

CaMg₂Al₁₆O₂₇

hP94

(187) $P-6m2 - n^9kji^6h^6g^4ba$ **CaMg₂Al₁₆O₂₇** [1], magnetoplumbite family

Structural features: Close-packed O₄ and CaO₃ layers in h₃c₄ stacking; Al in octahedral and tetrahedral, Mg in tetrahedral voids. Intergrowth of spinel-type (edge-linked AlO₆ octahedra sharing vertices with single MgO₄ tetrahedra) and so-called R slabs containing units of two face-linked AlO₆ octahedra, AlO₄ tetrahedra (statistical occupation of two face-sharing tetrahedra) and Ca atoms.

Iyi N. et al. (1995) [1]

Al₁₆Ca_{0.97}Mg₂O₂₇ $a = 0.559$, $c = 3.1288$ nm, $c/a = 5.597$, $V = 0.8467$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6n	.m.	0.1637	0.8363	0.4296		non-coplanar triangle Al ₃
Al2	6n	.m.	0.1644	0.8356	0.09903		octahedron O ₆
O3	6n	.m.	0.1824	0.8176	0.21653		tetrahedron Al ₃ Mg
O4	6n	.m.	0.4862	0.5138	0.13922		tetrahedron MgAl ₃
Al5	6n	.m.	0.5	0.5	0.24896		octahedron O ₆
O6	6n	.m.	0.5121	0.4879	0.35988		tetrahedron Al ₄
O7	6n	.m.	0.8225	0.1775	0.28716		tetrahedron Al ₄
O8	6n	.m.	0.833	0.167	0.07198		non-coplanar triangle Al ₃
Al9	6n	.m.	0.8352	0.1648	0.40076		octahedron O ₆
O10	3k	mm2	0.4855	0.5145	$\frac{1}{2}$		
O11	3j	mm2	0.5141	0.4859	0		
Al12	2i	3m.	$\frac{2}{3}$	$\frac{1}{3}$	0.04303		octahedron O ₆
Mg13	2i	3m.	$\frac{2}{3}$	$\frac{1}{3}$	0.1545		tetrahedron O ₄
O14	2i	3m.	$\frac{2}{3}$	$\frac{1}{3}$	0.219		tetrahedron Al ₃ Mg
Al15	2i	3m.	$\frac{2}{3}$	$\frac{1}{3}$	0.32407		octahedron O ₆
O16	2i	3m.	$\frac{2}{3}$	$\frac{1}{3}$	0.4308		tetrahedron Al ₄
Al17	2i	3m.	$\frac{2}{3}$	$\frac{1}{3}$	0.494	0.5	
Al18	2h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.00757	0.5	
O19	2h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0743		tetrahedron Al ₄
Al20	2h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.17647		octahedron O ₆
O21	2h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2872		tetrahedron Al ₄
Al22	2h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.343		tetrahedron O ₄
Al23	2h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.46073		octahedron O ₆
O24	2g	3m.	0	0	0.1333		tetrahedron MgAl ₃
Mg25	2g	3m.	0	0	0.1915		tetrahedron O ₄
Al26	2g	3m.	0	0	0.30423		tetrahedron O ₄
O27	2g	3m.	0	0	0.3652		tetrahedron Al ₄
Ca28	1b	-6m2	0	0	$\frac{1}{2}$		anticuboctahedron O ₁₂
Ca29	1a	-6m2	0	0	0	0.93	anticuboctahedron O ₁₂

Experimental: single crystal, diffractometer, X-rays, wR = 0.054

Remarks: Phase referred to as CAM-II; homogeneity range CaMg_{2-3x}Al_{16+2x}O₂₇, 0 < x < 0.2. No attempt was made to distinguish Al and Mg in the refinement; the authors state that Mg occupies former sites Al(4) and Al(9). Short interatomic distances for partly occupied site(s). Space group (194) $P6_3/mmc$ was tested and rejected (weak symmetry-forbidden reflections).

References: [1] Iyi N., Göbbels M., Matsui Y. (1995), J. Solid State Chem. 120, 364-371.