

$\text{Pr}_3\text{NbCl}_6\text{O}_4$ $hP28$ $(176) P6_3/m - h^4dc$ **$\text{Pr}_3\text{NbO}_4\text{Cl}_6$** [1]

Structural features: $\text{Pr}(\text{Cl}_6\text{O}_2)\text{Cl}$ monocapped square antiprisms ($\text{Pr}(\text{Cl}_4\text{O}_2)\text{Cl}_3$ tricapped trigonal prisms) share atoms to form a 3D-framework; Nb in trigonal bipyramidal voids. Infinite chains of vertex-linked NbO_5 trigonal bipyramids.

Brixner L.H. et al. (1983) [1]

 $\text{Cl}_6\text{NbO}_4\text{Pr}_3$ $a = 1.27301$, $c = 0.39626$ nm, $c/a = 0.311$, $V = 0.5561$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	$6h$	$m..$	0.0704	0.4436	$1/4$		non-coplanar triangle Pr_2O
Cl2	$6h$	$m..$	0.2484	0.1425	$1/4$		4-vertex polyhedron Pr_3O
Pr3	$6h$	$m..$	0.28163	0.39752	$1/4$		non-colinear O_2
O4	$6h$	$m..$	0.5095	0.2016	$1/4$		single atom Nb
Nb5	$2d$	$-6..$	$2/3$	$1/3$	$1/4$		trigonal bipyramid O_5
O6	$2c$	$-6..$	$1/3$	$2/3$	$1/4$		colinear Nb_2

Transformation from published data: origin shift $0\ 0\ 1/2$ Experimental: single crystal, diffractometer, X-rays, $R = 0.017$

References: [1] Brixner L.H., Calabrese J.C., Foris C.M. (1983), Mater. Res. Bull. 18, 1493-1498.