

Cubic CuPt [$L1_3(I)$, $D4$] Structure: AB_cF32_227_c_d-001

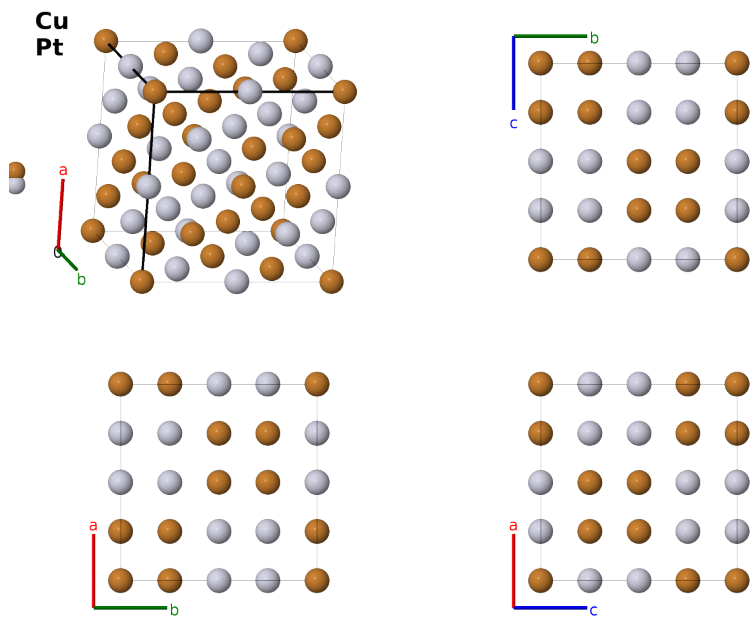
This structure previously used the label(s) **AB_cF32_227_c_d**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/0HDN>

https://aflow.org/prototype-encyclopedia/AB_cF32_227_c_d-001



Prototype	CuPt
AFLOW prototype label	AB_cF32_227_c_d-001
<i>Strukturbericht</i> designation	$L1_3(I)$
Pearson symbol	cF32
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB_cF32_227_c_d-001 --params=a</code>

- (Johansson, 1929) described two possible structures for CuPt. (Ewald, 1929) and later (Villars, 2007) used the description to determine the space group and atomic positions. This page describes the cubic structure, which (Ewald, 1929) labeled *Strukturbericht* $L1_1$. The other structure is rhombohedral, and was listed as $L1_1$. (Villars, 2007) prefers the later structure, listing the current one as “superceded.”

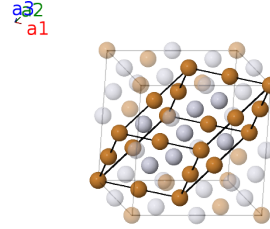
- (Barrett, 1980) noted that even slight additions of platinum above stoichiometry will cause a change in the crystal structure.
- This structure is equivalent to the $D4$ structure of (Lu, 1991).
- It should not be confused with the CuPt_3 structure, which has also been given the $L1_3$ label, and which we will often refer to as $L1_3(II)$.

Face-centered Cubic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(16c) Cu I
$\mathbf{B}_2$	$=$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}}$	(16c) Cu I
$\mathbf{B}_3$	$=$	$\frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16c) Cu I
$\mathbf{B}_4$	$=$	$\frac{1}{2}\mathbf{a}_1$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16c) Cu I
$\mathbf{B}_5$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(16d) Pt I
$\mathbf{B}_6$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(16d) Pt I
$\mathbf{B}_7$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16d) Pt I
$\mathbf{B}_8$	$=$	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16d) Pt I

References

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Found in

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