

$\text{Ag}_{2.5}\text{Bi}_{24}\text{Cl}_{15.5}\text{O}_{29.5}$ *hP83*(189) *P-62m - k<sup>6:4</sup>j<sup>2</sup>ig<sup>2</sup>f<sup>3</sup>e***Ag<sub>5</sub>[Bi<sub>48</sub>O<sub>59</sub>Cl<sub>30</sub>]Cl [1]**

Structural features: BiO<sub>n</sub> polyhedra (mainly :BiO<sub>4</sub> square  $\psi$ -pyramids) share atoms to form a 3D-framework; triple chains of edge- and vertex-linked AgCl<sub>5</sub> square pyramids in large channels parallel to [001], additional Cl in these and other channels (partial disorder).

Aurivillius B. (1990) [1]

 $\text{Ag}_{2.40}\text{Bi}_{24}\text{Cl}_{15.70}\text{O}_{30}$  $a = 2.00893$ ,  $c = 0.38589$  nm,  $c/a = 0.192$ ,  $V = 1.3487$  nm<sup>3</sup>,  $Z = 1$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>k</i>	<i>m</i> ..	0.081	0.537	$\frac{1}{2}$		tetrahedron Bi <sub>4</sub>
Cl2	6 <i>k</i>	<i>m</i> ..	0.107	0.2172	$\frac{1}{2}$		non-colinear Ag <sub>2</sub>
Bi3	6 <i>k</i>	<i>m</i> ..	0.1886	0.5329	$\frac{1}{2}$		non-coplanar square O <sub>4</sub>
O4	6 <i>k</i>	<i>m</i> ..	0.1911	0.4153	$\frac{1}{2}$		tetrahedron Bi <sub>4</sub>
Bi5	6 <i>k</i>	<i>m</i> ..	0.3081	0.4207	$\frac{1}{2}$	0.5	
Bi6	6 <i>k</i>	<i>m</i> ..	0.3409	0.4353	$\frac{1}{2}$	0.5	
Bi7	6 <i>j</i>	<i>m</i> ..	0.1342	0.3606	0		non-coplanar square O <sub>4</sub>
O8	6 <i>j</i>	<i>m</i> ..	0.1426	0.4715	0		non-coplanar triangle Bi <sub>3</sub>
O9	6 <i>j</i>	<i>m</i> ..	0.2488	0.359	0		tetrahedron Bi <sub>4</sub>
Cl10	6 <i>j</i>	<i>m</i> ..	0.3318	0.5551	0		
O11	6 <i>i</i>	.. <i>m</i>	0.587	0	0.09	0.5	
Cl12	3 <i>g</i>	<i>m2m</i>	0.3334	0	$\frac{1}{2}$		non-coplanar square Bi <sub>4</sub>
O13	3 <i>g</i>	<i>m2m</i>	0.6928	0	$\frac{1}{2}$		
Ag14	3 <i>f</i>	<i>m2m</i>	0.1327	0	0	0.8	
Bi15	3 <i>f</i>	<i>m2m</i>	0.4747	0	0		
Bi16	3 <i>f</i>	<i>m2m</i>	0.7529	0	0		non-coplanar square O <sub>4</sub>
Cl17	2 <i>e</i>	3. <i>m</i>	0	0	0.083	0.35	

Transformation from published data: origin shift 0 0  $\frac{1}{2}$ 

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

Remarks: O vacancies not located. Partial occupation of site Cl17 by O or Ag could not be excluded. Average structure; the superstructure was refined in the same space group with double cell volume (new axes a,b,2c). Short interatomic distances for partly occupied site(s).

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