

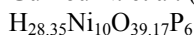
*hP*124

(176) $P6_3/m - i^4h^{12}f$



Structural features: $\text{Ni}(\text{O}_3[\text{OH}]_3)$, $\text{Ni}(\text{O}_4[\text{OH}]_2)$ and $\text{Ni}(\text{O}_4[\text{OH}][\text{OH}_2])$ octahedra share faces, edges and vertices to form a 3D-framework; P in tetrahedral voids (single PO_4 and $\text{P}(\text{O}_3[\text{OH}])$ tetrahedra), additional H_2O in large channels parallel to $[001]$.

Guillou N. et al. (2001) [1]



$a = 1.8209$, $c = 0.63898$ nm, $c/a = 0.351$, $V = 1.8348$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.0545	0.4482	0.05		single atom P
(OH ₂)2	12 <i>i</i>	1	0.089	0.157	0.038	0.35	single atom (OH ₂)
Ni3	12 <i>i</i>	1	0.1442	0.5757	0.0154		octahedron (OH) ₂ O ₄
O4	12 <i>i</i>	1	0.5478	0.2422	0.045		single atom P
P5	6 <i>h</i>	<i>m</i> ..	0.0041	0.4138	$\frac{1}{4}$		tetrahedron O ₄
(OH ₂)6	6 <i>h</i>	<i>m</i> ..	0.024	0.204	$\frac{1}{4}$	0.42	non-colinear (OH ₂) ₂
(OH)7	6 <i>h</i>	<i>m</i> ..	0.108	0.615	$\frac{1}{4}$		non-colinear Ni ₂
(OH ₂)8	6 <i>h</i>	<i>m</i> ..	0.184	0.3731	$\frac{1}{4}$	0.938	single atom (OH ₂)
(OH)9	6 <i>h</i>	<i>m</i> ..	0.2337	0.5864	$\frac{1}{4}$		non-coplanar square Ni ₄
(OH ₂)10	6 <i>h</i>	<i>m</i> ..	0.309	0.284	$\frac{1}{4}$		single atom Ni
M11	6 <i>h</i>	<i>m</i> ..	0.357	0.038	$\frac{1}{4}$		single atom P
(OH)12	6 <i>h</i>	<i>m</i> ..	0.412	0.186	$\frac{1}{4}$		single atom P
Ni13	6 <i>h</i>	<i>m</i> ..	0.4324	0.3973	$\frac{1}{4}$		octahedron O ₄ (OH ₂)(OH)
O14	6 <i>h</i>	<i>m</i> ..	0.5072	0.0782	$\frac{1}{4}$		single atom P
P15	6 <i>h</i>	<i>m</i> ..	0.511	0.2544	$\frac{1}{4}$		tetrahedron O ₃ (OH)
O16	6 <i>h</i>	<i>m</i> ..	0.523	0.342	$\frac{1}{4}$		single atom P
Ni17	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.102	0.5	7-vertex polyhedron Ni(OH) ₃ O ₃

M11 = 0.667O + 0.333OH

Transformation from published data: $y, x, -z$

Experimental: powder, diffractometer, X-rays, $R_B = 0.068$

Remarks: 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] Guillou N., Forster P.M., Gao Q., Cheetham A.K., Férey G. (2001), Mater. Sci. Forum 378/381, 576-581. [2] Guillou N., Gao Q., Forster P.M., Chang J.S., Noguès M., Park S.E., Férey G., Cheetham A.K. (2001), Angew. Chem. Int. Ed. 40, 2831-2834.