$K_5W_{12}AlO_{40}[H_2O]_{17}$	*hP*246	(180) $P6_222 - k^{17}ji^2hgfda$

$K_5[AlW_{12}O_{40}]\cdot 17H_2O$ α [1]

Structural features: $AlW_{12}O_{40}$ Keggin units (twelve edge- and vertex-linked WO_6 octahedra sharing vertices with a central AlO_4 tetrahedron; α-isomer) in a quartz-like arrangement (3D-framework with twisted chains); K and H_2O between the units and in large channels parallel to [001].

Weinstock I.A. et al. (1999) [1]

$AlH_{34}K_5O_{57}W_{12}$

a = 1.9072, c = 1.25658 nm, c/a = 0.659, V = 3.9583 nm^3, Z = 3

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*k*	1	0.0601	0.477	0.24723		single atom Al
O2	12*k*	1	0.0667	0.3795	0.0805		non-colinear W_2
O3	12*k*	1	0.093	0.3673	0.28733		non-colinear W_2
$(OH_2)4$	12*k*	1	0.121	0.2373	0.20403		single atom (OH_2)
$(OH_2)5$	12*k*	1	0.1435	0.0977	0.1475	0.5	single atom (OH_2)
W6	12*k*	1	0.1532	0.4486	0.17723		octahedron O_6
$(OH_2)7$	12*k*	1	0.166	0.1394	0.0243	0.5	single atom (OH_2)
O8	12*k*	1	0.1769	0.5323	0.0773		non-colinear W_2
O9	12*k*	1	0.2088	0.5237	0.28973		non-colinear W_2
O10	12*k*	1	0.2235	0.4214	0.14753		single atom W
O11	12*k*	1	0.2985	0.3102	0.1209		single atom W
$(OH_2)12$	12*k*	1	0.3452	0.4649	0.31773		
W13	12*k*	1	0.3721	0.0088	0.30493		octahedron O_6
O14	12*k*	1	0.409	0.4742	0.0694		non-colinear W_2
O15	12*k*	1	0.4662	0.0918	0.22703		non-colinear W_2
W16	12*k*	1	0.5665	0.1479	0.29953		octahedron O_6
O17	12*k*	1	0.6204	0.2216	0.20823		single atom W
$(OH_2)18$	6*j*	..2	0.2042	0.4083	$^1/_2$		non-colinear O_2
K19	6*i*	..2	0.1363	0.2726	0	0.551	cuboctahedron $(OH_2)_6O_6$
K20	6*i*	..2	0.6301	0.2602	0		8-vertex polyhedron $O_6(OH_2)_2$
$(OH_2)21$	6*h*	.2.	0.2048	0	$^1/_2$		non-colinear $(OH_2)_2$
K22	6*g*	.2.	0.2593	0	0	0.449	tetrahedron $O_2(OH_2)_2$
K23	6*f*	2..	$^1/_2$	0	0.0524	0.5	
Al24	3*d*	222	$^1/_2$	0	$^1/_2$		tetrahedron O_4
$(OH_2)25$	3*a*	222	0	0	0		square antiprism $(OH_2)_8$

Transformation from published data: origin shift 0 0 $^1/_2$

Experimental: single crystal, diffractometer, X-rays, R = 0.034, T = 173 K

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. 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] Weinstock I.A., Cowan J.J., Barbuzzi E.M.G., Zeng H., Hill C.L. (1999), J. Am. Chem. Soc. 121, 4608-4617.