$HBa_5Nb_3O_3F_{20}$	*hP*62	(176) $P6_3/m$ – i^2h^5fdb

$Ba_5Nb_3O_3F_{18}(HF_2)$ [1]
Structural features: Single $Nb[F_5(F,O)_2]$ pentagonal bipyramids and F-H-F units.

Crosnier Lopez M.P. et al. (1993) [1]
$Ba_5F_{20}Nb_3O_3$
a = 1.1935, c = 0.7852 nm, c/a = 0.658, V = 0.9686 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	12*i*	1	0.2776	0.0515	0.01		single atom Nb
F2	12*i*	1	0.4901	0.098	0.0989		single atom Nb
M3	6*h*	*m*..	0.1152	0.4137	$^1/_4$		single atom Nb
M4	6*h*	*m*..	0.1413	0.0002	$^1/_4$		single atom Nb
Nb5	6*h*	*m*..	0.3285	0.0466	$^1/_4$		pentagonal bipyramid F_7
Ba6	6*h*	*m*..	0.3599	0.4395	$^1/_4$		pentacapped trigonal prism F_{11}
F7	6*h*	*m*..	0.4075	0.2434	$^1/_4$		single atom Nb
F8	4*f*	3..	$^1/_3$	$^2/_3$	0.1093		single atom F
Ba9	2*d*	-6..	$^2/_3$	$^1/_3$	$^1/_4$		pentacapped trigonal prism F_{11}
Ba10	2*b*	-3..	0	0	0		icosahedron F_{12}

M3 = 0.5F + 0.5O; M4 = 0.5F + 0.5O
Transformation from published data: origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.025, T = 293 K

Remarks: H not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Space group (173) $P6_3$ was tested and rejected.

References: [1] Crosnier Lopez M.P., Duroy H., Fourquet J.L. (1993), J. Solid State Chem. 107, 211-217.