

α -Li₃BN₂ Structure:

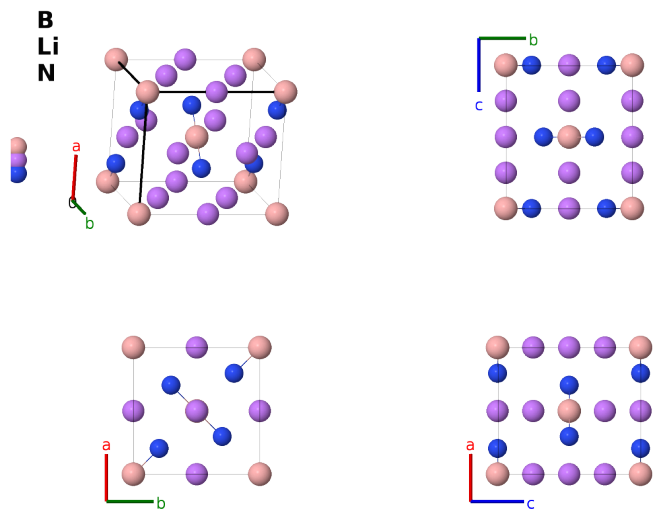
AB3C2_tP12_136_a_bd_f-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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.

<https://aflow.org/prototype-encyclopedia/2PDY>

https://aflow.org/prototype-encyclopedia/AB3C2_tP12_136_a_bd_f-001



Prototype	BLi ₃ N ₂
AFLOW prototype label	AB3C2_tP12_136_a_bd_f-001
ICSD	655673
CCDC	1765880
Pearson symbol	tP12
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	<pre>aflow --proto=AB3C2_tP12_136_a_bd_f-001 --params=a,c/a,x₄</pre>

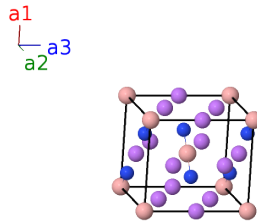
- (Yamane, 1987) find a phase transition from α - to β -Li₃BN₂ at 1135K. The β -Li₃BN₂ phase has space group $P2_1/c$ #14 and four formula units in a monoclinic cell, compared to two units in the α - phase, but they did not describe the atomic positions for β -Li₃BN₂.
- (Yamane, 1987) put this in space group $P4_22_12$ #94, but the positions of the lithium atoms are such that there is an inversion site, placing the system in space group $P4_2/mnm$ #136. (Cenzual, 1991)

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
$\mathbf{B}_1$	$=$	0	$=$	0	(2a) B I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a) B I
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2b) Li I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(2b) Li I
$\mathbf{B}_5$	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d) Li II
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d) Li II
$\mathbf{B}_7$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d) Li II
$\mathbf{B}_8$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d) Li II
$\mathbf{B}_9$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}}$	(4f) N I
$\mathbf{B}_{10}$	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}}$	(4f) N I
$\mathbf{B}_{11}$	$=$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f) N I
$\mathbf{B}_{12}$	$=$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f) N I

References

- [1] H. Yamane, S. Kikkawa, and M. Koizumi, *High- and low-temperature phases of lithium boron nitride, Li_3BN_2 : Preparation, phase relation, crystal structure, and ionic conductivity*, J. Solid State Chem. **71**, 1–11 (1987), doi:10.1016/0022-4596(87)90135-6.

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.

First cited in

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