

MgNi ₃ B ₂	<i>hP</i> 18	(180) <i>P</i> 6 ₂ 22 – ifda
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MgNi_{2.5}B₂ [2]; Li_{1.2}Ni_{2.5}B₂ [2]

Structural features: Kagomé-mesh Ni₃ layers and MgB₂ layers alternate along [001]. BNi₆ trigonal prisms share edges to form infinite slabs. Deformation derivative of CeCo₃B₂ with formation of B₂ pairs perpendicular to [001].

Gross K.J. et al. (1998) [1]

B₂MgNi₃

$a = 0.48799$, $c = 0.87859$ nm, $c/a = 1.800$, $V = 0.1812$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
B1	6 <i>i</i>	..2	0.6146	0.2292	0		7-vertex polyhedron BNi ₆
Ni2	6 <i>f</i>	2..	$\frac{1}{2}$	0	0.208		tetrahedron B ₄
Ni3	3 <i>d</i>	222	$\frac{1}{2}$	0	$\frac{1}{2}$		14-vertex Frank-Kasper B ₄ Ni ₆ Mg ₄
Mg4	3 <i>a</i>	222	0	0	0		pseudo Frank-Kasper B ₆ Ni ₁₂ Mg ₂

Experimental: powder, diffractometer, X-rays, R_B = 0.042

Remarks: Refinement of the site occupancies showed no significant deviation from unity.

References: [1] Gross K.J., Züttel A., Schlapbach L. (1998), J. Alloys Compd. 274, 234-238. [2] Jung W. (1977), Z. Naturforsch. B 32, 1371-1374.