β-$PdCl_2$ Structure: A2B_hR18_148_2f_f-001

This structure originally had the label `A2B_hR18_148_2f_f`. Calls to that address will be redirected here.

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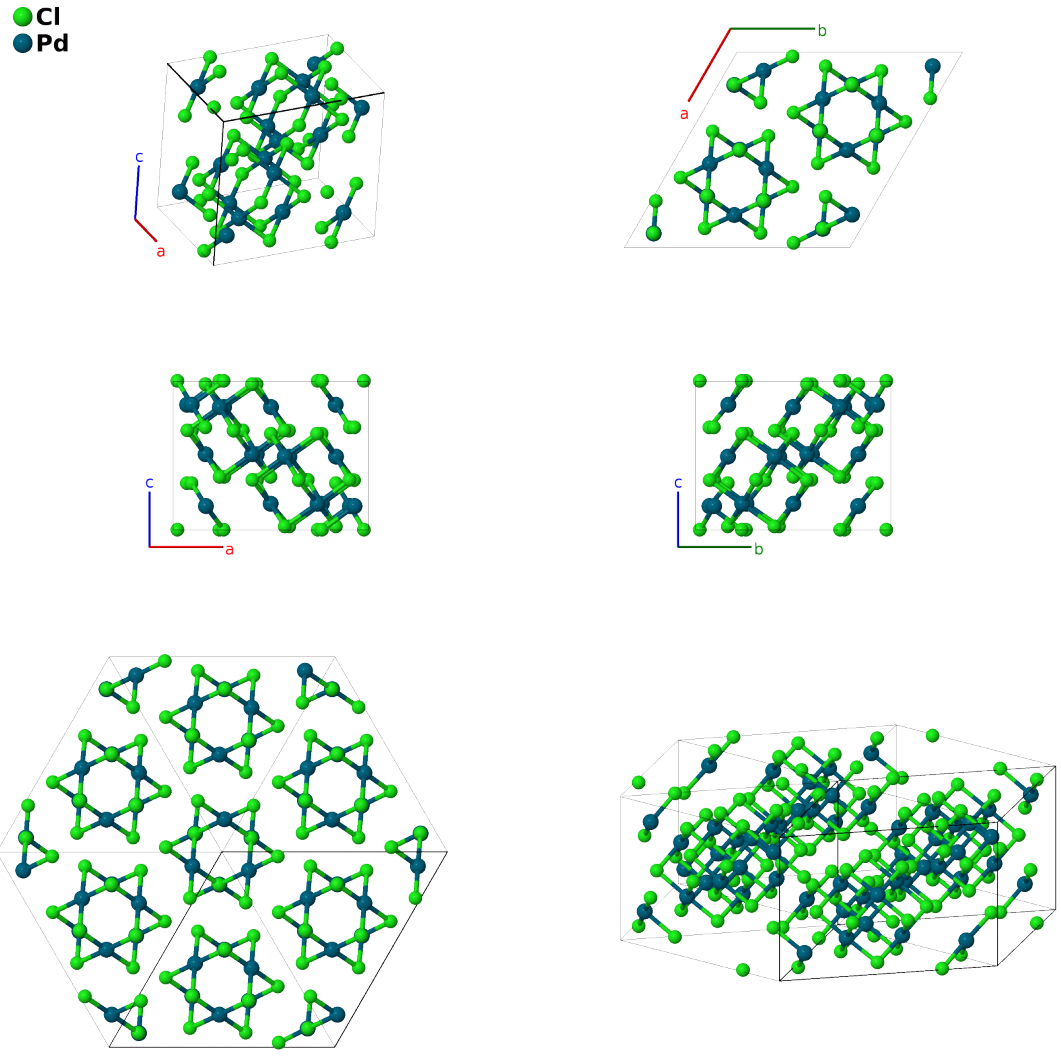
https://aflow.org/p/8GMP

https://aflow.org/p/A2B_hR18_148_2f_f-001



Prototype	Cl_2Pd
AFLOW prototype label	A2B_hR18_148_2f_f-001
ICSD	404624
Pearson symbol	hR18
Space group number	148

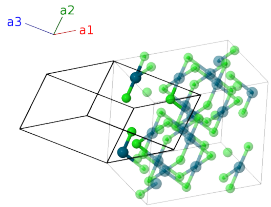
Space group symbol $R\bar{3}$

AFLOW prototype command `aflow --proto=A2B_hR18_148_2f_f-001 --params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

- $PdCl_2$ is known to exist in four different structures at ambient pressure (Evers, 2010):
  - orthorhombic α-$PdCl_2$,
  - rhombohedral β-$PdCl_2$ (this structure),
  - monoclinic γ-$PdCl_2$, and
  - monoclinic δ-$PdCl_2$.
- (Dell'Amico, 1996) did the original assessment of the crystal structure of β-$PdCl_2$, but it is difficult to determine the Wyckoff positions from this paper. We relied on (Villars, 2010) for the Wyckoff positions.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_1 - 2y_1 + z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	Cl I
$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + y_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_1 - z_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_1 - y_1 - z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	Cl I
$\mathbf{B_3}$	=	$y_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1 - y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_1 + y_1 - 2z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	Cl I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_1 - 2y_1 + z_1)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	Cl I
$\mathbf{B_5}$	=	$-z_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - y_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_1 - z_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_1 - y_1 - z_1)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	Cl I
$\mathbf{B_6}$	=	$-y_1\,\mathbf{a}_1 - z_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_1 + y_1 - 2z_1)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	Cl I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 - 2y_2 + z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B_8}$	=	$z_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_2 - y_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B_9}$	=	$y_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 + y_2 - 2z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B_{10}}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 - 2y_2 + z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B_{11}}$	=	$-z_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_2 - z_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_2 - y_2 - z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	Cl II

$$\mathbf{B_{12}} = -y_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_2 - y_2)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_2 + y_2 - 2z_2)\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_2 + y_2 + z_2)\;\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Cl II}$$

$$\mathbf{B_{13}} = x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_3 - z_3)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_3 + y_3 + z_3)\;\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd I}$$

$$\mathbf{B_{14}} = z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_3 - z_3)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_3 + y_3 + z_3)\;\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd I}$$

$$\mathbf{B_{15}} = y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_3 - y_3)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_3 + y_3 + z_3)\;\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd I}$$

$$\mathbf{B_{16}} = -x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_3 - z_3)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_3 + y_3 + z_3)\;\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd I}$$

$$\mathbf{B_{17}} = -z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3 = \tfrac{1}{2}a\,(y_3 - z_3)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_3 + y_3 + z_3)\;\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd I}$$

$$\mathbf{B_{18}} = -y_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_3 - y_3)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_3 + y_3 + z_3)\;\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Pd I}$$

References

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