AuMn₃ Structure:
AB3_tP12_123_ae_cghi-001

https://aflow.org/p/U1FT

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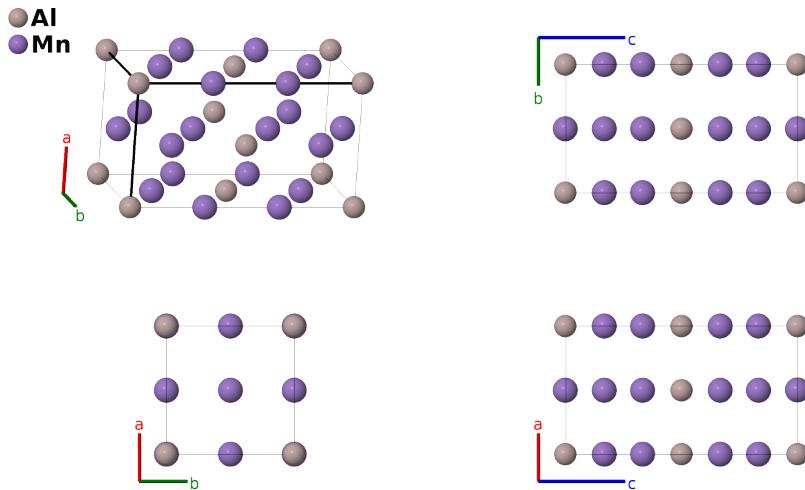
Prototype	AuMn₃
AFLOW prototype label	AB3_tP12_123_ae_cghi-001
ICSD	150552
Pearson symbol	tP12
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	aflow --proto=AB3_tP12_123_ae_cghi-001 --params=$a, c/a, z_4, z_5, z_6$

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
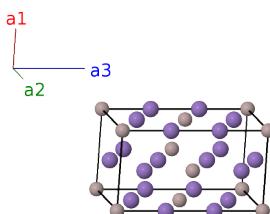
Basis vectors

		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.