$Al_{12}W$ Structure: A12B_cI26_204_g_a-001

This structure originally had the label `A12B_cI26_204_g_a`. Calls to that address will be redirected here.

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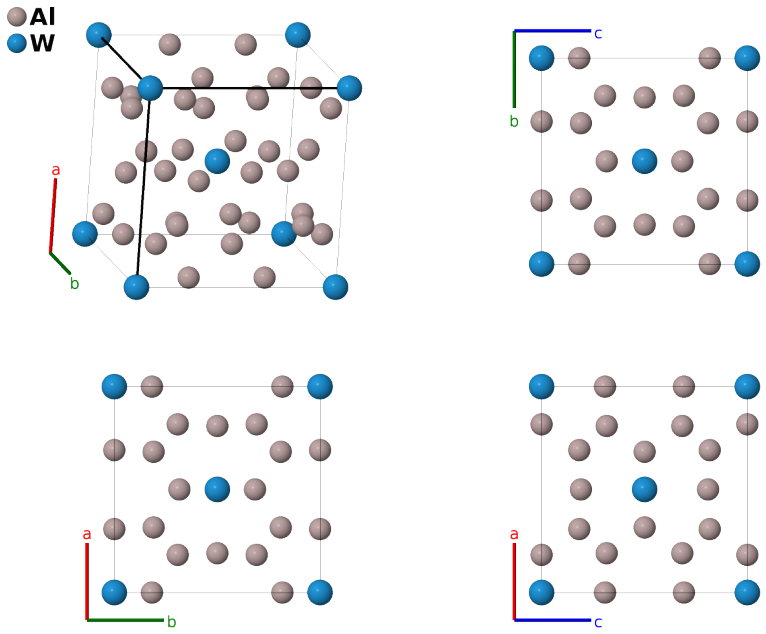
https://aflow.org/p/JDL2

https://aflow.org/p/A12B_cI26_204_g_a-001

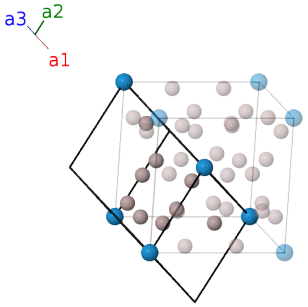


Prototype	$Al_{12}W$
AFLOW prototype label	A12B_cI26_204_g_a-001
ICSD	58207
Pearson symbol	cI26
Space group number	204
Space group symbol	$Im\bar{3}$
AFLOW prototype command	`aflow --proto=A12B_cI26_204_g_a-001 --params=`a, y_2, z_2

Other compounds with this structure
$Al_{12}Mo$, $Al_{12}Mn$, $Al_{12}Re$, $Al_{12}Te$

Body-centered Cubic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}a\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	W I
$\mathbf{B_2}$	=	$(y_2+z_2)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{y}} + az_2\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_3}$	=	$-(y_2-z_2)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{y}} + az_2\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_4}$	=	$(y_2-z_2)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{y}} - az_2\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_5}$	=	$-(y_2+z_2)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{y}} - az_2\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_6}$	=	$y_2\,\mathbf{a}_1 + (y_2+z_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$az_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_7}$	=	$-y_2\,\mathbf{a}_1 - (y_2-z_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$az_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_8}$	=	$y_2\,\mathbf{a}_1 + (y_2-z_2)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-az_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_9}$	=	$-y_2\,\mathbf{a}_1 - (y_2+z_2)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-az_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_{10}}$	=	$z_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + (y_2+z_2)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + az_2\,\hat{\mathbf{y}}$	(24g)	Al I
$\mathbf{B_{11}}$	=	$z_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - (y_2-z_2)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + az_2\,\hat{\mathbf{y}}$	(24g)	Al I
$\mathbf{B_{12}}$	=	$-z_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + (y_2-z_2)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - az_2\,\hat{\mathbf{y}}$	(24g)	Al I
$\mathbf{B_{13}}$	=	$-z_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - (y_2+z_2)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} - az_2\,\hat{\mathbf{y}}$	(24g)	Al I

References

[1] J. Adam and J. B. Rich, *The crystal structure of WAl_{12}, $MoAl_{12}$ and (Mn, Cr)Al_{12}*, Acta Cryst. **7**, 813–816 (1954), doi:10.1107/S0365110X54002514.