# $Li_2Sb$ Structure: A2B_hP18_190_gh_bf-001

This structure originally had the label `A2B_hP18_190_gh_bf`. Calls to that address will be redirected here.

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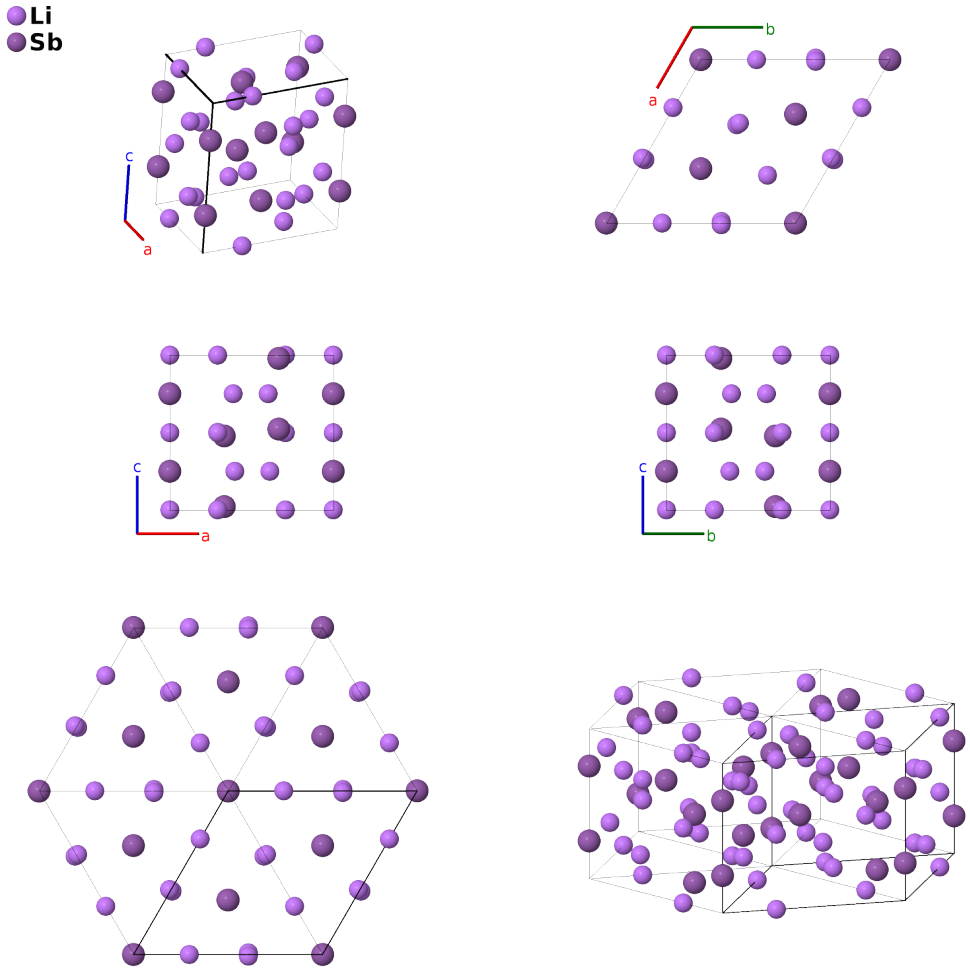
https://aflow.org/p/DA98

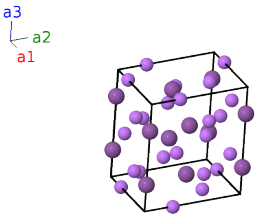
https://aflow.org/p/A2B_hP18_190_gh_bf-001




| | |
|---|---|
| **Prototype** | $Li_2Sb$ |
| **AFLOW prototype label** | A2B_hP18_190_gh_bf-001 |
| **ICSD** | 100020 |
| **Pearson symbol** | hP18 |
| **Space group number** | 190 |
| **Space group symbol** | $P\bar{6}2c$ |
| **AFLOW prototype command** | `aflow --proto=A2B_hP18_190_gh_bf-001 --params=`$a, c/a, z_2, x_3, x_4, y_4$ |

## Hexagonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$




## Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{1}{4}c\,\hat{\mathbf{z}}$ | (2b) | Sb I |
| $\mathbf{B_2}$ | = | $\frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{3}{4}c\,\hat{\mathbf{z}}$ | (2b) | Sb I |
| $\mathbf{B_3}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (4f) | Sb II |
| $\mathbf{B_4}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (4f) | Sb II |
| $\mathbf{B_5}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$ | (4f) | Sb II |
| $\mathbf{B_6}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (4f) | Sb II |
| $\mathbf{B_7}$ | = | $x_3\,\mathbf{a}_1$ | = | $\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$ | (6g) | Li I |
| $\mathbf{B_8}$ | = | $x_3\,\mathbf{a}_2$ | = | $\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$ | (6g) | Li I |
| $\mathbf{B_9}$ | = | $-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$ | = | $-ax_3\,\hat{\mathbf{x}}$ | (6g) | Li I |
| $\mathbf{B_{10}}$ | = | $x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6g) | Li I |
| $\mathbf{B_{11}}$ | = | $x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6g) | Li I |
| $\mathbf{B_{12}}$ | = | $-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6g) | Li I |
| $\mathbf{B_{13}}$ | = | $x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6h) | Li II |
| $\mathbf{B_{14}}$ | = | $-y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6h) | Li II |
| $\mathbf{B_{15}}$ | = | $-(x_4 - y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6h) | Li II |
| $\mathbf{B_{16}}$ | = | $y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (6h) | Li II |
| $\mathbf{B_{17}}$ | = | $(x_4 - y_4)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (6h) | Li II |
| $\mathbf{B_{18}}$ | = | $-x_4\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (6h) | Li II |

## References


[1] W. Müller, *Darstellung und Struktur der Phase $Li_2Sb$*, Z. Naturforsch. B **32**, 357–359 (1977).