

Co_{5.5}[PHO₃]₄[OH]₃

hP52

(186) $P6_3mc - d^2c^4b^2$ **Co₁₁(HPO₃)₈(OH)₆** [1]

Structural features: Columns of edge- and face-linked Co(O₄[OH]₂) octahedra are interconnected via common vertices and P(HO₃) tetrahedra (partial orientational disorder) to form a 3D-framework with large channels parallel to [001]. Variant of Zn₁₁(HPO₃)₈(OH)₆.

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

Co_{5.50}H₇O₁₅P₄ $a = 1.28244$, $c = 0.49734$ nm, $c/a = 0.388$, $V = 0.7084$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Co1	12 <i>d</i>	1	0.0772	0.4311	0.2513	0.917	octahedron O ₆
O2	12 <i>d</i>	1	0.343	0.0762	0.3993		single atom P
O3	6 <i>c</i>	. <i>m</i> .	0.2037	0.7963	0.4823		single atom P
O4	6 <i>c</i>	. <i>m</i> .	0.39847	0.60153	0.0879		
O5	6 <i>c</i>	. <i>m</i> .	0.5325	0.4675	0.0523		non-coplanar square Co ₄
P6	6 <i>c</i>	. <i>m</i> .	0.83845	0.16155	0.2246		non-coplanar triangle O ₃
P7	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0	0.2	
P8	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1757	0.8	
H9	6 <i>c</i>	. <i>m</i> .	0.558	0.442	0.2216		
H10	6 <i>c</i>	. <i>m</i> .	0.8955	0.1045	0.1313		
H11	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.4472	0.8	
H12	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.7286	0.2	

Transformation from published data: origin shift 0 0 0.9987

Experimental: powder, diffractometer, X-rays, R_B = 0.079

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] Marcos M.D., Amoros P., Beltran Porter A., Martinez Manez R., Attfield J.P. (1993), Chem. Mater. 5, 121-128.