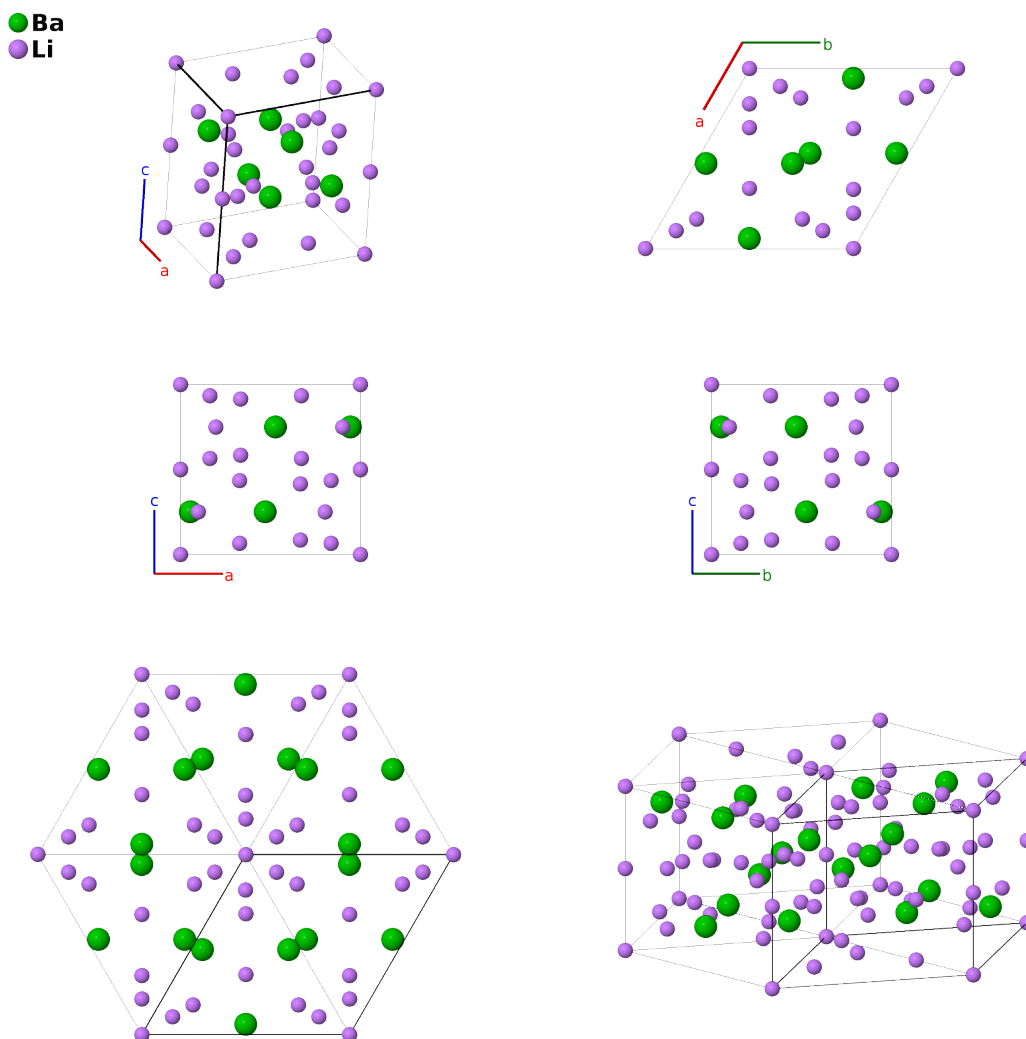


BaLi₄ Structure: AB4_hP30_194_h_afhk-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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

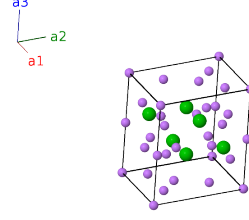
https://aflow.org/p/AB4_hP30_194_h_afhk-001



Prototype	BaLi ₄
AFLOW prototype label	AB4_hP30_194_h_afhk-001
ICSD	409902
Pearson symbol	hP30
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=AB4_hP30_194_h_afhk-001 --params=a, c/a, z₂, x₃, x₄, x₅, z₅</code>

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(2a)	Li I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Li 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)	Li II
\mathbf{B}_4	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Li 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)	Li II
\mathbf{B}_6	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Li II
\mathbf{B}_7	$x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2} ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ax_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Ba I
\mathbf{B}_8	$-2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2} ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ax_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Ba I
\mathbf{B}_9	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3} ax_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Ba I
\mathbf{B}_{10}	$-x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2} ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ax_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Ba I
\mathbf{B}_{11}	$2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2} ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ax_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Ba I
\mathbf{B}_{12}	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\sqrt{3} ax_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Ba I
\mathbf{B}_{13}	$x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2} ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ax_4 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Li III
\mathbf{B}_{14}	$-2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2} ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ax_4 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Li III
\mathbf{B}_{15}	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3} ax_4 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h)	Li III
\mathbf{B}_{16}	$-x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2} ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ax_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Li III
\mathbf{B}_{17}	$2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2} ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ax_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Li III
\mathbf{B}_{18}	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\sqrt{3} ax_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h)	Li III
\mathbf{B}_{19}	$x_5 \mathbf{a}_1 + 2x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{3}{2} ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12k)	Li IV
\mathbf{B}_{20}	$-2x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{3}{2} ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12k)	Li IV
\mathbf{B}_{21}	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\sqrt{3} ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12k)	Li IV
\mathbf{B}_{22}	$-x_5 \mathbf{a}_1 - 2x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{3}{2} ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Li IV
\mathbf{B}_{23}	$2x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{2} ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Li IV
\mathbf{B}_{24}	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\sqrt{3} ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Li IV
\mathbf{B}_{25}	$2x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{3}{2} ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(12k)	Li IV
\mathbf{B}_{26}	$-x_5 \mathbf{a}_1 - 2x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-\frac{3}{2} ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(12k)	Li IV
\mathbf{B}_{27}	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\sqrt{3} ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(12k)	Li IV
\mathbf{B}_{28}	$-2x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{3}{2} ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Li IV
\mathbf{B}_{29}	$x_5 \mathbf{a}_1 + 2x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{2} ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Li IV
\mathbf{B}_{30}	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\sqrt{3} ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Li IV

References

- [1] V. Smetana, V. Babizhetskyy, C. Hoch, and A. Simon, *Refinement of the crystal structure of barium tetralithium, BaLi₄*, *Z. Kristallogr.* **221**, 434 (2006), doi:10.1524/ncrs.2006.0142.