

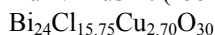
*hP89*

(189)  $P\text{-}62m - k^4j^6i^3gf^2e$

### **Cu<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; units of three edge-linked CuCl<sub>4</sub> tetrahedra share vertices to form infinite chains in large channels parallel to [001], additional Cl in these and other channels (partial disorder).

Aurivillius B. (1990) [1]



$a = 2.00248$ ,  $c = 0.3868$  nm,  $c/a = 0.193$ ,  $V = 1.3432$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Bi1	6 <i>k</i>	<i>m</i> ..	0.1328	0.3586	$\frac{1}{2}$		non-coplanar square O <sub>4</sub>
O2	6 <i>k</i>	<i>m</i> ..	0.1376	0.4694	$\frac{1}{2}$		non-coplanar triangle Bi <sub>3</sub>
O3	6 <i>k</i>	<i>m</i> ..	0.2478	0.3589	$\frac{1}{2}$		tetrahedron Bi <sub>4</sub>
Cl4	6 <i>k</i>	<i>m</i> ..	0.331	0.554	$\frac{1}{2}$		
O5	6 <i>j</i>	<i>m</i> ..	0.0845	0.5381	0		tetrahedron Bi <sub>4</sub>
Cl6	6 <i>j</i>	<i>m</i> ..	0.1087	0.2178	0		
O7	6 <i>j</i>	<i>m</i> ..	0.1886	0.4153	0		tetrahedron Bi <sub>4</sub>
Bi8	6 <i>j</i>	<i>m</i> ..	0.189	0.5321	0		non-coplanar square O <sub>4</sub>
Bi9	6 <i>j</i>	<i>m</i> ..	0.3076	0.4196	0	0.5	
Bi10	6 <i>j</i>	<i>m</i> ..	0.3373	0.4324	0	0.5	
Cu11	6 <i>i</i>	.. <i>m</i>	0.1031	0	0.118	0.45	
Bi12	6 <i>i</i>	.. <i>m</i>	0.4749	0	0.459	0.5	
O13	6 <i>i</i>	.. <i>m</i>	0.587	0	0.413	0.5	
Bi14	3 <i>g</i>	<i>m2m</i>	0.7556	0	$\frac{1}{2}$		non-coplanar square O <sub>4</sub>
Cl15	3 <i>f</i>	<i>m2m</i>	0.3318	0	0		non-coplanar square Bi <sub>4</sub>
O16	3 <i>f</i>	<i>m2m</i>	0.6946	0	0		
Cl17	2 <i>e</i>	3.. <i>m</i>	0	0	0.362	0.375	single atom Cl

Experimental: single crystal, diffractometer, X-rays, R = 0.049

Remarks: O vacancies not located. Partial occupation of site Cl17 by O or Cu 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.