α-Li_3BN_2 Structure: AB3C2_tP12_136_a_bd_f-001

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https://aflow.org/p/2PDY

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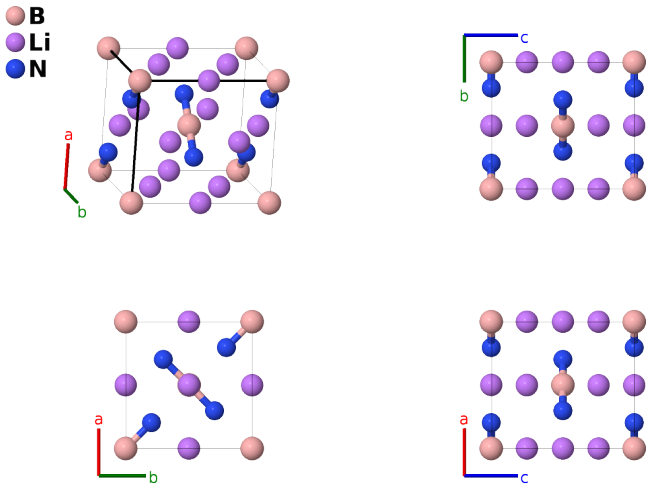
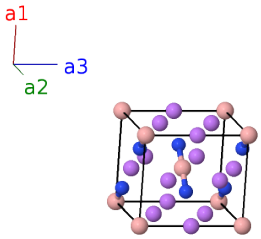


Prototype	BLi_3N_2
AFLOW prototype label	AB3C2_tP12_136_a_bd_f-001
ICSD	655673
Pearson symbol	tP12
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	`aflow --proto=AB3C2_tP12_136_a_bd_f-001 --params=`$a, c/a, x_4$

- (Yamane, 1987) find a phase transition from α- to β-Li_3BN_2 at 1135K. The β-Li_3BN_2 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-Li_3BN_2.
- (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 cite, 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
$\mathbf{B_{11}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	N I
$\mathbf{B_{12}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(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.