

$\text{K}_6\text{W}_{12}\text{CoO}_{40}[\text{H}_2\text{O}]_{16}$ $hP192$ $(180) P6_222 - k^{14}; 2\text{gdc}$ **$\text{K}_6[\text{CoW}_{12}\text{O}_{40}] \cdot 16\text{H}_2\text{O}$ [1]**

Structural features: $\text{Co}^{2+}\text{W}_{12}\text{O}_{40}$ Keggin units (twelve edge- and vertex-linked WO_6 octahedra sharing vertices with a central CoO_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].

Nolan A.L. et al. (2000) [1]

 $\text{CoH}_{12}\text{K}_5\text{O}_{46}\text{W}_{12}$ $a = 1.9118$, $c = 1.2383$ nm, $c/a = 0.648$, $V = 3.9196$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 <i>k</i>	1	0.0635	0.3789	0.08287		non-colinear W_2
O2	12 <i>k</i>	1	0.0675	0.4749	0.25577		tetrahedron CoW_3
O3	12 <i>k</i>	1	0.0951	0.3655	0.28667		non-colinear W_2
W4	12 <i>k</i>	1	0.15309	0.4513	0.17962		octahedron O_6
O5	12 <i>k</i>	1	0.175	0.5337	0.07667		non-colinear W_2
O6	12 <i>k</i>	1	0.2102	0.5248	0.29177		non-colinear W_2
O7	12 <i>k</i>	1	0.2205	0.4215	0.15517		single atom W
O8	12 <i>k</i>	1	0.2993	0.3103	0.11853		single atom W
(OH_2)9	12 <i>k</i>	1	0.3466	0.4611	0.31593		single atom K
W10	12 <i>k</i>	1	0.37288	0.01009	0.30505		octahedron O_6
O11	12 <i>k</i>	1	0.4104	0.4738	0.07043		non-colinear W_2
O12	12 <i>k</i>	1	0.4651	0.0928	0.2201		non-colinear W_2
W13	12 <i>k</i>	1	0.56422	0.14419	0.29656		octahedron O_6
O14	12 <i>k</i>	1	0.6177	0.2185	0.2036		single atom W
K15	6 <i>i</i>	.2	0.1431	0.2862	0		4-vertex polyhedron O_4
K16	6 <i>i</i>	.2	0.6354	0.2708	0		8-vertex polyhedron $\text{O}_6(\text{OH}_2)_2$
(OH_2)17	6 <i>g</i>	.2	0.2709	0	0		non-colinear O_2
Co18	3 <i>d</i>	222	$\frac{1}{2}$	0	$\frac{1}{2}$		tetrahedron O_4
K19	3 <i>c</i>	222	$\frac{1}{2}$	0	0		tetrahedron $(\text{OH}_2)_4$

Experimental: single crystal, diffractometer, X-rays, $R = 0.045$

Remarks: Minor part of K and main part of H_2O not located. 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] Nolan A.L., Allen C.C., Burns R.C., Craig D.C., Lawrance G.A. (2000), Aust. J. Chem. 53, 59-66.