

$\text{Mg}_2\text{Cu}_6\text{Al}_5$ *cP39**(200) Pm-3 – jihgfa***Mg₂Cu₆Al₅** [1]

Structural features: AlCu_{12} icosahedra and empty Cu_6 octahedra in a CsCl-type arrangement, separated by additional Al and Mg atoms. Ordering variant of $\text{Mg}_2\text{Zn}_{11}$.

Samson S. (1949) [1]

 $\text{Al}_5\text{Cu}_6\text{Mg}_2$ $a = 0.8311 \text{ nm}$, $V = 0.5741 \text{ nm}^3$, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cu1	12 <i>j</i>	<i>m</i> ..	0	0.164	0.257		icosahedron $\text{Al}_4\text{Cu}_5\text{Mg}_3$
Al2	8 <i>i</i>	.3.	0.285	0.285	0.285		icosahedron $\text{Cu}_6\text{Al}_3\text{Mg}_3$
Cu3	6 <i>h</i>	<i>mm</i> 2..	0.275	$\frac{1}{2}$	$\frac{1}{2}$		10-vertex polyhedron Al_6Cu_4
Al4	6 <i>g</i>	<i>mm</i> 2..	0.34	$\frac{1}{2}$	0		pseudo Frank-Kasper $\text{Cu}_4\text{Al}_5\text{Mg}_4$
Mg5	6 <i>f</i>	<i>mm</i> 2..	0.18	0	$\frac{1}{2}$		7-capped pentagonal prism $\text{Cu}_8\text{Al}_8\text{Mg}$
Al6	1 <i>a</i>	<i>m</i> -3.	0	0	0		icosahedron Cu_{12}

Transformation from published data: *y*,*x*,*-z*; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, Weissenberg and rotation photographs, X-rays

References: [1] Samson S. (1949), Acta Chem. Scand. 3, 809-834.