

MgZn₂ [2], Laves phase 2H, Friauf phase hexagonal, Strukturbericht notation C14; WFe₂ [3]

Structural features: Mg(Mg₄Zn₁₂) Friauf polyhedra (Zn₁₂ truncated tetrahedron + Mg₄ tetrahedron) share the hexagonal faces of the truncated tetrahedra to form a 3D-framework. Zn₄ tetrahedra share faces and vertices to form infinite columns parallel to [001]. Kagomé-mesh Zn₃ and puckered triangle-mesh Mg₂Zn layers alternate along [001]. Laves-type slabs in h stacking. Tetrahedrally close-packed structure (Frank-Kasper phase). See Fig. III.21.

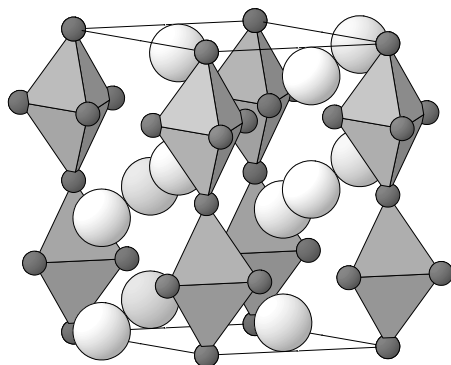


Fig. III.21. **MgZn₂**

Arrangement of Zn₄ tetrahedra (Zn atoms small) and Mg atoms (large).

Wandahl G., Christensen A.N. (1989) [1]

MgZn₂

$a = 0.52234$, $c = 0.85562$ nm, $c/a = 1.638$, $V = 0.2022$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zn1	6h	<i>mm</i> 2	0.1697	0.3394	$\frac{1}{4}$		icosahedron Zn ₆ Mg ₆
Mg2	4f	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5629		16-vertex Frank-Kasper Zn ₁₂ Mg ₄
Zn3	2a	-3 <i>m</i> .	0	0	0		icosahedron Zn ₆ Mg ₆

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

Experimental: single crystal, diffractometer, neutrons, R = 0.030

Remarks: Strukturbericht notation C41 was defined on WFe₂.

References: [1] Wandahl G., Christensen A.N. (1989), Acta Chem. Scand. 43, 296-297. [2] (1931), Strukturberichte 1, 180,228. [3] Arnfelt H., Westgren A. (1935), Jernkontorets Ann. 1935, 185-196.