

NaZnB[PO₄]₂[H₂O]*hP*84(178) *P*6₁22 – c⁵b³a**NaZn[BP₂O₈]·H₂O** [1]

Structural features: BO₄ and PO₄ tetrahedra share vertices to form infinite twisted chains, which are interconnected via ZnO₄ tetrahedra to form a 3D-framework with channels of approximately hexagonal cross-section parallel to [001].

Boy I. et al. (2001) [1]

BH₂NaO₉P₂Zn*a* = 0.95404, *c* = 1.4778 nm, *c/a* = 1.549, *V* = 1.1649 nm³, *Z* = 6

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>c</i>	1	0.214	0.011	0.394		non-colinear BP
O2	12 <i>c</i>	1	0.367	0.295	0.3673		single atom P
P3	12 <i>c</i>	1	0.3886	0.1581	0.4019		tetrahedron O ₄
O4	12 <i>c</i>	1	0.444	0.183	0.5082		non-colinear BP
O5	12 <i>c</i>	1	0.526	0.16	0.3599		single atom P
Na6	6 <i>b</i>	..2	0.195	0.39	¹ / ₄		non-colinear (OH ₂) ₂
Zn7	6 <i>b</i>	..2	0.5149	0.0298	¹ / ₄		tetrahedron O ₄
B8	6 <i>b</i>	..2	0.834	0.668	¹ / ₄		tetrahedron O ₄
(OH ₂)9	6 <i>a</i>	.2.	0.238	0	0		non-colinear Na ₂

Experimental: powder, diffractometer, X-rays, wR_p = 0.052, T = 293 K

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Boy I., Stowasser F., Schäfer G., Kniep R. (2001), Chem. Eur. J. 7, 834-839.