Li_3N Structure: A3B_hP4_191_bc_a-001

This structure originally had the label `A3B_hP4_191_bc_a`. Calls to that address will be redirected here.

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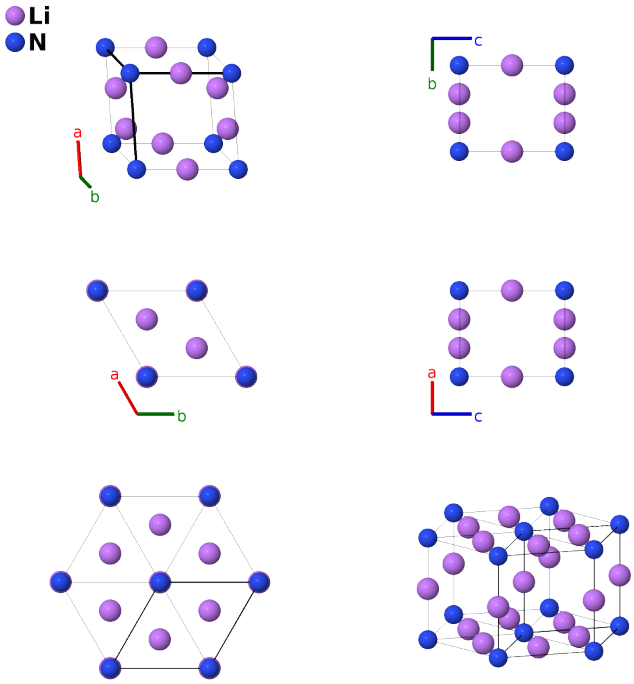
https://aflow.org/p/RYZL

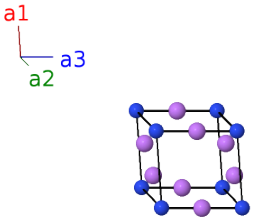
https://aflow.org/p/A3B_hP4_191_bc_a-001



Prototype	Li_3N
AFLOW prototype label	A3B_hP4_191_bc_a-001
ICSD	95939
Pearson symbol	hP4
Space group number	191
Space group symbol	$P6/mmm$
AFLOW prototype command	`aflow --proto=A3B_hP4_191_bc_a-001 --params=`$a, c/a$

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	(1a)	N I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Li I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Li II
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Li II

References

[1] D. H. Gregory, P. M. O'Meara, A. G. Gordon, J. P. Hodges, S. Short, and J. D. Jorgensen, *Structure of Lithium Nitride and Transition-Metal-Doped Derivatives, $Li_{3-x-y}M_xN$ (M = Ni, Cu): A Powder Neutron Diffraction Study*, Chem. Mater. **14**, 2063–2070 (2002), doi:10.1021/cm010718t.

Found in

[1] P. Villars, K. Cenzual, J. Daams, R. Gladyshevskii, O. Shcherban, V. Dubenskyy, N. Melnichenko-Koblyuk, O. Pavlyuk, I. Savysyuk, S. Stoyko, and L. Sysa, *Structure Types. Part 3: Space Groups (194)$P6_3/mmc$-(190)P-62c·Li_3N* (2006). Landolt-Börnstein - Group III Condensed Matter 43A6 (Springer-Verlag Berlin Heidelberg).