

$\text{Mg}_8\text{Cu}_2\text{Al}_4\text{Si}_7$ $hP21$ (174) $P-6 - k^3j^3eda$ **$\text{Mg}_{12-x}\text{Cu}_2\text{Al}_x\text{Si}_7$** [1]

Structural features: Infinite columns of base-linked $\text{Si}(\text{Mg}_4\text{Al}_2)(\text{Mg}_2\text{Cu})$, $\text{SiMg}_6(\text{MgAlCu})$ and SiMg_6Al_3 tricapped trigonal prisms (partial substitution of Al for Mg ignored) share atoms to form a 3D-framework with AlB_2 -type (BaLiSi) columns (4 prisms in the triangular cross-section). CuSi_3 trigonal units.

Arnberg L., Aurivillius B. (1980) [1]

$\text{Al}_4\text{Cu}_2\text{Mg}_8\text{Si}_7$

$a = 1.03932$, $c = 0.40173$ nm, $c/a = 0.387$, $V = 0.3758$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	$3k$	$m..$	0.04567	0.19203	$\frac{1}{2}$		7-capped pentagonal prism $\text{Si}_5\text{Cu}_2\text{Mg}_8\text{Al}_2$
Si2	$3k$	$m..$	0.08227	0.46583	$\frac{1}{2}$		tricapped trigonal prism CuAl_2Mg_6
Mg3	$3k$	$m..$	0.45447	0.32533	$\frac{1}{2}$		pseudo Frank-Kasper $\text{Si}_6\text{Al}_4\text{Mg}_8$
Si4	$3j$	$m..$	0.24887	0.19543	0		tricapped trigonal prism CuAlMg_7
Mg5	$3j$	$m..$	0.29987	0.47383	0		7-capped pentagonal prism $\text{Si}_5\text{Cu}_2\text{Mg}_8\text{Al}_2$
Al6	$3j$	$m..$	0.42617	0.09083	0		tetrahedron Si_4
Si7	$1e$	$-6..$	$\frac{2}{3}$	$\frac{1}{3}$	0		tricapped trigonal prism Al_3Mg_6
Cu8	$1d$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		tricapped trigonal prism Si_3Mg_6
Cu9	$1a$	$-6..$	0	0	0		tricapped trigonal prism Si_3Mg_6

$\text{M1} = 0.667\text{Mg} + 0.333\text{Al}$

Transformation from published data: origin shift $\frac{1}{3} \frac{2}{3} 0$

Experimental: single crystal, diffractometer, X-rays, $R = 0.109$

Remarks: Phase referred to as $h\text{-(AlCuMgSi)}$. The authors suggest correct space group may be (176) $P6_3/m$ and the structure partly disordered.

References: [1] Arnberg L., Aurivillius B. (1980), Acta Chem. Scand. A 34, 1-5.