α-$LiNH_2$ Structure: A2BC_tI32_82_2g_ace_g-001

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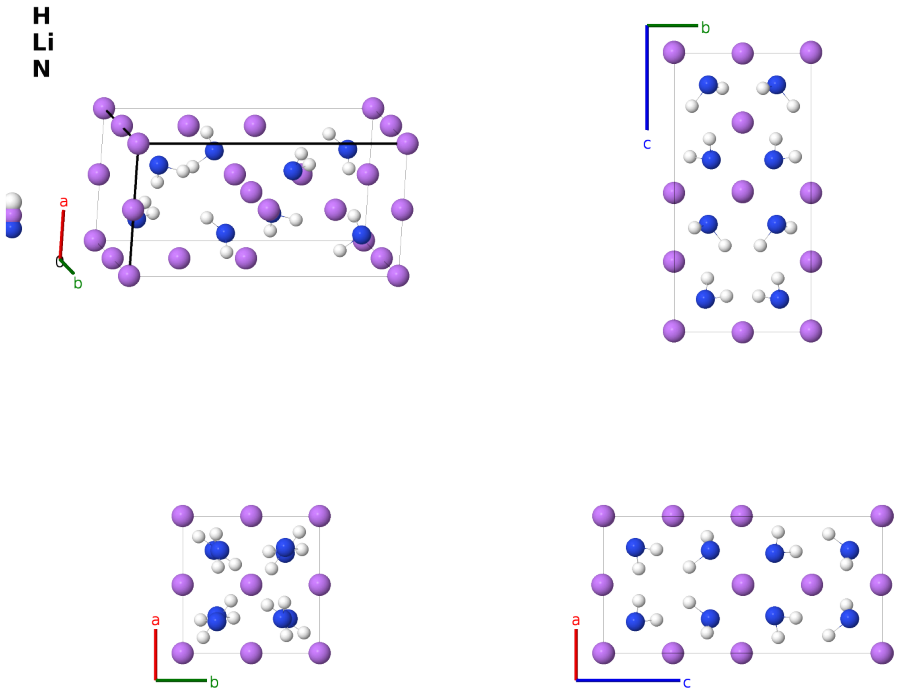
https://aflow.org/prototype-encyclopedia/UMLP

https://aflow.org/prototype-encyclopedia/A2BC_tI32_82_2g_ace_g-001

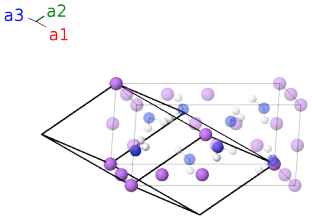


Prototype	H_2LiN
AFLOW prototype label	A2BC_tI32_82_2g_ace_g-001
ICSD	154395
CCDC	1671029
Pearson symbol	tI32
Space group number	82
Space group symbol	$I\bar{4}$
AFLOW prototype command	`aflow --proto=A2BC_tI32_82_2g_ace_g-001 --params=`$a, c/a, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- Under pressure $LiNH_2$ has at least three phases (Yamawaki, 2014): tetragonal α-$LiNiH_2$, or Phase I, the ground state, stable up to 10GPa. (this structure)
- Monoclinic Phase II, stable between 10 and 13 GPa.
- β-$LiNH_2$, or Phase III, is stable above 13 GPa. The structure is very uncertain. (Yamawaki, 2014) discuss two possible structures: orthorhombic space group $Pccn$ #56 and body-centered orthorhombic space group $Iba2$ #45.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Li I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Li II
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	Li III
$\mathbf{B_4}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	Li III
$\mathbf{B_5}$	=	$(y_4+z_4)\,\mathbf{a}_1 + (x_4+z_4)\,\mathbf{a}_2 + (x_4+y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8g)	H I
$\mathbf{B_6}$	=	$-(y_4-z_4)\,\mathbf{a}_1 - (x_4-z_4)\,\mathbf{a}_2 - (x_4+y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8g)	H I
$\mathbf{B_7}$	=	$-(x_4+z_4)\,\mathbf{a}_1 + (y_4-z_4)\,\mathbf{a}_2 - (x_4-y_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8g)	H I
$\mathbf{B_8}$	=	$(x_4-z_4)\,\mathbf{a}_1 - (y_4+z_4)\,\mathbf{a}_2 + (x_4-y_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8g)	H I
$\mathbf{B_9}$	=	$(y_5+z_5)\,\mathbf{a}_1 + (x_5+z_5)\,\mathbf{a}_2 + (x_5+y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8g)	H II
$\mathbf{B_{10}}$	=	$-(y_5-z_5)\,\mathbf{a}_1 - (x_5-z_5)\,\mathbf{a}_2 - (x_5+y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8g)	H II
$\mathbf{B_{11}}$	=	$-(x_5+z_5)\,\mathbf{a}_1 + (y_5-z_5)\,\mathbf{a}_2 - (x_5-y_5)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8g)	H II
$\mathbf{B_{12}}$	=	$(x_5-z_5)\,\mathbf{a}_1 - (y_5+z_5)\,\mathbf{a}_2 + (x_5-y_5)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8g)	H II
$\mathbf{B_{13}}$	=	$(y_6+z_6)\,\mathbf{a}_1 + (x_6+z_6)\,\mathbf{a}_2 + (x_6+y_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8g)	N I
$\mathbf{B_{14}}$	=	$-(y_6-z_6)\,\mathbf{a}_1 - (x_6-z_6)\,\mathbf{a}_2 - (x_6+y_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8g)	N I
$\mathbf{B_{15}}$	=	$-(x_6+z_6)\,\mathbf{a}_1 + (y_6-z_6)\,\mathbf{a}_2 - (x_6-y_6)\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8g)	N I

$$\mathbf{B_{16}} = (x_6 - z_6)\,\mathbf{a}_1 - (y_6 + z_6)\,\mathbf{a}_2 + (x_6 - y_6)\,\mathbf{a}_3 = -ay_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad (8g) \quad \text{N I}$$

References

[1] J. B. Yang, X. D. Zhou, Q. Cai, W. J. James, and W. B. Yelon, *Crystal and electronic structures of $LiNH_2$*, Appl. Phys. Lett. **88**, 041914 (2006), doi:10.1063/1.2163258.

[2] H. Yamawaki, H. Fujihisa, Y. Gotoh, and S. Nakano, *Structure of Intermediate Phase II of $LiNH_2$ under High Pressure*, J. Phys. Chem. B **118**, 9991–9996 (2014), doi:10.1021/jp505133q.

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