

Pr₃WO₆Cl₃ [1]; La₂ThTaO₆Cl₃ [2]

Structural features: Pr(O₆Cl₄) polyhedra (an O₄ square on one side, an O₂Cl₃ pentagon capped by an additional Cl on the other side) share atoms to form a 3D-framework; W in trigonal prismatic (O₆) voids. Single WO₆ trigonal prisms. See Fig. IV.58.

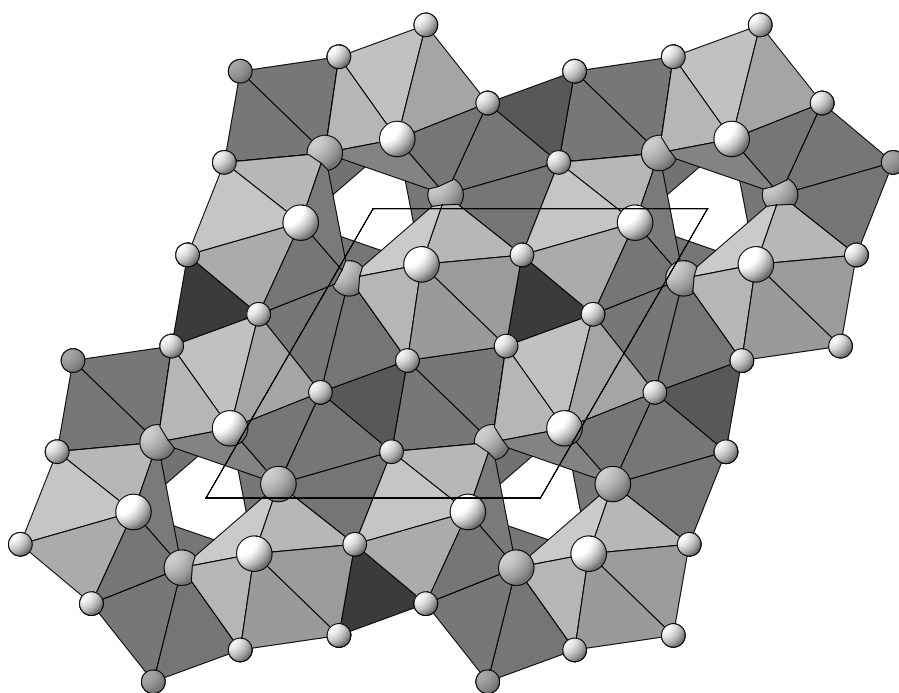


Fig. IV.58. **Pr₃WO₆Cl₃**

Arrangement of Pr(O₆Cl₄) polyhedra (light) (O atoms small, Cl atoms large) and WO₆ trigonal prisms (dark) viewed along [001].

Polianskaia T.M. et al. (1969) [1]

Cl₃O₆Pr₃W

$a = 0.9314$, $c = 0.5369$ nm, $c/a = 0.576$, $V = 0.4034$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.16	0.525	0.022		single atom W
Cl2	6h	$m..$	0.1925	0.2408	$\frac{1}{4}$		single atom Pr
Pr3	6h	$m..$	0.404	0.0904	$\frac{1}{4}$		10-vertex polyhedron O ₆ Cl ₄
W4	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism O ₆

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

Experimental: single crystal, precession photographs, X-rays, $R = 0.121$

Remarks: Space group (173) $P6_3$ was tested and rejected ($R = 0.14$).

References: [1] Polianskaia T.M., Borisov S.V., Belov N.V. (1969), Dokl. Akad. Nauk SSSR 187, 1043-1046. [2] Schaffrath U., Gruehn R. (1988), J. Less-Common Met. 137, 61-73.