$BaAl_2O_4$	*hP*18	(182) $P6_322$ – hgfb

$BaAl_2O_4$ [1]
Structural features: AlO_4 tetrahedra (splitting of one O site) share vertices to form a 3D-framework; Ba in channels delimited by 6-rings parallel to [001].

Perrotta A.J., Smith J.V. (1968) [1]
Al_2BaO_4
$a = 0.5218$, $c = 0.8781$ nm, $c/a = 1.683$, $V = 0.2071$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	6*h*	..2	0.371	0.742	$^1/_4$	0.333	
O2	6*g*	.2.	0.36	0	0		non-colinear Al_2
Al3	4*f*	3..	$^1/_3$	$^2/_3$	0.054		
Ba4	2*b*	3.2	0	0	$^1/_4$		

Experimental: single crystal, diffractometer, X-rays, R = 0.086

Remarks: Short interatomic distances for partly occupied site(s). Additional reflections could be indexed with a 4-fold supercell (new axes 2a,2b,c). The superstructure was refined in space group (173) $P6_3$ in [2].

References: [1] Perrotta A.J., Smith J.V. (1968), Bull. Soc. Fr. Mineral. Cristallogr. 91, 85-87. [2] Huang S.Y., Von Der Mühll R., Ravez J., Chaminade J.P., Hagenmuller P., Couzi M. (1994), J. Solid State Chem. 109, 97-105.