Li_2Pd_3B Structure: AB2C3_cP24_212_a_c_d-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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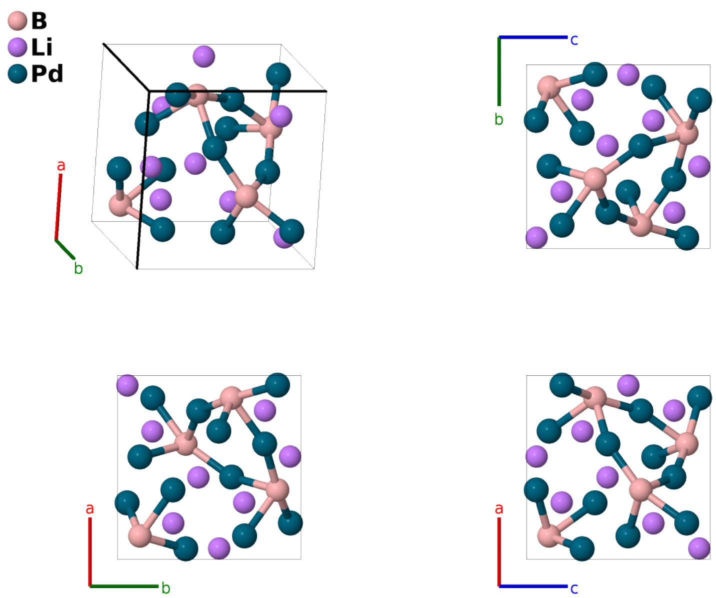
https://aflow.org/p/K791

https://aflow.org/p/AB2C3_cP24_212_a_c_d-001



Prototype	BLi_2Pt_3
AFLOW prototype label	AB2C3_cP24_212_a_c_d-001
ICSD	84931
Pearson symbol	cP24
Space group number	212
Space group symbol	$P4_332$
AFLOW prototype command	`aflow --proto=AB2C3_cP24_212_a_c_d-001` `--params=`a, x_2, y_3

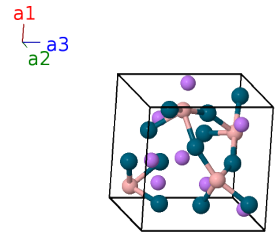
Other compounds with this structure

Li_2Pt_3B

- This structure can also be expressed in the enantiomorphic space group $P4_132$ #213.

Simple Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B_2}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + \frac{5}{8}a\,\hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B_3}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{5}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B_4}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{5}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{7}{8}a\,\hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	Li I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Li I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Li I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	Li I
$\mathbf{B_9}$	=	$\left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8c)	Li I
$\mathbf{B_{10}}$	=	$-\left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8c)	Li I
$\mathbf{B_{11}}$	=	$\left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{3}{4}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8c)	Li I
$\mathbf{B_{12}}$	=	$-\left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{3}{4}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8c)	Li I
$\mathbf{B_{13}}$	=	$\frac{1}{8}\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(12d)	Pd I
$\mathbf{B_{14}}$	=	$\frac{3}{8}\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - \left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} - a\left(y_3 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(12d)	Pd I
$\mathbf{B_{15}}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(12d)	Pd I
$\mathbf{B_{16}}$	=	$\frac{5}{8}\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{5}{8}a\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(y_3 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(12d)	Pd I
$\mathbf{B_{17}}$	=	$-\left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(12d)	Pd I
$\mathbf{B_{18}}$	=	$-\left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(12d)	Pd I
$\mathbf{B_{19}}$	=	$\left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Pd I
$\mathbf{B_{20}}$	=	$\left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{5}{8}a\,\hat{\mathbf{y}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Pd I
$\mathbf{B_{21}}$	=	$y_3\,\mathbf{a}_1 - \left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(12d)	Pd I
$\mathbf{B_{22}}$	=	$-y_3\,\mathbf{a}_1 - \left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - a\left(y_3 - \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(12d)	Pd I
$\mathbf{B_{23}}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{7}{8}a\,\hat{\mathbf{z}}$	(12d)	Pd I
$\mathbf{B_{24}}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_3 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{5}{8}a\,\hat{\mathbf{z}}$	(12d)	Pd I

References

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