

$\text{Pb}_2\text{Cl}_3[\text{OH}]$	$hP18$	$(174) P-6 - k^3j^3$
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**Pb<sub>2</sub>(OH)Cl<sub>3</sub>** [1], penfieldite

Structural features: Double infinite chains of vertex-linked  $:\text{Pb}([\text{OH}]\text{Cl}_2)$  and  $:\text{Pb}([\text{OH}]_2\text{Cl})$   $\psi$ -tetrahedra parallel to [001]; additional Cl complete square antiprismatic (bicapped trigonal prismatic) coordination around Pb.

Merlino S. et al. (1995) [1]

$\text{Cl}_3\text{HOPb}_2$

$a = 1.1393$ ,  $c = 0.4024$  nm,  $c/a = 0.353$ ,  $V = 0.4523$  nm<sup>3</sup>,  $Z = 3$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Pb1	$3k$	$m..$	0.2739	0.1743	$\frac{1}{2}$		square antiprism (OH)Cl <sub>7</sub>
Cl2	$3k$	$m..$	0.2948	0.4676	$\frac{1}{2}$		square pyramid Pb <sub>5</sub>
(OH)3	$3k$	$m..$	0.41	0.062	$\frac{1}{2}$		non-coplanar triangle Pb <sub>3</sub>
Cl4	$3j$	$m..$	0.0505	0.1941	0		non-coplanar triangle Pb <sub>3</sub>
Pb5	$3j$	$m..$	0.0835	0.4614	0		square antiprism (OH) <sub>2</sub> Cl <sub>6</sub>
Cl6	$3j$	$m..$	0.4683	0.3212	0		non-colinear Pb <sub>2</sub>

Transformation from published data:  $y, x, z$ ; origin shift  $0\ 0\ \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.041$

Remarks: Natural specimen from Baratti beach, Piombino, Tuscany, Italy. Composition  $\text{Pb}_2\text{Cl}_{2.88}\text{F}_{0.03}(\text{OH})_{1.09}$  from electron microprobe analysis. Average structure; additional reflections could be indexed with a 12- or 15-fold supercell (new axes  $a, b, 12c$  and  $a, b, 15c$ , respectively). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Merlino S., Pasero M., Perchiazzi N., Gianfagna A. (1995), Mineral. Mag. 59, 341-347.