$K_5W_{12}BO_{40}[H_2O]_{16}$	*hP*207	(180) $P6_222 - k^{14}ji^2hgfd$

$K_5[BW_{12}O_{40}]\cdot 16H_2O$ [1]
Structural features: $BW_{12}O_{40}$ Keggin units (twelve edge- and vertex-linked WO_6 octahedra sharing vertices with a central BO_4 tetrahedron; α-isomer) in a quartz-like arrangement (3D-framework with twisted chains); K and H_2O between the units, additional H_2O in channels parallel to [001].

Fletcher H. et al. (2001) [1]
$BH_{20.02}K_{4.99}O_{50.01}W_{12}$
a = 1.897, c = 1.2414 nm, c/a = 0.654, V = 3.8688 nm^3, Z = 3

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*k*	1	0.0551	0.4809	0.23927		single atom B
O2	12*k*	1	0.0673	0.3785	0.07447		non-colinear W_2
O3	12*k*	1	0.0918	0.3678	0.28607		non-colinear W_2
W4	12*k*	1	0.15078	0.44594	0.17574		octahedron O_6
O5	12*k*	1	0.1798	0.5309	0.07507		non-colinear W_2
O6	12*k*	1	0.2046	0.5236	0.28697		non-colinear W_2
O7	12*k*	1	0.223	0.419	0.15347		single atom W
O8	12*k*	1	0.3008	0.3114	0.12433		single atom W
W9	12*k*	1	0.37332	0.00723	0.30232		octahedron O_6
O10	12*k*	1	0.4066	0.4735	0.07213		non-colinear W_2
O11	12*k*	1	0.4675	0.091	0.2268		non-colinear W_2
W12	12*k*	1	0.56844	0.14873	0.30205		octahedron O_6
O13	12*k*	1	0.6199	0.2225	0.2064		single atom W
M14	12*k*	1	0.6512	0.1213	0.00917		
(OH_2)15	6*j*	..2	0.1995	0.399	$^1/_2$		non-colinear O_2
M16	6*i*	..2	0.1305	0.261	0		non-colinear $(OH_2)_2$
K17	6*i*	..2	0.6313	0.2626	0		8-vertex polyhedron $O_6(OH_2)_2$
(OH_2)18	6*h*	.2.	0.204	0	$^1/_2$		non-colinear $(OH_2)_2$
(OH_2)19	6*g*	.2.	0.275	0	0		non-colinear O_2
M20	6*f*	2..	$^1/_2$	0	0.0448	0.5	
B21	3*d*	222	$^1/_2$	0	$^1/_2$		tetrahedron O_4

M14 = 0.70OH_2 + 0.30K; M16 = 0.52OH_2 + 0.48K; M20 = 0.83K + 0.17OH_2
Experimental: single crystal, diffractometer, X-rays, R = 0.036, T = 294 K

Remarks: Part of H_2O not located. We assume that in the cif file deposited for [1] the occupancy of former OKW1 is misprinted as 1 instead of 0.5 (too short interatomic distances otherwise). Ambiguous data: the authors state that only 8.08 H_2O per formula unit were located, however, the published data (after correction of the misprint) correspond to ~10 H_2O per formula unit; other partial occupancies possibly omitted. 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] Fletcher H., Allen C.C., Burns R.C., Craig D.C. (2001), Acta Crystallogr. C 57, 505-507.