

 $hP26$ $(186) P6_3mc - c^3b^3a$

Al₂O₃·0.2H₂O [2], tohdite

Structural features: Close-packed (O,OH) layers in hc stacking; Al in octahedral and tetrahedral voids. Infinite slabs of edge-linked AlO₆ octahedra are interconnected via additional AlO₆ octahedra and AlO₄ tetrahedra to form a 3D-framework.

Yamaguchi G. et al. (1969) [1]

Al₅O₈

$a = 0.5575$, $c = 0.8761$ nm, $c/a = 1.571$, $V = 0.2358$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	6c	.m.	0.1647	0.8353	0.3708		octahedron O ₆
O2	6c	.m.	0.5098	0.4902	0.0143		tetrahedron Al ₄
O3	6c	.m.	0.8291	0.1709	0.2666		non-coplanar triangle Al ₃
Al4	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0611		tetrahedron O ₄
O5	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2638		tetrahedron Al ₄
Al6	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6533		octahedron O ₆
O7	2a	3m.	0	0	0.0		non-coplanar triangle Al ₃

Experimental: powder, diffractometer, X-rays, $R_B = 0.080$

Remarks: H not located. Space group (159) $P31c$ was tested and rejected. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Yamaguchi G., Okumiya M., Ono S. (1969), Bull. Chem. Soc. Jpn. 42, 2247-2249. [2] Yamaguchi G., Yanagida H., Ono S. (1964), Bull. Chem. Soc. Jpn. 37, 1555-1557.