

Al₈Mo₃ Structure:

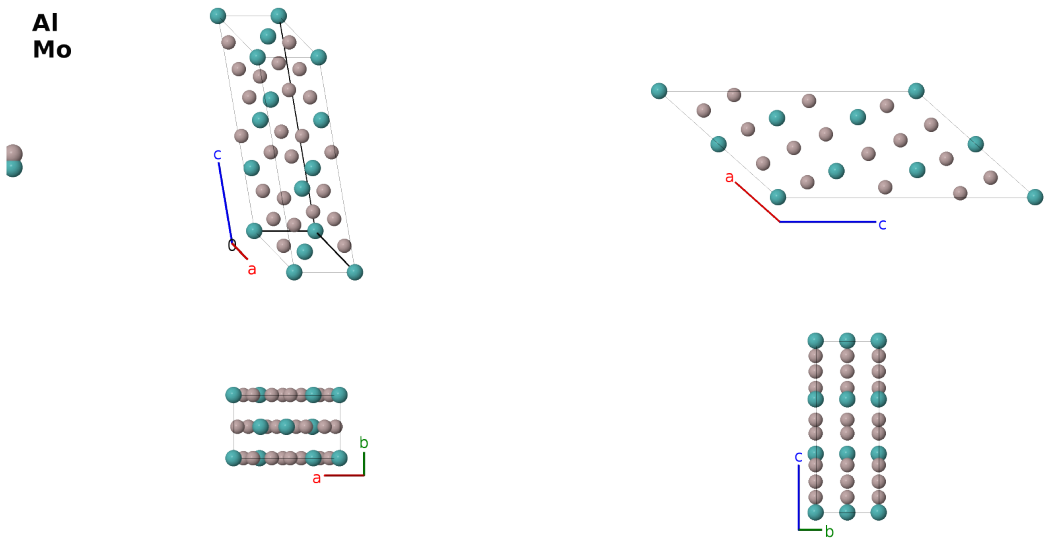
A8B3_mC22_12_4i_ai-001

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<https://aflow.org/prototype-encyclopedia/1Y1T>

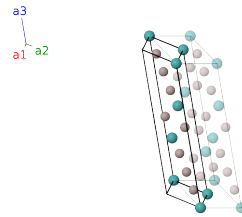
https://aflow.org/prototype-encyclopedia/A8B3_mC22_12_4i_ai-001



Prototype	Al ₈ Mo ₃
AFLOW prototype label	A8B3_mC22_12_4i_ai-001
ICSD	58002
CCDC	1622039
Pearson symbol	mC22
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<pre>aflow --proto=A8B3_mC22_12_4i_ai-001 --params=a, b/a, c/a, β, $x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6$</pre>

- There is no ICSD entry on file for (Oster, 2017), so we use the similar entry from (Forsyth, 1962).

Base-centered Monoclinic primitive vectors

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


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) Mo I
$\mathbf{B}_2$	=	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4i) Al I
$\mathbf{B}_3$	=	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4i) Al I
$\mathbf{B}_4$	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Al II
$\mathbf{B}_5$	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Al II
$\mathbf{B}_6$	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Al III
$\mathbf{B}_7$	=	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Al III
$\mathbf{B}_8$	=	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i) Al IV
$\mathbf{B}_9$	=	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i) Al IV
$\mathbf{B}_{10}$	=	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4i) Mo II
$\mathbf{B}_{11}$	=	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4i) Mo II

References

- [1] M. Oster, J. Tapp, A. Hagenow, and A. Möller, *Thermal oxidation of the intermetallic phases Al_8Mo_3 and AlMo_3* , J. Solid State Chem. **251**, 233–236 (2017), doi:10.1016/j.jssc.2017.04.029.
- [2] J. B. Forsyth and G. Gran, *The structure of the intermetallic phase $\gamma(\text{Mo-Al})\text{-Mo}_3\text{Al}_8$* , Acta Cryst. **15**, 100–104 (1960), doi:10.1107/S0365110X62000304.

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