

$\text{Na}_4\text{V}_2\text{O}_7[\text{H}_2\text{O}]_{18}$ $hP110$ $(176) P6_3/m - i^6h^4f^2eb$ $\text{Na}_4\text{V}_2\text{O}_7(\text{H}_2\text{O})_{18}$ [1]

Structural features: Units of two vertex-linked VO_4 tetrahedra (partial orientational disorder) and units of two face-linked $\text{Na}(\text{OH}_2)_6$ octahedra (in part forming infinite columns of face-linked $\text{Na}(\text{OH}_2)_6$ octahedra with $2/3$ occupation).

Björnberg A. (1979) [1]

 $\text{H}_{36}\text{Na}_4\text{O}_{25}\text{V}_2$ $a = 0.92478$, $c = 1.6591$ nm, $c/a = 1.794$, $V = 1.2288$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.0008	0.1996	0.0897		non-colinear Na ₂
O2	12i	1	0.338	0.462	0.0709		single atom Na
O3	12i	1	0.4755	0.2824	0.1376	0.333	
O4	12i	1	0.5036	0.2945	0.0824	0.167	
O5	12i	1	0.5271	0.1519	0.1413	0.333	
O6	12i	1	0.537	0.1589	0.0916	0.167	
O7	6h	$m..$	0.1395	0.4696	$1/4$		non-colinear Na ₂
O8	6h	$m..$	0.2265	0.2105	$1/4$		non-colinear Na ₂
O9	6h	$m..$	0.5596	0.2851	$1/4$	0.167	
O10	6h	$m..$	0.6401	0.2139	$1/4$	0.167	
Na11	4f	3..	$1/3$	$2/3$	0.1528		octahedron O ₆
V12	4f	3..	$1/3$	$2/3$	0.65121		
Na13	4e	3..	0	0	0.1828	0.5	7-vertex polyhedron NaO ₆
Na14	2b	-3..	0	0	0		octahedron O ₆
H15	12i	1	0.025	0.588	0.095		
H16	12i	1	0.096	0.29	0.087		
H17	12i	1	0.295	0.056	0.065		
H18	12i	1	0.305	0.237	0.213		
H19	12i	1	0.363	0.478	0.03		
H20	6h	$m..$	0.029	0.402	$1/4$		
H21	6h	$m..$	0.149	0.393	$1/4$		

Transformation from published data: origin shift 0 0 $1/2$

Experimental: single crystal, diffractometer, X-rays, R = 0.061, T = 292 K

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] Björnberg A. (1979), Acta Chem. Scand. A 33, 539-546.