

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

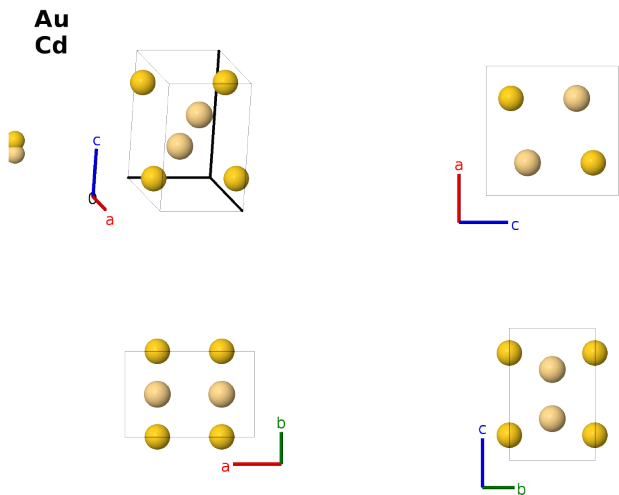
This structure previously used the label(s) **AB_oP4_51_e_f**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/WLS6>

https://aflow.org/prototype-encyclopedia/AB_oP4_51_e_f-001



Prototype	AuCd
AFLOW prototype label	AB_oP4_51_e_f-001
<i>Strukturbericht</i> designation	<i>B19</i>
ICSD	58409
CCDC	1622424
Pearson symbol	oP4
Space group number	51
Space group symbol	<i>Pmma</i>
AFLOW prototype command	<code>aflow --proto=AB_oP4_51_e_f-001 --params=a,b/a,c/a,z₁,z₂</code>

Other compounds with this structure

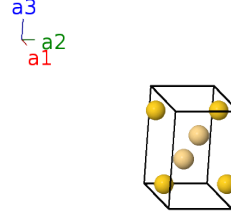
AuTi (H.T.), CdMg, IrMo, IrW, MoPt (H.T.), MoRh, NbPt, NbRh, TiPb, TiPd, TiPt, VPt (L.T.)

- 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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + cz_1 \hat{\mathbf{z}}$	(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-cadmium 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, Toronto, 1972), chap. 7, pp. 313–314.

First cited in

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