Th_3Pd_5 Structure: A5B3_hP8_189_cf_g-001

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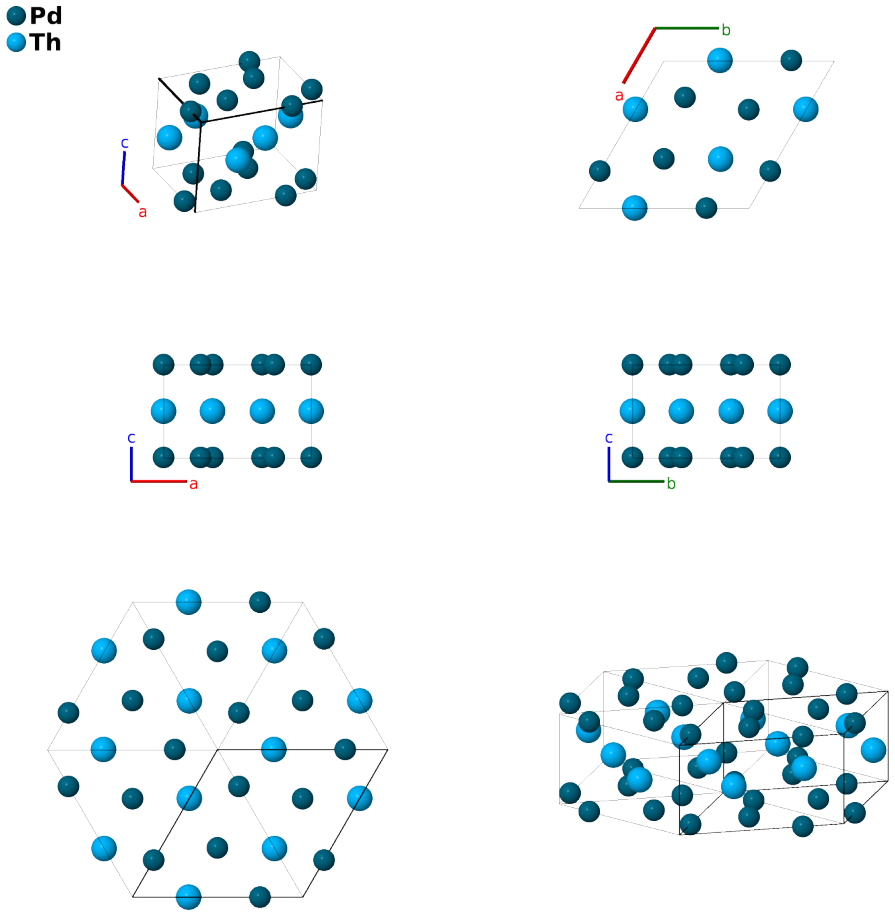
https://aflow.org/p/K8CX

https://aflow.org/p/A5B3_hP8_189_cf_g-001



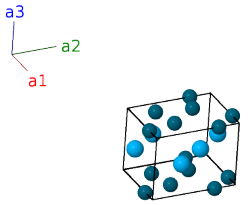
Prototype	Pd_5Th_3
AFLOW prototype label	A5B3_hP8_189_cf_g-001
ICSD	649755
Pearson symbol	hP8
Space group number	189
Space group symbol	$P\bar{6}2m$
AFLOW prototype command	`aflow --proto=A5B3_hP8_189_cf_g-001 --params=`$a, c/a, x_2, x_3$

Other compounds with this structure
Th_3Pt_5, Yb_3Ge_5

- 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

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



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 Th_3Pd_5 and Th_3Pt_5*, 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.