

NdNiInH <sub>1.7</sub>	<i>hP</i> 19	(189) <i>P</i> -62 <i>m</i> – khgfda
------------------------	--------------	--------------------------------------

**NdNiInH<sub>1.7</sub>** [1]

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

Bulyk I.I. et al. (1999) [1]

H<sub>1.67</sub>InNdNi

$a = 0.7256$ ,  $c = 0.4633$  nm,  $c/a = 0.639$ ,  $V = 0.2112$  nm<sup>3</sup>,  $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
H1	6 <i>k</i>	<i>m</i> ..	0.3518	0.4286	$\frac{1}{2}$	0.5	single atom H
H2	4 <i>h</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1343	0.5	single atom H
In3	3 <i>g</i>	<i>m2m</i>	0.232	0	$\frac{1}{2}$		non-colinear H <sub>2</sub>
Nd4	3 <i>f</i>	<i>m2m</i>	0.5841	0	0		non-coplanar square H <sub>4</sub>
Ni5	2 <i>d</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		trigonal bipyramid H <sub>5</sub>
Ni6	1 <i>a</i>	-62 <i>m</i>	0	0	0		tricapped trigonal prism In <sub>6</sub> Nd <sub>3</sub>

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

Experimental: powder, diffractometer, X-rays

Remarks: H could not be located with certainty, alternative models are also proposed. Short interatomic distances for partly occupied site(s).

References: [1] Bulyk I.I., Yartys V.A., Denys R.V., Kalychak Y.M., Harris I.R. (1999), J. Alloys Compd. 284, 256-261.