



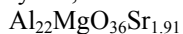
hP66

(187) *P-6m2* – $n^6k^2j^3i^3h^3g^4e$

Sr₂MgAl₂₂O₃₆ [1]

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids, (Al,Mg) in tetrahedral voids) alternate with SrO layers (split O site, Sr near BR positions) and so-called R slabs containing units of two face-linked AlO₆ octahedra, AlO₄ tetrahedra (statistical occupation of two face-sharing tetrahedra) and Sr atoms, along [001]. Magnetoplumbite- and β alumina-type slabs, SrAl₁₂O₁₉ + SrMgAl₁₀O₁₇.

Iyi N., Göbbels M. (1996) [1]



$a = 0.5583$, $c = 2.2225$ nm, $c/a = 3.981$, $V = 0.5999$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>n</i>	. <i>m</i> .	0.1527	0.8473	0.1962		tetrahedron Al ₄
Al2	6 <i>n</i>	. <i>m</i> .	0.1667	0.8333	0.3554		octahedron O ₆
O3	6 <i>n</i>	. <i>m</i> .	0.4949	0.5051	0.3988		non-coplanar triangle Al ₃
O4	6 <i>n</i>	. <i>m</i> .	0.503	0.497	0.101		non-coplanar triangle Al ₃
Al5	6 <i>n</i>	. <i>m</i> .	0.8316	0.1684	0.1405		octahedron O ₆
O6	6 <i>n</i>	. <i>m</i> .	0.844	0.156	0.2997		tetrahedron Al ₄
Sr7	3 <i>k</i>	<i>mm</i> 2	0.3105	0.6895	$\frac{1}{2}$	0.303	
O8	3 <i>k</i>	<i>mm</i> 2	0.6359	0.3641	$\frac{1}{2}$	0.333	
O9	3 <i>j</i>	<i>mm</i> 2	0.1807	0.8193	0		
O10	2 <i>i</i>	3 <i>m</i> .	$\frac{2}{3}$	$\frac{1}{3}$	0.1917		tetrahedron Al ₄
Al11	2 <i>i</i>	3 <i>m</i> .	$\frac{2}{3}$	$\frac{1}{3}$	0.2729		tetrahedron O ₄
Al12	2 <i>i</i>	3 <i>m</i> .	$\frac{2}{3}$	$\frac{1}{3}$	0.4249		
Al13	2 <i>h</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0589		octahedron O ₆
M14	2 <i>h</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.2202		tetrahedron O ₄
O15	2 <i>h</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.305		tetrahedron Al ₄
Al16	2 <i>g</i>	3 <i>m</i> .	0	0	0.01	0.5	
O17	2 <i>g</i>	3 <i>m</i> .	0	0	0.1002		tetrahedron Al ₄
Al18	2 <i>g</i>	3 <i>m</i> .	0	0	0.2478		octahedron O ₆
O19	2 <i>g</i>	3 <i>m</i> .	0	0	0.3936		non-coplanar triangle Al ₃
Sr20	1 <i>e</i>	-6 <i>m</i> 2	$\frac{2}{3}$	$\frac{1}{3}$	0		anticuboctahedron O ₁₂

M14 = 0.5Al + 0.5Mg

Experimental: single crystal, diffractometer, X-rays, R = 0.058

Remarks: We assigned an approximate value to the Al/Mg ratio of site M14 based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Iyi N., Göbbels M. (1996), J. Solid State Chem. 122, 46-52.