

$\text{H}_{1.67}\text{Ni}_{6.67}[\text{AsO}_4]_4[\text{OH}]_3$  $hP120$  $(186) P6_3mc - d^4c^{10}b^4a^2$  $\text{Ni}_{6.67}\text{H}_{1.67}(\text{AsO}_4)_4(\text{OH})_3$  [1]

Structural features: Columns of edge- and face-linked  $\text{Ni}(\text{O},\text{OH})_6$  octahedra are interconnected via common vertices and  $\text{AsO}_4$  tetrahedra to form a 3D-framework; additional Ni in channels parallel to [001] (infinite columns of face-linked  $\text{O}_6$  octahedra, partial disorder).

Marcos M.D. et al. (1995) [1]

 $\text{As}_4\text{H}_3\text{Ni}_{6.67}\text{O}_{19}$  $a = 1.26953$ ,  $c = 0.50311$  nm,  $c/a = 0.396$ ,  $V = 0.7022$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ni1	12 <i>d</i>	1	0.075	0.431	0.008	0.16	
O2	12 <i>d</i>	1	0.341	0.0615	0.045	0.778	
O3	12 <i>d</i>	1	0.363	0.082	0.158	0.222	
Ni4	12 <i>d</i>	1	0.426	0.0748	0.382	0.84	
O5	6 <i>c</i>	. <i>m</i> .	0.0716	0.9284	0.301	0.778	
O6	6 <i>c</i>	. <i>m</i> .	0.0816	0.9184	0.428	0.222	
As7	6 <i>c</i>	. <i>m</i> .	0.1489	0.8511	0.35198	0.778	
As8	6 <i>c</i>	. <i>m</i> .	0.1603	0.8397	0.442	0.222	
O9	6 <i>c</i>	. <i>m</i> .	0.182	0.818	0.113	0.222	
O10	6 <i>c</i>	. <i>m</i> .	0.1922	0.8078	0.071	0.778	
(OH)11	6 <i>c</i>	. <i>m</i> .	0.4744	0.5256	0.203	0.91	
(OH)12	6 <i>c</i>	. <i>m</i> .	0.477	0.523	0.323	0.09	
O13	6 <i>c</i>	. <i>m</i> .	0.5915	0.4085	0.231	0.66	
O14	6 <i>c</i>	. <i>m</i> .	0.6074	0.3926	0.425	0.34	
O15	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.297	0.66	
O16	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.367	0.34	
As17	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.632	0.66	
As18	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.705	0.34	
Ni19	2 <i>a</i>	3 <i>m</i> .	0	0	0.0	0.333	
Ni20	2 <i>a</i>	3 <i>m</i> .	0	0	0.124	0.333	

Transformation from published data: origin shift 0 0 0.561

Experimental: powder, diffractometer, X-rays,  $R_B = 0.037$ 

Remarks: H not belonging to OH was not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 3 of [1] the Wyckoff position of former Ni2 is misprinted as 2*d* instead of 2*a*. An (almost) ordered structure was refined in the same space group for composition  $\text{Ni}_{13.16}\text{H}_{3.68}(\text{AsO}_4)_8(\text{OH})_6$ .

References: [1] Marcos M.D., Amoros P., Beltran D., Beltran A., Attfield J.P. (1995), J. Mater. Chem. 5, 917-925.