

MnAl₆ (*D*2_h) Structure: A6B_oC28_63_efg_c-001

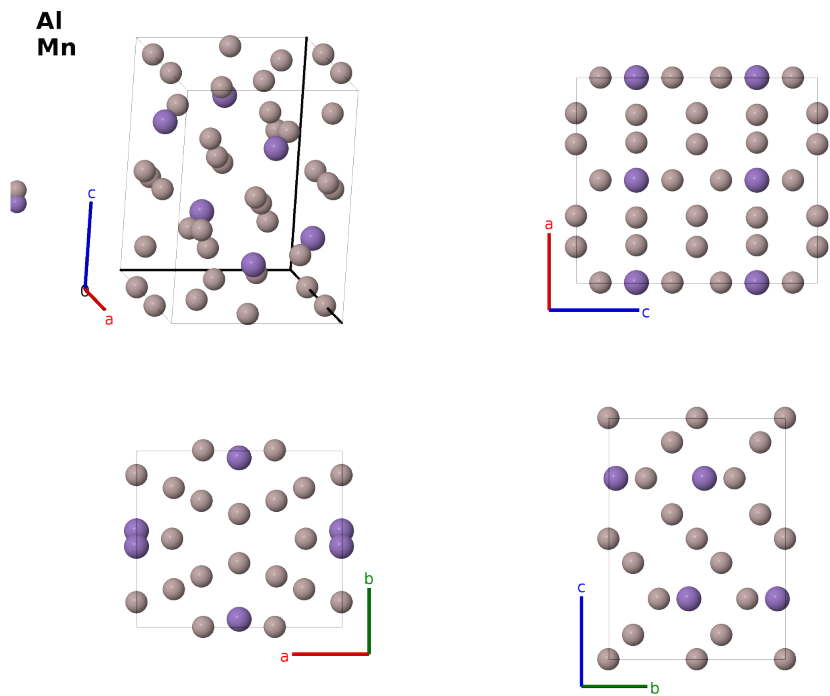
This structure previously used the label(s) **A6B_oC28_63_efg_c**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/386R>

https://aflow.org/prototype-encyclopedia/A6B_oC28_63_efg_c-001



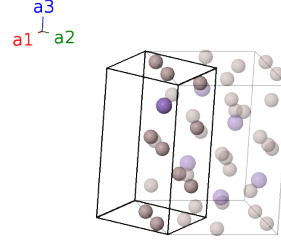
Prototype	Al ₆ Mn
AFLOW prototype label	A6B_oC28_63_efg_c-001
<i>Strukturbericht</i> designation	<i>D</i> 2 _h
ICSD	57973
CCDC	1622011
Pearson symbol	oC28
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=A6B_oC28_63_efg_c-001</code> <code>--params=a, b/a, c/a, y₁, x₂, y₃, z₃, x₄, y₄</code>

Other compounds with this structure

FeAl₆, ReAl₆, TcAl₆

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Mn I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Mn I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}}$	(8e)	Al I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8e)	Al I
$\mathbf{B}_5$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}}$	(8e)	Al I
$\mathbf{B}_6$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8e)	Al I
$\mathbf{B}_7$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8f)	Al II
$\mathbf{B}_8$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Al II
$\mathbf{B}_9$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Al II
$\mathbf{B}_{10}$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8f)	Al II
$\mathbf{B}_{11}$	$= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	Al III
$\mathbf{B}_{12}$	$= -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	Al III
$\mathbf{B}_{13}$	$= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	Al III
$\mathbf{B}_{14}$	$= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	Al III

References

- [1] A. Kontio and P. Coppens, *New study of the structure of MnAl₆*, Acta Crystallogr. Sect. B **37**, 433–435 (1981), doi:10.1107/S0567740881003191.

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