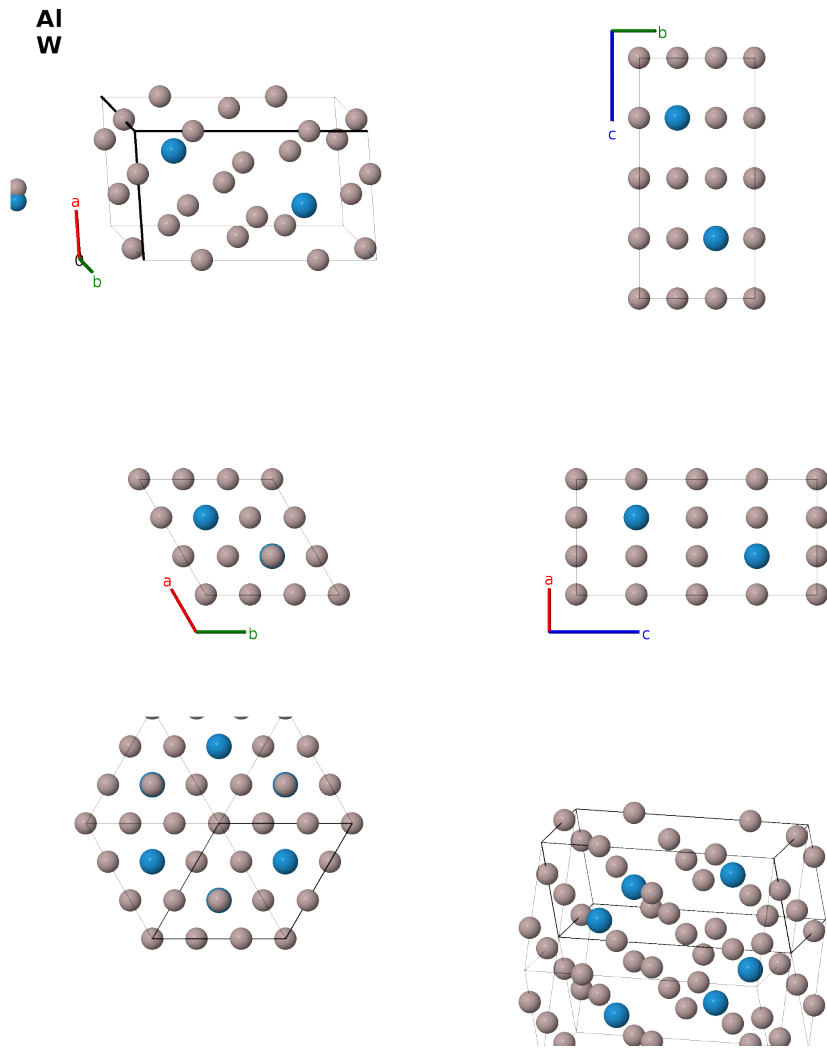
A5B_hP12_182_bcg_d-001

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<https://aflow.org/prototype-encyclopedia/BQ6N>

https://aflow.org/prototype-encyclopedia/A5B_hP12_182_bcg_d-001



Prototype	Al ₅ W
AFLOW prototype label	A5B_hP12_182_bcg_d-001
ICSD	58206
CCDC	1622234
Pearson symbol	hP12

Space group number	182
Space group symbol	$P6_322$
AFLOW prototype command	<code>aflow --proto=A5B_hP12_182_bcg_d-001</code> <code>--params=a, c/a, x₄</code>

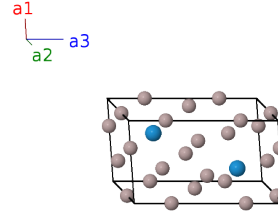
Other compounds with this structure

MoAl₅

- Although (Adam, 1955) state that 'Spatial considerations rule out space group [$P6_322$ #182] and so put this crystal in space group $P6_3$ #173, their coordinates are in fact consistent with space group $P6_322$. (Cenzual, 1991)

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(2b)	Al I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(2b)	Al I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Al II
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Al II
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2d)	W I
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2d)	W I
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$	(6g)	Al III
$\mathbf{B}_8$	$= x_4 \mathbf{a}_2$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$	(6g)	Al III
$\mathbf{B}_9$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}}$	(6g)	Al III
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	Al III
$\mathbf{B}_{11}$	$= -x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	Al III
$\mathbf{B}_{12}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	Al III

References

- [1] J. Adam and J. B. Rich, *The crystal structure of WAl₅*, Acta Cryst. **8**, 349–350 (1955), doi:10.1107/S0365110X55001060.

Found in

- [1] K. Cenzual, L. M. Gelato, M. Penzo, and E. Parthé, *Inorganic structure types with revised space groups. I*, Acta Crystallogr. Sect. B **47**, 433–439 (1991), doi:10.1107/S0108768191000903.

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