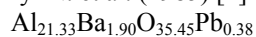


hP89

(187) $P-6m2 - n^9k^2j^3i^2h^3g^5$ **(Ba,Pb)_{2.34}Al₂₁O_{33.84} form II [1]**

Structural features: Spinel-type slabs (close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and BaO layers (split O site, Ba near BR position) alternate along [001]; additional Ba and Pb are accommodated inside the slabs, accompanied by complex defects.

Iyi N. et al. (1985) [1]

a = 0.56003, c = 2.2922 nm, c/a = 4.093, V = 0.6226 nm³, Z = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	6n	.m.	0.16843	0.83157	0.1515	0.66	7-vertex polyhedron O ₆ Al tetrahedron Al ₄
O2	6n	.m.	0.17933	0.82067	0.3048		
Al3	6n	.m.	0.18983	0.81017	0.0694	0.317	tetrahedron Al ₄ octahedron O ₆
O4	6n	.m.	0.49403	0.50597	0.2062		
Al5	6n	.m.	0.49933	0.50067	0.3573		
Al6	6n	.m.	0.64173	0.35827	0.0741	0.332	
O7	6n	.m.	0.82733	0.17267	0.0827	0.278	non-coplanar triangle Al ₃
O8	6n	.m.	0.82753	0.17247	0.3996		
O9	6n	.m.	0.83863	0.16137	0.108	0.793	
O10	3k	mm2	0.01933	0.98067	¹ / ₂	0.333	
Ba11	3k	mm2	0.65353	0.34647	¹ / ₂	0.334	tetrahedron O ₂ Al ₂ non-colinear O ₂
Ba12	3j	mm2	0.01033	0.98967	0	0.228	
O13	3j	mm2	0.24933	0.75067	0	0.33	tetrahedron O ₄ tetrahedron Al ₄
O14	3j	mm2	0.59433	0.40567	0	0.393	
Al15	2i	3m.	² / ₃	¹ / ₃	0.2302		trigonal prism Al ₆ octahedron O ₆
O16	2i	3m.	² / ₃	¹ / ₃	0.3102		
O17	2h	3m.	¹ / ₃	² / ₃	0.1131		non-coplanar triangle Al ₃
Al18	2h	3m.	¹ / ₃	² / ₃	0.2532		
O19	2h	3m.	¹ / ₃	² / ₃	0.3962		
O20	2g	3m.	0	0	0.2004	0.93	
Ba21	2g	3m.	0	0	0.2202	0.106	
Pb22	2g	3m.	0	0	0.2422	0.188	
Al23	2g	3m.	0	0	0.2767	0.74	
Al24	2g	3m.	0	0	0.4249		

Transformation from published data: origin shift ²/₃ ¹/₃ 0

Experimental: single crystal, diffractometer, X-rays, R = 0.030

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Iyi N., Inoue Z., Takekawa S., Kimura S. (1985), J. Solid State Chem. 60, 41-50.