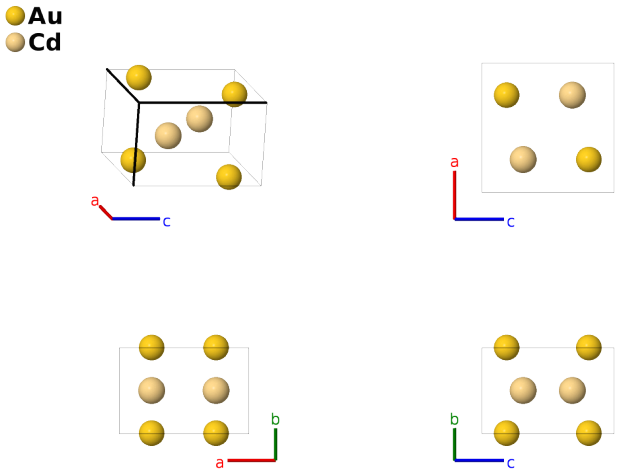
β'-AuCd ($B19$) Structure: AB_oP4_51_e_f-001

This structure originally had the label `AB_oP4_51_e_f`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/WLS6

https://aflow.org/p/AB_oP4_51_e_f-001

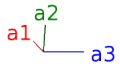


Prototype	AuCd
AFLOW prototype label	AB_oP4_51_e_f-001
***Strukturbericht* designation**	$B19$
ICSD	58409
Pearson symbol	oP4
Space group number	51
Space group symbol	$Pmma$
AFLOW prototype command	`aflow --proto=AB_oP4_51_e_f-001 --params=`$a, b/a, c/a, z_1, z_2$

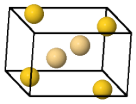
Other compounds with this structure
AuTi (H.T.), CdMg, IrMo, IrW, MoPt (H.T.), NbPt, NbRh, PbTi, PtTi, PtV (L.T.)

- When $a = b = c$, $z_1 = 1/4$, and $z_2 = 3/4$ the atoms are on the sites of a face-centered cubic lattice.
- When $a = c$, $z_1 = 1/4$, and $z_2 = 3/4$ the system reduces to the $L1_0$ (AuCu) structure.
- When $a/b = (8/3)^{2/3}$, $c/b = 3^{1/2}$, $z_1 = 1/3$, and $z_2 = 5/6$, the atoms are on the sites of the hcp structure.
- Finally, when $z_2 = 1/2 + z_1$ the atoms are at the positions of the α-U ($A20$) structure.

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
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + z_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + cz_1\,\hat{\mathbf{z}}$	(2e)	Au I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 - z_1\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - cz_1\,\hat{\mathbf{z}}$	(2e)	Au I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2f)	Cd I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2f)	Cd I

References

[1] L.-C. Chang, *Atomic displacements and crystallographic mechanisms in diffusionless transformation of gold-cadium single crystals containing 47.5 atomic per cent cadmium*, Acta Cryst. **4**, 320–324 (1951), doi:10.1107/S0365110X51001057.

Found in

[1] W. B. Pearson, *The Crystal Chemistry and Physics of Metals and Alloys* (Wiley Interscience, New York, London, Sydney, Tornoto, 1972), chap. 7, pp. 313–314.