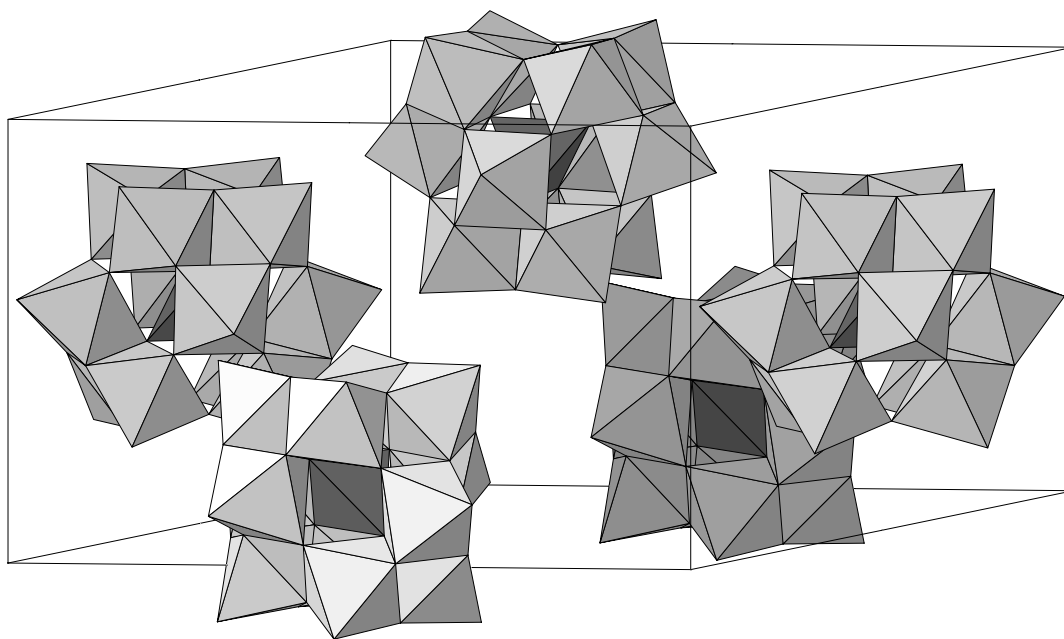


**K<sub>5</sub>[CoW<sub>12</sub>O<sub>40</sub>]·16H<sub>2</sub>O [1]**

Structural features: Co<sup>3+</sup>W<sub>12</sub>O<sub>40</sub> Keggin units (twelve edge- and vertex-linked WO<sub>6</sub> octahedra sharing vertices with a central CoO<sub>4</sub> tetrahedron;  $\alpha$ -isomer) in a quartz-like arrangement (3D-framework with twisted chains and channels parallel to [001]). See Fig. IV.46.

Fig. IV.46. **K<sub>5</sub>[CoW<sub>12</sub>O<sub>40</sub>]·16H<sub>2</sub>O**

Arrangement of Keggin units: a CoO<sub>4</sub> tetrahedron (dark) surrounded by twelve WO<sub>6</sub> octahedra (light). For clarity, K atoms and H<sub>2</sub>O molecules are omitted.

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

CoH<sub>5</sub>K<sub>4.50</sub>O<sub>42.50</sub>W<sub>12</sub>

$a = 1.9111$ ,  $c = 1.2509$  nm,  $c/a = 0.655$ ,  $V = 3.9566$  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	0.0638	0.477	0.25247		single atom Co
O2	12 <i>k</i>	1	0.0654	0.3816	0.08077		non-colinear W <sub>2</sub>
O3	12 <i>k</i>	1	0.0917	0.3665	0.28857		non-colinear W <sub>2</sub>
W4	12 <i>k</i>	1	0.15163	0.44723	0.17801		octahedron O <sub>6</sub>
O5	12 <i>k</i>	1	0.1755	0.5308	0.07897		non-colinear W <sub>2</sub>
O6	12 <i>k</i>	1	0.2073	0.5233	0.28827		non-colinear W <sub>2</sub>
O7	12 <i>k</i>	1	0.2209	0.4173	0.15077		single atom W
O8	12 <i>k</i>	1	0.3007	0.3139	0.12553		single atom W
M9	12 <i>k</i>	1	0.3428	0.4632	0.31407		
W10	12 <i>k</i>	1	0.37374	0.00882	0.30297		octahedron O <sub>6</sub>
O11	12 <i>k</i>	1	0.409	0.474	0.07013		non-colinear W <sub>2</sub>
O12	12 <i>k</i>	1	0.4658	0.0925	0.2239		non-colinear W <sub>2</sub>
W13	12 <i>k</i>	1	0.56691	0.14842	0.30043		octahedron O <sub>6</sub>
O14	12 <i>k</i>	1	0.6199	0.2219	0.2098		single atom W

K15	6i	..2	0.6303	0.2606	0		8-vertex polyhedron O <sub>6</sub> K <sub>2</sub>
M16	6f	2..	$\frac{1}{2}$	0	0.0566	0.5	
Co17	3d	222	$\frac{1}{2}$	0	$\frac{1}{2}$		tetrahedron O <sub>4</sub>

M9 = 0.5K + 0.5OH<sub>2</sub>; M16 = 0.5K + 0.5OH<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.032

Remarks: Minor part of K and main part of H<sub>2</sub>O not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 2 of [1] the occupancy of former KOw(1) is misprinted as implicit 1 instead of 0.5 (split site).

References: [1] Nolan A.L., Allen C.C., Burns R.C., Craig D.C., Lawrance G.A. (2000), Aust. J. Chem. 53, 59-66.