

$\text{Al}_{2.67}\text{O}_4$	$hP44$	$(186) P6_3mc - c^6b^3a$
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Al_2O_3 κ' [1]

Structural features: Close-packed O layers in hc stacking; Al in octahedral and tetrahedral voids (high degree of disorder).

Okumiyama M., Yamaguchi G. (1971) [1]

$\text{Al}_{2.56}\text{O}_4$

$a = 0.5544$, $c = 0.9024$ nm, $c/a = 1.628$, $V = 0.2402$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	6c	.m.	0.156	0.844	0.118	0.34	non-coplanar triangle Al ₃
Al2	6c	.m.	0.169	0.831	0.363	0.67	non-colinear Al ₂
O3	6c	.m.	0.500	0.500	0.006		non-coplanar triangle Al ₃
O4	6c	.m.	0.832	0.168	0.256		7-vertex polyhedron Al ₇
Al5	6c	.m.	0.833	0.167	0.061	0.08	10-vertex polyhedron Al ₆ O ₄
Al6	6c	.m.	0.884	0.116	0.448	0.12	single atom O
Al7	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.056	0.51	7-vertex polyhedron O ₄ Al ₃
O8	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.254		7-vertex polyhedron Al ₇
Al9	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.648	0.98	9-vertex polyhedron Al ₃ O ₆
O10	2a	3m.	0	0	0.0		non-coplanar triangle Al ₃

Experimental: powder, diffractometer, X-rays, R = 0.130

Remarks: Short interatomic distances: d(Al6-O10) = 0.121 nm. Short interatomic distances for partly occupied site(s).

References: [1] Okumiyama M., Yamaguchi G. (1971), Bull. Chem. Soc. Jpn. 44, 1567-1570.