

$\text{Zn}_{5.5}[\text{PHO}_3]_4[\text{OH}]_3$  $hP50$  $(186) P6_3mc - d^2c^4b$  **$\text{Zn}_{11}(\text{HPO}_3)_8(\text{OH})_6$**  [1]

Structural features: Columns of edge- and face-linked  $\text{Zn}(\text{O}_4[\text{OH}]_2)$  octahedra are interconnected via common vertices and  $\text{P}(\text{HO}_3)$  tetrahedra to form a 3D-framework with large channels parallel to  $[001]$ .

Marcos M.D. et al. (1993) [1]

 $\text{H}_7\text{O}_{15}\text{P}_4\text{Zn}_{5.50}$  $a = 1.2872$ ,  $c = 0.49772$  nm,  $c/a = 0.387$ ,  $V = 0.7142$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12d	1	0.0736	0.3437	0.1101		single atom P
Zn2	12d	1	0.42918	0.08062	0.2538	0.917	octahedron O <sub>6</sub>
P3	6c	.m.	0.16139	0.83861	0.2728		non-coplanar triangle O <sub>3</sub>
O4	6c	.m.	0.4747	0.5253	0.452		non-coplanar square Zn <sub>4</sub>
O5	6c	.m.	0.6013	0.3987	0.4148		single atom P
O6	6c	.m.	0.8019	0.1981	0.0358		single atom P
P7	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0		non-coplanar triangle O <sub>3</sub>
H8	6c	.m.	0.099	0.901	0.3238		
H9	6c	.m.	0.449	0.551	0.3138		
H10	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2838		

Transformation from published data:  $-x, -y, -z$ ; origin shift 0 0 0.2462Experimental: single crystal, diffractometer, X-rays,  $R = 0.030$ ,  $T = 293$  K

Remarks: Space group (194)  $P6_3/mmc$  was tested and rejected. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Marcos M.D., Amoros P., Le Bail A. (1993), J. Solid State Chem. 107, 250-257.