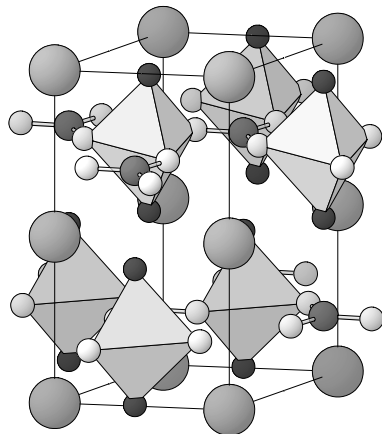


BaGa(BO₃)F₂ [1]

Structural features: Ga(O₃F₂) trigonal bipyramids and BO₃ trigonal units share vertices to form infinite layers; Ba between the layers. See Fig. IV.53.

Fig. IV.53. **BaGa(BO₃)F₂**

Arrangement of Ga(O₃F₂) trigonal bipyramids, BO₃ triangles (O atoms light, F atoms dark, B atoms medium) and Ba atoms (large).

Park H., Barbier J. (2000) [1]

BBaF₂GaO₃

$a = 0.4907$, $c = 0.962$ nm, $c/a = 1.960$, $V = 0.2006$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6 <i>h</i>	<i>m</i> ..	0.3775	0.0661	$\frac{1}{4}$		non-collinear BGa
F2	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0457		single atom Ga
B3	2 <i>d</i>	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		coplanar triangle O ₃
Ga4	2 <i>c</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal bipyramid O ₃ F ₂
Ba5	2 <i>b</i>	-3..	0	0	0		icosahedron F ₆ O ₆

Transformation from published data: $y, x, -z$

Experimental: twinned crystal, diffractometer, X-rays, wR = 0.039

References: [1] Park H., Barbier J. (2000), J. Solid State Chem. 155, 354-358.