Rhombohedral CuPt ($L1_1$) Structure: AB_hR2_166_a_b-001

This structure originally had the label `AB_hR2_166_a_b`. Calls to that address will be redirected here.

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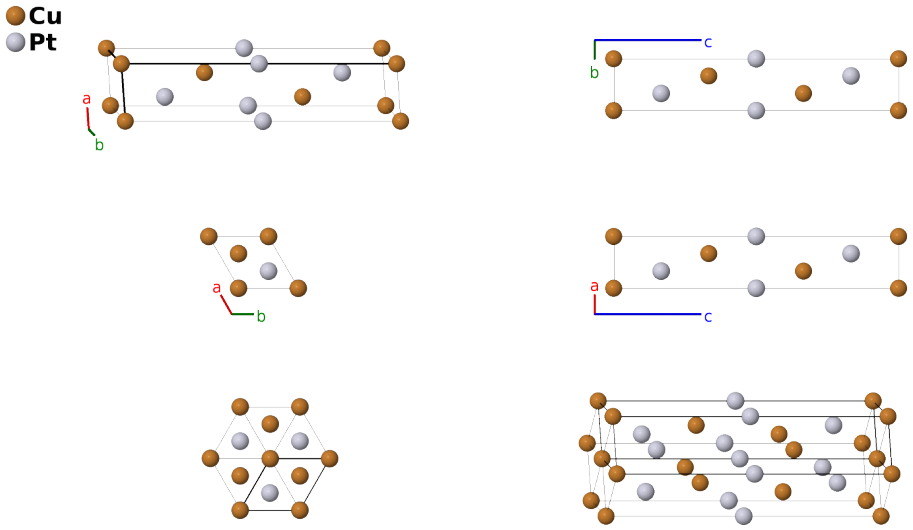
https://aflow.org/p/3A9R

https://aflow.org/p/AB_hR2_166_a_b-001



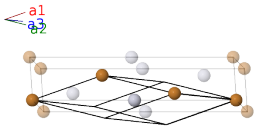
Prototype	CuPt
AFLOW prototype label	AB_hR2_166_a_b-001
***Strukturbericht* designation**	$L1_1$
ICSD	107118
Pearson symbol	hR2
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=AB_hR2_166_a_b-001 --params=`$a, c/a$

- (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 rhombohedral structure, which (Ewald, 1929) labeled *Strukturbericht* $L1_1$. The other structure is cubic, and was listed as $L1_3$.
- (Barrett, 1980) noted that even slight additions of platinum above stoichiometry will cause a change in the crystal structure.
- CuPt and KSH have the same AFLOW prototype label, AB_hR2_166_a_b. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

- This structure is given in the rhombohedral setting of space group $R\bar{3}m$ #166. The hexagonal setting may be obtained by adding `--hex` to the aflow command.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Pt I

References

[1] C. H. Johansson and J. O. Linde, *Gitterstruktur und elektrisches Leitvermögen der Mischkristallreihen Au-Cu, Pd-Cu und Pt-Cu*, Annalen der Physik **82**, 449–478 (1927), doi:10.1002/andp.19273870402.

[2] C. Barrett and T. B. Massalski, *Structure of Metals – Crystallographic Methods, Principles, and Data* (Pergammon Press, Oxford, New York, 1980).

Found in

[1] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).

[2] P. Villars, K. Cenzual, J. Daams, R. Gladyshevskii, O. Shcherban, V. Dubenskyy, N. Melnichenko-Koblyuk, O. Pavlyuk, I. Savysyuk, S. Stoyko, and L. Sysa, *Structure Types. Part 5: Space Groups (173) P63- (166) R-3m · CuPt: Datasheet from Landolt-Börnstein - Group III Condensed Matter · Volume 43A5: "Structure Types. Part 5: Space Groups (173) P63 - (166) R-3m" in SpringerMaterials*, doi:10.1007/978-3-540-46933-9_359. Copyright 2007 Springer-Verlag.