

Li₁₇Pb₄ Structure:

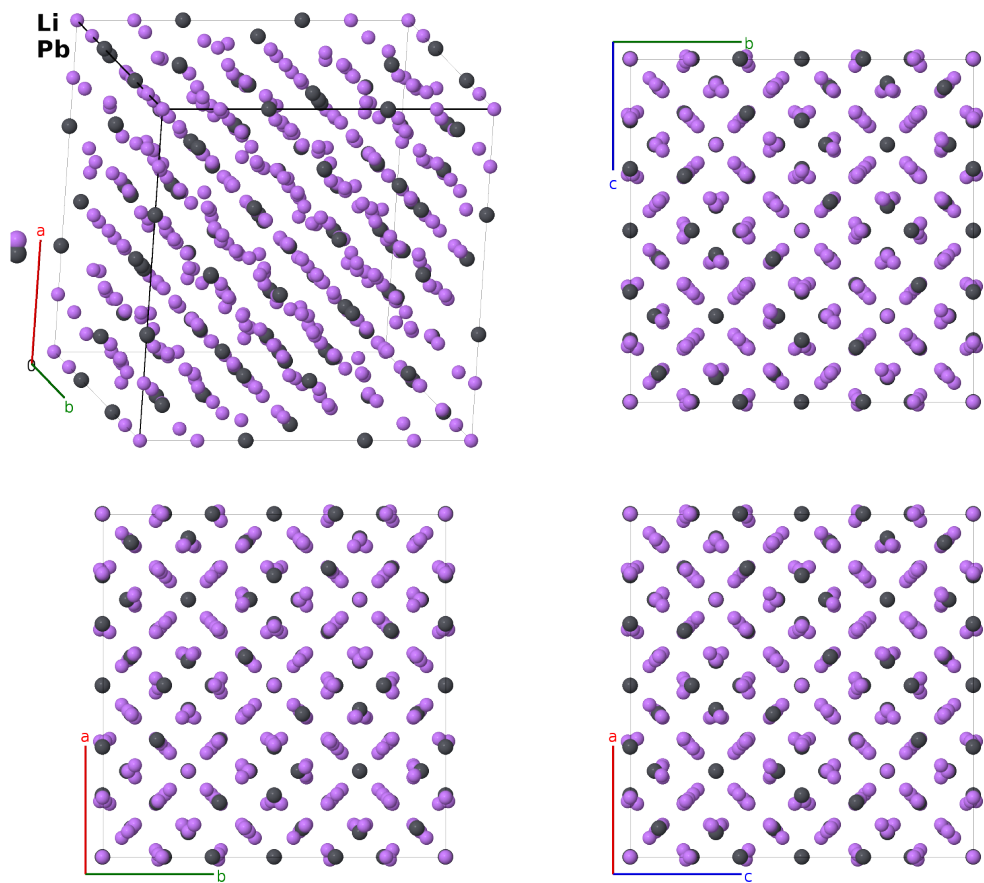
A17B4_cF420_216_a6efg4h_2efg-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/4E2L>

https://aflow.org/prototype-encyclopedia/A17B4_cF420_216_a6efg4h_2efg-001



Prototype	Li ₁₇ Pb ₄
AFLOW prototype label	A17B4_cF420_216_a6efg4h_2efg-001
ICSD	107216
CCDC	1664946
Pearson symbol	cF420
Space group number	216
Space group symbol	$F\bar{4}3m$

AFLOW prototype command `aflow --proto=A17B4_cF420_216_a6efg4h_2efg-001`
 `--params=a, x2, x3, x4, x5, x6, x7, x8, x9, x10, x11, x12, x13, x14, z14, x15, z15, x16, z16, x17, z17`

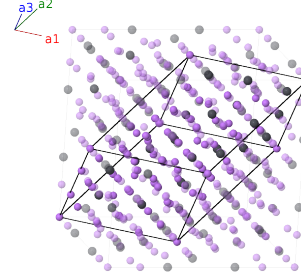
Other compounds with this structure

Li₁₇Ge₄, Li₁₇Si₄, Li₁₇Sn₄

- (Goward, 2001) propose this as a replacement for the Li₂₂Si₅ 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 Li₂₁M₅ or Li₂₂M₅ as needed. Phase diagrams quoted in (Villars, 2018) support this change.

Face-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}\end{aligned}$$



Basis vectors

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

$\mathbf{B}_{20} =$	$x_6 \mathbf{a}_1 - 3x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}}$	(16e)	Li VI
$\mathbf{B}_{21} =$	$-3x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}}$	(16e)	Li VI
$\mathbf{B}_{22} =$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(16e)	Li VII
$\mathbf{B}_{23} =$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - 3x_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(16e)	Li VII
$\mathbf{B}_{24} =$	$x_7 \mathbf{a}_1 - 3x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(16e)	Li VII
$\mathbf{B}_{25} =$	$-3x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(16e)	Li VII
$\mathbf{B}_{26} =$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}}$	(16e)	Pb I
$\mathbf{B}_{27} =$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - 3x_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}}$	(16e)	Pb I
$\mathbf{B}_{28} =$	$x_8 \mathbf{a}_1 - 3x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}}$	(16e)	Pb I
$\mathbf{B}_{29} =$	$-3x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}}$	(16e)	Pb I
$\mathbf{B}_{30} =$	$x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} + ax_9 \hat{\mathbf{z}}$	(16e)	Pb II
$\mathbf{B}_{31} =$	$x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - 3x_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} + ax_9 \hat{\mathbf{z}}$	(16e)	Pb II
$\mathbf{B}_{32} =$	$x_9 \mathbf{a}_1 - 3x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} - ax_9 \hat{\mathbf{z}}$	(16e)	Pb II
$\mathbf{B}_{33} =$	$-3x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} - ax_9 \hat{\mathbf{z}}$	(16e)	Pb II
$\mathbf{B}_{34} =$	$-x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}}$	(24f)	Li VIII
$\mathbf{B}_{35} =$	$x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - x_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}}$	(24f)	Li VIII
$\mathbf{B}_{36} =$	$x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{y}}$	(24f)	Li VIII
$\mathbf{B}_{37} =$	$-x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 - x_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{y}}$	(24f)	Li VIII
$\mathbf{B}_{38} =$	$x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 - x_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{z}}$	(24f)	Li VIII
$\mathbf{B}_{39} =$	$-x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{z}}$	(24f)	Li VIII
$\mathbf{B}_{40} =$	$-x_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + x_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}}$	(24f)	Pb III
$\mathbf{B}_{41} =$	$x_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - x_{11} \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}}$	(24f)	Pb III
$\mathbf{B}_{42} =$	$x_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 + x_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{y}}$	(24f)	Pb III
$\mathbf{B}_{43} =$	$-x_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 - x_{11} \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{y}}$	(24f)	Pb III
$\mathbf{B}_{44} =$	$x_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 - x_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{z}}$	(24f)	Pb III
$\mathbf{B}_{45} =$	$-x_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 + x_{11} \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{z}}$	(24f)	Pb III
$\mathbf{B}_{46} =$	$-\left(x_{12} - \frac{1}{2}\right) \mathbf{a}_1 + x_{12} \mathbf{a}_2 + x_{12} \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Li IX
$\mathbf{B}_{47} =$	$x_{12} \mathbf{a}_1 - \left(x_{12} - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_{12} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_{12} - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Li IX
$\mathbf{B}_{48} =$	$x_{12} \mathbf{a}_1 - \left(x_{12} - \frac{1}{2}\right) \mathbf{a}_2 + x_{12} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_{12} \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Li IX
$\mathbf{B}_{49} =$	$-\left(x_{12} - \frac{1}{2}\right) \mathbf{a}_1 + x_{12} \mathbf{a}_2 - \left(x_{12} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a \left(x_{12} - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Li IX
$\mathbf{B}_{50} =$	$x_{12} \mathbf{a}_1 + x_{12} \mathbf{a}_2 - \left(x_{12} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + ax_{12} \hat{\mathbf{z}}$	(24g)	Li IX
$\mathbf{B}_{51} =$	$-\left(x_{12} - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{12} - \frac{1}{2}\right) \mathbf{a}_2 + x_{12} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - a \left(x_{12} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24g)	Li IX
$\mathbf{B}_{52} =$	$-\left(x_{13} - \frac{1}{2}\right) \mathbf{a}_1 + x_{13} \mathbf{a}_2 + x_{13} \mathbf{a}_3$	$=$	$ax_{13} \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Pb IV
$\mathbf{B}_{53} =$	$x_{13} \mathbf{a}_1 - \left(x_{13} - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_{13} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_{13} - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Pb IV
$\mathbf{B}_{54} =$	$x_{13} \mathbf{a}_1 - \left(x_{13} - \frac{1}{2}\right) \mathbf{a}_2 + x_{13} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_{13} \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Pb IV
$\mathbf{B}_{55} =$	$-\left(x_{13} - \frac{1}{2}\right) \mathbf{a}_1 + x_{13} \mathbf{a}_2 - \left(x_{13} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a \left(x_{13} - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Pb IV
$\mathbf{B}_{56} =$	$x_{13} \mathbf{a}_1 + x_{13} \mathbf{a}_2 - \left(x_{13} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + ax_{13} \hat{\mathbf{z}}$	(24g)	Pb IV

$\mathbf{B}_{57}$	$= -\left(x_{13} - \frac{1}{2}\right) \mathbf{a}_1 - \frac{\left(x_{13} - \frac{1}{2}\right)}{x_{13}} \mathbf{a}_2 +$	$= \frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - a \left(x_{13} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24g)	Pb IV
$\mathbf{B}_{58}$	$= z_{14} \mathbf{a}_1 + z_{14} \mathbf{a}_2 + (2x_{14} - z_{14}) \mathbf{a}_3 =$	$ax_{14} \hat{\mathbf{x}} + ax_{14} \hat{\mathbf{y}} + az_{14} \hat{\mathbf{z}}$	(48h)	Li X
$\mathbf{B}_{59}$	$= z_{14} \mathbf{a}_1 + z_{14} \mathbf{a}_2 - (2x_{14} + z_{14}) \mathbf{a}_3 =$	$-ax_{14} \hat{\mathbf{x}} - ax_{14} \hat{\mathbf{y}} + az_{14} \hat{\mathbf{z}}$	(48h)	Li X
$\mathbf{B}_{60}$	$= \frac{(2x_{14} - z_{14}) \mathbf{a}_1 -}{(2x_{14} + z_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3} =$	$-ax_{14} \hat{\mathbf{x}} + ax_{14} \hat{\mathbf{y}} - az_{14} \hat{\mathbf{z}}$	(48h)	Li X
$\mathbf{B}_{61}$	$= \frac{-(2x_{14} + z_{14}) \mathbf{a}_1 +}{(2x_{14} - z_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3} =$	$ax_{14} \hat{\mathbf{x}} - ax_{14} \hat{\mathbf{y}} - az_{14} \hat{\mathbf{z}}$	(48h)	Li X
$\mathbf{B}_{62}$	$= (2x_{14} - z_{14}) \mathbf{a}_1 + z_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3 =$	$az_{14} \hat{\mathbf{x}} + ax_{14} \hat{\mathbf{y}} + ax_{14} \hat{\mathbf{z}}$	(48h)	Li X
$\mathbf{B}_{63}$	$= -(2x_{14} + z_{14}) \mathbf{a}_1 + z_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3 =$	$az_{14} \hat{\mathbf{x}} - ax_{14} \hat{\mathbf{y}} - ax_{14} \hat{\mathbf{z}}$	(48h)	Li X
$\mathbf{B}_{64}$	$= \frac{z_{14} \mathbf{a}_1 + (2x_{14} - z_{14}) \mathbf{a}_2 -}{(2x_{14} + z_{14}) \mathbf{a}_3} =$	$-az_{14} \hat{\mathbf{x}} - ax_{14} \hat{\mathbf{y}} + ax_{14} \hat{\mathbf{z}}$	(48h)	Li X
$\mathbf{B}_{65}$	$= \frac{z_{14} \mathbf{a}_1 - (2x_{14} + z_{14}) \mathbf{a}_2 +}{(2x_{14} - z_{14}) \mathbf{a}_3} =$	$-az_{14} \hat{\mathbf{x}} + ax_{14} \hat{\mathbf{y}} - ax_{14} \hat{\mathbf{z}}$	(48h)	Li X
$\mathbf{B}_{66}$	$= z_{14} \mathbf{a}_1 + (2x_{14} - z_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3 =$	$ax_{14} \hat{\mathbf{x}} + az_{14} \hat{\mathbf{y}} + ax_{14} \hat{\mathbf{z}}$	(48h)	Li X
$\mathbf{B}_{67}$	$= z_{14} \mathbf{a}_1 - (2x_{14} + z_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3 =$	$-ax_{14} \hat{\mathbf{x}} + az_{14} \hat{\mathbf{y}} - ax_{14} \hat{\mathbf{z}}$	(48h)	Li X
$\mathbf{B}_{68}$	$= \frac{-(2x_{14} + z_{14}) \mathbf{a}_1 + z_{14} \mathbf{a}_2 +}{(2x_{14} - z_{14}) \mathbf{a}_3} =$	$ax_{14} \hat{\mathbf{x}} - az_{14} \hat{\mathbf{y}} - ax_{14} \hat{\mathbf{z}}$	(48h)	Li X
$\mathbf{B}_{69}$	$= \frac{(2x_{14} - z_{14}) \mathbf{a}_1 + z_{14} \mathbf{a}_2 -}{(2x_{14} + z_{14}) \mathbf{a}_3} =$	$-ax_{14} \hat{\mathbf{x}} - az_{14} \hat{\mathbf{y}} + ax_{14} \hat{\mathbf{z}}$	(48h)	Li X
$\mathbf{B}_{70}$	$= z_{15} \mathbf{a}_1 + z_{15} \mathbf{a}_2 + (2x_{15} - z_{15}) \mathbf{a}_3 =$	$ax_{15} \hat{\mathbf{x}} + ax_{15} \hat{\mathbf{y}} + az_{15} \hat{\mathbf{z}}$	(48h)	Li XI
$\mathbf{B}_{71}$	$= z_{15} \mathbf{a}_1 + z_{15} \mathbf{a}_2 - (2x_{15} + z_{15}) \mathbf{a}_3 =$	$-ax_{15} \hat{\mathbf{x}} - ax_{15} \hat{\mathbf{y}} + az_{15} \hat{\mathbf{z}}$	(48h)	Li XI
$\mathbf{B}_{72}$	$= \frac{(2x_{15} - z_{15}) \mathbf{a}_1 -}{(2x_{15} + z_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3} =$	$-ax_{15} \hat{\mathbf{x}} + ax_{15} \hat{\mathbf{y}} - az_{15} \hat{\mathbf{z}}$	(48h)	Li XI
$\mathbf{B}_{73}$	$= \frac{-(2x_{15} + z_{15}) \mathbf{a}_1 +}{(2x_{15} - z_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3} =$	$ax_{15} \hat{\mathbf{x}} - ax_{15} \hat{\mathbf{y}} - az_{15} \hat{\mathbf{z}}$	(48h)	Li XI
$\mathbf{B}_{74}$	$= (2x_{15} - z_{15}) \mathbf{a}_1 + z_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 =$	$az_{15} \hat{\mathbf{x}} + ax_{15} \hat{\mathbf{y}} + ax_{15} \hat{\mathbf{z}}$	(48h)	Li XI
$\mathbf{B}_{75}$	$= -(2x_{15} + z_{15}) \mathbf{a}_1 + z_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 =$	$az_{15} \hat{\mathbf{x}} - ax_{15} \hat{\mathbf{y}} - ax_{15} \hat{\mathbf{z}}$	(48h)	Li XI
$\mathbf{B}_{76}$	$= \frac{z_{15} \mathbf{a}_1 + (2x_{15} - z_{15}) \mathbf{a}_2 -}{(2x_{15} + z_{15}) \mathbf{a}_3} =$	$-az_{15} \hat{\mathbf{x}} - ax_{15} \hat{\mathbf{y}} + ax_{15} \hat{\mathbf{z}}$	(48h)	Li XI
$\mathbf{B}_{77}$	$= \frac{z_{15} \mathbf{a}_1 - (2x_{15} + z_{15}) \mathbf{a}_2 +}{(2x_{15} - z_{15}) \mathbf{a}_3} =$	$-az_{15} \hat{\mathbf{x}} + ax_{15} \hat{\mathbf{y}} - ax_{15} \hat{\mathbf{z}}$	(48h)	Li XI
$\mathbf{B}_{78}$	$= z_{15} \mathbf{a}_1 + (2x_{15} - z_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3 =$	$ax_{15} \hat{\mathbf{x}} + az_{15} \hat{\mathbf{y}} + ax_{15} \hat{\mathbf{z}}$	(48h)	Li XI
$\mathbf{B}_{79}$	$= z_{15} \mathbf{a}_1 - (2x_{15} + z_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3 =$	$-ax_{15} \hat{\mathbf{x}} + az_{15} \hat{\mathbf{y}} - ax_{15} \hat{\mathbf{z}}$	(48h)	Li XI
$\mathbf{B}_{80}$	$= \frac{-(2x_{15} + z_{15}) \mathbf{a}_1 + z_{15} \mathbf{a}_2 +}{(2x_{15} - z_{15}) \mathbf{a}_3} =$	$ax_{15} \hat{\mathbf{x}} - az_{15} \hat{\mathbf{y}} - ax_{15} \hat{\mathbf{z}}$	(48h)	Li XI
$\mathbf{B}_{81}$	$= \frac{(2x_{15} - z_{15}) \mathbf{a}_1 + z_{15} \mathbf{a}_2 -}{(2x_{15} + z_{15}) \mathbf{a}_3} =$	$-ax_{15} \hat{\mathbf{x}} - az_{15} \hat{\mathbf{y}} + ax_{15} \hat{\mathbf{z}}$	(48h)	Li XI
$\mathbf{B}_{82}$	$= z_{16} \mathbf{a}_1 + z_{16} \mathbf{a}_2 + (2x_{16} - z_{16}) \mathbf{a}_3 =$	$ax_{16} \hat{\mathbf{x}} + ax_{16} \hat{\mathbf{y}} + az_{16} \hat{\mathbf{z}}$	(48h)	Li XII
$\mathbf{B}_{83}$	$= z_{16} \mathbf{a}_1 + z_{16} \mathbf{a}_2 - (2x_{16} + z_{16}) \mathbf{a}_3 =$	$-ax_{16} \hat{\mathbf{x}} - ax_{16} \hat{\mathbf{y}} + az_{16} \hat{\mathbf{z}}$	(48h)	Li XII
$\mathbf{B}_{84}$	$= \frac{(2x_{16} - z_{16}) \mathbf{a}_1 -}{(2x_{16} + z_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3} =$	$-ax_{16} \hat{\mathbf{x}} + ax_{16} \hat{\mathbf{y}} - az_{16} \hat{\mathbf{z}}$	(48h)	Li XII
$\mathbf{B}_{85}$	$= \frac{-(2x_{16} + z_{16}) \mathbf{a}_1 +}{(2x_{16} - z_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3} =$	$ax_{16} \hat{\mathbf{x}} - ax_{16} \hat{\mathbf{y}} - az_{16} \hat{\mathbf{z}}$	(48h)	Li XII
$\mathbf{B}_{86}$	$= (2x_{16} - z_{16}) \mathbf{a}_1 + z_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3 =$	$az_{16} \hat{\mathbf{x}} + ax_{16} \hat{\mathbf{y}} + ax_{16} \hat{\mathbf{z}}$	(48h)	Li XII

$$\begin{aligned}
\mathbf{B}_{87} &= -(2x_{16} + z_{16}) \mathbf{a}_1 + z_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3 = az_{16} \hat{\mathbf{x}} - ax_{16} \hat{\mathbf{y}} - ax_{16} \hat{\mathbf{z}} & (48h) & \text{Li XII} \\
\mathbf{B}_{88} &= z_{16} \mathbf{a}_1 + (2x_{16} - z_{16}) \mathbf{a}_2 - (2x_{16} + z_{16}) \mathbf{a}_3 = -az_{16} \hat{\mathbf{x}} - ax_{16} \hat{\mathbf{y}} + ax_{16} \hat{\mathbf{z}} & (48h) & \text{Li XII} \\
\mathbf{B}_{89} &= z_{16} \mathbf{a}_1 - (2x_{16} + z_{16}) \mathbf{a}_2 + (2x_{16} - z_{16}) \mathbf{a}_3 = -az_{16} \hat{\mathbf{x}} + ax_{16} \hat{\mathbf{y}} - ax_{16} \hat{\mathbf{z}} & (48h) & \text{Li XII} \\
\mathbf{B}_{90} &= z_{16} \mathbf{a}_1 + (2x_{16} - z_{16}) \mathbf{a}_2 + 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}_{91} &= z_{16} \mathbf{a}_1 - (2x_{16} + z_{16}) \mathbf{a}_2 + 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}_{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.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.