

Mg₂NiH_{0.3}*hP21*(180) *P6₂22* – jfdca**Mg₂NiH_{0.3}** [1]Structural features: Filled-up derivative of Mg₂Ni with H between two Mg atoms.

Noréus D., Werner P.E. (1982) [1]

H_{0.30}Mg₂Ni $a = 0.52315$, $c = 1.3404$ nm, $c/a = 2.562$, $V = 0.3177$ nm³, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Mg1	6 <i>j</i>	..2	0.16	0.32	$\frac{1}{2}$	0.6	icosahedron Ni ₄ Mg ₅ H ₃
Mg2	6 <i>f</i>	2..	$\frac{1}{2}$	0	0.3609		single atom H
H3	3 <i>d</i>	222	$\frac{1}{2}$	0	$\frac{1}{2}$		colinear Mg ₂
Ni4	3 <i>c</i>	222	$\frac{1}{2}$	0	0		bicapped square antiprism Ni ₂ Mg ₈
Ni5	3 <i>a</i>	222	0	0	0		bicapped square antiprism Ni ₂ Mg ₈

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

Experimental: powder, film, X-rays, R = 0.200

Remarks: In [1] the atom coordinates of the H site are misprinted as 0 0 $\frac{1}{2}$ instead of $\frac{1}{2}$ 0 0 (agreement with Wyckoff position 3*c*; checked on the drawing of the structure).

References: [1] Noréus D., Werner P.E. (1982), Acta Chem. Scand. A 36, 847-851.