$CdPt_3$ ("New" $L1_3$) Structure: AB3_oC8_65_a_bf-001

This structure originally had the label `AB3_oC8_65_a_bf`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

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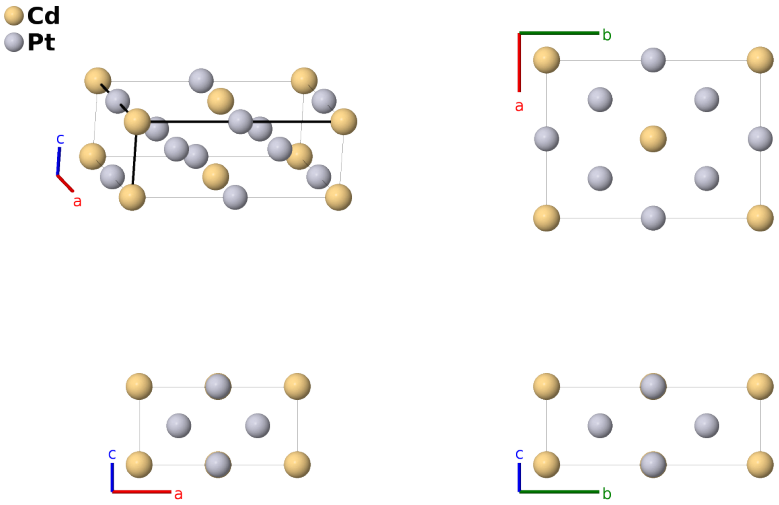
https://aflow.org/p/JBK1

https://aflow.org/p/AB3_oC8_65_a_bf-001

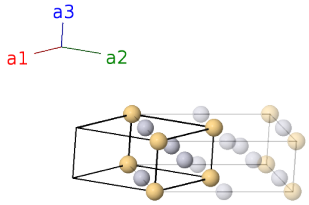


Prototype	$CdPt_3$
AFLOW prototype label	AB3_oC8_65_a_bf-001
***Strukturbericht* designation**	$L1_3$
ICSD	none
Pearson symbol	oC8
Space group number	65
Space group symbol	$Cmmm$
AFLOW prototype command	`aflow --proto=AB3_oC8_65_a_bf-001 --params=`$a, b/a, c/a$

- This is *not* the $L1_3$ CuPt structure labeled by (Ewald, 1931) as $L1_3$. That structure is now considered obsolete.
- This structure has not been experimentally confirmed, but it has frequently been predicted as a low energy structure. (Hart, 2009) has a review of these calculations. It was originally given the $L1_3$ designation. As this has been frequently used in the literature (*e.g.* Mehl, 2017), we will continue to used it despite the possible confusion.
- Data for this structure comes from the supplemental material of (Hart, 2013).

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Cd I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2b)	Pt I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	Pt II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	Pt II

References

[1] G. L. W. Hart, *Verifying predictions of the $L1_3$ crystal structure in Cd-Pt and Pd-Pt by exhaustive enumeration*, Phys. Rev. B **80**, 014106 (2009), doi:10.1103/PhysRevB.80.014106.

[2] G. L. W. Hart, S. Curtarolo, T. B. Massalski, and O. Levy, *Comprehensive Search for New Phases and Compounds in Binary Alloy Systems Based on Platinum-Group Metals, Using a Computational First-Principles Approach*, Phys. Rev. X **3**, 041305 (2013), doi:10.1103/PhysRevX.3.041035.

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

[4] M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW library of crystallographic prototypes: part 1*, Comp. Mater. Sci. **136**, S1–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.