$BaMg_3Al_{14}O_{25}$	*hP*88	(187) *P*-6*m*2 – $n^9ki^5h^4g^5fca$

$Ba_2Mg_6Al_{28}O_{50}$ [1]

Structural features: Spinel-type slabs (six close-packed O layers in c stacking, Al in octahedral and outer tetrahedral, (Al,Mg) and Mg in inner tetrahedral voids) and BaO layers (Ba at and near BR positions) alternate along [001]. Infinite slabs of edge-linked AlO_6 octahedra sharing vertices with single MgO_4 and $(Al,Mg)O_4$ tetrahedra are interconnected via units of two vertex-linked AlO_4 tetrahedra to form a 3D-framework.

Iyi N. et al. (1998) [1]

$Al_{14.10}Ba_{0.94}Mg_{2.50}O_{25}$

a = 0.5638, c = 3.1983 nm, c/a = 5.673, V = 0.8804 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6*n*	.*m*.	0.15563	0.84437	0.285		tetrahedron $MgAl_3$
O2	6*n*	.*m*.	0.16813	0.83187	0.0724		non-coplanar triangle Al_3
Al3	6*n*	.*m*.	0.16813	0.83187	0.3981		octahedron O_6
O4	6*n*	.*m*.	0.49373	0.50627	0.4282		non-coplanar triangle Al_3
Al5	6*n*	.*m*.	0.50133	0.49867	0.1028		octahedron O_6
O6	6*n*	.*m*.	0.52013	0.47987	0.2168		tetrahedron Al_3Mg
O7	6*n*	.*m*.	0.81673	0.18327	0.1436		tetrahedron Al_4
Al8	6*n*	.*m*.	0.83493	0.16507	0.2495	0.95	octahedron O_6
O9	6*n*	.*m*.	0.84363	0.15637	0.36		tetrahedron Al_4
Ba10	3*k*	*mm*2	0.32333	0.67667	$^1/_2$	0.29	
O11	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.0759		non-coplanar triangle Al_3
Al12	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.1785		octahedron O_6
O13	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.2806		tetrahedron Al_4
M14	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.34	0.88	tetrahedron O_4
Al15	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.4475		tetrahedron O_4
O16	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.1379		tetrahedron $MgAl_3$
Mg17	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.1928	0.87	tetrahedron O_4
Mg18	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.3044		tetrahedron O_4
O19	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.3682		tetrahedron Al_3Mg
Al20	2*g*	3*m*.	0	0	0.054		tetrahedron O_4
M21	2*g*	3*m*.	0	0	0.1583		tetrahedron O_4
O22	2*g*	3*m*.	0	0	0.2161		tetrahedron Al_4
Al23	2*g*	3*m*.	0	0	0.3232		octahedron O_6
O24	2*g*	3*m*.	0	0	0.4242		non-coplanar triangle Al_3
O25	1*f*	-6*m*2	$^2/_3$	$^1/_3$	$^1/_2$		colinear Al_2
Ba26	1*c*	-6*m*2	$^1/_3$	$^2/_3$	0		trigonal prism O_6
O27	1*a*	-6*m*2	0	0	0		colinear Al_2

M14 = 0.667Al + 0.333Mg; M21 = 0.667Al + 0.333Mg

Transformation from published data: -*x*,-*y*,-*z*; origin shift $^2/_3$ $^1/_3$ $^1/_2$

Experimental: single crystal, diffractometer, X-rays, R = 0.048

Remarks: Phase referred to as BAM-II. Composition $Ba_{1.84}Mg_{5.0}Al_{28.8}O_{50}$ from electron microprobe analysis. Refinement considering f(Al) for the cation sites in the spinel-type slabs; the authors state that Mg substitutes for Al mainly on former sites Al4 and Al5, and partly on sites Al6 and Al9. We assigned approximate values to the Al/Mg distribution based on the authors' conclusions, assuming 5 Mg per unit cell. Short interatomic distances for partly occupied site(s).

References: [1] Iyi N., Göbbels M., Kimura S. (1998), J. Solid State Chem. 136, 258-262.