

Mg₂₈Al₄₅ [1]

Structural features: 672 icosahedra and 252 Friauf polyhedra in the unit cell.

Samson S. (1965) [1]

Al₄₅Mg₂₈ $a = 2.8239 \text{ nm}$, $V = 22.5189 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	192i	1	0.2036	0.2718	0.3399		
Al2	96h	..2	0	0.3867	0.6133		
Al3	96g	..m	0.0492	0.0492	0.127	0.25	
Mg4	96g	..m	0.0569	0.0569	0.4225		16-vertex Frank-Kasper Al ₁₂ Mg ₄
Mg5	96g	..m	0.0577	0.0577	0.1776	0.167	
Al6	96g	..m	0.0722	0.0722	0.2043	0.083	
Mg7	96g	..m	0.081	0.081	0.3106		
Al8	96g	..m	0.0831	0.0831	0.0428	0.083	
Al9	96g	..m	0.0925	0.0925	0.0222	0.5	
Al10	96g	..m	0.1101	0.1101	0.2293	0.167	
Mg11	96g	..m	0.2568	0.2568	0.1321	0.75	
Al12	96g	..m	0.2666	0.2666	0.1386	0.25	
Al13	96g	..m	0.2715	0.2715	0.4071		icosahedron Al ₆ Mg ₆
Mg14	96g	..m	0.3042	0.3042	0.0361	0.5	
Al15	96g	..m	0.3059	0.3059	0.0589	0.5	
Al16	96g	..m	0.3424	0.3424	0.1364		
Mg17	48f	2.mm	0.4896	1/8	1/8		16-vertex Frank-Kasper Al ₁₂ Mg ₄
Al18	32e	.3m	0.0206	0.0206	0.0206	0.5	tetrahedron AlMg ₃
Mg19	32e	.3m	0.2442	0.2442	0.2442		
Mg20	32e	.3m	0.3088	0.3088	0.3088		16-vertex Frank-Kasper Al ₁₂ Mg ₄
Al21	32e	.3m	0.4098	0.4098	0.4098		icosahedron Al ₆ Mg ₆
Al22	16d	-.3m	1/2	1/2	1/2		icosahedron Al ₆ Mg ₆
Mg23	8a	-43m	1/8	1/8	1/8		

Transformation from published data (origin choice 1): origin shift $\frac{5}{8} \frac{5}{8} \frac{5}{8}$

Experimental: single crystal, manual diffractometer, X-rays, R = 0.061

Remarks: The distribution of Mg and Al could not be determined with certainty. Short interatomic distances for partly occupied site(s). Identical to the phase called Mg₂Al₃ in [2], Mg₅Al₈ in [3].

References: [1] Samson S. (1965), Acta Crystallogr. 19, 401-413. [2] Perlitz H. (1944), Nature (London) 154, 607. [3] Riederer K. (1936), Z. Metallkd. 28, 312-317.