

α -PdCl₂ (*C*50) Structure: A2B_oP6_58_g_a-001

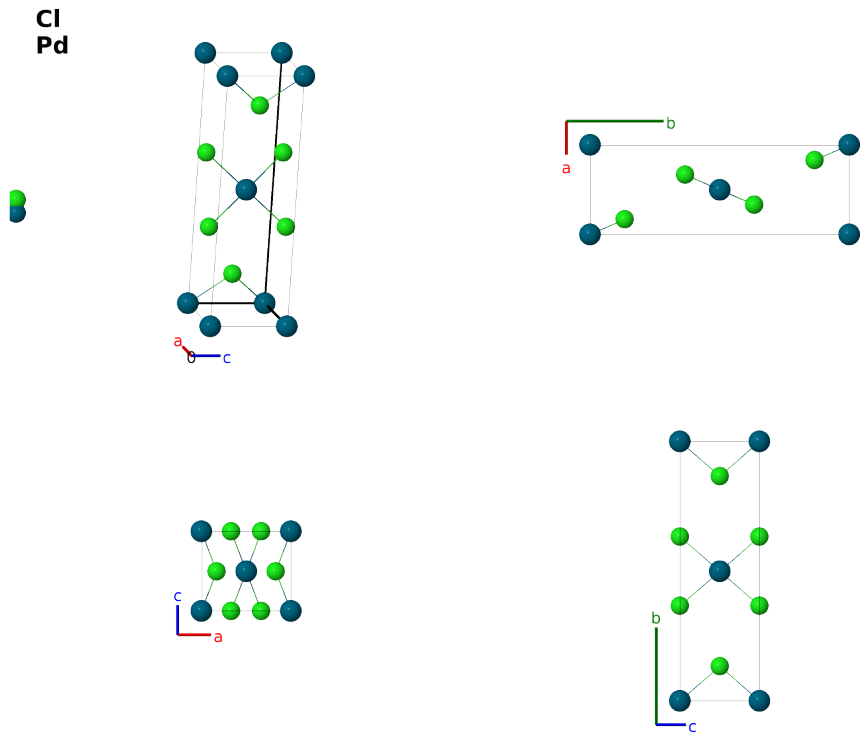
This structure previously used the label(s) **A2B_oP6_58_g_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/HU31>

https://aflow.org/prototype-encyclopedia/A2B_oP6_58_g_a-001

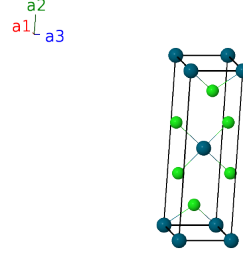


Prototype	Cl ₂ Pd
AFLOW prototype label	A2B_oP6_58_g_a-001
<i>Strukturbericht</i> designation	<i>C</i> 50
ICSD	421213
CCDC	1733313
Pearson symbol	oP6
Space group number	58
Space group symbol	<i>Pnnm</i>
AFLOW prototype command	<code>aflow --proto=A2B_oP6_58_g_a-001 --params=a, b/a, c/a, x₂, y₂</code>

- PdCl₂ is known to exist in four different structures at ambient pressure (Evers, 2010):
 - orthorhombic α -PdCl₂ (this structure),
 - rhombohedral β -PdCl₂,
 - monoclinic γ -PdCl₂, and
 - monoclinic δ -PdCl₂.
- 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

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	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
$\mathbf{B}_5$	$=$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g) Cl I
$\mathbf{B}_6$	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(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 -PdCl₂ and γ -PdCl₂: Phases with Negative Thermal Expansion in One Direction*, Angew. Chem. Int. Ed. **49**, 5677–5682 (2010), doi:10.1002/anie.201000680.

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