δ-Pd_2Cl Structure: A2B_mP6_10_mn_bc-001

This structure previously used the label(s) `A2B_mP6_10_mn_bg`. Calls to these addresses will be redirected here.

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https://aflow.org/prototype-encyclopedia/ZWXH

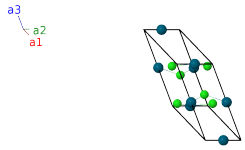
https://aflow.org/prototype-encyclopedia/A2B_mP6_10_mn_bc-001

Prototype	Cl_2Pd
AFLOW prototype label	A2B_mP6_10_mn_bc-001
ICSD	421220
CCDC	1733320
Pearson symbol	mP6
Space group number	10
Space group symbol	$P2/m$
AFLOW prototype command	`aflow --proto=A2B_mP6_10_mn_bc-001 --params=`$a, b/a, c/a, \beta, x_3, z_3, x_4, z_4$

- $PdCl_2$ is known to exist in four different structures at ambient pressure (Evers, 2010):
  - orthorhombic α-$PdCl_2$,
  - rhombohedral β-$PdCl_2$,
  - monoclinic γ-$PdCl_2$, and
  - monoclinic δ-$PdCl_2$ (this structure).
- (Evers, 2010) use the unique-axis c setting of space group $P2/m$ #10. We have switched this to our standard unique-axis b setting. Data was taken at 793K.

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
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(1b)	Pd I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(1c)	Pd II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2m)	Cl I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(2m)	Cl I
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(2n)	Cl II
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(2n)	Cl II

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.

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