

Pd₅Pu₃ Structure: A5B3_oC32_63_cfg_ce-001

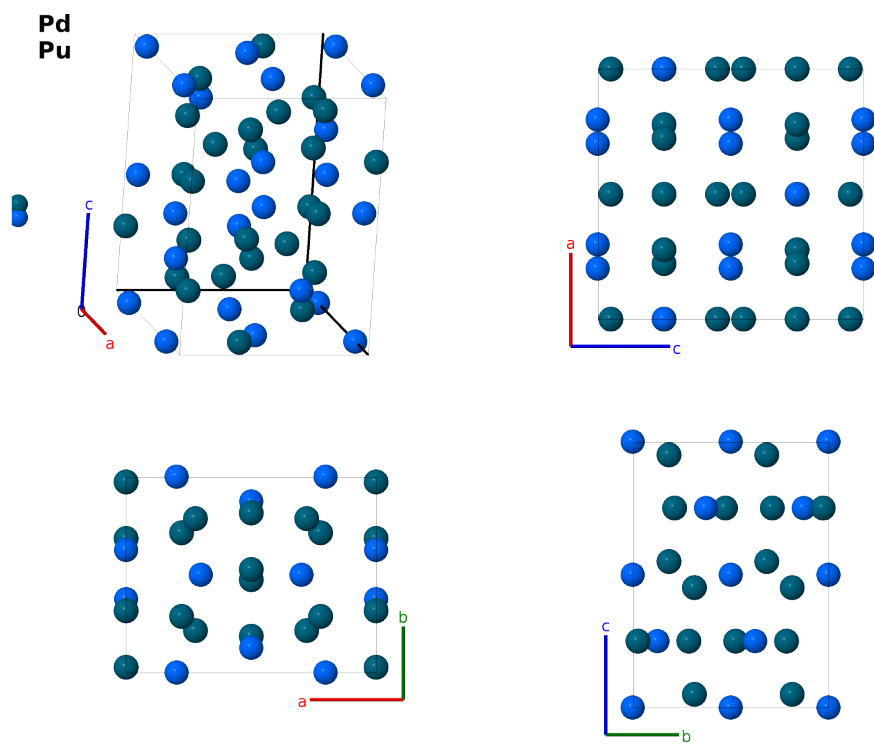
This structure previously used the label(s) **A5B3_oC32.63_cfg.ce**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/9AGN>

https://aflow.org/prototype-encyclopedia/A5B3_oC32_63_cfg_ce-001



Prototype	Pd ₅ Pu ₃
AFLOW prototype label	A5B3_oC32_63_cfg_ce-001
ICSD	350
CCDC	1590886
Pearson symbol	oC32
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=A5B3_oC32_63_cfg_ce-001</code> <code>--params=a,b/a,c/a,y₁,y₂,x₃,y₄,z₄,x₅,y₅</code>

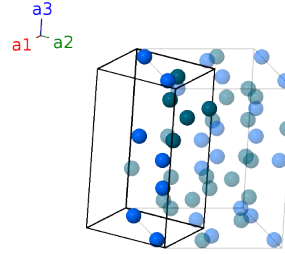
Other compounds with this structure

Ga₅U₃, Ga₅Zr₃, In₅Ce₃, In₅Dy₃, In₅Er₃, In₅Gd₃, In₅Ho₃, In₅La₃, In₅Lu₃, In₅Nd₃, In₅Pr₃, In₅Sm₃, In₅Tb₃, In₅Th₃, In₅Y₃, Pb₅Ba₃, Pd₅Dy₃, Pd₅Er₃, Pd₅Gd₃, Pd₅Ho₃, Pd₅Lu₃, Pd₅Sc₃, Pd₅Tb₃, Pd₅Tm₃, Pd₅Y₃, Pd₅Yb₃, Rh₅Zr₃, Sn₅La₃, Sn₅Sr₃, Sn₅Yb₃, (Mg_xSn_{1-x})₅La₃

- Although (Massalski, 1990) lists Pd₅Pu₃ 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 Ga₅Zr₃, but at the time of publication the exact structure of that phase had not been solved.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



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
$\mathbf{B}_{10}$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Pd II
$\mathbf{B}_{11}$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(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), 2nd 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.

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