Al$_4$W Structure:
A4B_mC30_8_2a5b_ab-001

https://aflow.org/p/10PS

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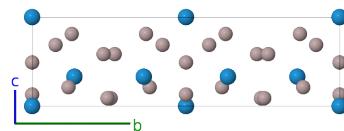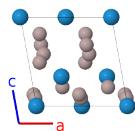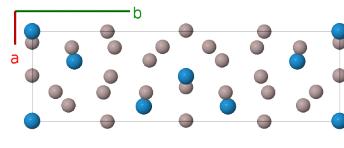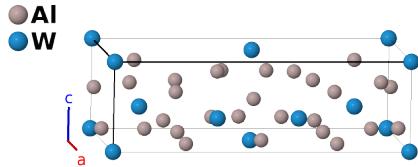
Prototype	Al$_4$W
AFLOW prototype label	A4B_mC30_8_2a5b_ab-001
ICSD	58205
Pearson symbol	mC30
Space group number	8
Space group symbol	Cm
AFLOW prototype command	aflow --proto=A4B_mC30_8_2a5b_ab-001

--params=$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8,$ y_8, z_8, x_9, y_9, z_9


Other compounds with this structure

Al$_4$Rh, Al$_4$Mo

- Space group Cm #8 allows arbitrary origins for the x and z coordinates. Here we use this to place the W-I atom at the origin.

Base-centered Monoclinic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}
$$
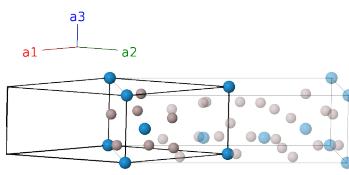
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_1} + x_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	$=$	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B_2}$	$=$	$x_2\,\mathbf{a_1} + x_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al II
$\mathbf{B_3}$	$=$	$x_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2a)	W I
$\mathbf{B_4}$	$=$	$(x_4 - y_4)\,\mathbf{a_1} + (x_4 + y_4)\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4b)	Al III
$\mathbf{B_5}$	$=$	$(x_4 + y_4)\,\mathbf{a_1} + (x_4 - y_4)\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4b)	Al III
$\mathbf{B_6}$	$=$	$(x_5 - y_5)\,\mathbf{a_1} + (x_5 + y_5)\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4b)	Al IV
$\mathbf{B_7}$	$=$	$(x_5 + y_5)\,\mathbf{a_1} + (x_5 - y_5)\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4b)	Al IV
$\mathbf{B_8}$	$=$	$(x_6 - y_6)\,\mathbf{a_1} + (x_6 + y_6)\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4b)	Al V
$\mathbf{B_9}$	$=$	$(x_6 + y_6)\,\mathbf{a_1} + (x_6 - y_6)\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4b)	Al V
$\mathbf{B_{10}}$	$=$	$(x_7 - y_7)\,\mathbf{a_1} + (x_7 + y_7)\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	$=$	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4b)	Al VI
$\mathbf{B_{11}}$	$=$	$(x_7 + y_7)\,\mathbf{a_1} + (x_7 - y_7)\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	$=$	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4b)	Al VI
$\mathbf{B_{12}}$	$=$	$(x_8 - y_8)\,\mathbf{a_1} + (x_8 + y_8)\,\mathbf{a_2} + z_8\,\mathbf{a_3}$	$=$	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4b)	Al VII
$\mathbf{B_{13}}$	$=$	$(x_8 + y_8)\,\mathbf{a_1} + (x_8 - y_8)\,\mathbf{a_2} + z_8\,\mathbf{a_3}$	$=$	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4b)	Al VII
$\mathbf{B_{14}}$	$=$	$(x_9 - y_9)\,\mathbf{a_1} + (x_9 + y_9)\,\mathbf{a_2} + z_9\,\mathbf{a_3}$	$=$	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4b)	W II
$\mathbf{B_{15}}$	$=$	$(x_9 + y_9)\,\mathbf{a_1} + (x_9 - y_9)\,\mathbf{a_2} + z_9\,\mathbf{a_3}$	$=$	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4b)	W II

References

[1] J. A. Bland and D. Clark, *Studies of aluminum-rich alloys with the transition metals manganese and tungsten. I. The crystal structure of ϵ(W-Al)-WAl$_4$*, Acta Cryst. **11**, 231–236 (1958), doi:10.1107/S0365110X58000608.

Found in

[1] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Aluminum-Tungsten Binary Phase Diagram (1990 Okamoto H.). Copyright ©2006-2018 ASM International.