$L1_a$ (disputed $CuPt_3$ Structure): AB7_cF32_225_a_bd-001

This structure originally had the label `AB7_cF32_225_b_ad`. Calls to that address will be redirected here.

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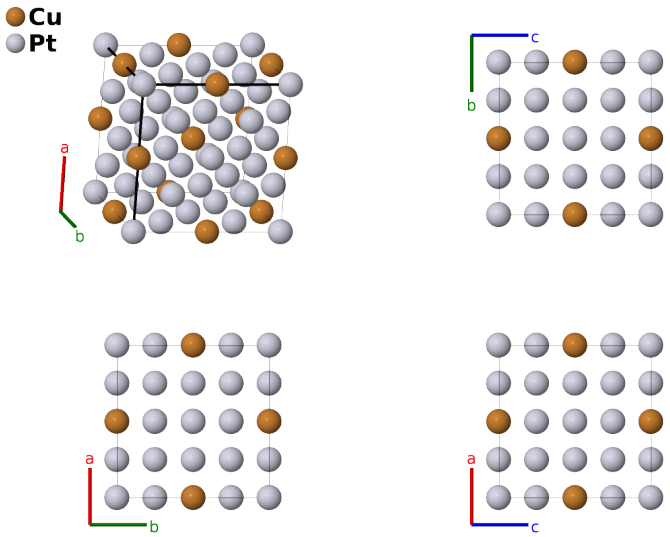
https://aflow.org/p/3APN

https://aflow.org/p/AB7_cF32_225_a_bd-001



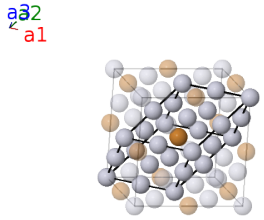
Prototype	$CuPt_3$
AFLOW prototype label	AB7_cF32_225_a_bd-001
***Strukturbericht* designation**	$L1_a$
ICSD	none
Pearson symbol	cF32
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB7_cF32_225_a_bd-001 --params=`a

- According to (Tang, 1951), the (24d) sites have the composition $Pt_{0.8}Cu_{0.2}$ in stoichiometric $CuPt_3$. Here we use "Pt" to specify the atoms on this site.
- (Tang, 1951) states that the crystal structure of $CuPt_3$ must be cubic, but (Mshumi, 2014) argue that it is orthorhombic, and is in fact the $L1_3$ structure.
- (Smithells, 1955) gave this structure the $L1_a$ designation as part of his extension of the original *Strukturbericht* labels. He does note that an alternative orthorhombic structure had been proposed.
- (Smithells, 1955) assigns this structure to space group $F432$ #209, but the positions given by (Tang, 1951) are also consistent with $Fm\bar{3}m$ #225, so we assign this structure to the higher symmetry space group.

- (Tang, 1951) does not give the lattice constant, so we use the value estimated by (Smithells, 1955).
- The Wyckoff positions are identical to those of the Ca_7Ge structure.

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	(4a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	Pt I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Pt II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Pt II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Pt II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Pt II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(24d)	Pt II
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(24d)	Pt II

References

[1] Y.-C. Tang, *A cubic structure for the phase Pt_3Cu*, Acta Cryst. **4**, 377–378 (1951), doi:10.1107/S0365110X51001185.

[2] C. J. Smithells, *Metals Reference Book* (Butterworths Scientific, London, 1955), second edn.

Found in

[1] C. Mshumi, C. I. Lang, L. R. Richey, K. C. Erb, C. W. Rosenbrock, L. J.Nelson, R. R. Vanfleet, H. T. Stokes, B. J. Campbell, and G. L. W. Hart, *Revisiting the $CuPt_3$ prototype and the $L1_3$ structure*, Acta Mat. **73**, 326–336 (2014), doi:10.1016/j.actamat.2014.03.029.