

Pb<sub>12</sub>[CO<sub>3</sub>][ClO<sub>4</sub>]<sub>10</sub>[OH]<sub>12</sub>[H<sub>2</sub>O]<sub>6</sub>

*hP*180

(176) *P*6<sub>3</sub>/*m* – i<sup>10</sup>h<sup>6</sup>f<sup>4</sup>eba

[Pb<sub>4</sub>(OH)<sub>4</sub>]<sub>3</sub>(CO<sub>3</sub>)(ClO<sub>4</sub>)<sub>10</sub>·6H<sub>2</sub>O [1]

Structural features: (Pb<sub>4</sub>[OH]<sub>4</sub>) cubic clusters (a Pb<sub>4</sub> tetrahedron with one OH above each face), ClO<sub>4</sub> tetrahedra (partial orientational disorder) and CO<sub>3</sub> trigonal units (perpendicular to [001]); H<sub>2</sub>O between the units.

Hong S.H., Olin B. (1973) [1]

CCl<sub>10</sub>H<sub>24</sub>O<sub>61</sub>Pb<sub>12</sub>

*a* = 1.4121, *c* = 1.6316 nm, *c/a* = 1.155, *V* = 2.8176 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cl1	12 <i>i</i>	1	0.0063	0.3335	0.0928		tetrahedron O <sub>4</sub>
O2	12 <i>i</i>	1	0.062	0.3713	0.0195		single atom Cl
O3	12 <i>i</i>	1	0.0674	0.3233	0.153		single atom Cl
O4	12 <i>i</i>	1	0.0946	0.0017	0.0376	0.5	non-collinear ClO
Pb5	12 <i>i</i>	1	0.22033	0.22285	0.13474		non-coplanar triangle (OH) <sub>3</sub>
O6	12 <i>i</i>	1	0.3288	0.093	0.0803		single atom Cl
(OH <sub>2</sub> )7	12 <i>i</i>	1	0.3304	0.4613	0.0978		single atom Pb
(OH)8	12 <i>i</i>	1	0.4191	0.3282	0.1668		single atom Pb
O9	12 <i>i</i>	1	0.4277	0.0179	0.1168		single atom Cl
O10	12 <i>i</i>	1	0.5758	0.3369	0.0346		single atom Cl
O11	6 <i>h</i>	<i>m</i> ..	0.0422	0.1099	<sup>1</sup> / <sub>4</sub>		single atom C
Pb12	6 <i>h</i>	<i>m</i> ..	0.05022	0.57673	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle (OH) <sub>3</sub>
(OH)13	6 <i>h</i>	<i>m</i> ..	0.2427	0.3329	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle Pb <sub>3</sub>
(OH)14	6 <i>h</i>	<i>m</i> ..	0.2611	0.146	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle Pb <sub>3</sub>
O15	6 <i>h</i>	<i>m</i> ..	0.2657	0.5538	<sup>1</sup> / <sub>4</sub>		
Pb16	6 <i>h</i>	<i>m</i> ..	0.44783	0.21413	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle (OH) <sub>3</sub>
O17	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.141	0.5	single atom Cl
Cl18	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.2296	0.5	
Cl19	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5632		tetrahedron O <sub>4</sub>
O20	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6519		single atom Cl
O21	4 <i>e</i>	3..	0	0	0.09	0.5	single atom Cl
Cl22	2 <i>b</i>	-3..	0	0	0		square prism (cube) O <sub>8</sub>
C23	2 <i>a</i>	-6..	0	0	<sup>1</sup> / <sub>4</sub>		coplanar triangle O <sub>3</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.060

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Hong S.H., Olin B. (1973), Acta Chem. Scand. 27, 2309-2320.