

LaNiInH <sub>1.63</sub>	<i>hP</i> 16	(189) <i>P</i> -62 <i>m</i> – hgf <sup>2</sup> da
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**LaNiInH<sub>1.63</sub>** [1]

Structural features: Filled-up derivative of ZrNiAl with H in tetrahedral (La<sub>3</sub>Ni) and octahedral (La<sub>3</sub>NiIn<sub>2</sub>) voids; H<sub>2</sub> pairs (0.171 nm).

Denys R.V. et al. (2003) [1]

D<sub>1.64</sub>InLaNi

$a = 0.73874$ ,  $c = 0.46816$  nm,  $c/a = 0.634$ ,  $V = 0.2213$  nm<sup>3</sup>,  $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
D1	4 <i>h</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.183	0.96	colinear NiD
In2	3 <i>g</i>	<i>m2m</i>	0.247	0	$\frac{1}{2}$		non-colinear D <sub>2</sub>
D3	3 <i>f</i>	<i>m2m</i>	0.226	0	0	0.36	single atom Ni
La4	3 <i>f</i>	<i>m2m</i>	0.603	0	0		trigonal prism D <sub>6</sub>
Ni5	2 <i>d</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		colinear D <sub>2</sub>
Ni6	1 <i>a</i>	-62 <i>m</i>	0	0	0		coplanar triangle D <sub>3</sub>

Transformation from published data: origin shift 0 0  $\frac{1}{2}$

Experimental: powder, diffractometer, neutrons, R<sub>p</sub> = 0.031, T = 298 K, p(H<sub>2</sub>) = 0.46 MPa

References: [1] Denys R.V., Riabov A.B., Yartys V.A., Hauback B.C., Brinks H.W. (2003), J. Alloys Compd. 356/357, 65-68.