

# Li<sub>2</sub>Si<sub>2</sub>O<sub>5</sub> Structure:

## A2B5C2\_oC36\_37\_d\_c2d\_d-001

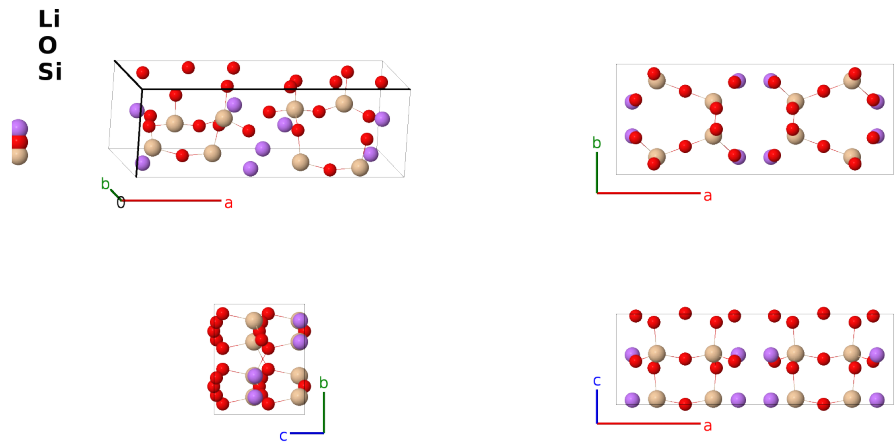
This structure previously used the label(s) **A2B5C2\_oC36\_37\_d\_c2d\_d**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/JE1T>

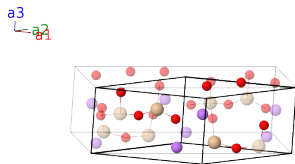
[https://aflow.org/prototype-encyclopedia/A2B5C2\\_oC36\\_37\\_d\\_c2d\\_d-001](https://aflow.org/prototype-encyclopedia/A2B5C2_oC36_37_d_c2d_d-001)



|                         |                                                                                                                                                                                                                                                                                               |
|-------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype               | Li <sub>2</sub> O <sub>5</sub> Si <sub>2</sub>                                                                                                                                                                                                                                                |
| AFLOW prototype label   | A2B5C2_oC36_37_d_c2d_d-001                                                                                                                                                                                                                                                                    |
| ICSD                    | 78562                                                                                                                                                                                                                                                                                         |
| CCDC                    | 1638838                                                                                                                                                                                                                                                                                       |
| Pearson symbol          | oC36                                                                                                                                                                                                                                                                                          |
| Space group number      | 37                                                                                                                                                                                                                                                                                            |
| Space group symbol      | <i>Ccc2</i>                                                                                                                                                                                                                                                                                   |
| AFLOW prototype command | <code>aflow --proto=A2B5C2_oC36_37_d_c2d_d-001</code><br><code>--params=a, b/a, c/a, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub></code> |

Base-centered Orthorhombic primitive vectors

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



## Basis vectors

|                   | Lattice<br>coordinates                                                                      |     | Cartesian<br>coordinates                                                                                | Wyckoff<br>position | Atom<br>type |
|-------------------|---------------------------------------------------------------------------------------------|-----|---------------------------------------------------------------------------------------------------------|---------------------|--------------|
| $\mathbf{B}_1$    | $= \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$                                             | $=$ | $\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$                 | (4c)                | O I          |
| $\mathbf{B}_2$    | $= \frac{1}{2} \mathbf{a}_1 + (z_1 + \frac{1}{2}) \mathbf{a}_3$                             | $=$ | $\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4c)                | O I          |
| $\mathbf{B}_3$    | $= (x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$                  | $=$ | $ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$                                 | (8d)                | Li I         |
| $\mathbf{B}_4$    | $= -(x_2 - y_2) \mathbf{a}_1 - (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$                 | $=$ | $-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$                                | (8d)                | Li I         |
| $\mathbf{B}_5$    | $= (x_2 + y_2) \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$                 | (8d)                | Li I         |
| $\mathbf{B}_6$    | $= -(x_2 + y_2) \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$                | (8d)                | Li I         |
| $\mathbf{B}_7$    | $= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$                  | $=$ | $ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$                                 | (8d)                | O II         |
| $\mathbf{B}_8$    | $= -(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$                 | $=$ | $-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$                                | (8d)                | O II         |
| $\mathbf{B}_9$    | $= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$                 | (8d)                | O II         |
| $\mathbf{B}_{10}$ | $= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$                | (8d)                | O II         |
| $\mathbf{B}_{11}$ | $= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$                  | $=$ | $ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$                                 | (8d)                | O III        |
| $\mathbf{B}_{12}$ | $= -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$                 | $=$ | $-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$                                | (8d)                | O III        |
| $\mathbf{B}_{13}$ | $= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$                 | (8d)                | O III        |
| $\mathbf{B}_{14}$ | $= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$                | (8d)                | O III        |
| $\mathbf{B}_{15}$ | $= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$                  | $=$ | $ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$                                 | (8d)                | Si I         |
| $\mathbf{B}_{16}$ | $= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$                 | $=$ | $-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$                                | (8d)                | Si I         |
| $\mathbf{B}_{17}$ | $= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$                 | (8d)                | Si I         |
| $\mathbf{B}_{18}$ | $= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$                | (8d)                | Si I         |

## References

- [1] B. H. W. S. de Jong, P. G. G. Slaats, H. T. J. Supér, N. Veldman, and A. L. Spek, *Extended structures in crystalline phyllosilicates: silica ring systems in lithium, rubidium, cesium, and cesium/lithium phyllosilicate*, J. Non-Cryst. Solids **176**, 164–171 (1994), doi:10.1016/0022-3093(94)90074-4.

## Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

## First cited in

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