$Mg(Cu_{0.54}Al_{0.46})_2$	*hP*36	(187) *P*-6*m*2 – $n^2kji^3h^3g^3$

Mn(Cu,Al)$_2$ 6H [1], Laves phase 6H
Structural features: $(Cu,Al)_4$ tetrahedra share faces and vertices to form a 3D-framework. Laves-type slabs in hch_3c stacking. Tetrahedrally close-packed structure (Frank-Kasper phase).

Kitano Y. et al. (1977) [1]
$Al_{0.92}Cu_{1.08}Mg$
a = 0.510, c = 2.50 nm, c/a = 4.902, V = 0.5631 nm^3, Z = 12

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	6*n*	.*m*.	0.16667	0.83333	0.16667		icosahedron Cu_6Mg_6
M2	6*n*	.*m*.	0.5	0.5	0.33333		icosahedron Cu_6Mg_6
M3	3*k*	*mm*2	0.83333	0.16667	$^1/_2$		icosahedron Cu_6Mg_6
M4	3*j*	*mm*2	0.5	0.5	0		icosahedron Cu_6Mg_6
Mg5	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.10417		16-vertex Frank-Kasper $Cu_{12}Mg_4$
Mg6	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.22917		16-vertex Frank-Kasper $Cu_{12}Mg_4$
M7	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.41667		icosahedron Cu_6Mg_6
M8	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.08333		icosahedron Cu_6Mg_6
M9	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.25		icosahedron Cu_6Mg_6
Mg10	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.4375		16-vertex Frank-Kasper $Cu_{12}Mg_4$
Mg11	2*g*	3*m*.	0	0	0.0625		16-vertex Frank-Kasper $Cu_{12}Mg_4$
Mg12	2*g*	3*m*.	0	0	0.27083		16-vertex Frank-Kasper $Cu_{12}Mg_4$
Mg13	2*g*	3*m*.	0	0	0.39583		16-vertex Frank-Kasper $Cu_{12}Mg_4$

M1 = 0.54Cu + 0.46Al; M2 = 0.54Cu + 0.46Al; M3 = 0.54Cu + 0.46Al; M4 = 0.54Cu + 0.46Al; M7 = 0.54Cu + 0.46Al; M8 = 0.54Cu + 0.46Al; M9 = 0.54Cu + 0.46Al
Transformation from published data: -*x*,-*y*,-*z*; origin shift $^1/_3$ $^2/_3$ $^1/_2$
Experimental: foil, electron diffraction

Remarks: Idealized coordinates. We assigned an approximate Al/Cu ratio to sites M based on the nominal composition (multiphase sample).

References: [1] Kitano Y., Komura Y., Kajiwara H. (1977), Trans. Jpn. Inst. Met. 18, 39-45.