

$\text{Pb}_5[\text{CO}_3]_3\text{O}[\text{OH}]_2$ *hP*126(185) $P6_3cm - d^4c^9b^4a^4$ **Pb₅(CO₃)₃O(OH)₂** [1], plumbonacrite

Structural features: O(OH)₃Pb₇ clusters (a central OPb₄ tetrahedron sharing edges with three (OH)Pb₃ non-planar trigonal units) and CO₃ trigonal units (perpendicular to [001]) share atoms to form infinite slabs (Pb electron lone-pairs in the interlayers).

Krivovichev S.V., Burns P.C. (2000) [1]

 $\text{C}_3\text{H}_2\text{O}_{12}\text{Pb}_5$ $a = 0.90921$, $c = 2.4923$ nm, $c/a = 2.741$, $V = 1.7843$ nm³, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.138	0.323	0.3345	0.5	single atom C
O2	12 <i>d</i>	1	0.199	0.525	0.0164		single atom C
O3	12 <i>d</i>	1	0.332	0.522	0.1576		single atom C
Pb4	12 <i>d</i>	1	0.3477	0.4265	0.4264		
O5	6 <i>c</i>	.. <i>m</i>	0.138	0	0.0126		single atom C
O6	6 <i>c</i>	.. <i>m</i>	0.143	0	0.637		single atom C
Pb7	6 <i>c</i>	.. <i>m</i>	0.2466	0	0.735		single atom O
(OH)8	6 <i>c</i>	.. <i>m</i>	0.289	0	0.2121		single atom Pb
Pb9	6 <i>c</i>	.. <i>m</i>	0.3219	0	0.534		single atom (OH)
C10	6 <i>c</i>	.. <i>m</i>	0.323	0	0.337		non-coplanar triangle O ₃
(OH)11	6 <i>c</i>	.. <i>m</i>	0.351	0	0.4437		single atom Pb
Pb12	6 <i>c</i>	.. <i>m</i>	0.3537	0	0.1281		single atom (OH)
O13	6 <i>c</i>	.. <i>m</i>	0.469	0	0.3294		single atom C
C14	4 <i>b</i>	3.. _{1/3}	_{1/3}	_{2/3}	0.021		non-coplanar triangle O ₃
C15	4 <i>b</i>	3.. _{1/3}	_{1/3}	_{2/3}	0.147		non-coplanar triangle O ₃
Pb16	4 <i>b</i>	3.. _{1/3}	_{1/3}	_{2/3}	0.3148		single atom O
O17	4 <i>b</i>	3.. _{1/3}	_{1/3}	_{2/3}	0.401		tetrahedron Pb ₄
C18	2 <i>a</i>	3.. <i>m</i>	0	0	0.0		non-coplanar triangle O ₃
C19	2 <i>a</i>	3.. <i>m</i>	0	0	0.145		non-coplanar triangle O ₃
O20	2 <i>a</i>	3.. <i>m</i>	0	0	0.255		tetrahedron Pb ₄
Pb21	2 <i>a</i>	3.. <i>m</i>	0	0	0.3521		single atom O

Transformation from published data: origin shift 0 0 0.465

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

Remarks: Metastable phase. The atom arrangement within one structural slab was determined in [2]. 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] Krivovichev S.V., Burns P.C. (2000), Mineral. Mag. 64, 1069-1075. [2] Cowley J.M. (1956), Acta Crystallogr. 9, 391-396.