$BaAl[BO_3]F_2$	*hP*16	(174) *P*-6 – kjihgdcba

$BaAl(BO_3)F_2$ [1]
Structural features: $Al(O_3F_2)$ trigonal bipyramids and BO_3 trigonal units share vertices to form infinite slabs.

Hu Z.G. et al. (2003) [1]
$AlBBaF_2O_3$
a = 0.48879, c = 0.9403 nm, c/a = 1.924, V = 0.1946 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	3*k*	*m*..	0.28417	0.00833	$^1/_2$		non-colinear BAl
O2	3*j*	*m*..	0.04727	0.39003	0		non-colinear BAl
Ba3	2*i*	3..	$^2/_3$	$^1/_3$	0.25026		icosahedron F_6O_6
F4	2*h*	3..	$^1/_3$	$^2/_3$	0.2962		single atom Al
F5	2*g*	3..	0	0	0.1862		single atom Al
Al6	1*d*	-6..	$^1/_3$	$^2/_3$	$^1/_2$		trigonal bipyramid O_3F_2
B7	1*c*	-6..	$^1/_3$	$^2/_3$	0		coplanar triangle O_3
B8	1*b*	-6..	0	0	$^1/_2$		coplanar triangle O_3
Al9	1*a*	-6..	0	0	0		trigonal bipyramid F_2O_3

Transformation from published data: origin shift $^1/_3$ $^2/_3$ $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.024, T = 296 K

Remarks: Supersedes a structure proposal in space group (176) $P6_3/m$ in [2]. Space groups (143) *P*3 and (173) $P6_3$ were tested and rejected (R = 0.061 for the latter).

References: [1] Hu Z.G., Maramatsu K., Kanehisa N., Yoshimura M., Mori Y., Sasaki T., Kai Y. (2003), Z. Kristallogr., New Cryst. Struct. 218, 1-2. [2] Park H., Barbier J. (2000), J. Solid State Chem. 155, 354-358.