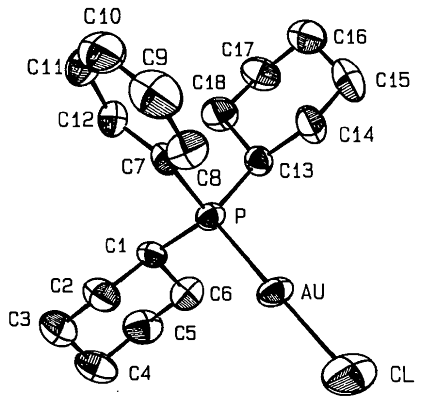

Fig. 1. Labeling of atoms in $Cy_2PhPAuCl$ (50% probability ellipsoids).

complex $(Cy_2PhP)_2AuCl$ has been determined and shows a large increase in the Au—Cl distance [2·744 (2) Å] (Muir, Cuadrado, Muir & Barnes, 1988) compared to $Cy_2PhPAuCl$ [Au—Cl 2·281 (3) Å].

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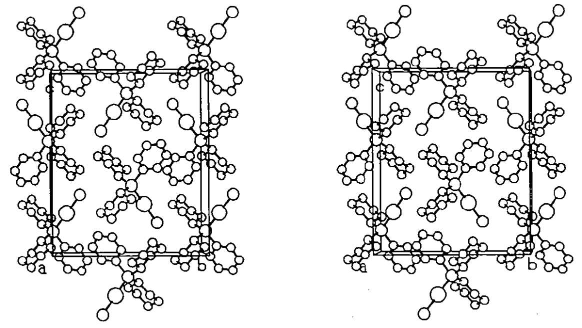

Fig. 2. Stereo packing diagram of $Cy_2PhPAuCl$ in the unit cell.

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Structure of Hexaaquadichloropraseodymium(III) Chloride

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Abstract. $[PrCl_2(H_2O)_6]Cl$, $M_r = 355{\cdot}4$, monoclinic, $P2/n$, $a = 8{\cdot}019\ (3)$, $b = 6{\cdot}599\ (3)$, $c = 9{\cdot}729\ (2)$ Å, $\beta = 93{\cdot}75\ (2)^\circ$, $V = 513{\cdot}7\ (7)$ Å^3, $Z = 2$, $D_x = 2{\cdot}297$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 54{\cdot}86$ cm^{-1}, $F(000) = 340$, room temperature, $R = 0{\cdot}051$ for 1233 observed reflections. The complex is isostructural with Nd, Sm, Gd, Dy and Lu analogues. The cation has C_2 symmetry and the geometry around the eight-coordinated Pr^{III} atom, located on a twofold axis, is a square antiprism. The Pr—Cl (coordinated) distance and the average Pr—O distances are 2·834 (2) and 2·472 Å, respectively.

Experimental. The compound was crystallized from the solution in which a tetranuclear Pr^{III} complex (Xu, Lin, Wu, Xu & Chen, 1991) was synthesized. A

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Table 1. *Fractional atomic coordinates and equivalent isotropic temperature factors* (Å^2)

$$B_{eq} = (4/3)[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)].$$

	x	y	z	B_{eq}
Pr	0·25	0·14699 (8)	0·25	0·61
Cl(1)	0·2399 (3)	−0·1728 (3)	0·4436 (2)	1·99
Cl(2)	0·25	0·3780 (5)	0·75	2·19
O(1)	−0·0481 (7)	0·0441 (9)	0·2161 (6)	2·06
O(2)	0·0865 (7)	0·4284 (9)	0·1466 (6)	2·08
O(3)	0·3937 (7)	0·2994 (9)	0·0571 (5)	2·04

Table 2. *Bond distances* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

Pr—Cl(1)	2·834 (2)	Pr—O(1)	2·486 (6)
Pr—O(2)	2·451 (6)	Pr—O(3)	2·479 (6)
Cl(1)—Pr—O(1)	79·4 (1)	Cl(1)—Pr—O(2)	143·1 (1)
Cl(1)—Pr—O(3)	147·2 (1)	Cl(1)—Pr—Cl(1)*	83·7 (1)
Cl(1)—Pr—O(1)*	77·1 (1)	Cl(1)—Pr—O(2)*	109·2 (1)
Cl(1)—Pr—O(3)*	76·3 (1)	O(1)—Pr—O(2)	70·6 (2)
O(1)—Pr—O(3)	120·1 (2)	O(1)—Pr—O(1)*	148·3 (2)
O(1)—Pr—O(2)*	138·2 (2)	O(1)—Pr—O(3)*	73·8 (2)
O(2)—Pr—O(3)	69·2 (2)	O(2)—Pr—O(2)*	81·5 (2)
O(2)—Pr—O(3)*	75·0 (2)	O(3)—Pr—O(3)*	132·1 (2)

* Atoms are in equivalent positions (0·5 − x, y, 0·5 − z).

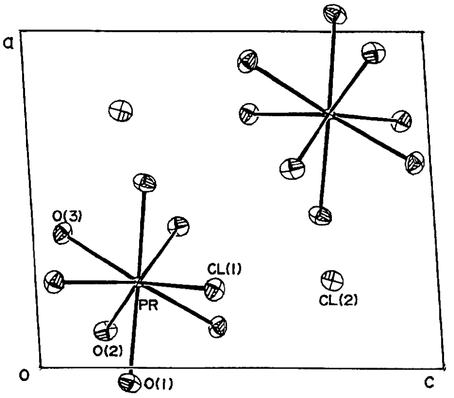

Fig. 1. Crystal structure viewed along the **b*** axis together with the atomic numbering system.

greenish crystal sealed in a Lindemann capillary with dimensions 0·40 × 0·45 × 0·50 mm was mounted on an Enraf–Nonius CAD-4 diffractometer. Unit-cell parameters were determined by least-squares fit of 2θ values of 25 reflections ($20 \leq 2\theta \leq 30°$). Intensity data were collected by the ω–2θ-scan technique using graphite-monochromated Mo $K\alpha$ radiation; the scan rate was variable (0·8–5·6° min^{-1}) and the scan width was $\Delta\omega = (0·80 + 0·35\tan\theta)°$. A total of 1310 independent reflections were measured with 2θ up to 54° and index range h = 10 to 10, k = 0 to 8, l = 0 to 12. 1233 observed reflections [$|F_o| \geq 3\sigma(F_o)$] were employed in the refinements. Three standard reflections were measured every hour, no intensity variation was observed. Usual Lp, empirical absorption ($T_{\max} = 0·9977$, $T_{\min} = 0·6902$) and extinction corrections (secondary-extinction coefficient 1·39309 × 10^{-5}) were carried out. The structure was solved by the Patterson method, followed by Fourier syntheses, and refined by full-matrix least squares with anisotropic temperature factors for non-H atoms using *SDP* (Enraf–Nonius, 1983). The function $\sum w(|F_o| - |F_c|)^2$ was minimized, where $w = 1$. No H atoms were refined. Final refinement reached convergence with $R = 0·051$ and $wR = 0·060$, $(\Delta/\sigma)_{\max} = 0·07$. Maximum and minimum heights in final difference Fourier map 2·18 and −3·60 e Å^{-3} (near the Pr position). Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV, p. 71). Atomic coordinates are given in Table 1.* Bond lengths and angles are listed in Table 2. The crystal structure is illustrated in Fig. 1 together with the atomic numbering scheme.

Related literature. The structures of some lanthanide(III) chloride hydrates have been reported, among which the compounds of three lighter lanthanides are heptahydrated [La (Bakakin, Klevtsova & Solov'eva, 1974; Habenschuss & Spedding, 1979), Ce (Peterson, Onstott & Von Dreele, 1979), Pr (Habenschuss & Spedding, 1978)], while others are hexahydrated [Nd, Sm, Gd and Lu (Habenschuus & Spedding, 1980), Dy (Rogers, 1987)]. This work shows that the hexahydrate of Pr^{III} chloride, as well as the heptahydrate, is stable. The differences in coordinated bond lengths between the present compound and other lanthanide compounds agree well with the lanthanide contraction.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53677 (6 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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