

| | | |
|--|---------------|---|
| Na(Zn _{0.8} Co _{0.2})[PO ₄][H ₂ O] | <i>hP</i> 132 | (178) <i>P</i> 6 ₁ 22 – c ¹⁰ b ² |
|--|---------------|---|

Na₆[Co_{0.2}Zn_{0.8}PO₄]₆·6H₂O [2]

Structural features: PO₄ and (Zn,Co)O₄ tetrahedra share vertices to form a 3D-framework; Na and H₂O in cavities interconnected via 6- and 8-rings (partial disorder).

Helliwell M. et al. (1999) [1]

Co_{0.16}H₂NaO₅PZn_{0.84}

a = 1.0464, *c* = 1.5056 nm, *c/a* = 1.439, *V* = 1.4277 nm³, *Z* = 12

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|---------------------|-------------|------|----------|----------|-----------------------------|------|--------------------------------|
| Na1 | 12 <i>c</i> | 1 | 0.091 | 0.018 | 0.538 | 0.32 | |
| O2 | 12 <i>c</i> | 1 | 0.1174 | 0.4286 | 0.0181 | | non-colinear PZn |
| O3 | 12 <i>c</i> | 1 | 0.1978 | 0.2469 | 0.0535 | | non-colinear PZn |
| Na4 | 12 <i>c</i> | 1 | 0.212 | 0.185 | 0.549 | 0.18 | |
| P5 | 12 <i>c</i> | 1 | 0.2406 | 0.4097 | 0.05934 | | tetrahedron O ₄ |
| O6 | 12 <i>c</i> | 1 | 0.2646 | 0.4612 | 0.1553 | | single atom P |
| O7 | 12 <i>c</i> | 1 | 0.3838 | 0.5081 | 0.0088 | | non-colinear PZn |
| (OH ₂)8 | 12 <i>c</i> | 1 | 0.414 | 0.102 | 0.50967 | 0.66 | single atom (OH ₂) |
| (OH ₂)9 | 12 <i>c</i> | 1 | 0.416 | 0.173 | 0.564 | 0.34 | |
| Na10 | 12 <i>c</i> | 1 | 0.6631 | 0.2974 | 0.0765 | 0.5 | |
| M11 | 6 <i>b</i> | ..2 | 0.15823 | 0.31646 | ¹ / ₄ | | tetrahedron O ₄ |
| M12 | 6 <i>b</i> | ..2 | 0.50727 | 0.01454 | ¹ / ₄ | | tetrahedron O ₄ |

M11 = 0.88Zn + 0.12Co; M12 = 0.81Zn + 0.19Co

Transformation from published data (*P*6₅22): new axes -a,-b,-c; origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.051, T = 294 K

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Co could not be located in [2] (atom coordinates not published).

References: [1] Helliwell M., Helliwell J.R., Kaucic V., Logar N.Z., Barba L., Busetto E., Lausi A. (1999), *Acta Crystallogr. B* 55, 327-332. [2] Zabukovec Logar N., Rajic N., Kaucic V., Golic L. (1995), *J. Chem. Soc., Chem. Commun.* 1995, 353-354.