

$\text{Li}_5\text{Ni}_3\text{N}_3$	$hP11$	(189) $P\text{-}62m\text{-}gf^2c$
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**$\text{Li}_5\text{Ni}_3\text{N}_3$  [2]**

Structural features:  $\text{N}(\text{Li}_4\text{Ni}_2)$  octahedra share vertices to form a 3D-framework.

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

$\text{Li}_5\text{N}_3\text{Ni}_3$

$a = 0.6475$ ,  $c = 0.3555$  nm,  $c/a = 0.549$ ,  $V = 0.1291$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ni1	$3g$	$m2m$	0.3557	0	$\frac{1}{2}$		non-colinear $\text{N}_2$
N2	$3f$	$m2m$	0.3537	0	0		octahedron $\text{Ni}_2\text{Li}_4$
Li3	$3f$	$m2m$	0.7281	0	0		non-colinear $\text{N}_2$
Li4	$2c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	0		coplanar triangle $\text{N}_3$

Transformation from published data:  $-x, -y, -z$ ; origin shift  $0\ 0\ \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.035$ ,  $T = 293$  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. [2] Klatyk J., Höhn P., Kniep R. (1998), Z. Kristallogr., New Cryst. Struct. 213, 31.