| $Ag_5Bi_{48}Cl_{31}O_{59}$ | *hP*146 | (189) *P*-62*m* – $l^4k^5j^5i^4g^2f^2e$ |
|---|---|---|

**$Ag_5[Bi_{48}O_{59}Cl_{30}]Cl$** [1]
Structural features: $BiO_n$ polyhedra (mainly :$BiO_4$ square ψ-pyramids) share atoms to form a 3D-framework; triple chains of edge- and vertex-linked $AgCl_5$ square pyramids in large channels parallel to [001], additional Cl in these and other channels.

Aurivillius B. (1990) [1]
$Ag_{4.80}Bi_{47.82}Cl_{31.50}O_{60}$
$a$ = 2.00893, $c$ = 0.77178 nm, $c/a$ = 0.384, $V$ = 2.6975 nm$^3$, $Z$ = 1

| site | Wyck. | sym. | *x* | *y* | *z* | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| O1 | 12*l* | 1 | 0.111 | 0.3588 | 0.24 | | non-coplanar triangle $Bi_3$ |
| Cl2 | 12*l* | 1 | 0.224 | 0.555 | 0.252 | | single atom Bi |
| Bi3 | 12*l* | 1 | 0.2265 | 0.3606 | 0.2472 | | non-coplanar square $O_4$ |
| O4 | 12*l* | 1 | 0.3271 | 0.4686 | 0.25 | | non-coplanar triangle $Bi_3$ |
| O5 | 6*k* | *m*.. | 0.069 | 0.541 | $^1/_2$ | | non-coplanar triangle $Bi_3$ |
| Cl6 | 6*k* | *m*.. | 0.1032 | 0.2135 | $^1/_2$ | | non-colinear $Ag_2$ |
| Bi7 | 6*k* | *m*.. | 0.1117 | 0.4202 | $^1/_2$ | | non-coplanar square $O_4$ |
| O8 | 6*k* | *m*.. | 0.228 | 0.424 | $^1/_2$ | | tetrahedron $Bi_4$ |
| Bi9 | 6*k* | *m*.. | 0.3486 | 0.5352 | $^1/_2$ | | non-coplanar square $O_4$ |
| O10 | 6*j* | *m*.. | 0.0916 | 0.5442 | 0 | | non-colinear $Bi_2$ |
| Bi11 | 6*j* | *m*.. | 0.0953 | 0.4358 | 0 | 0.97 | tricapped trigonal prism $O_7Cl_2$ |
| Cl12 | 6*j* | *m*.. | 0.1148 | 0.2198 | 0 | | non-colinear $Ag_2$ |
| O13 | 6*j* | *m*.. | 0.223 | 0.407 | 0 | | non-colinear $Bi_2$ |
| Bi14 | 6*j* | *m*.. | 0.3399 | 0.5309 | 0 | | non-coplanar square $O_4$ |
| Bi15 | 6*i* | ..*m* | 0.2472 | 0 | 0.247 | | non-coplanar square $O_4$ |
| O16 | 6*i* | ..*m* | 0.416 | 0 | 0.2 | | non-coplanar triangle $Bi_3$ |
| Bi17 | 6*i* | ..*m* | 0.5252 | 0 | 0.2563 | | non-coplanar triangle $O_3$ |
| Ag18 | 6*i* | ..*m* | 0.8674 | 0 | 0.252 | 0.8 | square pyramid $Cl_5$ |
| O19 | 3*g* | *m*2*m* | 0.31 | 0 | $^1/_2$ | | tetrahedron $Bi_4$ |
| Cl20 | 3*g* | *m*2*m* | 0.662 | 0 | $^1/_2$ | | pseudo Frank-Kasper $Bi_8O_8Cl_4$ |
| O21 | 3*f* | *m*2*m* | 0.304 | 0 | 0 | | tetrahedron $Bi_4$ |
| Cl22 | 3*f* | *m*2*m* | 0.6681 | 0 | 0 | | pseudo Frank-Kasper $Bi_8O_8Cl_4$ |
| Cl23 | 2*e* | 3.*m* | 0 | 0 | 0.212 | 0.75 | tetrahedron $Ag_3Cl$ |

Transformation from published data: -*x*,-*y*,-*z*; origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.058

Remarks: O vacancies not located. Space groups (150) *P*321 and (157) *P*31*m* were tested and rejected. The average structure was refined in 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.