β-$LiNH_2$ ($Iba2$) Structure: A2BC_oI32_45_2c_c_c-001

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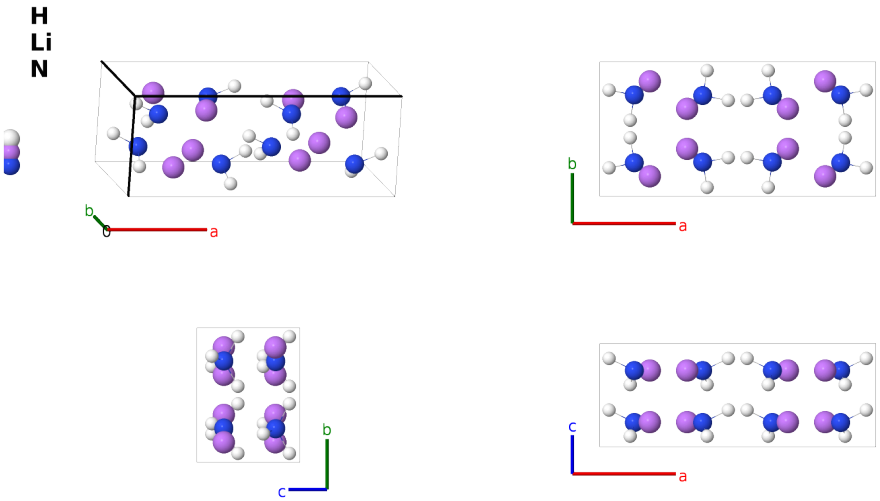
https://aflow.org/prototype-encyclopedia/ZBD3

https://aflow.org/prototype-encyclopedia/A2BC_oI32_45_2c_c_c-001

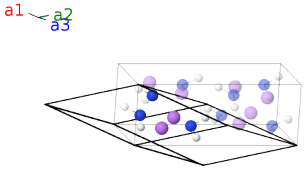


Prototype	H_2LiN
AFLOW prototype label	A2BC_oI32_45_2c_c_c-001
ICSD	116487
CCDC	2273728
Pearson symbol	oI32
Space group number	45
Space group symbol	$Iba2$
AFLOW prototype command	`aflow --proto=A2BC_oI32_45_2c_c_c-001 --params=`$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

- 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.
- 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 (this structure).

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$(y_1+z_1)\,\mathbf{a}_1+(x_1+z_1)\,\mathbf{a}_2+(x_1+y_1)\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}}+by_1\,\hat{\mathbf{y}}+cz_1\,\hat{\mathbf{z}}$	(8c)	H I
$\mathbf{B_2}$	=	$-(y_1-z_1)\,\mathbf{a}_1-(x_1-z_1)\,\mathbf{a}_2-(x_1+y_1)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}}-by_1\,\hat{\mathbf{y}}+cz_1\,\hat{\mathbf{z}}$	(8c)	H I
$\mathbf{B_3}$	=	$\left(-y_1+z_1+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_1+z_1+\frac{1}{2}\right)\,\mathbf{a}_2+(x_1-y_1)\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}}-by_1\,\hat{\mathbf{y}}+c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	H I
$\mathbf{B_4}$	=	$\left(y_1+z_1+\frac{1}{2}\right)\,\mathbf{a}_1+\left(-x_1+z_1+\frac{1}{2}\right)\,\mathbf{a}_2-(x_1-y_1)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}}+by_1\,\hat{\mathbf{y}}+c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	H I
$\mathbf{B_5}$	=	$(y_2+z_2)\,\mathbf{a}_1+(x_2+z_2)\,\mathbf{a}_2+(x_2+y_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}+by_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(8c)	H II
$\mathbf{B_6}$	=	$-(y_2-z_2)\,\mathbf{a}_1-(x_2-z_2)\,\mathbf{a}_2-(x_2+y_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}-by_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(8c)	H II
$\mathbf{B_7}$	=	$\left(-y_2+z_2+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_2+z_2+\frac{1}{2}\right)\,\mathbf{a}_2+(x_2-y_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}-by_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	H II
$\mathbf{B_8}$	=	$\left(y_2+z_2+\frac{1}{2}\right)\,\mathbf{a}_1+\left(-x_2+z_2+\frac{1}{2}\right)\,\mathbf{a}_2-(x_2-y_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}+by_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	H II
$\mathbf{B_9}$	=	$(y_3+z_3)\,\mathbf{a}_1+(x_3+z_3)\,\mathbf{a}_2+(x_3+y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}+by_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(8c)	Li I
$\mathbf{B_{10}}$	=	$-(y_3-z_3)\,\mathbf{a}_1-(x_3-z_3)\,\mathbf{a}_2-(x_3+y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(8c)	Li I
$\mathbf{B_{11}}$	=	$\left(-y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2+(x_3-y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Li I
$\mathbf{B_{12}}$	=	$\left(y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(-x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2-(x_3-y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}+by_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Li I
$\mathbf{B_{13}}$	=	$(y_4+z_4)\,\mathbf{a}_1+(x_4+z_4)\,\mathbf{a}_2+(x_4+y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_{14}}$	=	$-(y_4-z_4)\,\mathbf{a}_1-(x_4-z_4)\,\mathbf{a}_2-(x_4+y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_{15}}$	=	$\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2+(x_4-y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_{16}}$	=	$\left(y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(-x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2-(x_4-y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	N I

References

[1] 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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