

H₇[H₃O][NH₄]Ni₉[PO₄]₇[OH]_{1.5}F_{4.5}[H₂O]₆*hP*141(183) *P6mm* – f⁶e⁶d⁶cb²a²**(H₃O,NH₄)₄Ni₁₈(HPO₄)₁₄(OH)₃F₉·12H₂O** [1]Structural features: Ni(O,OH,F)₆ octahedra and PO₄ tetrahedra share atoms to form a 3D-framework (partial disorder) with large channels parallel to [001].

Guillou N. et al. (1999) [1]

F_{4.50}H_{16.50}Ni₉O_{36.50}P₇*a* = 1.9652, *c* = 0.5018 nm, *c/a* = 0.255, *V* = 1.6783 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(OH ₂)1	12 <i>f</i>	1	0.0525	0.3364	0.3726	0.5	single atom O
O2	12 <i>f</i>	1	0.0733	0.4293	0.7148		non-colinear P ₂
Ni3	12 <i>f</i>	1	0.0898	0.49549	0.0411	0.5	non-coplanar triangle OPNi
O4	12 <i>f</i>	1	0.1607	0.4507	0.2312		single atom P
Ni5	12 <i>f</i>	1	0.17709	0.51083	0.57		octahedron O ₄ F ₂
O6	6 <i>e</i>	. <i>m</i> .	0.169	0.831	0.0411		single atom P
P7	6 <i>e</i>	. <i>m</i> .	0.21421	0.78581	0.0619		tetrahedron O ₄
O8	6 <i>e</i>	. <i>m</i> .	0.2319	0.7681	0.7937		single atom P
O9	6 <i>e</i>	. <i>m</i> .	0.2907	0.7092	0.4497		single atom P
M10	6 <i>e</i>	. <i>m</i> .	0.4102	0.5898	0.8334		non-coplanar square Ni ₄
F11	6 <i>e</i>	. <i>m</i> .	0.4342	0.5658	0.3591		non-coplanar square Ni ₄
(OH ₂)12	6 <i>d</i>	.. <i>m</i>	0.2474	0	0.044		non-colinear (OH ₂) ₂
O13	6 <i>d</i>	.. <i>m</i>	0.2986	0	0.5282	0.5	non-colinear (OH ₂) ₂
O14	6 <i>d</i>	.. <i>m</i>	0.3742	0	0.1192	0.5	
P15	6 <i>d</i>	.. <i>m</i>	0.379	0	0.5375	0.5	single atom O
O16	6 <i>d</i>	.. <i>m</i>	0.4023	0	0.268	0.5	
P17	6 <i>d</i>	.. <i>m</i>	0.4135	0	0.8634	0.5	non-coplanar triangle O ₃
O18	3 <i>c</i>	2 <i>mm</i>	¹ / ₂	0	0.9243		trigonal prism P ₂ Ni ₄
O19	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.0518		single atom P
P20	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.3725		tetrahedron O ₄
(OH ₃)21	1 <i>a</i>	6 <i>mm</i>	0	0	0.0		single atom (OH ₃)
(OH ₃)22	1 <i>a</i>	6 <i>mm</i>	0	0	0.651		single atom (OH ₃)

M10 = 0.5F + 0.5OH

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.512Experimental: single crystal, diffractometer, X-rays, synchrotron, *R* = 0.095, *T* = 160 K

Remarks: NH₄ and H belonging to PO₄ were not located. We assigned an approximate value to the F/OH ratio of site M10 (not bonded to P) based on the nominal composition. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. An incommensurate superlattice was observed for some crystals.

References: [1] Guillou N., Gao Q., Nogues M., Morris R.E., Hervieu M., Férey G., Cheetham A.K. (1999), C. R. Acad. Sci., Ser. IIc 2, 387-392.