



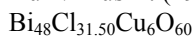
*hP*152

(189) *P*-62*m* – $1^4k^5j^5i^5g^2fe$

Cu₅[Bi₄₈O₅₉Cl₃₀]Cl [1]

Structural features: BiO_n polyhedra (mainly :BiO₄ square ψ -pyramids) share atoms to form a 3D-framework; units of three edge-linked CuCl₄ tetrahedra share vertices to form infinite chains in large channels parallel to [001], additional Cl in these and other channels.

Aurivillius B. (1990) [1]



$a = 2.00248$, $c = 0.7736$ nm, $c/a = 0.386$, $V = 2.6865$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Bi1	12 <i>l</i>	1	0.1328	0.3586	0.2512		non-coplanar square O ₄
O2	12 <i>l</i>	1	0.1372	0.4684	0.25		non-coplanar triangle Bi ₃
O3	12 <i>l</i>	1	0.2437	0.3589	0.231		non-coplanar triangle Bi ₃
Cl4	12 <i>l</i>	1	0.3308	0.5535	0.258		non-coplanar triangle Bi ₃
O5	6 <i>k</i>	<i>m</i> ..	0.086	0.538	$\frac{1}{2}$		tetrahedron Bi ₄
Cl6	6 <i>k</i>	<i>m</i> ..	0.1088	0.2164	$\frac{1}{2}$		
O7	6 <i>k</i>	<i>m</i> ..	0.176	0.402	$\frac{1}{2}$		non-colinear Bi ₂
Bi8	6 <i>k</i>	<i>m</i> ..	0.1908	0.5311	$\frac{1}{2}$		non-coplanar square O ₄
Bi9	6 <i>k</i>	<i>m</i> ..	0.336	0.4324	$\frac{1}{2}$		tricapped trigonal prism O ₇ Cl ₂
O10	6 <i>j</i>	<i>m</i> ..	0.081	0.538	0		non-coplanar triangle Bi ₃
Cl11	6 <i>j</i>	<i>m</i> ..	0.108	0.2188	0		
Bi12	6 <i>j</i>	<i>m</i> ..	0.1876	0.5331	0		non-coplanar square O ₄
O13	6 <i>j</i>	<i>m</i> ..	0.194	0.423	0		tetrahedron Bi ₄
Bi14	6 <i>j</i>	<i>m</i> ..	0.3075	0.4188	0		non-coplanar square O ₄
Cu15	6 <i>i</i>	.. <i>m</i>	0.1011	0	0.041	0.5	
Cu16	6 <i>i</i>	.. <i>m</i>	0.1051	0	0.421	0.5	
Bi17	6 <i>i</i>	.. <i>m</i>	0.4749	0	0.2451		5-vertex polyhedron O ₅
O18	6 <i>i</i>	.. <i>m</i>	0.585	0	0.289		non-coplanar triangle Bi ₃
Bi19	6 <i>i</i>	.. <i>m</i>	0.7557	0	0.2522		non-coplanar square O ₄
Cl20	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.3269	0	$\frac{1}{2}$		pseudo Frank-Kasper O ₈ Bi ₈ Cl ₄
O21	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.699	0	$\frac{1}{2}$		tetrahedron Bi ₄
Cl22	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.337	0	0		pseudo Frank-Kasper Bi ₈ O ₈ Cl ₄
O23	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.679	0	0		non-colinear Bi ₂
Cl24	2 <i>e</i>	3.. <i>m</i>	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) *P*6₃22 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.