Au_5Mn_2 Structure: A5B2_mC14_12_a2i_i-001

This structure originally had the label `A5B2_mC14_12_a2i_i`. Calls to that address will be redirected here.

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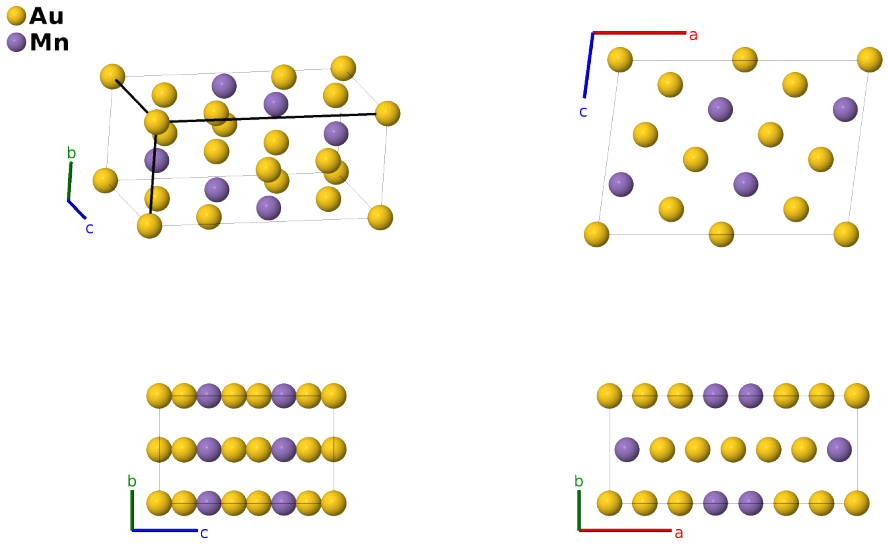
https://aflow.org/p/9H7D

https://aflow.org/p/A5B2_mC14_12_a2i_i-001

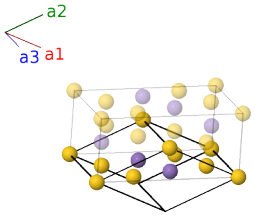


Prototype	Au_5Mn_2
AFLOW prototype label	A5B2_mC14_12_a2i_i-001
ICSD	144447
Pearson symbol	mC14
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A5B2_mC14_12_a2i_i-001 --params=`$a, b/a, c/a, \beta, x_2, z_2, x_3, z_3, x_4, z_4$

- 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 $C2/m$ #12.

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



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, Tornoto, 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, Tornoto, 1972).