$Al_6[BO_3]_5F_3$	*hP*58	(176) $P6_3/m$ – i^3h^3f

$Al_6(BO_3)_5F_3$ [2], jeremejevite
Structural features: $Al(O_5F)$ octahedra share edges and vertices to form a 3D-framework; B in trigonal voids. Single BO_3 trigonal units.

Sokolova E.V. et al. (1987) [1]
$Al_6B_5F_3O_{15}$
a = 0.8552, c = 0.8187 nm, c/a = 0.957, V = 0.5185 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*i*	1	0.1501	0.5894	0.0535		single atom B
O2	12*i*	1	0.2847	0.1962	0.1019		single atom B
Al3	12*i*	1	0.3529	0.0159	0.0754		octahedron FO_5
O4	6*h*	*m*..	0.1145	0.3033	$^1/_4$		single atom B
B5	6*h*	*m*..	0.23	0.232	$^1/_4$		coplanar triangle O_3
F6	6*h*	*m*..	0.5006	0.1146	$^1/_4$		non-colinear Al_2
B7	4*f*	3..	$^1/_3$	$^2/_3$	0.057		non-coplanar triangle O_3

Transformation from published data: *y*,*x*,-*z*; origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.038

Remarks: In [1] the number of formula units per cell Z is misprinted as 12 instead of 2.

References: [1] Sokolova E.V., Egorov Tismenko Y.K., Kargaltsev S.V., Klyakhin V.A., Urusov V.S. (1987), Vestn. Mosk. Univ., Ser. 4: Geol. 1987(3), 82-84. [2] Rodellas C., Garcia Blanco S., Vegas A. (1983), Z. Kristallogr. 165, 255-260.