

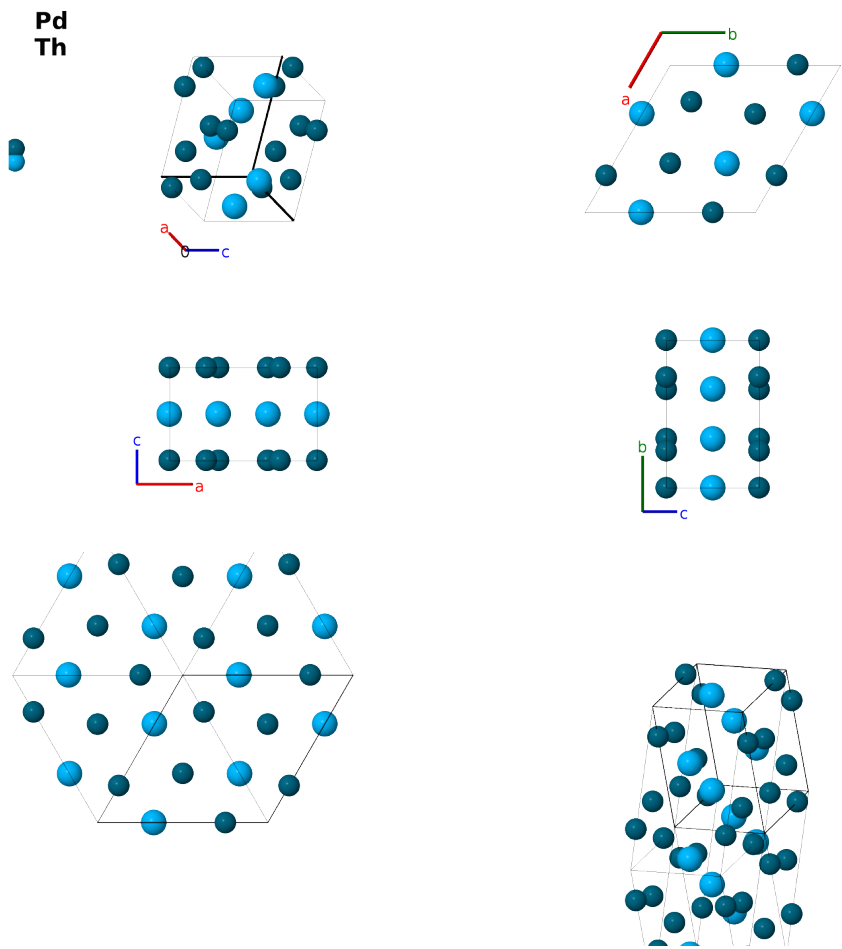
Th₃Pd₅ Structure: A5B3_hP8_189_cf_g-001

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<https://aflow.org/prototype-encyclopedia/K8CX>

https://aflow.org/prototype-encyclopedia/A5B3_hP8_189_cf_g-001



Prototype	Pd ₅ Th ₃
AFLOW prototype label	A5B3_hP8_189_cf_g-001
ICSD	649755
CCDC	1763878
Pearson symbol	hP8
Space group number	189
Space group symbol	$P\bar{6}2m$

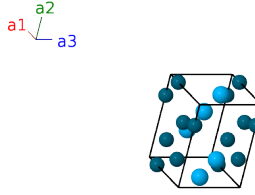
AFLOW prototype command `aflow --proto=A5B3_hP8_189_cf_g-001`
 `--params=a, c/a, x2, x3`

Other compounds with this structure

Th₃Pt₅, Yb₃Ge₅

- The ICSD entry uses the data from (Thomson, 1963), but relabels palladium as platinum and puts the thorium atom on the (3f) site with palladium/platinum on the (3g) site. We use the published data.

Hexagonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}}$	(2c)	Pd I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}}$	(2c)	Pd I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1$	$=$	$\frac{1}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}}$	(3f)	Pd II
$\mathbf{B}_4$	$= x_2 \mathbf{a}_2$	$=$	$\frac{1}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}}$	(3f)	Pd II
$\mathbf{B}_5$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}}$	(3f)	Pd II
$\mathbf{B}_6$	$= x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3g)	Th I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3g)	Th I
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3g)	Th I

References

- [1] J. R. Thomson, *The crystal structure of Th₃Pd₅ and Th₃Pt₅*, Acta Cryst. **16**, 320–321 (1963), doi:10.1107/S0365110X63000864.

Found in

- [1] J. R. Thomson, *Alloys of thorium with certain transition metals: III. The system thorium-palladium*, J. Less-Common Met. **6**, 94–99 (1964), doi:10.1016/0022-5088(64)90113-4.

First cited in

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