Pd$_{15}$P$_2$ Structure:
A2B15_hR17_148_c_ac2f-001

https://aflow.org/p/Z055

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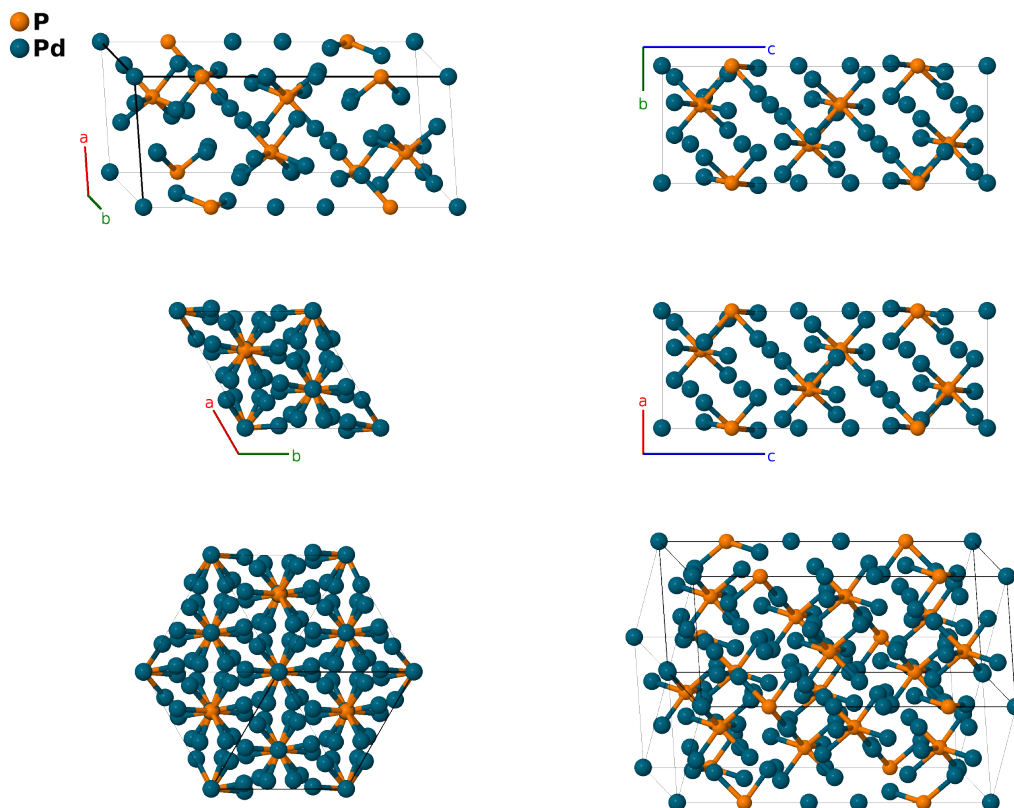
Prototype	P$_2$Pd$_{15}$
AFLOW prototype label	A2B15_hR17_148_c_ac2f-001
ICSD	1096
Pearson symbol	hR17
Space group number	148
Space group symbol	$R\overline{3}$
AFLOW prototype command	aflow --proto=A2B15_hR17_148_c_ac2f-001
	--params=$a, c/a, x_2, x_3, x_4, y_4, z_4, x_5, y_5, z_5$

- We have shifted the origin of the system from that used by (Andersson, 1977), moving the Pd-I atom (her Pd(4)) to the (1a) Wyckoff position.

- Hexagonal settings for rhombohedral structures can be obtained with the option --hex.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_2} = \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_3} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$
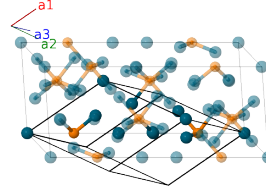
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(1a)	Pd I
$\mathbf{B_2}$	$=$	$x_2\,\mathbf{a_1} + x_2\,\mathbf{a_2} + x_2\,\mathbf{a_3}$	$=$	$cx_2\,\hat{\mathbf{z}}$	(2c)	P I
$\mathbf{B_3}$	$=$	$-x_2\,\mathbf{a_1} - x_2\,\mathbf{a_2} - x_2\,\mathbf{a_3}$	$=$	$-cx_2\,\hat{\mathbf{z}}$	(2c)	P I
$\mathbf{B_4}$	$=$	$x_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + x_3\,\mathbf{a_3}$	$=$	$cx_3\,\hat{\mathbf{z}}$	(2c)	Pd II
$\mathbf{B_5}$	$=$	$-x_3\,\mathbf{a_1} - x_3\,\mathbf{a_2} - x_3\,\mathbf{a_3}$	$=$	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Pd II
$\mathbf{B_6}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 - z_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_4 - 2y_4 + z_4\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B_7}$	$=$	$z_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + y_4\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(y_4 - z_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_4 - y_4 - z_4\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B_8}$	$=$	$y_4\,\mathbf{a_1} + z_4\,\mathbf{a_2} + x_4\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_4 - y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_4 + y_4 - 2z_4\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B_9}$	$=$	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_4 - z_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_4 - 2y_4 + z_4\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B_{10}}$	$=$	$-z_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} - y_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(y_4 - z_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(2x_4 - y_4 - z_4\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B_{11}}$	$=$	$-y_4\,\mathbf{a_1} - z_4\,\mathbf{a_2} - x_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 - y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_4 + y_4 - 2z_4\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B_{12}}$	$=$	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5 - z_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_5 - 2y_5 + z_5\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_5 + y_5 + z_5\right)\hat{\mathbf{z}}$	(6f)	Pd IV
$\mathbf{B_{13}}$	$=$	$z_5\,\mathbf{a_1} + x_5\,\mathbf{a_2} + y_5\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(y_5 - z_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_5 - y_5 - z_5\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_5 + y_5 + z_5\right)\hat{\mathbf{z}}$	(6f)	Pd IV
$\mathbf{B_{14}}$	$=$	$y_5\,\mathbf{a_1} + z_5\,\mathbf{a_2} + x_5\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_5 - y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_5 + y_5 - 2z_5\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_5 + y_5 + z_5\right)\hat{\mathbf{z}}$	(6f)	Pd IV
$\mathbf{B_{15}}$	$=$	$-x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_5 - z_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_5 - 2y_5 + z_5\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_5 + y_5 + z_5\right)\hat{\mathbf{z}}$	(6f)	Pd IV
$\mathbf{B_{16}}$	$=$	$-z_5\,\mathbf{a_1} - x_5\,\mathbf{a_2} - y_5\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(y_5 - z_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(2x_5 - y_5 - z_5\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_5 + y_5 + z_5\right)\hat{\mathbf{z}}$	(6f)	Pd IV
$\mathbf{B_{17}}$	$=$	$-y_5\,\mathbf{a_1} - z_5\,\mathbf{a_2} - x_5\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5 - y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_5 + y_5 - 2z_5\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_5 + y_5 + z_5\right)\hat{\mathbf{z}}$	(6f)	Pd IV

References

[1] Y. Andersson, *The Crystal Structure of $Pd_{15}P_2$*, Acta Chem. Scand. **31a**, 354–358 (1977), doi:10.3891/acta.chem.scand.31a-0354.