

$\text{H}_3\text{Na}_7\text{W}_9\text{SiO}_{34}[\text{H}_2\text{O}]_9$  $hP120$  $(186) P6_3mc - d^4c^{11}b^3$  **$\text{Na}_7\text{H}_3[\text{SiW}_9\text{O}_{34}] \cdot 9\text{H}_2\text{O}$**   $\alpha$  [1]

Structural features:  $\text{SiW}_9\text{O}_{31}(\text{OH})_3$  units (a 3-ring of edge-linked  $\text{W}(\text{O}_4[\text{OH}]_2)$  octahedra sharing vertices with a 6-ring of vertex-linked  $\text{WO}_6$  octahedra and a central  $\text{SiO}_4$  tetrahedron) in a Mg-type (h.c.p.) arrangement.

Hubert V., Hartl H. (1996) [1]

 $\text{H}_{21}\text{Na}_7\text{O}_{43}\text{SiW}_9$  $a = 1.4394$ ,  $c = 1.2337$  nm,  $c/a = 0.857$ ,  $V = 2.2136$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12d	1	0.061	0.429	0.28		single atom W
W2	12d	1	0.0843	0.4276	0.1553		octahedron $\text{O}_6$
O3	12d	1	0.32	0.018	0.107		single atom W
O4	12d	1	0.46	0.14	0.483		single atom W
O5	6c	.m.	0.202	0.798	0.168		non-colinear $\text{W}_2$
( $\text{OH}_2$ )6	6c	.m.	0.2415	0.7585	0.386		square pyramid $\text{Na}_2\text{O}_3$
O7	6c	.m.	0.395	0.605	0.165		single atom Si
O8	6c	.m.	0.497	0.503	0.106		non-colinear $\text{W}_2$
Na9	6c	.m.	0.513	0.487	0.397		6-vertex polyhedron $\text{O}_5(\text{OH})$
( $\text{OH}_2$ )10	6c	.m.	0.599	0.401	0.109		trigonal bipyramid $\text{Na}_3\text{O}(\text{OH})$
( $\text{OH}$ )11	6c	.m.	0.602	0.398	0.322		non-colinear $\text{W}_2$
W12	6c	.m.	0.7459	0.254	0.401		octahedron $\text{O}_4(\text{OH})_2$
Na13	6c	.m.	0.7845	0.2155	0.091		octahedron $\text{O}_3(\text{OH}_2)_3$
O14	6c	.m.	0.793	0.207	0.296		single atom W
( $\text{OH}_2$ )15	6c	.m.	0.888	0.112	0.245		single atom O
O16	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0		single atom Si
Si17	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.123		tetrahedron $\text{O}_4$
Na18	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.483		octahedron ( $\text{OH}_2$ ) <sub>6</sub>

Transformation from published data:  $-x, -y, -z$ ; origin shift 0 0 0.011Experimental: single crystal, diffractometer, X-rays,  $R = 0.048$ ,  $T = 293$  K

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Hubert V., Hartl H. (1996), Z. Naturforsch. B 51, 969-974.