LiBC Structure: ABC_hP6_194_c_d_a-001

This structure previously used the label(s) `ABC_hP6_194_c_d_a`. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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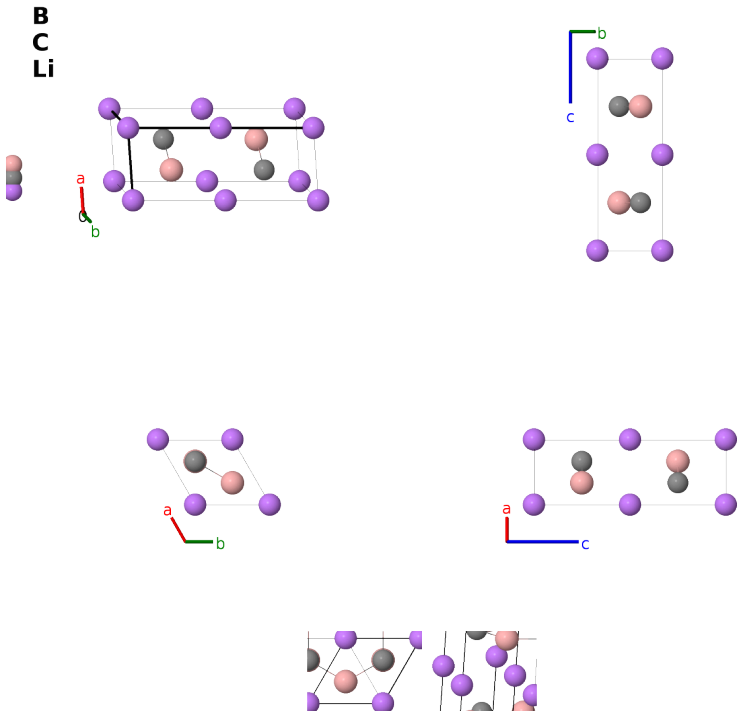
https://aflow.org/prototype-encyclopedia/F0CN

https://aflow.org/prototype-encyclopedia/ABC_hP6_194_c_d_a-001



Prototype	BCLi
AFLOW prototype label	ABC_hP6_194_c_d_a-001
ICSD	78731
CCDC	1639002
Pearson symbol	hP6
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=ABC_hP6_194_c_d_a-001 --params=`$a, c/a$

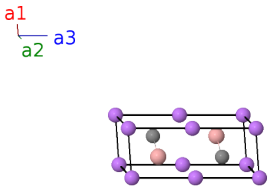
Other compounds with this structure

AgAsBa, AgAsEu, AgAsSr, AgBaBi, AgBaP, AgBaSb, AgBiCa, AgBiEu, AgBiSr, AgEuP, AgEuSb, AgPSr, AgSbSr, AlAuCe, AlAuTi, AlCeIr, AlDyZn, AlErZn, AlGaYb, AlGdZn, AlMnPt, AlPtTi, AlTmZn, AlYZn, AsAuBa, AsAuCa, AsAuEu, AsBaCu, AsBeNa, AsCaCu, AsCePd, AsCuEu, AsCuSr, AsHgK, AsKZn, AsLaPd, AsNdPd, AsPdSr, AsPtSr, AsSrZn, AuBaBi, AuBaP, AuBaSb, AuBiSr, AuCaP, AuCePb, AuCeSn, AuDySn, AuEuP, AuEuSb, AuGaTi, AuHoSn, AuKTe, AuLaPb, AuLiSn, AuNaTe, AuNdPb, AuNdSn, AuPbPr, AuPbSm, AuPdSn, AuPrSn, AuRbTe, AuSbSr, AuSmSn, AuSnTb, AuSnU, AuSnY, BaBiCu, BaCdGe, BaCuP, BaCuSb, BaGeZn, BaHgSn, BaLiP, BaLiSb, BaPbZn, BaSiZn, BaSnZn, BCLi, BeGeLa, BeHfSi, BeNaSb, BeSiZr, BiCaCu, BiCuEu, BiCuSr, BiCuYb, BiEuZn, BiSrZn, CaCuP, CaCuSb, CaGeZn, CaHgPb, CaHgSn, CaPbZn, CaSiZn, CaSnZn, CdCeTl, CdLaTl, CdNdTl, CdPrTl, CdSmTl, CeCuGe, CeCuIn, CeCuPb, CeCuSi, CeCuSn, CeGaZn, CeGeNi, CeHSe, CeInZn, CeNiSn, CePdSb, CePPd, CeTlZn, CoCrGe, CoFeGe, CoGeMn, CoGeU, CoMnSi, CoMnSn, CoNiSb, CoNiSn, CrFeSb, CsSbZn, CuDyGa, CuDyPb, CuDySi, CuDySn, CuErPb, CuErSi, CuErSn, CuEuP, CuEuSb, CuGaHf, CuGaU, CuGaZr, CuGdPb, CuGdSi, CuGdSn, CuGeHo, CuGeTm, CuGeYb, CuHoPb, CuHoSi, CuHoSn, CuKSe, CuKTe, CuLaPb, CuLaSi, CuLaSn, CuLuSi, CuLuSn, CuMnSb, CuNdSi, CuNdSn, CuPbPr, CuPbSm, CuPbYb, CuPrSi, CuPrSn, CuPSr, CuSbSr, CuSbYb, CuScSn, CuSiSm, CuSiTb, CuSiTm, CuSiY, CuSiYb, CuSmSn, CuSnTb, CuSnTm, CuSnU, CuSnY, DyGaZn, DyInZn, DyPdSb, DyTlZn, ErGaZn, ErInZn, ErTlZn, EuGeZn, EuPPd, EuPPt, EuSbZn, EuSiZn, FeGeMn, FeGeNi, FeMnSb, FeSbV, FLaSe, GaGdZn, GaLaZn, GaMnNi, GaMnPd, GaMnPt, GaNbRh, GaPrZn, GaPtTi, GaSmZn, GaTmZn, GaYZn, GdInZn, GdPdSb, GdPPd, GdTlZn, GeMnNi, GeNiU, HgKSb, HgPbYb, HoInZn, InLaZn, InNdZn, InPrZn, InSmZn, InYbZn, KLiS, KNaS, KPZn, KSbZn, LaNiSb, LaPdSb, LaPPd, LaTlZn, LiPSr, MnNiSi, MnSbZn, NdPdSb, NdPPd, NdTlZn, NiPtSn, NiPZr, NiSbV, PbSrZn, PdPrSb, PdSbSm, PdSbTb, PdSbU, PdSnU, PPdPr, PPdSm, PSrZn, RbSbZn, SbSrZn, SiSrZn, SmTlZn, SnSrZn

- This is the parent of the $Li_{1-x}BC$ Structure. The ICSD lists several different structure types for these compounds, but the Wykcoff positions are fixed so the only difference between the structures are the lattice constants. We lump all these structures together under one prototype. The order of the elements is alphabetical, we do not distinguish which element is on the (2a) site.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	B I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	B I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2d)	C I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(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.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017