

Cu_{12.7}Cr₁₉Al_{83.8}

hP244

(176) $P6_3/m - i^{14}h^{11}fcb$ a**Al_{72.6}Cr_{16.4}Cu_{11.0} ζ-phase [1]**

Structural features: A dense 3D-framework with mainly icosahedral coordination.

Sugiyama K. et al. (2002) [1]

Al_{83.57}Cr_{19.38}Cu_{12.56} $a = 1.7714$, $c = 1.2591$ nm, $c/a = 0.711$, $V = 3.4216$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cu1	12i	1	0.0128	0.14217	0.04496		pseudo Frank-Kasper Al ₈ Cu ₃
M2	12i	1	0.0349	0.27734	0.13913		14-vertex Frank-Kasper Cu ₂ Al ₁₀ Cr ₂
M3	12i	1	0.05868	0.43306	0.0633		14-vertex Frank-Kasper CuAl ₁₀ Cr ₃
Al4	12i	1	0.08511	0.60192	0.06911		tricapped pentagonal prism Cr ₂ Al ₁₀ Cu
Al5	12i	1	0.12278	0.13522	0.14831		icosahedron Cu ₆ Al ₅ Cr
Al6	12i	1	0.20409	0.40931	0.0697		tricapped pentagonal prism Cr ₂ Al ₁₀ Cu
Al7	12i	1	0.21855	0.56895	0.13809		pseudo Frank-Kasper Al ₇ Cu ₂ Cr ₂
M8	12i	1	0.26648	0.1331	0.06415		14-vertex Frank-Kasper Cu ₃ Al ₉ Cr ₂
Al9	12i	1	0.27689	0.29283	0.06732		tricapped pentagonal prism Cr ₂ Al ₁₀ Cu
Cr10	12i	1	0.40189	0.10652	0.07818		icosahedron Al ₁₁ Cr
Al11	12i	1	0.42106	0.26744	0.13729		14-vertex polyhedron CuAl ₁₀ Cr ₃
Al12	12i	1	0.53646	0.07851	0.13713		14-vertex polyhedron CuAl ₁₀ Cr ₃
Cu13	12i	1	0.5382	0.3553	0.034	0.052	bicapped square prism Al ₁₀
Al14	12i	1	0.5594	0.24174	0.06094		15-vertex Frank-Kasper Al ₁₁ Cu ₂ Cr ₂
Cr15	6h	m..	0.07798	0.53505	1/4		icosahedron Al ₁₁ Cr
Cr16	6h	m..	0.14686	0.42182	1/4		icosahedron Al ₁₁ Cr
M17	6h	m..	0.15523	0.02445	1/4		14-vertex Frank-Kasper Cu ₃ Al ₁₀ Cr
Al18	6h	m..	0.1886	0.30582	1/4		12-vertex polyhedron Cr ₂ Al ₁₀
Cr19	6h	m..	0.26767	0.2249	1/4		icosahedron Al ₁₁ Cu
Al20	6h	m..	0.30812	0.49706	1/4		tricapped pentagonal prism Cr ₂ CuAl ₁₀
M21	6h	m..	0.32738	0.12061	1/4		icosahedron Cr ₄ Al ₇ Cu
Al22	6h	m..	0.38195	0.38087	1/4		12-vertex polyhedron Cr ₂ Al ₁₀
M23	6h	m..	0.3891	0.01748	1/4		icosahedron Cr ₅ Al ₇
Cr24	6h	m..	0.49364	0.18529	1/4		icosahedron Al ₁₀ Cr ₂
Al25	6h	m..	0.58045	0.34795	1/4		14-vertex polyhedron Cr ₂ Al ₁₀ Cu ₂
M26	4f	3..	1/3	2/3	0.0463		bicapped square prism Al ₆ Cu ₄
Cu27	2c	-6..	1/3	2/3	1/4	0.202	pseudo Frank-Kasper Al ₁₁
Al28	2b	-3..	0	0	0		rhombic dodecahedron Cu ₈ Al ₆
Cu29	2a	-6..	0	0	1/4		tricapped trigonal prism Cu ₃ Al ₆

M2 = 0.945Al + 0.055Cu; M3 = 0.874Al + 0.126Cu; M8 = 0.881Al + 0.119Cu; M17 = 0.540Cu + 0.460Cr; M21 = 0.862Al + 0.138Cu; M23 = 0.796Al + 0.204Cu; M26 = 0.700Al + 0.300Cu

Transformation from published data: $y, x, -z$

Experimental: single crystal, diffractometer, X-rays, R = 0.033

References: [1] Sugiyama K., Saito H., Hiraga K. (2002), J. Alloys Compd. 342, 148-152.