

$K_4Ca_{10}[P_2O_7]_6[H_2O]_9$	<i>hP88</i>	(185) $P6_3cm - d^4c^6b$
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$K_4Ca_{10}(P_2O_7)_6 \cdot 9H_2O$ [1]

Structural features: Units of two vertex-linked PO_4 tetrahedra (perpendicular to [001]) share atoms with CaO_6 octahedra and $CaO_6(OH_2)$ monocapped trigonal prisms to form a 3D-framework; K and additional H_2O in channels parallel to [001] (partial disorder).

Mathew M., Ammon H.L. (1995) [1]

$Ca_{10}H_{18}K_4O_{51}P_{12}$

$a = 1.1761$, $c = 0.977$ nm, $c/a = 0.831$, $V = 1.1703$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.1455	0.3796	0.2274		single atom P
O2	12 <i>d</i>	1	0.1503	0.6251	0.1389		single atom P
P3	12 <i>d</i>	1	0.2891	0.4337	0.2497		tetrahedron O ₄
O4	12 <i>d</i>	1	0.3336	0.4894	0.3937		single atom P
K5	6 <i>c</i>	.. <i>m</i>	0.055	0	0.2509	0.167	
(OH ₂)6	6 <i>c</i>	.. <i>m</i>	0.1822	0	0.0169		tetrahedron CaK(OH ₂) ₂
(OH ₂)7	6 <i>c</i>	.. <i>m</i>	0.252	0	0.4469	0.5	
K8	6 <i>c</i>	.. <i>m</i>	0.298	0	0.4472	0.5	
Ca9	6 <i>c</i>	.. <i>m</i>	0.3966	0	0.0759		monocapped trigonal prism O ₆ (OH ₂)
O10	6 <i>c</i>	.. <i>m</i>	0.6945	0	0.242		non-colinear P ₂
Ca11	4 <i>b</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0		octahedron O ₆

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.2501

Experimental: single crystal, diffractometer, X-rays, R = 0.028, T = 293 K

Remarks: Partial occupancy of site K5 by OH₂ alone and partial substitution by K on site (OH₂)7 could not be excluded. 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] Mathew M., Ammon H.L. (1995), J. Chem. Crystallogr. 25, 219-222.