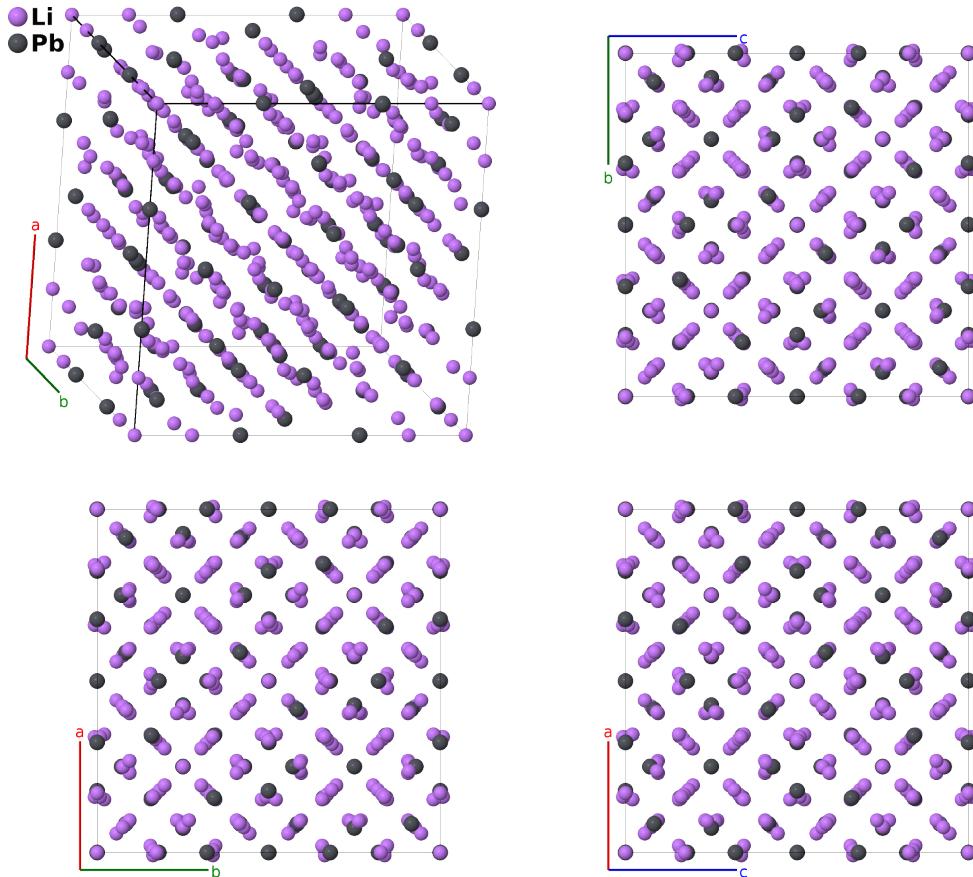


$\text{Li}_{17}\text{Pb}_4$ Structure: A17B4_cF420_216_a6efg4h_2efg-001

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

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



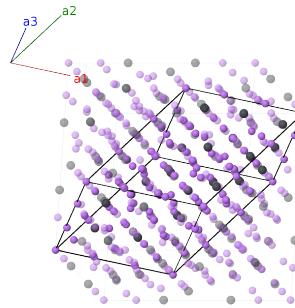
Prototype	$\text{Li}_{17}\text{Pb}_4$
AFLOW prototype label	A17B4_cF420_216_a6efg4h_2efg-001
ICSD	107216
Pearson symbol	cF420
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	<pre>aflow --proto=A17B4_cF420_216_a6efg4h_2efg-001 --params=a, x₂, x₃, x₄, x₅, x₆, x₇, x₈, x₉, x₁₀, x₁₁, x₁₂, x₁₃, x₁₄, z₁₄, x₁₅, z₁₅, x₁₆, z₁₆, x₁₇, z₁₇</pre>

Other compounds with this structure
 $\text{Li}_{17}\text{Ge}_4$, $\text{Li}_{17}\text{Si}_4$, $\text{Li}_{17}\text{Sn}_4$

- (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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	=	0	=	0	(4a)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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)
\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
$\mathbf{B}_{46} =$	$-(x_{12} - \frac{1}{2}) \mathbf{a}_1 + x_{12} \mathbf{a}_2 + x_{12} \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Li IX
$\mathbf{B}_{47} =$	$x_{12} \mathbf{a}_1 - (x_{12} - \frac{1}{2}) \mathbf{a}_2 - (x_{12} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{12} - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Li IX
$\mathbf{B}_{48} =$	$x_{12} \mathbf{a}_1 - (x_{12} - \frac{1}{2}) \mathbf{a}_2 + x_{12} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_{12} \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Li IX
$\mathbf{B}_{49} =$	$-(x_{12} - \frac{1}{2}) \mathbf{a}_1 + x_{12} \mathbf{a}_2 - (x_{12} - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(x_{12} - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Li IX
$\mathbf{B}_{50} =$	$x_{12} \mathbf{a}_1 + x_{12} \mathbf{a}_2 - (x_{12} - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + ax_{12} \hat{\mathbf{z}}$	(24g)	Li IX
$\mathbf{B}_{51} =$	$-(x_{12} - \frac{1}{2}) \mathbf{a}_1 - (x_{12} - \frac{1}{2}) \mathbf{a}_2 + x_{12} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - a(x_{12} - \frac{1}{2}) \hat{\mathbf{z}}$	(24g)	Li IX
$\mathbf{B}_{52} =$	$-(x_{13} - \frac{1}{2}) \mathbf{a}_1 + x_{13} \mathbf{a}_2 + x_{13} \mathbf{a}_3$	$=$	$ax_{13} \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Pb IV
$\mathbf{B}_{53} =$	$x_{13} \mathbf{a}_1 - (x_{13} - \frac{1}{2}) \mathbf{a}_2 - (x_{13} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{13} - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Pb IV
$\mathbf{B}_{54} =$	$x_{13} \mathbf{a}_1 - (x_{13} - \frac{1}{2}) \mathbf{a}_2 + x_{13} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_{13} \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Pb IV
$\mathbf{B}_{55} =$	$-(x_{13} - \frac{1}{2}) \mathbf{a}_1 + x_{13} \mathbf{a}_2 - (x_{13} - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(x_{13} - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Pb IV
$\mathbf{B}_{56} =$	$x_{13} \mathbf{a}_1 + x_{13} \mathbf{a}_2 - (x_{13} - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + ax_{13} \hat{\mathbf{z}}$	(24g)	Pb IV
$\mathbf{B}_{57} =$	$-(x_{13} - \frac{1}{2}) \mathbf{a}_1 - (x_{13} - \frac{1}{2}) \mathbf{a}_2 + x_{13} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - a(x_{13} - \frac{1}{2}) \hat{\mathbf{z}}$	(24g)	Pb IV
$\mathbf{B}_{58} =$	$z_{14} \mathbf{a}_1 + z_{14} \mathbf{a}_2 + (2x_{14} - z_{14}) \mathbf{a}_3$	$=$	$az_{14} \hat{\mathbf{x}} + ax_{14} \hat{\mathbf{y}} + az_{14} \hat{\mathbf{z}}$	(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
$\mathbf{B}_{60} =$	$(2x_{14} - z_{14}) \mathbf{a}_1 - (2x_{14} + z_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$-ax_{14} \hat{\mathbf{x}} + ax_{14} \hat{\mathbf{y}} - az_{14} \hat{\mathbf{z}}$	(48h)	Li X
$\mathbf{B}_{61} =$	$-(2x_{14} + z_{14}) \mathbf{a}_1 + (2x_{14} - z_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$ax_{14} \hat{\mathbf{x}} - ax_{14} \hat{\mathbf{y}} - az_{14} \hat{\mathbf{z}}$	(48h)	Li X

\mathbf{B}_{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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	Li XIII

References

- [1] G. R. Goward, N. J. Taylor, D. C. S. Souza, and L. F. Nazar, *The true crystal structure of Li₁₇M₄ (M=Ge, Sn, Pb)-revised from Li₂₂M₅*, 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.