

NaZn[PO₄][H₂O]*hP*126(178) *P*6₁22 – c⁸b⁴a**NaZnPO₄·H₂O** [1]

Structural features: PO₄ and ZnO₄ tetrahedra share vertices to form a 3D-framework; Na and H₂O in cavities interconnected via 6- and 8-rings (partial disorder).

Harrison W.T.A. et al. (1996) [1]

H_{1.52}Na_{0.51}O_{4.76}PZn*a* = 1.04797, *c* = 1.5089 nm, *c/a* = 1.44, *V* = 1.4351 nm³, *Z* = 12

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>c</i>	1	0.2466	0.0485	0.38517		non-colinear PZn
Na2	12 <i>c</i>	1	0.336	0.602	0.09833	0.24	
P3	12 <i>c</i>	1	0.4088	0.1676	0.39243		tetrahedron O ₄
(OH ₂)4	12 <i>c</i>	1	0.41	0.108	0.00567	0.29	
(OH ₂)5	12 <i>c</i>	1	0.425	0.178	0.04967	0.3	
O6	12 <i>c</i>	1	0.429	0.311	0.35253		non-colinear PZn
O7	12 <i>c</i>	1	0.4597	0.195	0.48943		single atom P
O8	12 <i>c</i>	1	0.511	0.127	0.34233		non-colinear PZn
(OH ₂)9	6 <i>b</i>	..2	0.035	0.07	¹ / ₄	0.1	non-colinear (OH ₂) ₂
Zn10	6 <i>b</i>	..2	0.4929	0.9858	¹ / ₄		tetrahedron O ₄
Na11	6 <i>b</i>	..2	0.668	0.336	¹ / ₄	0.53	
Zn12	6 <i>b</i>	..2	0.8413	0.6827	¹ / ₄		tetrahedron O ₄
(OH ₂)13	6 <i>a</i>	.2.	0.076	0	0	0.24	non-colinear (OH ₂) ₂

Experimental: single crystal, diffractometer, X-rays, wR = 0.052, T = 298 K

Remarks: Part of Na and H₂O not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 1 of [1] the *y*-coordinate of former O(5) is misprinted as 0.033 instead of 0.035 (agreement with Wyckoff position 6*b*).

References: [1] Harrison W.T.A., Gier T.E., Stucky G.D., Broach R.W., Bedard R.A. (1996), Chem. Mater. 8, 145-151.