$Mg_2NiH_{0.3}$	*hP*36	(180) $P6_222$ – kjifca

$Mg_2NiH_{0.3}$ [1]
Structural features: Filled-up derivative of Mg_2Ni with H in trigonal (Mg_2Ni) and tetrahedral (Mg_2Ni_2) voids.

Soubeyroux J.L. et al. (1984) [1]
$D_{0.24}Mg_2Ni$
a = 0.5256, c = 1.3435 nm, c/a = 2.556, V = 0.3214 nm^3, Z = 6

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12*k*	1	0.32	0.2	0.04	0.052	square pyramid Ni_2DMg_2
Mg2	6*j*	..2	0.158	0.316	$^1/_2$		non-colinear D_2
D3	6*i*	..2	0.33	0.66	0	0.135	trigonal bipyramid $NiMg_2D_2$
Mg4	6*f*	2..	$^1/_2$	0	0.377		4-vertex polyhedron D_4
Ni5	3*c*	222	$^1/_2$	0	0		octahedron D_6
Ni6	3*a*	222	0	0	0		tetrahedron D_4

Transformation from published data: origin shift 0 0 $^1/_2$
Experimental: powder, diffractometer, neutrons, R_B = 0.050, T = 573 K

Remarks: Two alternative models gave similar R factors but too short Mg-D interatomic distances. A different hydrogen distribution is proposed in [2].

References: [1] Soubeyroux J.L., Fruchart D., Mikou A., Pezat M., Darriet B. (1984), Mater. Res. Bull. 19, 895-904. [2] Noréus D., Werner P.E. (1982), Acta Chem. Scand. A 36, 847-851.