$Cu_5Bi_{48}Cl_{31}O_{59}$	*hP*152	(189) *P*-62*m* – $l^4k^5j^5i^5g^2f^2e$

$Cu_5[Bi_{48}O_{59}Cl_{30}]Cl$ [1]
Structural features: BiO_n polyhedra (mainly :BiO_4 square ψ-pyramids) share atoms to form a 3D-framework; units of three edge-linked $CuCl_4$ tetrahedra share vertices to form infinite chains in large channels parallel to [001], additional Cl in these and other channels.

Aurivillius B. (1990) [1]
$Bi_{48}Cl_{31.50}Cu_6O_{60}$
a = 2.00248, c = 0.7736 nm, c/a = 0.386, V = 2.6865 nm^3, Z = 1

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Bi1	12*l*	1	0.1328	0.3586	0.2512		non-coplanar square O_4
O2	12*l*	1	0.1372	0.4684	0.25		non-coplanar triangle Bi_3
O3	12*l*	1	0.2437	0.3589	0.231		non-coplanar triangle Bi_3
Cl4	12*l*	1	0.3308	0.5535	0.258		non-coplanar triangle Bi_3
O5	6*k*	*m*..	0.086	0.538	$^1/_2$		tetrahedron Bi_4
Cl6	6*k*	*m*..	0.1088	0.2164	$^1/_2$		
O7	6*k*	*m*..	0.176	0.402	$^1/_2$		non-colinear Bi_2
Bi8	6*k*	*m*..	0.1908	0.5311	$^1/_2$		non-coplanar square O_4
Bi9	6*k*	*m*..	0.336	0.4324	$^1/_2$		tricapped trigonal prism O_7Cl_2
O10	6*j*	*m*..	0.081	0.538	0		non-coplanar triangle Bi_3
Cl11	6*j*	*m*..	0.108	0.2188	0		
Bi12	6*j*	*m*..	0.1876	0.5331	0		non-coplanar square O_4
O13	6*j*	*m*..	0.194	0.423	0		tetrahedron Bi_4
Bi14	6*j*	*m*..	0.3075	0.4188	0		non-coplanar square O_4
Cu15	6*i*	..*m*	0.1011	0	0.041	0.5	
Cu16	6*i*	..*m*	0.1051	0	0.421	0.5	
Bi17	6*i*	..*m*	0.4749	0	0.2451		5-vertex polyhedron O_5
O18	6*i*	..*m*	0.585	0	0.289		non-coplanar triangle Bi_3
Bi19	6*i*	..*m*	0.7557	0	0.2522		non-coplanar square O_4
Cl20	3*g*	*m*2*m*	0.3269	0	$^1/_2$		pseudo Frank-Kasper $O_8Bi_8Cl_4$
O21	3*g*	*m*2*m*	0.699	0	$^1/_2$		tetrahedron Bi_4
Cl22	3*f*	*m*2*m*	0.337	0	0		pseudo Frank-Kasper $Bi_8O_8Cl_4$
O23	3*f*	*m*2*m*	0.679	0	0		non-colinear Bi_2
Cl24	2*e*	3.*m*	0	0	0.185	0.75	non-coplanar triangle Cu_3

Experimental: single crystal, diffractometer, X-rays, R = 0.052

Remarks: O vacancies not located. Short interatomic distances for partly occupied site(s). Space group (182) $P6_322$ was tested and rejected. The average structure was refined space group (189) *P*-62*m* with half cell volume (new axes a,b,c/2).

References: [1] Aurivillius B. (1990), Acta Chem. Scand. 44, 111-122.