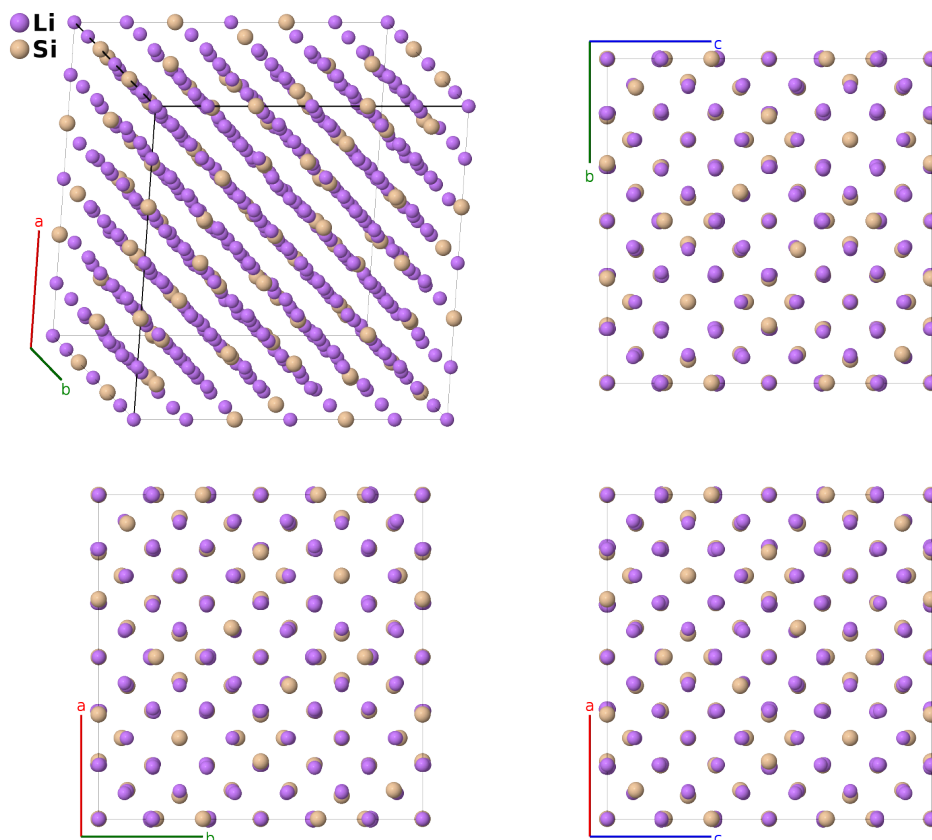


Li₂₂Si₅ Structure: A22B5_cF432_196_abcd6efg4h_2efg-001

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<https://aflow.org/p/GA7M>

https://aflow.org/p/A22B5_cF432_196_abcd6efg4h_2efg-001



Prototype	Li ₂₂ Si ₅
AFLOW prototype label	A22B5_cF432_196_abcd6efg4h_2efg-001
ICSD	24596
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>

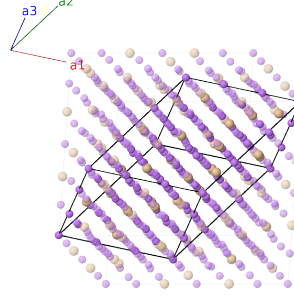
Other compounds with this structure

Li₂₂Ge₅, Li₂₂Pb₅, Li₂₂Sn₅, Li₂₂Tl₅

- 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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$=$	0	$=$	0	(4a) Li I
\mathbf{B}_2	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(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
\mathbf{B}_{22}	$=$	$x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - 3x_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} + ax_9 \hat{\mathbf{z}}$	(16e) Li IX
\mathbf{B}_{23}	$=$	$x_9 \mathbf{a}_1 - 3x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} - ax_9 \hat{\mathbf{z}}$	(16e) Li IX
\mathbf{B}_{24}	$=$	$-3x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} - ax_9 \hat{\mathbf{z}}$	(16e) Li IX
\mathbf{B}_{25}	$=$	$x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} + ax_{10} \hat{\mathbf{z}}$	(16e) Li X

$$\begin{aligned}
\mathbf{B}_{95} &= \begin{aligned} &-(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 \end{aligned} &= & ay_{19} \hat{\mathbf{x}} - az_{19} \hat{\mathbf{y}} - ax_{19} \hat{\mathbf{z}} & (48h) & \text{Li XV} \\
\mathbf{B}_{96} &= \begin{aligned} &(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 \end{aligned} &= & -ay_{19} \hat{\mathbf{x}} - az_{19} \hat{\mathbf{y}} + ax_{19} \hat{\mathbf{z}} & (48h) & \text{Li XV} \\
\mathbf{B}_{97} &= \begin{aligned} &(-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 \end{aligned} &= & ax_{20} \hat{\mathbf{x}} + ay_{20} \hat{\mathbf{y}} + az_{20} \hat{\mathbf{z}} & (48h) & \text{Li XVI} \\
\mathbf{B}_{98} &= \begin{aligned} &(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 \end{aligned} &= & -ax_{20} \hat{\mathbf{x}} - ay_{20} \hat{\mathbf{y}} + az_{20} \hat{\mathbf{z}} & (48h) & \text{Li XVI} \\
\mathbf{B}_{99} &= \begin{aligned} &(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 \end{aligned} &= & -ax_{20} \hat{\mathbf{x}} + ay_{20} \hat{\mathbf{y}} - az_{20} \hat{\mathbf{z}} & (48h) & \text{Li XVI} \\
\mathbf{B}_{100} &= \begin{aligned} &-(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 \end{aligned} &= & ax_{20} \hat{\mathbf{x}} - ay_{20} \hat{\mathbf{y}} - az_{20} \hat{\mathbf{z}} & (48h) & \text{Li XVI} \\
\mathbf{B}_{101} &= \begin{aligned} &(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 \end{aligned} &= & az_{20} \hat{\mathbf{x}} + ax_{20} \hat{\mathbf{y}} + ay_{20} \hat{\mathbf{z}} & (48h) & \text{Li XVI} \\
\mathbf{B}_{102} &= \begin{aligned} &-(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 \end{aligned} &= & az_{20} \hat{\mathbf{x}} - ax_{20} \hat{\mathbf{y}} - ay_{20} \hat{\mathbf{z}} & (48h) & \text{Li XVI} \\
\mathbf{B}_{103} &= \begin{aligned} &(-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 \end{aligned} &= & -az_{20} \hat{\mathbf{x}} - ax_{20} \hat{\mathbf{y}} + ay_{20} \hat{\mathbf{z}} & (48h) & \text{Li XVI} \\
\mathbf{B}_{104} &= \begin{aligned} &(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 \end{aligned} &= & -az_{20} \hat{\mathbf{x}} + ax_{20} \hat{\mathbf{y}} - ay_{20} \hat{\mathbf{z}} & (48h) & \text{Li XVI} \\
\mathbf{B}_{105} &= \begin{aligned} &(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 \end{aligned} &= & ay_{20} \hat{\mathbf{x}} + az_{20} \hat{\mathbf{y}} + ax_{20} \hat{\mathbf{z}} & (48h) & \text{Li XVI} \\
\mathbf{B}_{106} &= \begin{aligned} &(-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 \end{aligned} &= & -ay_{20} \hat{\mathbf{x}} + az_{20} \hat{\mathbf{y}} - ax_{20} \hat{\mathbf{z}} & (48h) & \text{Li XVI} \\
\mathbf{B}_{107} &= \begin{aligned} &-(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 \end{aligned} &= & ay_{20} \hat{\mathbf{x}} - az_{20} \hat{\mathbf{y}} - ax_{20} \hat{\mathbf{z}} & (48h) & \text{Li XVI} \\
\mathbf{B}_{108} &= \begin{aligned} &(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 \end{aligned} &= & -ay_{20} \hat{\mathbf{x}} - az_{20} \hat{\mathbf{y}} + ax_{20} \hat{\mathbf{z}} & (48h) & \text{Li XVI}
\end{aligned}$$

References

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