

AuMn₃ Structure:

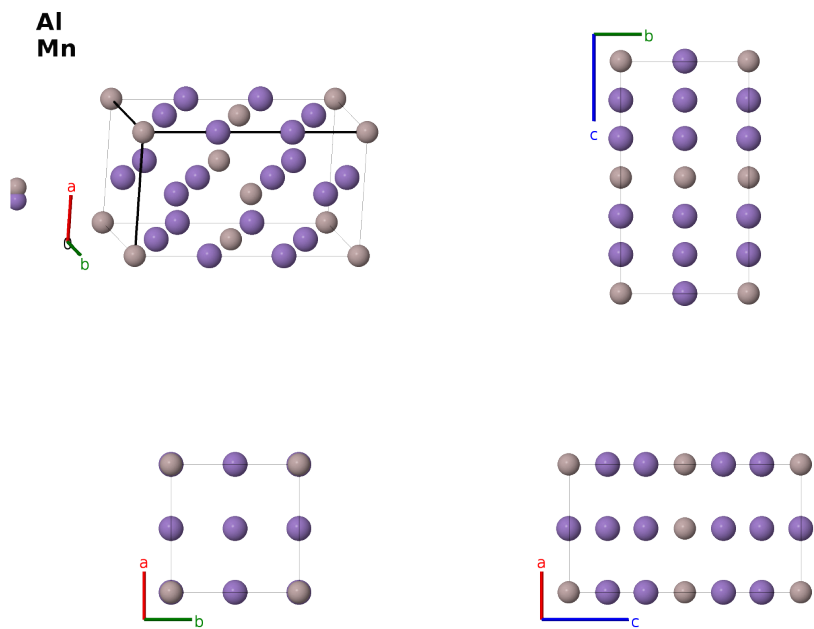
AB3_tP12_123_ae_cghi-001

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<https://aflow.org/prototype-encyclopedia/U1FT>

https://aflow.org/prototype-encyclopedia/AB3_tP12_123_ae_cghi-001

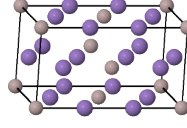


Prototype	AuMn ₃
AFLOW prototype label	AB3_tP12_123_ae_cghi-001
ICSD	150552
CCDC	1667715
Pearson symbol	tP12
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	<code>aflow --proto=AB3_tP12_123_ae_cghi-001</code> <code>--params=a, c/a, z₄, z₅, z₆</code>

Simple Tetragonal primitive vectors



$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(1a)	Al I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(1c)	Mn I
$\mathbf{B}_3$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2e)	Al II
$\mathbf{B}_4$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2e)	Al II
$\mathbf{B}_5$	$z_4 \mathbf{a}_3$	$=$	$cz_4 \hat{\mathbf{z}}$	(2g)	Mn II
$\mathbf{B}_6$	$-z_4 \mathbf{a}_3$	$=$	$-cz_4 \hat{\mathbf{z}}$	(2g)	Mn II
$\mathbf{B}_7$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(2h)	Mn III
$\mathbf{B}_8$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(2h)	Mn III
$\mathbf{B}_9$	$\frac{1}{2} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4i)	Mn IV
$\mathbf{B}_{10}$	$\frac{1}{2} \mathbf{a}_1 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + cz_6 \hat{\mathbf{z}}$	(4i)	Mn IV
$\mathbf{B}_{11}$	$\frac{1}{2} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4i)	Mn IV
$\mathbf{B}_{12}$	$\frac{1}{2} \mathbf{a}_1 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_6 \hat{\mathbf{z}}$	(4i)	Mn IV

References

- [1] P. Gaunt and A. Eden, *The structure of AuMn₃*, Acta Cryst. **19**, 476–477 (1965), doi:10.1107/S0365110X6500364X.

Found in

- [1] <http://icsd.fiz-karlsruhe.de/>. ICSD Entry 150552.

First cited in

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