Li_7Pb_2 Structure: A7B2_hP9_164_ac2d_d-001

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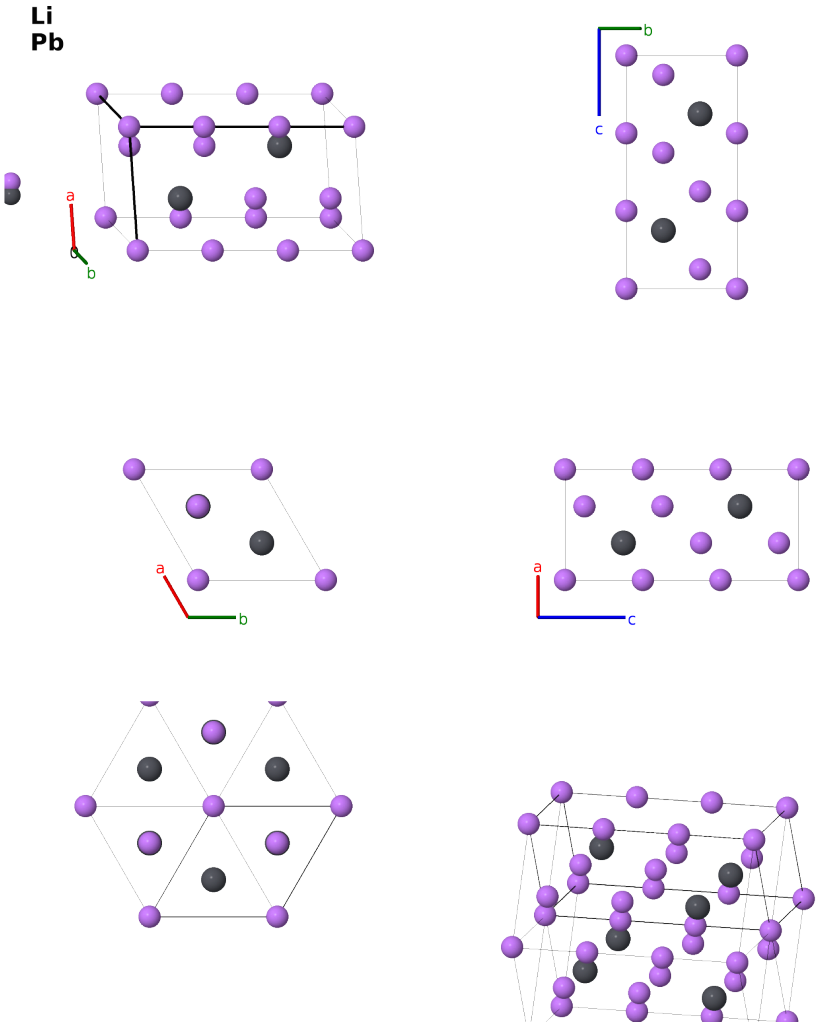
https://aflow.org/prototype-encyclopedia/FCSA

https://aflow.org/prototype-encyclopedia/A7B2_hP9_164_ac2d_d-001



Prototype	Li_7Pb_2
AFLOW prototype label	A7B2_hP9_164_ac2d_d-001
ICSD	104765
CCDC	1662667
Pearson symbol	hP9
Space group number	164

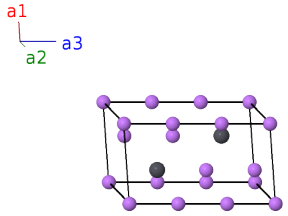
Space group symbol $P\bar{3}m1$

AFLOW prototype command `aflow --proto=A7B2_hP9_164_ac2d_d-001 --params=`$a, c/a, z_2, z_3, z_4, z_5$

- (Zalkin, 1956) put this structure in space group $P321$ #150, however the occupied Wyckoff positions are duplicated in the higher symmetry space group $P\bar{3}m1$ #164. Accordingly we use the higher symmetry space group.
- (Cenzual, 1991) note that the coordinate z_3 of the Li-III atom should be -1/12 rather than -1/2 as given in (Zalkin, 1956). This agrees with the figures in the original reference so we use that value.
- The ICSD entry is from (Zalkin, 1956).

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Li I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(2c)	Li II
$\mathbf{B_3}$	=	$-z_2\,\mathbf{a}_3$	=	$-cz_2\,\hat{\mathbf{z}}$	(2c)	Li II
$\mathbf{B_4}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2d)	Li III
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2d)	Li III
$\mathbf{B_6}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2d)	Li IV
$\mathbf{B_7}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2d)	Li IV
$\mathbf{B_8}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(2d)	Pb I
$\mathbf{B_9}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(2d)	Pb I

References

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[2] K. Cenzual, L. M. Gelato, M. Penzo, and E. Parthé, *Inorganic structure types with revised space groups. I*, Acta Crystallogr. Sect. B **47**, 433–439 (1991), doi:10.1107/S0108768191000903.

Found in

[1] J. Hauck and K. Mika, *Architecture of crystal structures from square planes*, Acta Crystallogr. Sect. B **56**, 750–765 (2000), doi:10.1107/S0108768100006480.

First cited in

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