

$\text{Mg}_{0.2}(\text{Al}_{0.4}\text{Si}_{0.6})\text{O}_2$ $hP12$ (180) $P6_222$ – ida**MgAl₂Si₃O₁₀** [1]

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a 3D-framework with twisted chains; Mg in narrow channels of hexagonal cross-section parallel to [001]. Filled-up derivative of SiO₂ β-quartz.

Schulz H. et al. (1971) [1]

 $\text{Al}_{0.40}\text{Mg}_{0.20}\text{O}_2\text{Si}_{0.60}$ $a = 0.5182$, $c = 0.536$ nm, $c/a = 1.034$, $V = 0.1246$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6i	..2	0.2044	0.4088	0		coplanar triangle Si ₂ Mg
M2	3d	222	1/2	0	1/2		tetrahedron O ₄
Mg3	3a	222	0	0	0	0.2	coplanar square Mg ₂ O ₂

 $\text{M2} = 0.6\text{Si} + 0.4\text{Al}$

Transformation from published data: origin shift 0 0 1/2

Experimental: single crystal, diffractometer, X-rays, R = 0.065

Remarks: Average structure. We assigned an approximate value to the Al/Si ratio of site M2 based on the nominal composition. Short interatomic distances for partly occupied site(s). Refinement considering partial occupation of Wyckoff position 3*b* by Mg (proposed in [2]) showed no significant deviation from zero occupancy. An alternative model with all sites in split positions gave R = 0.055.

References: [1] Schulz H., Hoffmann W., Muchow G.M. (1971), Z. Kristallogr. 134, 1-27. [2] Schulz H. (1971), Z. Kristallogr. 134, 253-261.