

NaZn[PO₄][H₂O]*hP90*(178) *P6₁22 – c⁶b³***NaZnPO₄·H₂O** [1]

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

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

H_{0.68}Na_{0.17}O_{4.34}PZn*a* = 1.0412, *c* = 1.5184 nm, *c/a* = 1.458, *V* = 1.4256 nm³, *Z* = 12

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|---------------------|-------------|------|----------|----------|-----------------------------|------|--------------------------------|
| O1 | 12 <i>c</i> | 1 | 0.1099 | 0.4229 | 0.0201 | | non-colinear PZn |
| O2 | 12 <i>c</i> | 1 | 0.1945 | 0.2464 | 0.0547 | | non-colinear PZn |
| P3 | 12 <i>c</i> | 1 | 0.23564 | 0.40605 | 0.06011 | | tetrahedron O ₄ |
| O4 | 12 <i>c</i> | 1 | 0.2621 | 0.4597 | 0.1566 | | single atom P |
| O5 | 12 <i>c</i> | 1 | 0.3738 | 0.503 | 0.0075 | | non-colinear PZn |
| (OH ₂)6 | 12 <i>c</i> | 1 | 0.4092 | 0.1205 | 0.51077 | 0.34 | single atom (OH ₂) |
| Zn7 | 6 <i>b</i> | ..2 | 0.15757 | 0.31514 | ¹ / ₄ | | tetrahedron O ₄ |
| Na8 | 6 <i>b</i> | ..2 | 0.3287 | 0.6575 | ¹ / ₄ | 0.34 | tetrahedron O ₄ |
| Zn9 | 6 <i>b</i> | ..2 | 0.50303 | 0.00607 | ¹ / ₄ | | tetrahedron O ₄ |

Transformation from published data (*P6₅22*): new axes -a,-b,-c

Experimental: single crystal, diffractometer, X-rays, R = 0.069

Remarks: Part of Na and H₂O not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

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