AuMn Structure: AB_oP2_47_a_h-001

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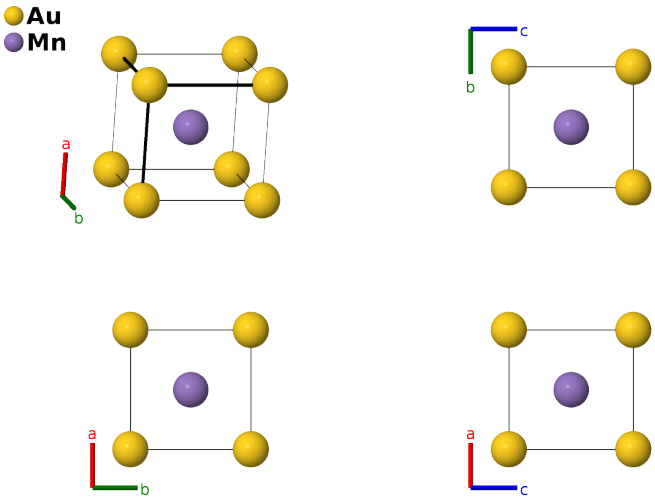
https://aflow.org/p/JM3Q

https://aflow.org/p/AB_oP2_47_a_h-001

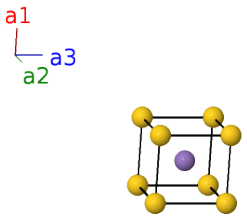


Prototype	AuMn
AFLOW prototype label	AB_oP2_47_a_h-001
ICSD	none
Pearson symbol	oP2
Space group number	47
Space group symbol	$Pmmm$
AFLOW prototype command	`aflow --proto=AB_oP2_47_a_h-001 --params=`$a, b/a, c/a$

- (Schubert, 1959) call this "AuMn (Mn)," and (Villars, 2018) shows it existing only on the manganese side of the phase diagram, while the gold-rich structure is not well determined. We present the ordered stoichiometric structure here, based on the comment in (Schubert, 1959) that this is an orthorhombic distortion of the $B2$ structure.
- Above 120K AuMn first transforms into a phase with uncertain structure, and above $\approx$ 300K it transforms into the CsCl ($B2$) structure (Villars,2018).

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Au I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1h)	Mn I

References

[1] K. Schubert, M. Balk, S. Bhan, H. Breimer, P. Esslinger, and E. Stolz, *Einige strukturelle Ergebnisse an metallischen Phasen IV*, Naturwissenschaften **46**, 647–648 (1959), doi:10.1007/BF00637995.

Found in

[1] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Gold-Manganese Binary Phase Diagram (1990 Massalski T.B.). Copyright ©2006-2018 ASM International.