

LiNiN	<i>hP3</i>	(187) <i>P-6m2</i> – cba
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# LiNiN [1]

Structural features: Close-packed Li and Ni layers in h stacking; N in trigonal voids in the Li layers. N(Li<sub>3</sub>Ni<sub>2</sub>) trigonal bipyramids share vertices to form a 3D-framework.

Barker M.G. et al. (1999) [1]

LiNNi

$a = 0.3758$ ,  $c = 0.354$  nm,  $c/a = 0.942$ ,  $V = 0.0433$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Li1	1 <i>c</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0		coplanar triangle N <sub>3</sub>
Ni2	1 <i>b</i>	-6 <i>m2</i>	0	0	$\frac{1}{2}$		colinear N <sub>2</sub>
N3	1 <i>a</i>	-6 <i>m2</i>	0	0	0		trigonal bipyramid Ni <sub>2</sub> Li <sub>3</sub>

Transformation from published data: origin shift  $\frac{2}{3} \frac{1}{3} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.037, T = 297 K

References: [1] Barker M.G., Blake A.J., Edwards P.P., Gregory D.H., Hamor T.A., Siddons D.J., Smith S.E. (1999), Chem. Commun. (Cambridge) 1999, 1187-1188.