

Li₂₂Si₅ Structure:

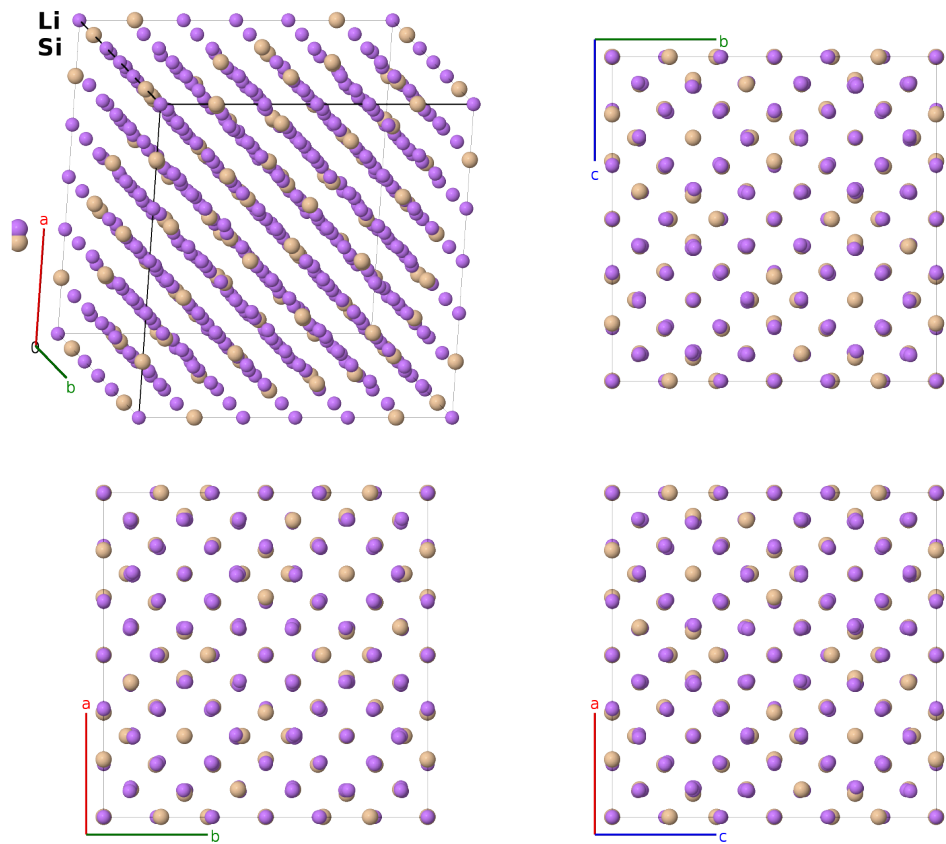
A22B5_cF432_196_abcd6efg4h_2efg-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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.
- 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/GA7M>

https://aflow.org/prototype-encyclopedia/A22B5_cF432_196_abcd6efg4h_2efg-001



Prototype	Li ₂₂ Si ₅
AFLOW prototype label	A22B5_cF432_196_abcd6efg4h_2efg-001
ICSD	24596
CCDC	1600618
Pearson symbol	cF432
Space group number	196
Space group symbol	<i>F</i> 23
AFLOW prototype command	<pre>aflow --proto=A22B5_cF432_196_abcd6efg4h_2efg-001 --params=a, x₅, x₆, x₇, x₈, x₉, x₁₀, x₁₁, x₁₂, x₁₃, x₁₄, x₁₅, x₁₆, x₁₇, y₁₇, z₁₇, x₁₈, y₁₈, z₁₈, x₁₉, y₁₉, z₁₉, x₂₀, y₂₀, z₂₀</pre>

Other compounds with this structure

$\text{Li}_{22}\text{Ge}_5$, $\text{Li}_{22}\text{Pb}_5$, $\text{Li}_{22}\text{Sn}_5$, $\text{Li}_{22}\text{Tl}_5$

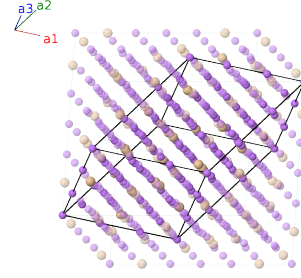
- The ICSD and other authorities use $\text{Li}_{22}\text{Pb}_5$ as the prototype for this structure, but (Goward, 2001) suggests that the true structure of that compound is $\text{Li}_{17}\text{Pb}_4$, changing the space group from $F32 \#196$ to $F\bar{4}3m$ $\text{Li}_{22}\text{Si}_5$ as the prototype.
- This is one of the few crystal structures where all of the Wyckoff positions in its space group are occupied.

Face-centered Cubic primitive vectors

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

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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(4a) Li I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(4b) Li II
$\mathbf{B}_3$	=	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(4c) Li III
$\mathbf{B}_4$	=	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{3}{4}a \hat{\mathbf{z}}$	(4d) Li IV
$\mathbf{B}_5$	=	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(16e) Li V
$\mathbf{B}_6$	=	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - 3x_5 \mathbf{a}_3$	=	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(16e) Li V
$\mathbf{B}_7$	=	$x_5 \mathbf{a}_1 - 3x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(16e) Li V
$\mathbf{B}_8$	=	$-3x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(16e) Li V
$\mathbf{B}_9$	=	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	=	$ax_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}}$	(16e) Li VI
$\mathbf{B}_{10}$	=	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - 3x_6 \mathbf{a}_3$	=	$-ax_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}}$	(16e) Li VI
$\mathbf{B}_{11}$	=	$x_6 \mathbf{a}_1 - 3x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	=	$-ax_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}}$	(16e) Li VI
$\mathbf{B}_{12}$	=	$-3x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	=	$ax_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}}$	(16e) Li VI
$\mathbf{B}_{13}$	=	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(16e) Li VII
$\mathbf{B}_{14}$	=	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - 3x_7 \mathbf{a}_3$	=	$-ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(16e) Li VII
$\mathbf{B}_{15}$	=	$x_7 \mathbf{a}_1 - 3x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$-ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(16e) Li VII
$\mathbf{B}_{16}$	=	$-3x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(16e) Li VII
$\mathbf{B}_{17}$	=	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	=	$ax_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}}$	(16e) Li VIII
$\mathbf{B}_{18}$	=	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - 3x_8 \mathbf{a}_3$	=	$-ax_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}}$	(16e) Li VIII
$\mathbf{B}_{19}$	=	$x_8 \mathbf{a}_1 - 3x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	=	$-ax_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}}$	(16e) Li VIII
$\mathbf{B}_{20}$	=	$-3x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	=	$ax_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}}$	(16e) Li VIII
$\mathbf{B}_{21}$	=	$x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	=	$ax_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} + ax_9 \hat{\mathbf{z}}$	(16e) Li IX

$$\begin{aligned}
\mathbf{B}_{59} &= x_{16} \mathbf{a}_1 + x_{16} \mathbf{a}_2 - \left(x_{16} - \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + a x_{16} \hat{\mathbf{z}} & (24g) & \text{Si IV} \\
\mathbf{B}_{60} &= -\left(x_{16} - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{16} - \frac{1}{2}\right) \mathbf{a}_2 + x_{16} \mathbf{a}_3 = \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} - a \left(x_{16} - \frac{1}{2}\right) \hat{\mathbf{z}} & (24g) & \text{Si IV} \\
\mathbf{B}_{61} &= (-x_{17} + y_{17} + z_{17}) \mathbf{a}_1 + (x_{17} - y_{17} + z_{17}) \mathbf{a}_2 + (x_{17} + y_{17} - z_{17}) \mathbf{a}_3 = a x_{17} \hat{\mathbf{x}} + a y_{17} \hat{\mathbf{y}} + a z_{17} \hat{\mathbf{z}} & (48h) & \text{Li XIII} \\
\mathbf{B}_{62} &= (x_{17} - y_{17} + z_{17}) \mathbf{a}_1 + (-x_{17} + y_{17} + z_{17}) \mathbf{a}_2 - (x_{17} + y_{17} + z_{17}) \mathbf{a}_3 = -a x_{17} \hat{\mathbf{x}} - a y_{17} \hat{\mathbf{y}} + a z_{17} \hat{\mathbf{z}} & (48h) & \text{Li XIII} \\
\mathbf{B}_{63} &= (x_{17} + y_{17} - z_{17}) \mathbf{a}_1 - (x_{17} + y_{17} + z_{17}) \mathbf{a}_2 + (-x_{17} + y_{17} + z_{17}) \mathbf{a}_3 = -a x_{17} \hat{\mathbf{x}} + a y_{17} \hat{\mathbf{y}} - a z_{17} \hat{\mathbf{z}} & (48h) & \text{Li XIII} \\
\mathbf{B}_{64} &= -(x_{17} + y_{17} + z_{17}) \mathbf{a}_1 + (x_{17} + y_{17} - z_{17}) \mathbf{a}_2 + (x_{17} - y_{17} + z_{17}) \mathbf{a}_3 = a x_{17} \hat{\mathbf{x}} - a y_{17} \hat{\mathbf{y}} - a z_{17} \hat{\mathbf{z}} & (48h) & \text{Li XIII} \\
\mathbf{B}_{65} &= (x_{17} + y_{17} - z_{17}) \mathbf{a}_1 + (-x_{17} + y_{17} + z_{17}) \mathbf{a}_2 + (x_{17} - y_{17} + z_{17}) \mathbf{a}_3 = a z_{17} \hat{\mathbf{x}} + a x_{17} \hat{\mathbf{y}} + a y_{17} \hat{\mathbf{z}} & (48h) & \text{Li XIII} \\
\mathbf{B}_{66} &= -(x_{17} + y_{17} + z_{17}) \mathbf{a}_1 + (x_{17} - y_{17} + z_{17}) \mathbf{a}_2 + (-x_{17} + y_{17} + z_{17}) \mathbf{a}_3 = a z_{17} \hat{\mathbf{x}} - a x_{17} \hat{\mathbf{y}} - a y_{17} \hat{\mathbf{z}} & (48h) & \text{Li XIII} \\
\mathbf{B}_{67} &= (-x_{17} + y_{17} + z_{17}) \mathbf{a}_1 + (x_{17} + y_{17} - z_{17}) \mathbf{a}_2 - (x_{17} + y_{17} + z_{17}) \mathbf{a}_3 = -a z_{17} \hat{\mathbf{x}} - a x_{17} \hat{\mathbf{y}} + a y_{17} \hat{\mathbf{z}} & (48h) & \text{Li XIII} \\
\mathbf{B}_{68} &= (x_{17} - y_{17} + z_{17}) \mathbf{a}_1 - (x_{17} + y_{17} + z_{17}) \mathbf{a}_2 + (x_{17} + y_{17} - z_{17}) \mathbf{a}_3 = -a z_{17} \hat{\mathbf{x}} + a x_{17} \hat{\mathbf{y}} - a y_{17} \hat{\mathbf{z}} & (48h) & \text{Li XIII} \\
\mathbf{B}_{69} &= (x_{17} - y_{17} + z_{17}) \mathbf{a}_1 + (x_{17} + y_{17} - z_{17}) \mathbf{a}_2 + (-x_{17} + y_{17} + z_{17}) \mathbf{a}_3 = a y_{17} \hat{\mathbf{x}} + a z_{17} \hat{\mathbf{y}} + a x_{17} \hat{\mathbf{z}} & (48h) & \text{Li XIII} \\
\mathbf{B}_{70} &= (-x_{17} + y_{17} + z_{17}) \mathbf{a}_1 - (x_{17} + y_{17} + z_{17}) \mathbf{a}_2 + (x_{17} - y_{17} + z_{17}) \mathbf{a}_3 = -a y_{17} \hat{\mathbf{x}} + a z_{17} \hat{\mathbf{y}} - a x_{17} \hat{\mathbf{z}} & (48h) & \text{Li XIII} \\
\mathbf{B}_{71} &= -(x_{17} + y_{17} + z_{17}) \mathbf{a}_1 + (-x_{17} + y_{17} + z_{17}) \mathbf{a}_2 + (x_{17} + y_{17} - z_{17}) \mathbf{a}_3 = a y_{17} \hat{\mathbf{x}} - a z_{17} \hat{\mathbf{y}} - a x_{17} \hat{\mathbf{z}} & (48h) & \text{Li XIII} \\
\mathbf{B}_{72} &= (x_{17} + y_{17} - z_{17}) \mathbf{a}_1 + (x_{17} - y_{17} + z_{17}) \mathbf{a}_2 - (x_{17} + y_{17} + z_{17}) \mathbf{a}_3 = -a y_{17} \hat{\mathbf{x}} - a z_{17} \hat{\mathbf{y}} + a x_{17} \hat{\mathbf{z}} & (48h) & \text{Li XIII} \\
\mathbf{B}_{73} &= (-x_{18} + y_{18} + z_{18}) \mathbf{a}_1 + (x_{18} - y_{18} + z_{18}) \mathbf{a}_2 + (x_{18} + y_{18} - z_{18}) \mathbf{a}_3 = a x_{18} \hat{\mathbf{x}} + a y_{18} \hat{\mathbf{y}} + a z_{18} \hat{\mathbf{z}} & (48h) & \text{Li XIV} \\
\mathbf{B}_{74} &= (x_{18} - y_{18} + z_{18}) \mathbf{a}_1 + (-x_{18} + y_{18} + z_{18}) \mathbf{a}_2 - (x_{18} + y_{18} + z_{18}) \mathbf{a}_3 = -a x_{18} \hat{\mathbf{x}} - a y_{18} \hat{\mathbf{y}} + a z_{18} \hat{\mathbf{z}} & (48h) & \text{Li XIV} \\
\mathbf{B}_{75} &= (x_{18} + y_{18} - z_{18}) \mathbf{a}_1 - (x_{18} + y_{18} + z_{18}) \mathbf{a}_2 + (-x_{18} + y_{18} + z_{18}) \mathbf{a}_3 = -a x_{18} \hat{\mathbf{x}} + a y_{18} \hat{\mathbf{y}} - a z_{18} \hat{\mathbf{z}} & (48h) & \text{Li XIV} \\
\mathbf{B}_{76} &= -(x_{18} + y_{18} + z_{18}) \mathbf{a}_1 + (x_{18} + y_{18} - z_{18}) \mathbf{a}_2 + (x_{18} - y_{18} + z_{18}) \mathbf{a}_3 = a x_{18} \hat{\mathbf{x}} - a y_{18} \hat{\mathbf{y}} - a z_{18} \hat{\mathbf{z}} & (48h) & \text{Li XIV}
\end{aligned}$$

$\mathbf{B}_{77}$	$=$	$(x_{18} + y_{18} - z_{18}) \mathbf{a}_1 +$ $(-x_{18} + y_{18} + z_{18}) \mathbf{a}_2 +$ $(x_{18} - y_{18} + z_{18}) \mathbf{a}_3$	$=$	$az_{18} \hat{\mathbf{x}} + ax_{18} \hat{\mathbf{y}} + ay_{18} \hat{\mathbf{z}}$	$(48h)$	Li XIV
$\mathbf{B}_{78}$	$=$	$-(x_{18} + y_{18} + z_{18}) \mathbf{a}_1 +$ $(x_{18} - y_{18} + z_{18}) \mathbf{a}_2 +$ $(-x_{18} + y_{18} + z_{18}) \mathbf{a}_3$	$=$	$az_{18} \hat{\mathbf{x}} - ax_{18} \hat{\mathbf{y}} - ay_{18} \hat{\mathbf{z}}$	$(48h)$	Li XIV
$\mathbf{B}_{79}$	$=$	$(-x_{18} + y_{18} + z_{18}) \mathbf{a}_1 +$ $(x_{18} + y_{18} - z_{18}) \mathbf{a}_2 -$ $(x_{18} + y_{18} + z_{18}) \mathbf{a}_3$	$=$	$-az_{18} \hat{\mathbf{x}} - ax_{18} \hat{\mathbf{y}} + ay_{18} \hat{\mathbf{z}}$	$(48h)$	Li XIV
$\mathbf{B}_{80}$	$=$	$(x_{18} - y_{18} + z_{18}) \mathbf{a}_1 -$ $(x_{18} + y_{18} + z_{18}) \mathbf{a}_2 +$ $(x_{18} + y_{18} - z_{18}) \mathbf{a}_3$	$=$	$-az_{18} \hat{\mathbf{x}} + ax_{18} \hat{\mathbf{y}} - ay_{18} \hat{\mathbf{z}}$	$(48h)$	Li XIV
$\mathbf{B}_{81}$	$=$	$(x_{18} - y_{18} + z_{18}) \mathbf{a}_1 +$ $(x_{18} + y_{18} - z_{18}) \mathbf{a}_2 +$ $(-x_{18} + y_{18} + z_{18}) \mathbf{a}_3$	$=$	$ay_{18} \hat{\mathbf{x}} + az_{18} \hat{\mathbf{y}} + ax_{18} \hat{\mathbf{z}}$	$(48h)$	Li XIV
$\mathbf{B}_{82}$	$=$	$(-x_{18} + y_{18} + z_{18}) \mathbf{a}_1 -$ $(x_{18} + y_{18} + z_{18}) \mathbf{a}_2 +$ $(x_{18} - y_{18} + z_{18}) \mathbf{a}_3$	$=$	$-ay_{18} \hat{\mathbf{x}} + az_{18} \hat{\mathbf{y}} - ax_{18} \hat{\mathbf{z}}$	$(48h)$	Li XIV
$\mathbf{B}_{83}$	$=$	$-(x_{18} + y_{18} + z_{18}) \mathbf{a}_1 +$ $(-x_{18} + y_{18} + z_{18}) \mathbf{a}_2 +$ $(x_{18} + y_{18} - z_{18}) \mathbf{a}_3$	$=$	$ay_{18} \hat{\mathbf{x}} - az_{18} \hat{\mathbf{y}} - ax_{18} \hat{\mathbf{z}}$	$(48h)$	Li XIV
$\mathbf{B}_{84}$	$=$	$(x_{18} + y_{18} - z_{18}) \mathbf{a}_1 +$ $(x_{18} - y_{18} + z_{18}) \mathbf{a}_2 -$ $(x_{18} + y_{18} + z_{18}) \mathbf{a}_3$	$=$	$-ay_{18} \hat{\mathbf{x}} - az_{18} \hat{\mathbf{y}} + ax_{18} \hat{\mathbf{z}}$	$(48h)$	Li XIV
$\mathbf{B}_{85}$	$=$	$(-x_{19} + y_{19} + z_{19}) \mathbf{a}_1 +$ $(x_{19} - y_{19} + z_{19}) \mathbf{a}_2 +$ $(x_{19} + y_{19} - z_{19}) \mathbf{a}_3$	$=$	$ax_{19} \hat{\mathbf{x}} + ay_{19} \hat{\mathbf{y}} + az_{19} \hat{\mathbf{z}}$	$(48h)$	Li XV
$\mathbf{B}_{86}$	$=$	$(x_{19} - y_{19} + z_{19}) \mathbf{a}_1 +$ $(-x_{19} + y_{19} + z_{19}) \mathbf{a}_2 -$ $(x_{19} + y_{19} + z_{19}) \mathbf{a}_3$	$=$	$-ax_{19} \hat{\mathbf{x}} - ay_{19} \hat{\mathbf{y}} + az_{19} \hat{\mathbf{z}}$	$(48h)$	Li XV
$\mathbf{B}_{87}$	$=$	$(x_{19} + y_{19} - z_{19}) \mathbf{a}_1 -$ $(x_{19} + y_{19} + z_{19}) \mathbf{a}_2 +$ $(-x_{19} + y_{19} + z_{19}) \mathbf{a}_3$	$=$	$-ax_{19} \hat{\mathbf{x}} + ay_{19} \hat{\mathbf{y}} - az_{19} \hat{\mathbf{z}}$	$(48h)$	Li XV
$\mathbf{B}_{88}$	$=$	$-(x_{19} + y_{19} + z_{19}) \mathbf{a}_1 +$ $(x_{19} + y_{19} - z_{19}) \mathbf{a}_2 +$ $(x_{19} - y_{19} + z_{19}) \mathbf{a}_3$	$=$	$ax_{19} \hat{\mathbf{x}} - ay_{19} \hat{\mathbf{y}} - az_{19} \hat{\mathbf{z}}$	$(48h)$	Li XV
$\mathbf{B}_{89}$	$=$	$(x_{19} + y_{19} - z_{19}) \mathbf{a}_1 +$ $(-x_{19} + y_{19} + z_{19}) \mathbf{a}_2 +$ $(x_{19} - y_{19} + z_{19}) \mathbf{a}_3$	$=$	$az_{19} \hat{\mathbf{x}} + ax_{19} \hat{\mathbf{y}} + ay_{19} \hat{\mathbf{z}}$	$(48h)$	Li XV
$\mathbf{B}_{90}$	$=$	$-(x_{19} + y_{19} + z_{19}) \mathbf{a}_1 +$ $(x_{19} - y_{19} + z_{19}) \mathbf{a}_2 +$ $(-x_{19} + y_{19} + z_{19}) \mathbf{a}_3$	$=$	$az_{19} \hat{\mathbf{x}} - ax_{19} \hat{\mathbf{y}} - ay_{19} \hat{\mathbf{z}}$	$(48h)$	Li XV
$\mathbf{B}_{91}$	$=$	$(-x_{19} + y_{19} + z_{19}) \mathbf{a}_1 +$ $(x_{19} + y_{19} - z_{19}) \mathbf{a}_2 -$ $(x_{19} + y_{19} + z_{19}) \mathbf{a}_3$	$=$	$-az_{19} \hat{\mathbf{x}} - ax_{19} \hat{\mathbf{y}} + ay_{19} \hat{\mathbf{z}}$	$(48h)$	Li XV
$\mathbf{B}_{92}$	$=$	$(x_{19} - y_{19} + z_{19}) \mathbf{a}_1 -$ $(x_{19} + y_{19} + z_{19}) \mathbf{a}_2 +$ $(x_{19} + y_{19} - z_{19}) \mathbf{a}_3$	$=$	$-az_{19} \hat{\mathbf{x}} + ax_{19} \hat{\mathbf{y}} - ay_{19} \hat{\mathbf{z}}$	$(48h)$	Li XV
$\mathbf{B}_{93}$	$=$	$(x_{19} - y_{19} + z_{19}) \mathbf{a}_1 +$ $(x_{19} + y_{19} - z_{19}) \mathbf{a}_2 +$ $(-x_{19} + y_{19} + z_{19}) \mathbf{a}_3$	$=$	$ay_{19} \hat{\mathbf{x}} + az_{19} \hat{\mathbf{y}} + ax_{19} \hat{\mathbf{z}}$	$(48h)$	Li XV

$\mathbf{B}_{94} =$	$(-x_{19} + y_{19} + z_{19}) \mathbf{a}_1 -$ $(x_{19} + y_{19} + z_{19}) \mathbf{a}_2 +$ $(x_{19} - y_{19} + z_{19}) \mathbf{a}_3$	$=$	$-ay_{19} \hat{\mathbf{x}} + az_{19} \hat{\mathbf{y}} - ax_{19} \hat{\mathbf{z}}$	$(48h)$	Li XV
$\mathbf{B}_{95} =$	$-(x_{19} + y_{19} + z_{19}) \mathbf{a}_1 +$ $(-x_{19} + y_{19} + z_{19}) \mathbf{a}_2 +$ $(x_{19} + y_{19} - z_{19}) \mathbf{a}_3$	$=$	$ay_{19} \hat{\mathbf{x}} - az_{19} \hat{\mathbf{y}} - ax_{19} \hat{\mathbf{z}}$	$(48h)$	Li XV
$\mathbf{B}_{96} =$	$(x_{19} + y_{19} - z_{19}) \mathbf{a}_1 +$ $(x_{19} - y_{19} + z_{19}) \mathbf{a}_2 -$ $(x_{19} + y_{19} + z_{19}) \mathbf{a}_3$	$=$	$-ay_{19} \hat{\mathbf{x}} - az_{19} \hat{\mathbf{y}} + ax_{19} \hat{\mathbf{z}}$	$(48h)$	Li XV
$\mathbf{B}_{97} =$	$(-x_{20} + y_{20} + z_{20}) \mathbf{a}_1 +$ $(x_{20} - y_{20} + z_{20}) \mathbf{a}_2 +$ $(x_{20} + y_{20} - z_{20}) \mathbf{a}_3$	$=$	$ax_{20} \hat{\mathbf{x}} + ay_{20} \hat{\mathbf{y}} + az_{20} \hat{\mathbf{z}}$	$(48h)$	Li XVI
$\mathbf{B}_{98} =$	$(x_{20} - y_{20} + z_{20}) \mathbf{a}_1 +$ $(-x_{20} + y_{20} + z_{20}) \mathbf{a}_2 -$ $(x_{20} + y_{20} + z_{20}) \mathbf{a}_3$	$=$	$-ax_{20} \hat{\mathbf{x}} - ay_{20} \hat{\mathbf{y}} + az_{20} \hat{\mathbf{z}}$	$(48h)$	Li XVI
$\mathbf{B}_{99} =$	$(x_{20} + y_{20} - z_{20}) \mathbf{a}_1 -$ $(x_{20} + y_{20} + z_{20}) \mathbf{a}_2 +$ $(-x_{20} + y_{20} + z_{20}) \mathbf{a}_3$	$=$	$-ax_{20} \hat{\mathbf{x}} + ay_{20} \hat{\mathbf{y}} - az_{20} \hat{\mathbf{z}}$	$(48h)$	Li XVI
$\mathbf{B}_{100} =$	$-(x_{20} + y_{20} + z_{20}) \mathbf{a}_1 +$ $(x_{20} + y_{20} - z_{20}) \mathbf{a}_2 +$ $(x_{20} - y_{20} + z_{20}) \mathbf{a}_3$	$=$	$ax_{20} \hat{\mathbf{x}} - ay_{20} \hat{\mathbf{y}} - az_{20} \hat{\mathbf{z}}$	$(48h)$	Li XVI
$\mathbf{B}_{101} =$	$(x_{20} + y_{20} - z_{20}) \mathbf{a}_1 +$ $(-x_{20} + y_{20} + z_{20}) \mathbf{a}_2 +$ $(x_{20} - y_{20} + z_{20}) \mathbf{a}_3$	$=$	$az_{20} \hat{\mathbf{x}} + ax_{20} \hat{\mathbf{y}} + ay_{20} \hat{\mathbf{z}}$	$(48h)$	Li XVI
$\mathbf{B}_{102} =$	$-(x_{20} + y_{20} + z_{20}) \mathbf{a}_1 +$ $(x_{20} - y_{20} + z_{20}) \mathbf{a}_2 +$ $(-x_{20} + y_{20} + z_{20}) \mathbf{a}_3$	$=$	$az_{20} \hat{\mathbf{x}} - ax_{20} \hat{\mathbf{y}} - ay_{20} \hat{\mathbf{z}}$	$(48h)$	Li XVI
$\mathbf{B}_{103} =$	$(-x_{20} + y_{20} + z_{20}) \mathbf{a}_1 +$ $(x_{20} + y_{20} - z_{20}) \mathbf{a}_2 -$ $(x_{20} + y_{20} + z_{20}) \mathbf{a}_3$	$=$	$-az_{20} \hat{\mathbf{x}} - ax_{20} \hat{\mathbf{y}} + ay_{20} \hat{\mathbf{z}}$	$(48h)$	Li XVI
$\mathbf{B}_{104} =$	$(x_{20} - y_{20} + z_{20}) \mathbf{a}_1 -$ $(x_{20} + y_{20} + z_{20}) \mathbf{a}_2 +$ $(x_{20} + y_{20} - z_{20}) \mathbf{a}_3$	$=$	$-az_{20} \hat{\mathbf{x}} + ax_{20} \hat{\mathbf{y}} - ay_{20} \hat{\mathbf{z}}$	$(48h)$	Li XVI
$\mathbf{B}_{105} =$	$(x_{20} - y_{20} + z_{20}) \mathbf{a}_1 +$ $(x_{20} + y_{20} - z_{20}) \mathbf{a}_2 +$ $(-x_{20} + y_{20} + z_{20}) \mathbf{a}_3$	$=$	$ay_{20} \hat{\mathbf{x}} + az_{20} \hat{\mathbf{y}} + ax_{20} \hat{\mathbf{z}}$	$(48h)$	Li XVI
$\mathbf{B}_{106} =$	$(-x_{20} + y_{20} + z_{20}) \mathbf{a}_1 -$ $(x_{20} + y_{20} + z_{20}) \mathbf{a}_2 +$ $(x_{20} - y_{20} + z_{20}) \mathbf{a}_3$	$=$	$-ay_{20} \hat{\mathbf{x}} + az_{20} \hat{\mathbf{y}} - ax_{20} \hat{\mathbf{z}}$	$(48h)$	Li XVI
$\mathbf{B}_{107} =$	$-(x_{20} + y_{20} + z_{20}) \mathbf{a}_1 +$ $(-x_{20} + y_{20} + z_{20}) \mathbf{a}_2 +$ $(x_{20} + y_{20} - z_{20}) \mathbf{a}_3$	$=$	$ay_{20} \hat{\mathbf{x}} - az_{20} \hat{\mathbf{y}} - ax_{20} \hat{\mathbf{z}}$	$(48h)$	Li XVI
$\mathbf{B}_{108} =$	$(x_{20} + y_{20} - z_{20}) \mathbf{a}_1 +$ $(x_{20} - y_{20} + z_{20}) \mathbf{a}_2 -$ $(x_{20} + y_{20} + z_{20}) \mathbf{a}_3$	$=$	$-ay_{20} \hat{\mathbf{x}} - az_{20} \hat{\mathbf{y}} + ax_{20} \hat{\mathbf{z}}$	$(48h)$	Li XVI

References

- [1] H. Axel, H. Schäfer, and A. Weiss, *Zur Kenntnis der Phase $Li_{22}Si_5$* , Z. Naturforsch. B **21**, 115–117 (1966), doi:10.1515/zn-1966-0204.

- [2] A. Zalkin and W. J. Ramsey, *Intermetallic compounds between lithium and lead. IV. The crystal structure of $Li_{22}Pb_5$* , J. Physic. Chem. **62**, 689–693 (1958), doi:10.1021/j150564a013.
- [3] 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.

Found in

- [1] *Inorganic Crystal Structure Database*. Entry 24596 ($Li_{22}Si_5$).

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.