

Cu₄Pd Structure:

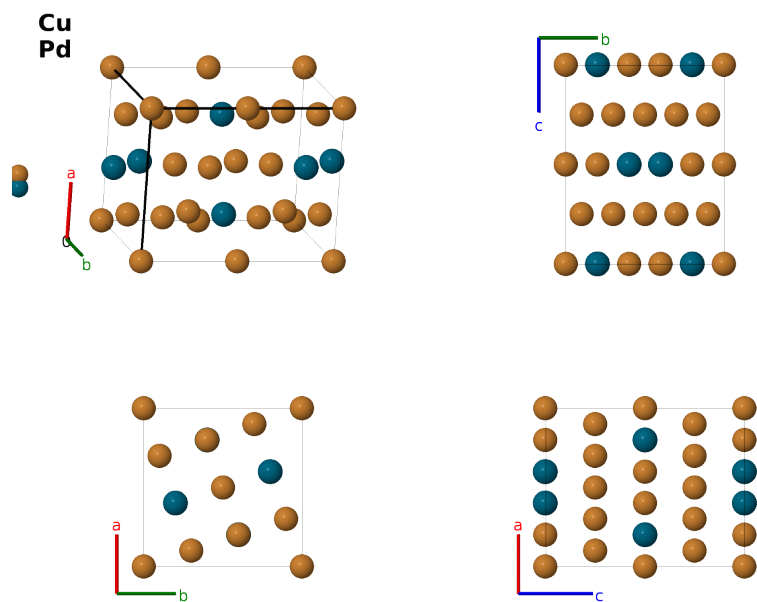
A4B_tP20_84_afjk_j-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/L3AR>

https://aflow.org/prototype-encyclopedia/A4B_tP20_84_afjk_j-001

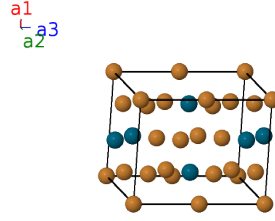


Prototype	Cu ₄ Pd
AFLOW prototype label	A4B_tP20_84_afjk_j-001
ICSD	103087
CCDC	1661043
Pearson symbol	tP20
Space group number	84
Space group symbol	$P4_2/m$
AFLOW prototype command	<code>aflow --proto=A4B_tP20_84_afjk_j-001</code> <code>--params=a, c/a, x₃, y₃, x₄, y₄, x₅, y₅, z₅</code>

- Above 476°C Cu₄Pd is completely disordered, with the atoms placed randomly on the sites of the face-centered cubic (A1) structure. Below that temperature it takes on this ordered tetragonal structure. (Geisler, 1954).
- The value of 0.25 for z₅ is not given in (Geisler, 1954), but we infer it from the description of the cell as a decoration of the face-centered cubic lattice.

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	Cu I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	Cu I
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	Cu II
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	Cu II
$\mathbf{B}_5$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}}$	Cu III
$\mathbf{B}_6$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}}$	Cu III
$\mathbf{B}_7$	$=$	$-y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	Cu III
$\mathbf{B}_8$	$=$	$y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	Cu III
$\mathbf{B}_9$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}}$	Pd I
$\mathbf{B}_{10}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}}$	Pd I
$\mathbf{B}_{11}$	$=$	$-y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	Pd I
$\mathbf{B}_{12}$	$=$	$y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	Pd I
$\mathbf{B}_{13}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	Cu IV
$\mathbf{B}_{14}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	Cu IV
$\mathbf{B}_{15}$	$=$	$-y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	Cu IV
$\mathbf{B}_{16}$	$=$	$y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	Cu IV
$\mathbf{B}_{17}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	Cu IV
$\mathbf{B}_{18}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	Cu IV
$\mathbf{B}_{19}$	$=$	$y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	Cu IV
$\mathbf{B}_{20}$	$=$	$-y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	Cu IV

References

- [1] A. H. Geisler and J. B. Newkirk, *Ordering Reaction of the Cu₄Pd Alloy*, JOM **6**, 1076–1082 (1954), doi:10.1007/BF03398349.

First cited in

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