

RbPr<sub>5</sub>C<sub>2</sub>Cl<sub>10</sub>

hP40

(176)  $P6_3/m - ih^2f^3e$ **RbPr<sub>5</sub>(C<sub>2</sub>)Cl<sub>10</sub>** [2]

Structural features: C<sub>2</sub>Pr<sub>5</sub>Cl<sub>21</sub> units (a C<sub>2</sub> dumbbell surrounded by a Pr<sub>5</sub> trigonal bipyramid, a Cl<sub>9</sub> tricapped trigonal prism and a Cl<sub>12</sub> polyhedron) share Cl atoms to form a 3D-framework.

Uhrlandt S., Meyer G. (1994) [1]

C<sub>2</sub>Cl<sub>9.98</sub>Pr<sub>5</sub>Rb<sub>0.93</sub> $a = 0.84499$ ,  $c = 1.4976$  nm,  $c/a = 1.772$ ,  $V = 0.9260$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cl1	12 <i>i</i>	1	0.3624	0.0187	0.0651		non-colinear Pr <sub>2</sub>
Pr2	6 <i>h</i>	<i>m</i> ..	0.0365	0.4171	<sup>1</sup> / <sub>4</sub>		tricapped trigonal prism C <sub>2</sub> Cl <sub>7</sub>
Cl3	6 <i>h</i>	<i>m</i> ..	0.254	0.2407	<sup>1</sup> / <sub>4</sub>		coplanar triangle Pr <sub>3</sub>
Pr4	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0478		single atom C
C5	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.2		single atom C
Cl6	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6854	0.49	single atom Cl
Rb7	4 <i>e</i>	3..	0	0	0.047	0.465	

Transformation from published data: *y*,*x*,*-z*; origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.083

Remarks: The same data are reported in [2] (atom coordinates deposited). Short interatomic distances for partly occupied site(s).

References: [1] Uhrlandt S., Meyer G. (1994), Z. Anorg. Allg. Chem. 620, 1872-1878. [2] Meyer G., Uhrlandt S. (1993), Angew. Chem. Int. Ed. Engl. 32, 1318-1319 (Angew. Chem. 105, 1379-1381).