

γ -PdCl₂ Structure: A2B_mP6_14_e_a-001

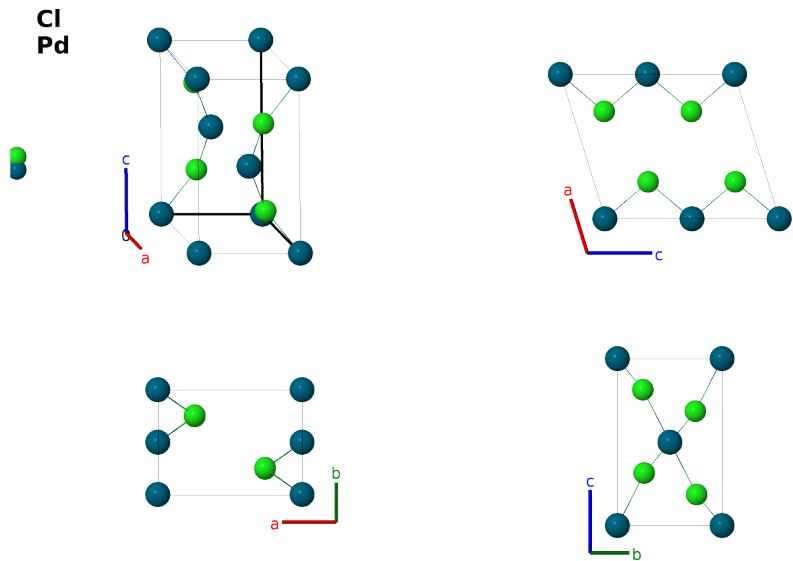
This structure previously used the label(s) **A2B_mP6_14_e_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/K9AG>

https://aflow.org/prototype-encyclopedia/A2B_mP6_14_e_a-001



Prototype	Cl ₂ Pd
AFLOW prototype label	A2B_mP6_14_e_a-001
ICSD	421221
CCDC	1733321
Pearson symbol	mP6
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	<pre>aflow --proto=A2B_mP6_14_e_a-001 --params=a,b/a,c/a,β,x_2,y_2,z_2</pre>

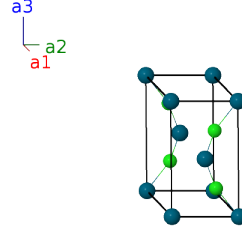
- PdCl₂ is known to exist in four different structures at ambient pressure (Evers, 2010):
 - orthorhombic α -PdCl₂,
 - rhombohedral β -PdCl₂,
 - monoclinic γ -PdCl₂ (this structure), and

– monoclinic δ -PdCl₂.

- (Evers, 2010) place the palladium atoms on the (2c) Wyckoff position. We have shifted the origin so that the palladium atoms are at the (2a) position.
- Data was taken at 300K.

Simple Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	Pd I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \cos \beta \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	(2a)	Pd I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B}_5$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B}_6$	$= x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	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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