LaB_2C_2 Structure: A2B2C_tP10_131_j_l_f-001

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https://aflow.org/p/XLRT

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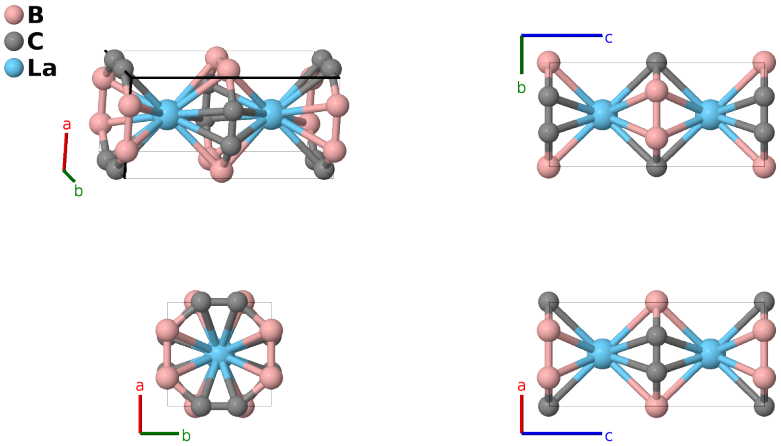


Prototype	B_2C_2La
AFLOW prototype label	A2B2C_tP10_131_j_l_f-001
ICSD	23300
Pearson symbol	tP10
Space group number	131
Space group symbol	$P4_2/mmc$
AFLOW prototype command	`aflow --proto=A2B2C_tP10_131_j_l_f-001 --params=`$a, c/a, x_2, x_3$

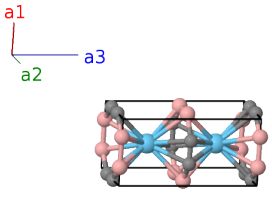
Other compounds with this structure

CaB_2C_2, CeB_2C_2, DyB_2C_2, EuB_2C_2, GdB_2C_2, HoB_2C_2, LuB_2C_2, NdB_2C_2, PrB_2C_2, SmB_2C_2, TbB_2C_2, TmB_2C_2, YB_2C_2, YbB_2C_2

- (Bauer, 1980) placed this structure in space group $P\bar{4}2c$ #112, with lanthanum atoms at the (2a) Wyckoff site, boron at (4h), and carbon at (4i). (Cenzual, 1991) showed that these Wyckoff positions imply an inversion site not present in $P\bar{4}2c$, and so the true space group is $P4_2/mmc$ #131.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2f)	La I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2f)	La I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1$	=	$ax_2\,\hat{\mathbf{x}}$	(4j)	B I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1$	=	$-ax_2\,\hat{\mathbf{x}}$	(4j)	B I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4j)	B I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4j)	B I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4l)	C I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4l)	C I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{y}}$	(4l)	C I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{y}}$	(4l)	C I

References

[1] J. Bauer and O. Bars, *The ordering of boron and carbon atoms in the LaB_2C_2 structure*, Acta Crystallogr. Sect. B **36**, 1540–1544 (1980), doi:10.1107/S0567740880006541.

Found in

[1] K. Cenzual, L. M. Gelato, M. Penzo, and E. Parthé, *Inorganic structure types with revised space groups. I*, Acta Crystallogr. Sect. B **47**, 433–439 (1991), doi:10.1107/S0108768191000903.