

$\text{H}_2\text{Pb}_5[\text{BO}_3]_3\text{O}[\text{OH}][\text{H}_2\text{O}]$	$hP126$	(185) $P6_3cm - d^4c^9b^4a^4$
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**$\text{Pb}_5\text{B}_3\text{O}_8(\text{OH})_3 \cdot \text{H}_2\text{O}$  [1]**

Structural features:  $\text{O}(\text{OH})_3\text{Pb}_7$  clusters (a central  $\text{OPb}_4$  tetrahedron sharing edges with three non-planar  $(\text{OH})\text{Pb}_3$  trigonal units) and  $\text{BO}_3$ ,  $\text{B}(\text{O}_2[\text{OH}])$  and  $\text{B}(\text{OH})_3$  trigonal units (perpendicular to  $[001]$ ) share atoms to form infinite slabs (Pb electron lone-pairs in the interlayers).

Rastsvetaeva R.K. et al. (1998) [1]

$\text{B}_3\text{H}_5\text{O}_{12}\text{Pb}_5$

$a = 0.9067$ ,  $c = 2.4637$  nm,  $c/a = 2.717$ ,  $V = 1.7541$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>d</i>	1	0.135	0.293	0.427		single atom B
O2	12 <i>d</i>	1	0.2	0.52	0.101		single atom B
O3	12 <i>d</i>	1	0.325	0.515	0.229		single atom B
Pb4	12 <i>d</i>	1	0.3438	0.4227	0.327	0.5	
(OH)5	6 <i>c</i>	.. <i>m</i>	0.154	0	0.736		single atom B
O6	6 <i>c</i>	.. <i>m</i>	0.156	0	0.111		single atom B
Pb7	6 <i>c</i>	.. <i>m</i>	0.2469	0	0.0179		6-vertex polyhedron $\text{O}_4(\text{OH})_2$
(OH)8	6 <i>c</i>	.. <i>m</i>	0.297	0	0.538		single atom Pb
B9	6 <i>c</i>	.. <i>m</i>	0.318	0	0.426		non-coplanar triangle $(\text{OH})\text{O}_2$
Pb10	6 <i>c</i>	.. <i>m</i>	0.3255	0	0.216		single atom $(\text{OH}_2)$
$(\text{OH}_2)11$	6 <i>c</i>	.. <i>m</i>	0.333	0	0.311		single atom Pb
$(\text{OH})12$	6 <i>c</i>	.. <i>m</i>	0.464	0	0.427		single atom B
Pb13	6 <i>c</i>	.. <i>m</i>	0.6495	0	0.1251		single atom (OH)
B14	4 <i>b</i>	3.. $\frac{1}{3}$	$\frac{1}{3}$	$\frac{2}{3}$	0.1		non-coplanar triangle $\text{O}_3$
B15	4 <i>b</i>	3.. $\frac{1}{3}$	$\frac{1}{3}$	$\frac{2}{3}$	0.228		non-coplanar triangle $\text{O}_3$
O16	4 <i>b</i>	3.. $\frac{1}{3}$	$\frac{1}{3}$	$\frac{2}{3}$	0.345		tetrahedron $\text{Pb}_4$
Pb17	4 <i>b</i>	3.. $\frac{1}{3}$	$\frac{1}{3}$	$\frac{2}{3}$	0.4373		single atom O
O18	2 <i>a</i>	3.. <i>m</i>	0	0	0.0		tetrahedron $\text{Pb}_4$
B19	2 <i>a</i>	3.. <i>m</i>	0	0	0.11		non-coplanar triangle $\text{O}_3$
B20	2 <i>a</i>	3.. <i>m</i>	0	0	0.235		non-coplanar triangle $(\text{OH})_3$
Pb21	2 <i>a</i>	3.. <i>m</i>	0	0	0.4		7-vertex polyhedron $\text{O}_7$

Transformation from published data:  $-x, -y, -z$ ; origin shift 0 0 0.6

Experimental: single crystal, diffractometer, X-rays,  $R = 0.067$

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] Rastsvetaeva R.K., Arakcheeva A.V., Pushcharovsky D.Y., Vinogradova S.A., Dimitrova O.V., Stefanovich S.Y. (1998), *Z. Kristallogr.* 213, 240-245.