

LaNi ₅ H ₇	<i>hP</i> 34	(186) <i>P</i> 6 ₃ <i>mc</i> – c ⁴ b ⁴ a
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LaNi₅H_{6.7} [1]

Structural features: Filled-up derivative of CaCu₅ with H in tetrahedral (Ni₄ and La₂Ni₂) and trigonal bipyramidal (La₂Ni₃) voids.

Lartigue C. et al. (1987) [1]

D₇LaNi₅

$a = 0.5409$, $c = 0.86$ nm, $c/a = 1.590$, $V = 0.2179$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
D1	6 <i>c</i>	. <i>m</i> .	0.1596	0.8404	0.2414	0.92	non-colinear D ₂
Ni2	6 <i>c</i>	. <i>m</i> .	0.4975	0.5025	0.2718		7-vertex polyhedron D ₇
D3	6 <i>c</i>	. <i>m</i> .	0.504	0.496	0.4662		coplanar triangle Ni ₃
D4	6 <i>c</i>	. <i>m</i> .	0.8404	0.1596	0.2414	0.08	non-colinear D ₂
Ni5	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0329		tetrahedron D ₄
D6	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.2081	0.2	7-vertex polyhedron Ni ₄ D ₃
Ni7	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5194		tetrahedron D ₄
D8	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.7081	0.8	7-vertex polyhedron Ni ₄ D ₃
La9	2 <i>a</i>	3 <i>m</i> .	0	0	0.0		18-vertex polyhedron D ₁₈

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.9782

Experimental: powder, diffractometer, neutrons, wR_p = 0.072

Remarks: Phase referred to as γ-LaNi₅H_x (β-LaNi₅H_x until the discovery of an intermediate LaNi₅H₃ phase). Supersedes an earlier refinement on the same diffraction data [2] where seven H sites were found. The authors state that space group (159) *P*31*c* could not be rejected ($R = 0.077$), however, the structure proposed in this space group presents strong pseudo-symmetry (186) *P*6₃*mc*.

References: [1] Lartigue C., Le Bail A., Percheron Guégan A. (1987), J. Less-Common Met. 129, 65-76.
[2] Lartigue C., Percheron Guégan A., Achard J.C., Soubeyroux J.L. (1985), J. Less-Common Met. 113, 127-148.