

$\text{H}_3\text{K}_6\text{BiCl}_8\text{F}_4$ $hP38$ $(186) P6_3mc - c^5b^3a$ **$\text{K}_6\text{H}_3\text{BiCl}_8\text{F}_4$ It [1]**

Structural features: BiCl_6 octahedra and $\text{F}(\text{FH})_3$ trigonal units (approximately planar FF_3 triangle) in a NiAs-type arrangement; additional Cl in columns of face-linked K_6 octahedra.

Udovenko A.A., Davidovich R.L. (1991) [1]

 $\text{BiCl}_8\text{F}_4\text{H}_3\text{K}_6$ $a = 0.9064, c = 1.4339 \text{ nm}, c/a = 1.582, V = 1.0202 \text{ nm}^3, Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
K1	$6c$	$.m.$	0.1792	0.8208	0.2517		square antiprism F_2Cl_6
K2	$6c$	$.m.$	0.5028	0.4972	0.014		square prism (cube) Cl_6F_2
F3	$6c$	$.m.$	0.5169	0.4831	0.2733		non-coplanar triangle FK_2
Cl4	$6c$	$.m.$	0.8592	0.1408	0.1072		single atom Bi
Cl5	$6c$	$.m.$	0.8593	0.1407	0.3918		single atom Bi
Cl6	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.1089		octahedron K_6
Cl7	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.395		octahedron K_6
F8	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.7611		non-coplanar triangle F_3
Bi9	$2a$	$3m.$	0	0	0.0		octahedron Cl_6
H10	$6c$	$.m.$	0.571	0.429	0.24		

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

Experimental: single crystal, diffractometer, X-rays, $wR = 0.026$, $T = 103 \text{ K}$

Remarks: Phase stable at $T < 130 \text{ K}$. Space groups (190) $P-62c$ and (194) $P6_3/mmc$ were tested and rejected ($R = 0.035$ and 0.037 , respectively). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Udovenko A.A., Davidovich R.L. (1991), Koord. Khim. 17, 1545-1546.