

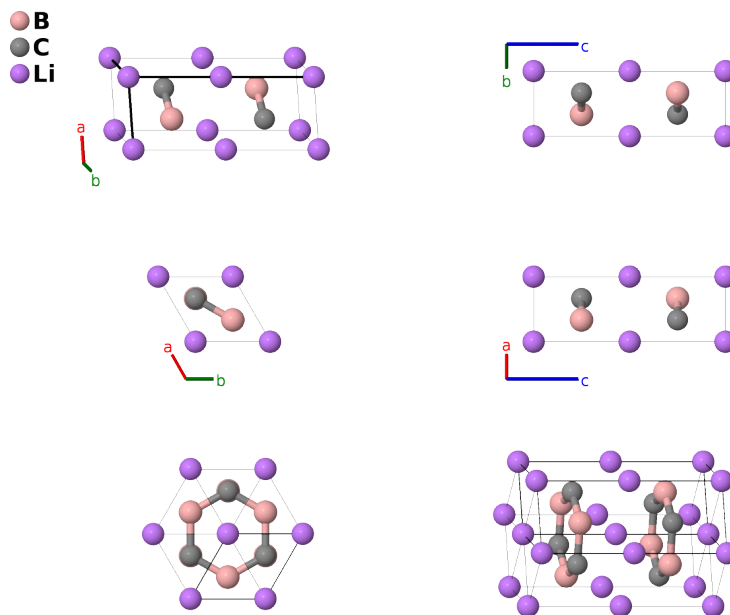
LiBC Structure: ABC_hP6_194_c_d_a-001

This structure originally had the label **ABC_hP6_194_c_d_a**. Calls to that address will be redirected here.

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<https://aflow.org/p/F0CN>

https://aflow.org/p/ABC_hP6_194_c_d_a-001



Prototype	BCLi
AFLOW prototype label	ABC_hP6_194_c_d_a-001
ICSD	78731
Pearson symbol	hP6
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=ABC_hP6_194_c_d_a-001 --params=a, c/a</code>

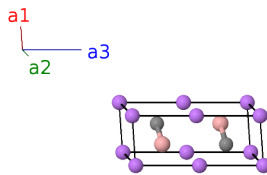
Other compounds with this structure

ZrBeSi, EuAuAs

- This is the parent of the Li_{1-x}BC Structure

Hexagonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	=	0	=	0	(2a) Li I
\mathbf{B}_2	=	$\frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}c\hat{z}$	(2a) Li I
\mathbf{B}_3	=	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{x} + \frac{\sqrt{3}}{6}a\hat{y} + \frac{1}{4}c\hat{z}$	(2c) B I
\mathbf{B}_4	=	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{x} - \frac{\sqrt{3}}{6}a\hat{y} + \frac{3}{4}c\hat{z}$	(2c) B I
\mathbf{B}_5	=	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{x} + \frac{\sqrt{3}}{6}a\hat{y} + \frac{3}{4}c\hat{z}$	(2d) C I
\mathbf{B}_6	=	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{x} - \frac{\sqrt{3}}{6}a\hat{y} + \frac{1}{4}c\hat{z}$	(2d) C I

References

- [1] M. Wörle, R. Nesper, G. Mair, M. Schwarz, and H. G. V. Schnering, *LiBC – ein vollständig interkalierter Heterographit*, *Z. Anorganische und Allgemeine Chemie* **621**, 1153–1159 (1995), doi:10.1002/zaac.19956210707.