γ-$PdCl_2$ Structure: A2B_mP6_14_e_a-001

This structure originally had the label `A2B_mP6_14_e_a`. Calls to that address will be redirected here.

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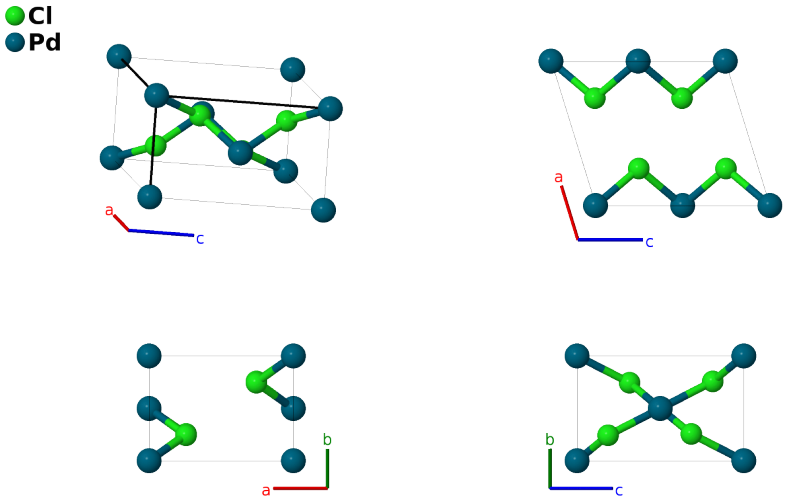
https://aflow.org/p/K9AG

https://aflow.org/p/A2B_mP6_14_e_a-001

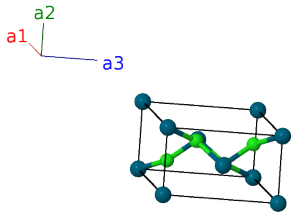


Prototype	Cl_2Pd
AFLOW prototype label	A2B_mP6_14_e_a-001
ICSD	421221
Pearson symbol	mP6
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	`aflow --proto=A2B_mP6_14_e_a-001 --params=`$a, b/a, c/a, \beta, x_2, y_2, z_2$

- $PdCl_2$ is known to exist in four different structures at ambient pressure (Evers, 2010):
  - orthorhombic α-$PdCl_2$,
  - rhombohedral β-$PdCl_2$,
  - monoclinic γ-$PdCl_2$ (this structure), and
  - monoclinic δ-$PdCl_2$.
- (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

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



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
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-\left(ax_2 + cz_2\cos\beta\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(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-$PdCl_2$ 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.