



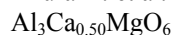
hP22

(176) $P6_3/m - h^3ca$

CaMg₂Al₆O₁₂ [1]

Structural features: Double infinite chains of edge-linked AlO_6 octahedra share vertices to form a 3D-framework; Mg in trigonal prismatic voids, Ca in channels of hexagonal cross-section parallel to [001] (partial disorder for the latter). Variant of $\text{Sr}_{0.5}\text{CaSc}_3\text{O}_6$.

Miura H. et al. (2000) [1]



$a = 0.87616$, $c = 0.2785$ nm, $c/a = 0.318$, $V = 0.1851$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Al1	6 <i>h</i>	<i>m</i> ..	0.01	0.352	$\frac{1}{4}$		octahedron O ₆
O2	6 <i>h</i>	<i>m</i> ..	0.197	0.306	$\frac{1}{4}$		non-coplanar triangle Al ₃
O3	6 <i>h</i>	<i>m</i> ..	0.601	0.134	$\frac{1}{4}$		square pyramid Al ₃ Mg ₂
Mg4	2 <i>c</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism O ₆
Ca5	2 <i>a</i>	-6..	0	0	$\frac{1}{4}$	0.5	

Transformation from published data: $y, x, -z$; origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, X-rays, $R_p = 0.051$

Remarks: Short interatomic distances for partly occupied site(s). In the abstract of [1] Mg is erroneously stated to be octahedrally coordinated instead of inside trigonal prisms.

References: [1] Miura H., Hamada Y., Suzuki T., Akaogi M., Miyajima N., Fujino K. (2000), *Am. Mineral.* 85, 1799-1803.