

Au₅Mn₂ Structure:

A5B2_mC14_12_a2i_i-001

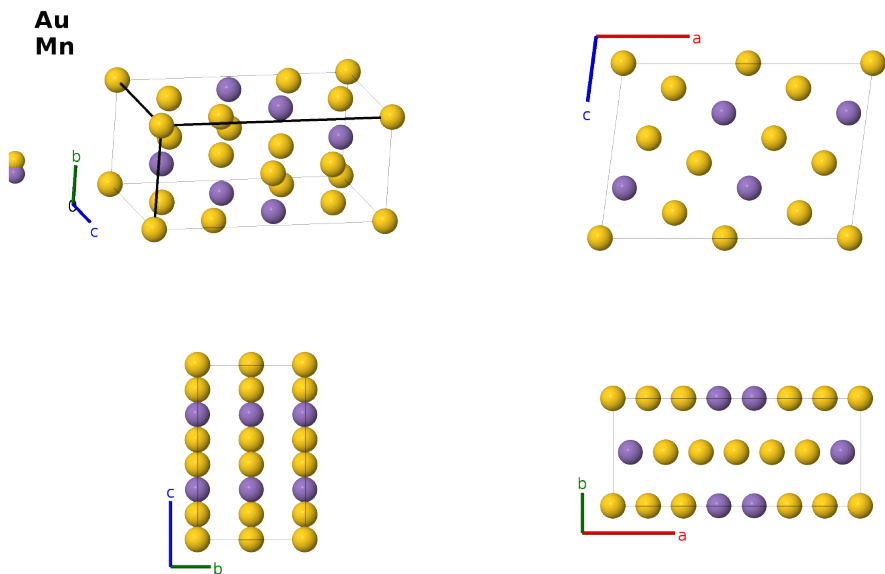
This structure previously used the label(s) **A5B2_mC14_12_a2i_i**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/9H7D>

https://aflow.org/prototype-encyclopedia/A5B2_mC14_12_a2i_i-001

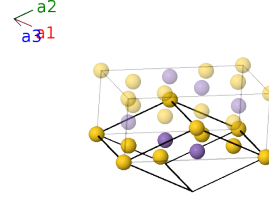


Prototype	Au ₅ Mn ₂
AFLOW prototype label	A5B2_mC14_12_a2i_i-001
ICSD	144447
CCDC	2229876
Pearson symbol	mC14
Space group number	12
Space group symbol	<i>C</i> 2/ <i>m</i>
AFLOW prototype command	<code>aflow --proto=A5B2_mC14_12_a2i_i-001</code> <code>--params=a,b/a,c/a,β,x₂,z₂,x₃,z₃,x₄,z₄</code>

- As noted by (Pearson, 1972), this structure is very nearly cubic close-packed. As such, it is frequently used for cluster expansion models.
- (Humble, 1964) puts this structure in space group *Cc* #5, but the coordinates given are consistent with space group *C*2/*m* #12.

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) Au 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) Au II
$\mathbf{B}_3$	=	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4i) Au II
$\mathbf{B}_4$	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Au III
$\mathbf{B}_5$	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Au III
$\mathbf{B}_6$	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Mn I
$\mathbf{B}_7$	=	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Mn I

References

- [1] S. G. Humble, *Establishment of an ordered phase of composition Au_5Mn_2 in the gold-manganese system*, Acta Cryst. **17**, 1485–1486 (1964), doi:10.1107/S0365110X64003723.
- [2] W. B. Pearson, *The Crystal Chemistry and Physics of Metals and Alloys* (Wiley Interscience, New York, London, Sydney, Toronto, 1972).

Found in

- [1] G. van Tendeloo, R. Wolf, and S. Amelinckx, *The Microstructure of the Alloy Au_5Mn_2 : A Domain Structure with 84 Variants*, Phys. Stat. Solidi A **40**, 531–550 (1977), doi:10.1002/pssa.2210400220.
- [2] W. B. Pearson, *The Crystal Chemistry and Physics of Metals and Alloys* (Wiley Interscience, New York, London, Sydney, Toronto, 1972).

First cited in

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