$LaNi_5H_5$	*hP*52	(186) $P6_3mc$ – dc^5b^4a

$LaNi_5H_5$ [1]
Structural features: Filled-up derivative of $CaCu_5$ with H in tetrahedral (Ni_4, $LaNi_3$ and La_2Ni_2) and trigonal bipyramidal (La_2Ni_3) voids.

Lartigue C. et al. (1985) [1]
D_5LaNi_5
a = 0.5395, c = 0.8484 nm, c/a = 1.573, V = 0.2139 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12*d*	1	0.0	0.48	0.456	0.39	
D2	6*c*	.*m*.	0.146	0.854	0.25	0.297	single atom D
D3	6*c*	.*m*.	0.225	0.775	0.167	0.113	non-colinear D_2
Ni4	6*c*	.*m*.	0.5	0.5	0.25		non-coplanar square D_4
D5	6*c*	.*m*.	0.775	0.225	0.167	0.113	non-colinear D_2
D6	6*c*	.*m*.	0.854	0.146	0.25	0.297	single atom D
Ni7	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.0		
D8	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.2	0.1	non-coplanar triangle D_3
Ni9	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.5		
D10	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.7	0.1	non-coplanar triangle D_3
La11	2*a*	3*m*.	0	0	0.0		

Transformation from published data: -*x*,-*y*,-*z*
Experimental: powder, diffractometer, neutrons, wR = 0.023, T = 363 K, p(H_2) = 2.40 MPa

Remarks: Short interatomic distances for partly occupied site(s). Space groups (163) $P\bar{3}1c$, (173) $P6_3$, (176) $P6_3/m$, (190) $P\bar{6}2c$, and (194) $P6_3/mmc$ were tested and rejected. Refinement on the same diffraction data in [2] revealed only five H sites.

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