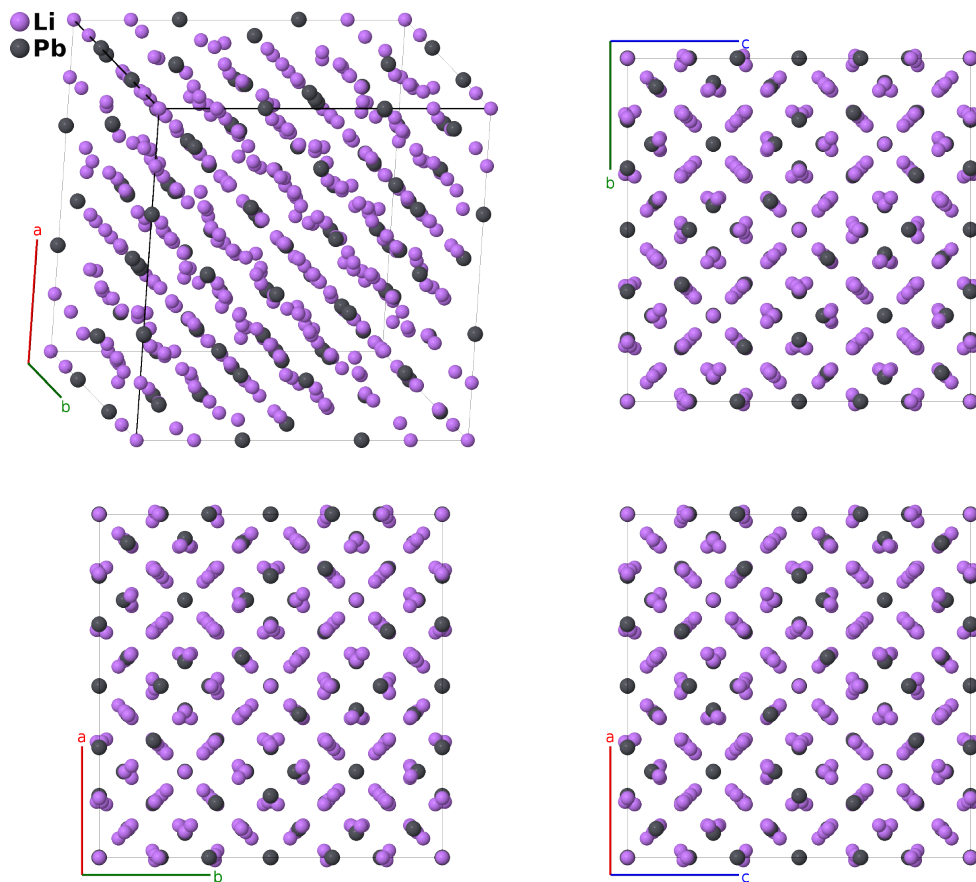


Li₁₇Pb₄ Structure: A17B4_cF420_216_a6efg4h_2efg-001

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.

<https://afLOW.org/p/4E2L>

https://afLOW.org/p/A17B4_cF420_216_a6efg4h_2efg-001



Prototype	Li ₁₇ Pb ₄
AFLOW prototype label	A17B4_cF420_216_a6efg4h_2efg-001
ICSD	107216
Pearson symbol	cF420
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	<pre>afLOW --proto=A17B4_cF420_216_a6efg4h_2efg-001 --params=a, x2, x3, x4, x5, x6, x7, x8, x9, x10, x11, x12, x13, x14, x14, x15, z15, x16, z16, x17, z17</pre>

Other compounds with this structure

Li₁₇Ge₄, Li₁₇Si₄, Li₁₇Sn₄

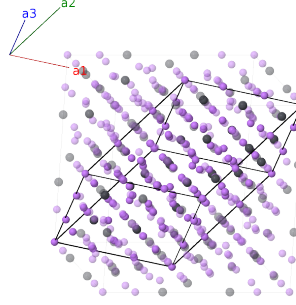
- (Goward, 2001) propose this as a replacement for the $\text{Li}_{22}\text{Si}_5$ structure. The change in stoichiometry is accounted for by placing extra lithium atoms on the the (4c) site (1/41/41/4) and an additional (16e) site (xxx), adjusting the stoichiometry to fit Li_{21}M_5 or Li_{22}M_5 as needed. Phase diagrams quoted in (Villars, 2018) support this change.

Face-centered Cubic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a \hat{y} + \frac{1}{2}a \hat{z}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{x} + \frac{1}{2}a \hat{z}$$

$$\mathbf{a}_3 = \frac{1}{2}a \hat{x} + \frac{1}{2}a \hat{y}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1 =$	0	$=$	0	(4a)	Li I
$\mathbf{B}_2 =$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{x} + ax_2 \hat{y} + ax_2 \hat{z}$	(16e)	Li II
$\mathbf{B}_3 =$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - 3x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{x} - ax_2 \hat{y} + ax_2 \hat{z}$	(16e)	Li II
$\mathbf{B}_4 =$	$x_2 \mathbf{a}_1 - 3x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{x} + ax_2 \hat{y} - ax_2 \hat{z}$	(16e)	Li II
$\mathbf{B}_5 =$	$-3x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{x} - ax_2 \hat{y} - ax_2 \hat{z}$	(16e)	Li II
$\mathbf{B}_6 =$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{x} + ax_3 \hat{y} + ax_3 \hat{z}$	(16e)	Li III
$\mathbf{B}_7 =$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - 3x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{x} - ax_3 \hat{y} + ax_3 \hat{z}$	(16e)	Li III
$\mathbf{B}_8 =$	$x_3 \mathbf{a}_1 - 3x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{x} + ax_3 \hat{y} - ax_3 \hat{z}$	(16e)	Li III
$\mathbf{B}_9 =$	$-3x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{x} - ax_3 \hat{y} - ax_3 \hat{z}$	(16e)	Li III
$\mathbf{B}_{10} =$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{x} + ax_4 \hat{y} + ax_4 \hat{z}$	(16e)	Li IV
$\mathbf{B}_{11} =$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - 3x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{x} - ax_4 \hat{y} + ax_4 \hat{z}$	(16e)	Li IV
$\mathbf{B}_{12} =$	$x_4 \mathbf{a}_1 - 3x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{x} + ax_4 \hat{y} - ax_4 \hat{z}$	(16e)	Li IV
$\mathbf{B}_{13} =$	$-3x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{x} - ax_4 \hat{y} - ax_4 \hat{z}$	(16e)	Li IV
$\mathbf{B}_{14} =$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{x} + ax_5 \hat{y} + ax_5 \hat{z}$	(16e)	Li V
$\mathbf{B}_{15} =$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - 3x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{x} - ax_5 \hat{y} + ax_5 \hat{z}$	(16e)	Li V
$\mathbf{B}_{16} =$	$x_5 \mathbf{a}_1 - 3x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{x} + ax_5 \hat{y} - ax_5 \hat{z}$	(16e)	Li V
$\mathbf{B}_{17} =$	$-3x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{x} - ax_5 \hat{y} - ax_5 \hat{z}$	(16e)	Li V
$\mathbf{B}_{18} =$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ax_6 \hat{x} + ax_6 \hat{y} + ax_6 \hat{z}$	(16e)	Li VI
$\mathbf{B}_{19} =$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - 3x_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{x} - ax_6 \hat{y} + ax_6 \hat{z}$	(16e)	Li VI
$\mathbf{B}_{20} =$	$x_6 \mathbf{a}_1 - 3x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{x} + ax_6 \hat{y} - ax_6 \hat{z}$	(16e)	Li VI
$\mathbf{B}_{21} =$	$-3x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ax_6 \hat{x} - ax_6 \hat{y} - ax_6 \hat{z}$	(16e)	Li VI
$\mathbf{B}_{22} =$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$ax_7 \hat{x} + ax_7 \hat{y} + ax_7 \hat{z}$	(16e)	Li VII
$\mathbf{B}_{23} =$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - 3x_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{x} - ax_7 \hat{y} + ax_7 \hat{z}$	(16e)	Li VII
$\mathbf{B}_{24} =$	$x_7 \mathbf{a}_1 - 3x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{x} + ax_7 \hat{y} - ax_7 \hat{z}$	(16e)	Li VII
$\mathbf{B}_{25} =$	$-3x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$ax_7 \hat{x} - ax_7 \hat{y} - ax_7 \hat{z}$	(16e)	Li VII
$\mathbf{B}_{26} =$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$ax_8 \hat{x} + ax_8 \hat{y} + ax_8 \hat{z}$	(16e)	Pb I

$$\begin{aligned}
\mathbf{B}_{92} &= - (2x_{16} + z_{16}) \mathbf{a}_1 + z_{16} \mathbf{a}_2 + (2x_{16} - z_{16}) \mathbf{a}_3 &= ax_{16} \hat{\mathbf{x}} - az_{16} \hat{\mathbf{y}} - ax_{16} \hat{\mathbf{z}} &(48h) & \text{Li XII} \\
\mathbf{B}_{93} &= (2x_{16} - z_{16}) \mathbf{a}_1 + z_{16} \mathbf{a}_2 - (2x_{16} + z_{16}) \mathbf{a}_3 &= -ax_{16} \hat{\mathbf{x}} - az_{16} \hat{\mathbf{y}} + ax_{16} \hat{\mathbf{z}} &(48h) & \text{Li XII} \\
\mathbf{B}_{94} &= z_{17} \mathbf{a}_1 + z_{17} \mathbf{a}_2 + (2x_{17} - z_{17}) \mathbf{a}_3 &= ax_{17} \hat{\mathbf{x}} + ax_{17} \hat{\mathbf{y}} + az_{17} \hat{\mathbf{z}} &(48h) & \text{Li XIII} \\
\mathbf{B}_{95} &= z_{17} \mathbf{a}_1 + z_{17} \mathbf{a}_2 - (2x_{17} + z_{17}) \mathbf{a}_3 &= -ax_{17} \hat{\mathbf{x}} - ax_{17} \hat{\mathbf{y}} + az_{17} \hat{\mathbf{z}} &(48h) & \text{Li XIII} \\
\mathbf{B}_{96} &= (2x_{17} - z_{17}) \mathbf{a}_1 - (2x_{17} + z_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 &= -ax_{17} \hat{\mathbf{x}} + ax_{17} \hat{\mathbf{y}} - az_{17} \hat{\mathbf{z}} &(48h) & \text{Li XIII} \\
\mathbf{B}_{97} &= - (2x_{17} + z_{17}) \mathbf{a}_1 + (2x_{17} - z_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 &= ax_{17} \hat{\mathbf{x}} - ax_{17} \hat{\mathbf{y}} - az_{17} \hat{\mathbf{z}} &(48h) & \text{Li XIII} \\
\mathbf{B}_{98} &= (2x_{17} - z_{17}) \mathbf{a}_1 + z_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3 &= az_{17} \hat{\mathbf{x}} + ax_{17} \hat{\mathbf{y}} + ax_{17} \hat{\mathbf{z}} &(48h) & \text{Li XIII} \\
\mathbf{B}_{99} &= - (2x_{17} + z_{17}) \mathbf{a}_1 + z_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3 &= az_{17} \hat{\mathbf{x}} - ax_{17} \hat{\mathbf{y}} - ax_{17} \hat{\mathbf{z}} &(48h) & \text{Li XIII} \\
\mathbf{B}_{100} &= z_{17} \mathbf{a}_1 + (2x_{17} - z_{17}) \mathbf{a}_2 - (2x_{17} + z_{17}) \mathbf{a}_3 &= -az_{17} \hat{\mathbf{x}} - ax_{17} \hat{\mathbf{y}} + ax_{17} \hat{\mathbf{z}} &(48h) & \text{Li XIII} \\
\mathbf{B}_{101} &= z_{17} \mathbf{a}_1 - (2x_{17} + z_{17}) \mathbf{a}_2 + (2x_{17} - z_{17}) \mathbf{a}_3 &= -az_{17} \hat{\mathbf{x}} + ax_{17} \hat{\mathbf{y}} - ax_{17} \hat{\mathbf{z}} &(48h) & \text{Li XIII} \\
\mathbf{B}_{102} &= z_{17} \mathbf{a}_1 + (2x_{17} - z_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 &= ax_{17} \hat{\mathbf{x}} + az_{17} \hat{\mathbf{y}} + ax_{17} \hat{\mathbf{z}} &(48h) & \text{Li XIII} \\
\mathbf{B}_{103} &= z_{17} \mathbf{a}_1 - (2x_{17} + z_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 &= -ax_{17} \hat{\mathbf{x}} + az_{17} \hat{\mathbf{y}} - ax_{17} \hat{\mathbf{z}} &(48h) & \text{Li XIII} \\
\mathbf{B}_{104} &= - (2x_{17} + z_{17}) \mathbf{a}_1 + z_{17} \mathbf{a}_2 + (2x_{17} - z_{17}) \mathbf{a}_3 &= ax_{17} \hat{\mathbf{x}} - az_{17} \hat{\mathbf{y}} - ax_{17} \hat{\mathbf{z}} &(48h) & \text{Li XIII} \\
\mathbf{B}_{105} &= (2x_{17} - z_{17}) \mathbf{a}_1 + z_{17} \mathbf{a}_2 - (2x_{17} + z_{17}) \mathbf{a}_3 &= -ax_{17} \hat{\mathbf{x}} - az_{17} \hat{\mathbf{y}} + ax_{17} \hat{\mathbf{z}} &(48h) & \text{Li XIII}
\end{aligned}$$

References

- [1] G. R. Goward, N. J. Taylor, D. C. S. Souza, and L. F. Nazar, *The true crystal structure of $Li_{17}M_4$ ($M=Ge, Sn, Pb$)-revised from $Li_{22}M_5$* , J. Alloys Compd. **329**, 82–91 (2001), doi:10.1016/S0925-8388(01)01567-5.
- [2] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Bismuth-Palladium Binary Phase Diagram (1994 Okamoto H.). Copyright ©2006-2018 ASM International.