Pd_4Se Structure: A4B_tP10_114_e_a-001

This structure previously used the label(s) `A4B_tP10_114_e_a`. Calls to these addresses will be redirected here.

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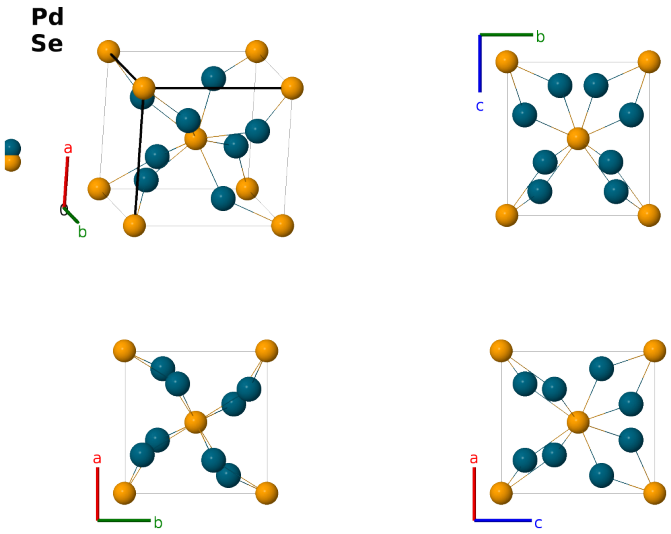
https://aflow.org/prototype-encyclopedia/C2PK

https://aflow.org/prototype-encyclopedia/A4B_tP10_114_e_a-001



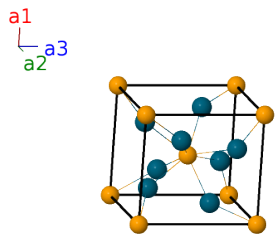
Prototype	Pd_4Se
AFLOW prototype label	A4B_tP10_114_e_a-001
ICSD	23864
CCDC	1599934
Pearson symbol	tP10
Space group number	114
Space group symbol	$P\bar{4}2_1c$
AFLOW prototype command	`aflow --proto=A4B_tP10_114_e_a-001 --params=`$a, c/a, x_2, y_2, z_2$

Other compounds with this structure

Pd_4S

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Se I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Se I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8e)	Pd I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8e)	Pd I
$\mathbf{B_5}$	=	$y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8e)	Pd I
$\mathbf{B_6}$	=	$-y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8e)	Pd I
$\mathbf{B_7}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Pd I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Pd I
$\mathbf{B_9}$	=	$-\left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Pd I
$\mathbf{B_{10}}$	=	$\left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Pd I

References

[1] F. Grand E. R, *The crystal structures of Pd_4Se and Pd_4S*, Acta Cryst. **15**, 11–13 (1962), doi:10.1107/S0365110X62000031.

[2] D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

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D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043