

$\text{H}_{1.84}\text{Ni}_{6.58}[\text{AsO}_4]_4[\text{OH}]_3$ $hP60$ $(186) P6_3mc - d^2c^5b^2a$ $\text{Ni}_{6.58}\text{H}_{1.84}(\text{AsO}_4)_4(\text{OH})_3$ [1]

Structural features: Columns of edge- and face-linked $\text{Ni}(\text{O}_4[\text{OH}]_2)$ octahedra are interconnected via common vertices and AsO_4 tetrahedra to form a 3D-framework; additional Ni in channels parallel to [001] (infinite columns of face-linked O_6 octahedra).

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

 $\text{As}_4\text{H}_3\text{Ni}_{6.58}\text{O}_{19}$ $a = 1.27018$, $c = 0.50322$ nm, $c/a = 0.396$, $V = 0.7031$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12d	1	0.0633	0.3395	0.493		non-coplanar triangle AsNi_2
Ni2	12d	1	0.4266	0.0752	0.33667		octahedron $\text{O}_4(\text{OH})_2$
O3	6c	.m.	0.0766	0.9234	0.262		coplanar triangle AsNi_2
As4	6c	.m.	0.15113	0.84887	0.3078		tetrahedron O_4
O5	6c	.m.	0.197	0.803	0.022		non-coplanar triangle AsNi_2
(OH)6	6c	.m.	0.4749	0.5251	0.152		non-coplanar square Ni_4
O7	6c	.m.	0.5952	0.4048	0.195		non-coplanar triangle AsNi_2
O8	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.253		single atom As
As9	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5959		tetrahedron O_4
Ni10	2a	3m.	0	0	0.0	0.58	octahedron O_6

Transformation from published data: origin shift 0 0 0.698

Experimental: powder, diffractometer, X-rays, $R_B = 0.046$

Remarks: H not belonging to OH was not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. A refinement on single-crystal X-ray diffraction data collected at 120 K is reported in [2].

References: [1] Marcos M.D., Amoros P., Beltran D., Beltran A., Attfield J.P. (1995), J. Mater. Chem. 5, 917-925. [2] Hughes R.W., Gerrard L.A., Price D.J., Weller M.T. (2003), Inorg. Chem. 42, 4160-4164.