

AuMn Structure:

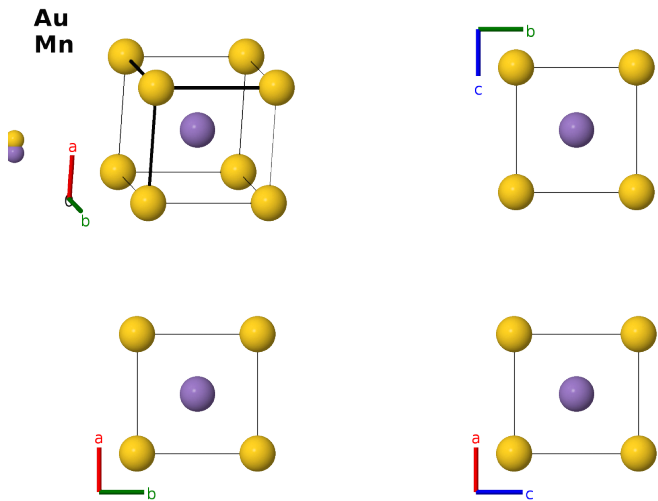
AB_oP2_47_a_h-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/JM3Q>

https://aflow.org/prototype-encyclopedia/AB_oP2_47_a_h-001

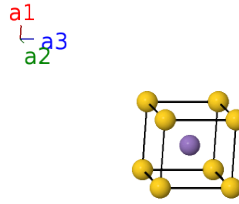


Prototype	AuMn
AFLOW prototype label	AB_oP2_47_a_h-001
Pearson symbol	oP2
Space group number	47
Space group symbol	$Pmmm$
AFLOW prototype command	<code>aflow --proto=AB_oP2_47_a_h-001</code> <code>--params=a, b/a, c/a</code>

- (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 ≈ 300 K it transforms into the CsCl ($B2$) structure (Villars, 2018).

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	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.

First cited in

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, *Comput. Mater. Sci.* **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.