

**K<sub>3</sub>W<sub>2</sub>Cl<sub>9</sub>** [2], Strukturbericht notation K7<sub>1</sub>

Structural features: Close-packed KCl<sub>3</sub> layers in hc<sub>2</sub> stacking; W in octahedral (Cl<sub>6</sub>) voids, leaving every third interlayer vacant. Units of two face-linked WCl<sub>6</sub> octahedra (W<sub>2</sub> dumbbells) in a Mg-type (h.c.p.) arrangement. Deformation derivative of Cs<sub>3</sub>Cr<sub>2</sub>Cl<sub>9</sub>. See Fig. IV.59.

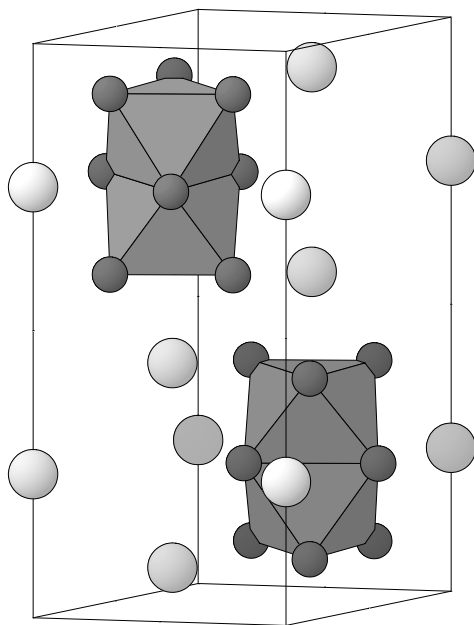


Fig. IV.59. **K<sub>3</sub>W<sub>2</sub>Cl<sub>9</sub>**

Arrangement of WCl<sub>6</sub> octahedra (Cl atoms small) and K atoms (large).

Watson W.H. Jr., Waser J. (1958) [1]

Cl<sub>9</sub>K<sub>3</sub>W<sub>2</sub>

$a = 0.7171$ ,  $c = 1.6258$  nm,  $c/a = 2.267$ ,  $V = 0.7240$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Cl1	12i	1	0.2158	0.3506	0.0926		single atom W
Cl2	6h	$m..$	0.4588	0.0116	$\frac{1}{4}$		non-colinear W <sub>2</sub>
W3	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1759		7-vertex polyhedron Cl <sub>6</sub> W
K4	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5718		tricapped trigonal prism Cl <sub>9</sub>
K5	2a	-6..	0	0	$\frac{1}{4}$		tricapped trigonal prism Cl <sub>9</sub>

Transformation from published data:  $y, x, -z$

Experimental: single crystal, Weissenberg photographs, X-rays,  $R = 0.119$

Remarks: In table 1 of [1] the Wyckoff letter of the 6-fold Cl site is misprinted as  $m$  instead of  $h$ .

References: [1] Watson W.H. Jr., Waser J. (1958), Acta Crystallogr. 11, 689-692. [2] Brosset C. (1936), Ark. Kemi Mineral. Geol. 12A(4), 1-8.