α-$PdCl_2$ ($C50$) Structure: A2B_oP6_58_g_a-001

This structure originally had the label `A2B_oP6_58_g_a`. Calls to that address will be redirected here.

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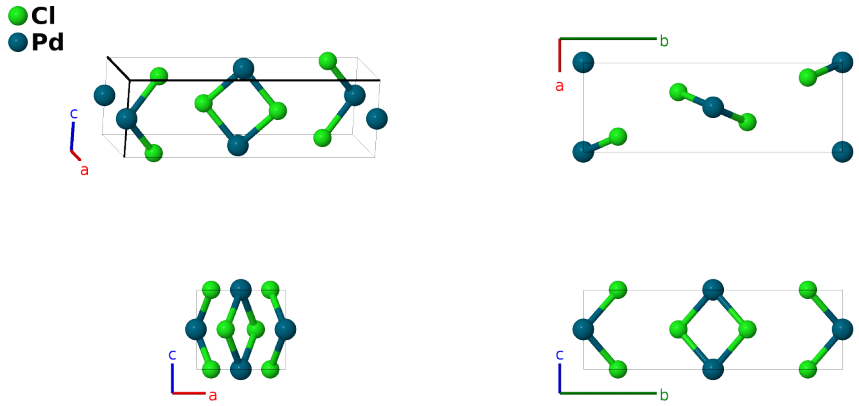
https://aflow.org/p/HU31

https://aflow.org/p/A2B_oP6_58_g_a-001

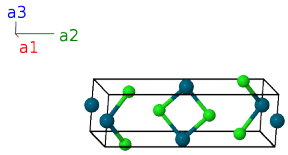


Prototype	Cl_2Pd
AFLOW prototype label	A2B_oP6_58_g_a-001
***Strukturbericht* designation**	$C50$
ICSD	421213
Pearson symbol	oP6
Space group number	58
Space group symbol	$Pnnm$
AFLOW prototype command	`aflow --proto=A2B_oP6_58_g_a-001 --params=`$a, b/a, c/a, x_2, y_2$

- $PdCl_2$ is known to exist in four different structures at ambient pressure (Evers, 2010):
  - orthorhombic α-$PdCl_2$ (this structure),
  - rhombohedral β-$PdCl_2$,
  - monoclinic γ-$PdCl_2$, and
  - monoclinic δ-$PdCl_2$.
- We use the data taken by (Evers, 2010) taken at 100K. They implicitly place the Pd atoms at the (2b) Wyckoff position. We have shifted the Pd atoms to the (2a) site.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Pd I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Pd I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}}$	(4g)	Cl I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}}$	(4g)	Cl I
$\mathbf{B_5}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	Cl I
$\mathbf{B_6}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	Cl I

References

[1] J.Evers, W. Beck, M. Göbel, S. Jakob, P. Mayer, G. Oehlinger, M. Rotter, and T. Klapötke, *The Structures of δ-$PdCl_2$ and γ-$PdCl_2$: Phases with Negative Thermal Expansion in One Direction*, Angew. Chem. Int. Ed. **49**, 5677–5682 (2010), doi:10.1002/anie.201000680.