$Hf_3Bi_{10}Cl_{18}$	*hP*64	(176) $P6_3/m$ – i^3h^4e

$BiBi_9(HfCl_6)_3$ [1]
Structural features: Distorted $HfCl_6$ octahedra and Bi_9 clusters (a Bi_6Bi_3 tricapped trigonal prism) in a Mg_3Cd-type (h.c.p.) arrangement; additional Bi in channels parallel to [001] (partial disorder). See Fig. IV.77.

Friedman R.M., Corbett J.D. (1973) [1]
$Bi_{10}Cl_{18}Hf_3$
a = 1.389, c = 1.0692 nm, c/a = 0.77, V = 1.7865 nm^3, Z = 2

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Cl1	12*i*	1	0.0658	0.4347	0.087		single atom Hf
Cl2	12*i*	1	0.1761	0.2591	0.0876		single atom Hf
Bi3	12*i*	1	0.5205	0.2141	0.0753		pseudo Frank-Kasper Bi_5Cl_6
Hf4	6*h*	*m*..	0.1193	0.34	$^1/_4$		octahedron Cl_6
Cl5	6*h*	*m*..	0.2601	0.0702	$^1/_4$		single atom Hf
Cl6	6*h*	*m*..	0.3054	0.5032	$^1/_4$		single atom Hf
Bi7	6*h*	*m*..	0.4877	0.3722	$^1/_4$		icosahedron Bi_4Cl_8
Bi8	4*e*	3..	0	0	0.1041	0.5	single atom Bi

Experimental: single crystal, diffractometer, X-rays, R = 0.093

Remarks: Short interatomic distances for partly occupied site(s). In table II of [1] the *y*-coordinate of former Cl(4) is misprinted as 0.2239 instead of 0.8239 (checked on interatomic distances).

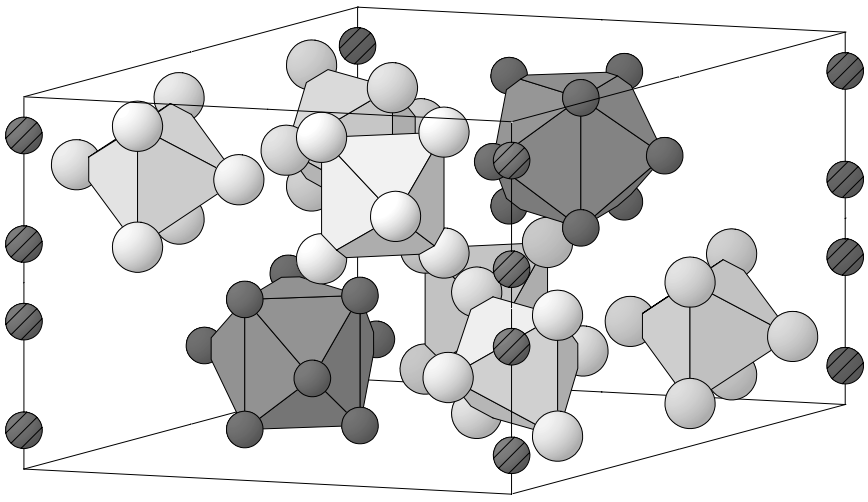

Fig. IV.77. **$BiBi_9(HfCl_6)_3$**

Arrangement of Bi_6Bi_3 tricapped trigonal prisms (dark) (Bi atoms small), $HfCl_6$ octahedra (light) (Cl atoms large) and additional Bi atoms (hatched; partly occupied sites). For clarity, atoms located in the cell but belonging to octahedra with the central Hf atom in a neighboring cell are omitted.

References: [1] Friedman R.M., Corbett J.D. (1973), Inorg. Chem. 12, 1134-1139.