

InB[PO₄]₂[H₂O]_{0.8}

hP90

(178) *P*6₁22 – c⁶b²a**In[BP₂O₈]·0.8H₂O** [1]

Structural features: BO₄ and PO₄ tetrahedra share vertices to form infinite twisted chains, which are interconnected via distorted InO₄ tetrahedra to form a 3D-framework with channels of approximately hexagonal cross-section parallel to [001]; H₂O between the chains (partial disorder).

Belokoneva E.L. et al. (2001) [1]

BH_{1.60}InO_{8.80}P₂*a* = 0.9581, *c* = 1.59 nm, *c/a* = 1.66, *V* = 1.2640 nm³, *Z* = 6

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>c</i>	1	0.063	0.377	0.05177		single atom P
O2	12 <i>c</i>	1	0.187	0.214	0.06367		non-colinear PB
P3	12 <i>c</i>	1	0.2108	0.3793	0.08273		tetrahedron O ₄
(OH ₂)4	12 <i>c</i>	1	0.36	0.18	0.55533	0.15	
O5	12 <i>c</i>	1	0.364	0.511	0.04467		single atom P
O6	12 <i>c</i>	1	0.409	0.176	0.01257		non-colinear BP
B7	6 <i>b</i>	..2	0.151	0.302	¹ / ₄		tetrahedron O ₄
In8	6 <i>b</i>	..2	0.4445	0.889	¹ / ₄		tetrahedron O ₄
(OH ₂)9	6 <i>a</i>	.2.	0.834	0	0	0.5	non-colinear (OH ₂) ₂

Transformation from published data: origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.071

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. 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] Belokoneva E.L., Gurbanova O.A., Dimitrova O.V., Stefanovich S.Y., Al Ama A.G. (2001), Zh. Neorg. Khim. 46, 1115-1120.