

$\text{Pr}_{1.29}\text{Cl}_3$ $hP10$ $(176) P6_3/m - hcb$ **PrCl_{2.33}** [1]

Structural features: Infinite columns of base-linked PrCl_6Cl_3 tricapped trigonal prisms share atoms to form a 3D-framework; additional Pr in channels of hexagonal cross-section parallel to [001] (partial disorder). Filled-up derivative of UCl_3 .

Meyer G. et al. (1989) [1]

 $\text{Cl}_3\text{Pr}_{1.29}$ $a = 0.7417$, $c = 0.4272$ nm, $c/a = 0.576$, $V = 0.2035$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	$6h$	$m..$	0.3883	0.0846	$\frac{1}{4}$		square pyramid Pr_5
Pr2	$2c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism Cl_9
Pr3	$2b$	$-3..$	0	0	0	0.29	square prism (cube) Pr_2Cl_6

Transformation from published data: $y, x, -z$ Experimental: single crystal, diffractometer, X-rays, $wR = 0.021$

Remarks: Phase stable at $867 < T < 932$ K, may be maintained metastable at rt. Short interatomic distances for partly occupied site(s).

References: [1] Meyer G., Schleid T., Krämer K. (1989), J. Less-Common Met. 149, 67-71.