

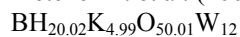
*hP*207

(180)  $P6_222 - k^{14}; j^2 hgfd$

### **K<sub>5</sub>[BW<sub>12</sub>O<sub>40</sub>]·16H<sub>2</sub>O [1]**

Structural features: BW<sub>12</sub>O<sub>40</sub> Keggin units (twelve edge- and vertex-linked WO<sub>6</sub> octahedra sharing vertices with a central BO<sub>4</sub> tetrahedron;  $\alpha$ -isomer) in a quartz-like arrangement (3D-framework with twisted chains); K and H<sub>2</sub>O between the units, additional H<sub>2</sub>O in channels parallel to [001].

Fletcher H. et al. (2001) [1]



$a = 1.897$ ,  $c = 1.2414$  nm,  $c/a = 0.654$ ,  $V = 3.8688$  nm<sup>3</sup>,  $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	1	0.0551	0.4809	0.23927		single atom B
O2	12 <i>k</i>	1	0.0673	0.3785	0.07447		non-colinear W <sub>2</sub>
O3	12 <i>k</i>	1	0.0918	0.3678	0.28607		non-colinear W <sub>2</sub>
W4	12 <i>k</i>	1	0.15078	0.44594	0.17574		octahedron O <sub>6</sub>
O5	12 <i>k</i>	1	0.1798	0.5309	0.07507		non-colinear W <sub>2</sub>
O6	12 <i>k</i>	1	0.2046	0.5236	0.28697		non-colinear W <sub>2</sub>
O7	12 <i>k</i>	1	0.223	0.419	0.15347		single atom W
O8	12 <i>k</i>	1	0.3008	0.3114	0.12433		single atom W
W9	12 <i>k</i>	1	0.37332	0.00723	0.30232		octahedron O <sub>6</sub>
O10	12 <i>k</i>	1	0.4066	0.4735	0.07213		non-colinear W <sub>2</sub>
O11	12 <i>k</i>	1	0.4675	0.091	0.2268		non-colinear W <sub>2</sub>
W12	12 <i>k</i>	1	0.56844	0.14873	0.30205		octahedron O <sub>6</sub>
O13	12 <i>k</i>	1	0.6199	0.2225	0.2064		single atom W
M14	12 <i>k</i>	1	0.6512	0.1213	0.00917		
(OH <sub>2</sub> )15	6 <i>j</i>	..2	0.1995	0.399	1/2		non-colinear O <sub>2</sub>
M16	6 <i>i</i>	..2	0.1305	0.261	0		non-colinear (OH <sub>2</sub> ) <sub>2</sub>
K17	6 <i>i</i>	..2	0.6313	0.2626	0		8-vertex polyhedron O <sub>6</sub> (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )18	6 <i>h</i>	..2	0.204	0	1/2		non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )19	6 <i>g</i>	..2	0.275	0	0		non-colinear O <sub>2</sub>
M20	6 <i>f</i>	2..	1/2	0	0.0448	0.5	
B21	3 <i>d</i>	222	1/2	0	1/2		tetrahedron O <sub>4</sub>

M14 = 0.70OH<sub>2</sub> + 0.30K; M16 = 0.52OH<sub>2</sub> + 0.48K; M20 = 0.83K + 0.17OH<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.036, T = 294 K

Remarks: Part of H<sub>2</sub>O 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<sub>2</sub>O per formula unit were located, however, the published data (after correction of the misprint) correspond to ~10 H<sub>2</sub>O 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.