$BaAl_2O_4$	*hP*14	(182) $P6_322$ – gfcb

$BaAl_2O_4$ [2], Strukturbericht notation $H2_8$
Structural features: AlO_4 tetrahedra share vertices to form a 3D-framework; Ba in channels delimited by 6-rings parallel to [001]. See Fig. IV.36.

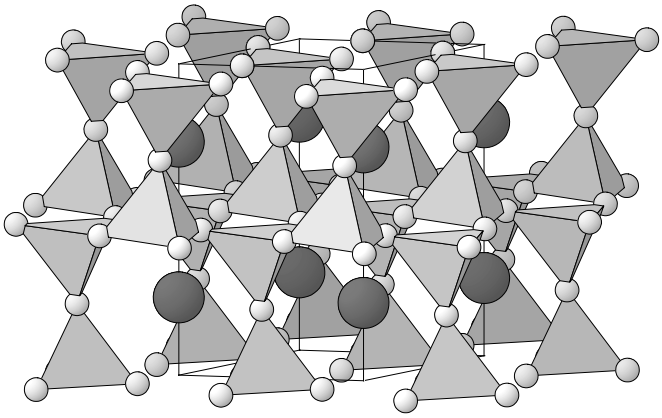

Fig. IV.36. **$BaAl_2O_4$**

Arrangement of AlO_4 tetrahedra (O atoms small) and Ba atoms (large).

Do Dinh C., Bertaut E.F. (1965) [1]
Al_2BaO_4
$a = 0.5227$, $c = 0.8802$ nm, $c/a = 1.684$, $V = 0.2083$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	6*g*	.2.	0.343	0	0		non-colinear Al_2
Al2	4*f*	3..	$^1/_3$	$^2/_3$	0.051		tetrahedron O_4
O3	2*c*	3.2	$^1/_3$	$^2/_3$	$^1/_4$		colinear Al_2
Ba4	2*b*	3.2	0	0	$^1/_4$		tricapped trigonal prism O_9

Experimental: powder, diffractometer, neutrons, R = 0.050

Remarks: Average structure; the superstructure was refined in space group (173) $P6_3$ (new axes 2a,2b,c) in [3]. In [1] the AlO_2 framework is erroneously stated to be identical to that formed by the SiO_4 tetrahedra in tridymite.

References: [1] Do Dinh C., Bertaut E.F. (1965), Bull. Soc. Fr. Mineral. Cristallogr. 88, 413-416. [2] Wallmark S., Westgren A. (1937), Ark. Kemi Mineral. Geol. 12B(35), 1-4. [3] Huang S.Y., Von Der Mühll R., Ravez J., Chaminade J.P., Hagenmuller P., Couzi M. (1994), J. Solid State Chem. 109, 97-105.