

LuMn ₅	<i>hP</i> 12	(186) <i>P6₃mc</i> – <i>cb</i> ² <i>a</i>
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LuMn₅ [1]

Structural features: Lu(Mn₁₆) and Mn(Lu₄Mn₁₂) Friauf polyhedra (Mn₁₂ truncated tetrahedron + Mn₄/Lu₄ tetrahedron) share faces of the truncated tetrahedra to form a 3D-framework. Kagomé-mesh Mn₃ and puckered triangle-mesh LuMn₂ layers alternate along [001]. Substitution derivative of MgZn₂ (hexagonal Laves phase). Tetrahedrally close-packed structure (Frank-Kasper phase).

Wang F.E., Gilfrich J.V. (1966) [1]

LuMn₅

a = 0.5186, *c* = 0.8566 nm, *c/a* = 1.652, *V* = 0.1995 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Mn1	6 <i>c</i>	. <i>m</i> .	0.833	0.167	0.232		icosahedron Mn ₉ Lu ₃
Mn2	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.043		16-vertex Frank-Kasper Mn ₁₂ Lu ₄
Lu3	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.435		16-vertex Frank-Kasper Mn ₁₆
Mn4	2 <i>a</i>	3 <i>m</i> .	0	0	0.000		icosahedron Mn ₉ Lu ₃

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.815

Experimental: single crystal, precession and Weissenberg photographs, X-rays, *R* = 0.090

Remarks: In table 3 of [1] the *z*-coordinate of former Mn(b) is misprinted as 0.358 instead of -0.358 (checked on interatomic distances); on page 479 the cell volume is misprinted as 184.7 Å³ instead of 199.5 Å³.

References: [1] Wang F.E., Gilfrich J.V. (1966), *Acta Crystallogr.* 21, 476-481.