Pd_5Pu_3 Structure: A5B3_oC32_63_cfg_ce-001

This structure originally had the label `A5B3_oC32_63_cfg_ce`. Calls to that address will be redirected here.

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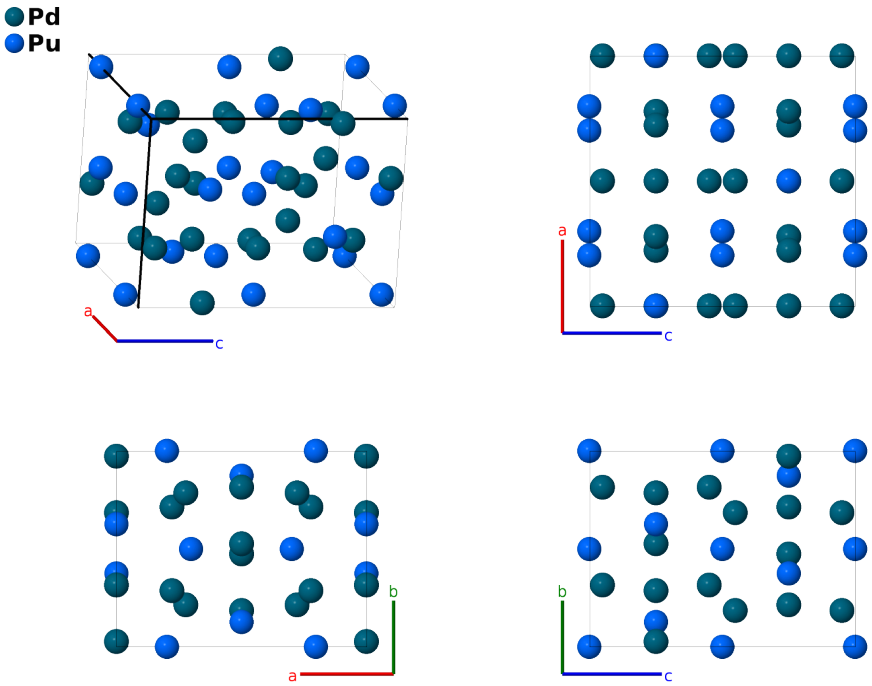
https://aflow.org/p/9AGN

https://aflow.org/p/A5B3_oC32_63_cfg_ce-001



Prototype	Pd_5Pu_3
AFLOW prototype label	A5B3_oC32_63_cfg_ce-001
ICSD	350
Pearson symbol	oC32
Space group number	63
Space group symbol	*Cmcm*
AFLOW prototype command	`aflow --proto=A5B3_oC32_63_cfg_ce-001 --params=`$a, b/a, c/a, y_1, y_2, x_3, y_4, z_4, x_5, y_5$

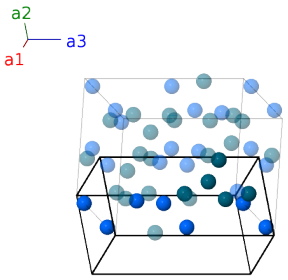
Other compounds with this structure

Ga_5U_3, Ga_5Zr_3, In_5Ce_3, In_5Dy_3, In_5Er_3, In_5Gd_3, In_5Ho_3, In_5La_3, In_5Lu_3, In_5Nd_3, In_5Pr_3, In_5Sm_3, In_5Tb_3, In_5Th_3, In_5Y_3, Pb_5Ba_3, Pd_5Dy_3, Pd_5Er_3, Pd_5Gd_3, Pd_5Ho_3, Pd_5Lu_3, Pd_5Sc_3, Pd_5Tb_3, Pd_5Tm_3, Pd_5Y_3, Pd_5Yb_3, Rh_5Zr_3, Sn_5La_3, Sn_5Sr_3, Sn_5Yb_3, $(Mg_xSn_{1-x})_5La_3$

- Although (Massalski, 1990) lists Pd_5Pu_3 as the prototype for many structures, it is not shown in the assessed Pd-Pu phase diagram, which is based on data from 1967.
- (Cromer, 1976) states that this phase may be isostructural with Ga_5Zr_3, but at the time of publication the exact structure of that phase had not been solved.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Pd I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Pd I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Pu I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Pu I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}}$	(8e)	Pu II
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8e)	Pu II
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(8e)	Pu II
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8e)	Pu II
$\mathbf{B_9}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8f)	Pd II
$\mathbf{B_{10}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Pd II
$\mathbf{B_{11}}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Pd II
$\mathbf{B_{12}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8f)	Pd II
$\mathbf{B_{13}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Pd III
$\mathbf{B_{14}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Pd III
$\mathbf{B_{15}}$	=	$-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Pd III
$\mathbf{B_{16}}$	=	$(x_5 + y_5)\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Pd III

References

[1] D. T. Cromer, *Plutonium-palladium Pu_3Pd_5*, Acta Crystallogr. Sect. B **32**, 1930–1932 (1976), doi:10.1107/S0567740876006778.

[2] T. B. Massalski, H. Okamoto, P. R. Subramanian, and L. Kacprzak, eds., *Binary Alloy Phase Diagrams*, vol. 1 (ASM International, Materials Park, Ohio, USA, 1990), 2^{nd} edn.

Found in

[1] A. Provino, N. S. Sangeetha, S. K. Dhar, V. Smetana, K. A. Gschneidner, V. K. Pecharsky, P. Manfrinetti, and A.-V. Mudring, *New R_3Pd_5 Compounds (R = Sc, Y, Gd-Lu): Formation and Stability, Crystal Structure, and Antiferromagnetism*, Crystal Growth & Design **16**, 6001–6015 (2016), doi:10.1021/acs.cgd.6b01045.