



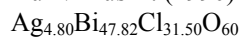
*hP*146

(189) *P*-62*m* – $1^4k^5j^5i^4g^2fe$

Ag₅[Bi₄₈O₅₉Cl₃₀]Cl [1]

Structural features: BiO_n polyhedra (mainly :BiO₄ square ψ -pyramids) share atoms to form a 3D-framework; triple chains of edge- and vertex-linked AgCl₅ square pyramids in large channels parallel to [001], additional Cl in these and other channels.

Aurivillius B. (1990) [1]



$a = 2.00893$, $c = 0.77178$ nm, $c/a = 0.384$, $V = 2.6975$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>l</i>	1	0.111	0.3588	0.24		non-coplanar triangle Bi ₃
Cl2	12 <i>l</i>	1	0.224	0.555	0.252		single atom Bi
Bi3	12 <i>l</i>	1	0.2265	0.3606	0.2472		non-coplanar square O ₄
O4	12 <i>l</i>	1	0.3271	0.4686	0.25		non-coplanar triangle Bi ₃
O5	6 <i>k</i>	<i>m</i> ..	0.069	0.541	$\frac{1}{2}$		non-coplanar triangle Bi ₃
Cl6	6 <i>k</i>	<i>m</i> ..	0.1032	0.2135	$\frac{1}{2}$		non-colinear Ag ₂
Bi7	6 <i>k</i>	<i>m</i> ..	0.1117	0.4202	$\frac{1}{2}$		non-coplanar square O ₄
O8	6 <i>k</i>	<i>m</i> ..	0.228	0.424	$\frac{1}{2}$		tetrahedron Bi ₄
Bi9	6 <i>k</i>	<i>m</i> ..	0.3486	0.5352	$\frac{1}{2}$		non-coplanar square O ₄
O10	6 <i>j</i>	<i>m</i> ..	0.0916	0.5442	0		non-colinear Bi ₂
Bi11	6 <i>j</i>	<i>m</i> ..	0.0953	0.4358	0	0.97	tricapped trigonal prism O ₇ Cl ₂
Cl12	6 <i>j</i>	<i>m</i> ..	0.1148	0.2198	0		non-colinear Ag ₂
O13	6 <i>j</i>	<i>m</i> ..	0.223	0.407	0		non-colinear Bi ₂
Bi14	6 <i>j</i>	<i>m</i> ..	0.3399	0.5309	0		non-coplanar square O ₄
Bi15	6 <i>i</i>	.. <i>m</i>	0.2472	0	0.247		non-coplanar square O ₄
O16	6 <i>i</i>	.. <i>m</i>	0.416	0	0.2		non-coplanar triangle Bi ₃
Bi17	6 <i>i</i>	.. <i>m</i>	0.5252	0	0.2563		non-coplanar triangle O ₃
Ag18	6 <i>i</i>	.. <i>m</i>	0.8674	0	0.252	0.8	square pyramid Cl ₅
O19	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.31	0	$\frac{1}{2}$		tetrahedron Bi ₄
Cl20	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.662	0	$\frac{1}{2}$		pseudo Frank-Kasper Bi ₈ O ₈ Cl ₄
O21	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.304	0	0		tetrahedron Bi ₄
Cl22	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.6681	0	0		pseudo Frank-Kasper Bi ₈ O ₈ Cl ₄
Cl23	2 <i>e</i>	3. <i>m</i>	0	0	0.212	0.75	tetrahedron Ag ₃ Cl

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 $\frac{1}{2}$

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.