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(*Trans*-dichloro-κCl)bis[(dicyclohexylphosphino)methane-$\kappa^2 P,P'$]ruthenium(II)

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Key indicators

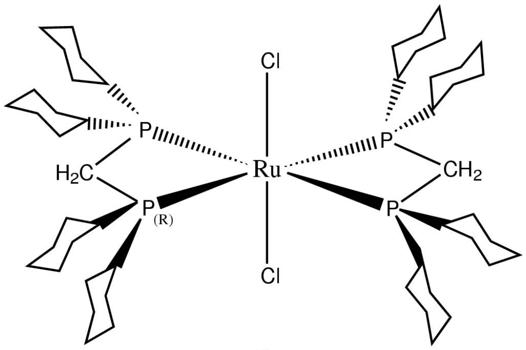
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.032
wR factor = 0.083
Data-to-parameter ratio = 18.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title complex, $[Ru(C_{25}H_{46}P_2)_2Cl_2]$ or $RuCl_2(dcpm)_2$ [dcpm is 1,2-bis(dicyclohexylphosphino)methane, $C_{25}H_{46}P_2$], the Ru atom (site symmetry $\overline{1}$) is in a octahedral coordination environment with two chelating dcpm ligands and two *trans* chloro ligands.

Comment

Ruthenium complexes containing chelating phosphine ligands play a prominent role as active catalysts in many fields (Collman, 1987 White & Coville, 1994). Many of these complexes have been prepared and characterized (Shawkataly *et al.*, 1998; Lucas *et al.*, 2000; Hockless *et al.*, 1996), but complexes containing dcpm [dcpm is 1,2-bis(dicyclohexylphosphino)methane, $C_{25}H_{46}P_2$] are uncommon (Joslin *et al.* 1991). Here, we report the synthesis and structure of the title compound, (I), (Fig. 1), which may serve as a useful precursor for the synthesis of further ruthenium complexes (Grocott & Wild, 1982; Nolan *et al.*, 1997; Volland *et al.*, 2004).



(I)

In (I) the central Ru(II) atom occupies an inversion centre and is coordinated by two *trans* chloro ligands and two *P,P*-chelating dcpm ligands, resulting in octahedral geometry for the ruthenium atom (Table 1). The Ru–Cl distances in (I) are comparable to those in related compounds (Blake *et al.*, 1993; Hockless *et al.*, 1996). The two Ru—P distances in (I) differ by 0.056 Å. The packing in (I) is shown in Fig. 2.

Experimental

Compound (I) was prepared from the reaction of the chelating phosphine ligand with ruthenium(III) chloride by a standard procedure (Grocott & Wild, 1982). Suitable crystals for single-crystal analysis were grown by diffusion of diethyl ether into a dichloromethane solution of (I) at room temperature. Yield 85%. Elemental analysis calcd for $C_{50}H_{92}Cl_2P_4Ru$: C 60.72%, H 9.37%, found: C 60.68%, H 9.35%.

Crystal data

$[Ru(C_{25}H_{46}P_2)_2Cl_2]$
$M_r = 989.09$
Monoclinic, $C2/c$
$a = 24.120\ (11)$ Å
$b = 10.732\ (5)$ Å
$c = 21.780\ (11)$ Å
$\beta = 108.098\ (8)^\circ$
$V = 5359\ (4)$ Å^3
$Z = 4$

$D_x = 1.226$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 858 reflections
$\theta = 2.7$–26.3°
$\mu = 0.54$ mm^{-1}
$T = 293\ (2)$ K
Block, orange
$0.30 \times 0.18 \times 0.12$ mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{\min} = 0.796$, $T_{\max} = 0.937$
13674 measured reflections

4717 independent reflections
3644 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.040$
$\theta_{\max} = 25.0^\circ$
$h = -28 \rightarrow 24$
$k = -12 \rightarrow 12$
$l = -25 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.083$
$S = 1.09$
4717 reflections
259 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 1.6382P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.30$ e Å^{-3}
$\Delta\rho_{\min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ru1—P2	2.3669 (12)	Ru1—Cl1	2.4334 (11)
Ru1—P1	2.3775 (10)		
P2—Ru1—P1	71.42 (4)	P2—C13—P1	97.10 (13)

H atoms were initially located in a difference Fourier map, then placed in ideal positions, with C—H = 0.97 Å, and refined as riding, with the constraint $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ applied.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART* **or SAINT?**; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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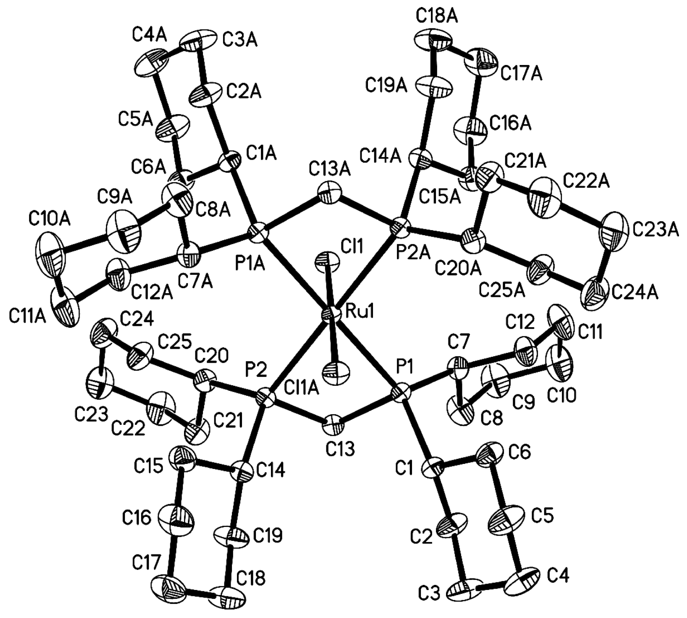

Figure 1
View of (I), with 30% displacement ellipsoids and H atoms omitted for clarity. Atoms with the suffix A are generated by the symmetry operation $1 - x, 2 - y, -z$.

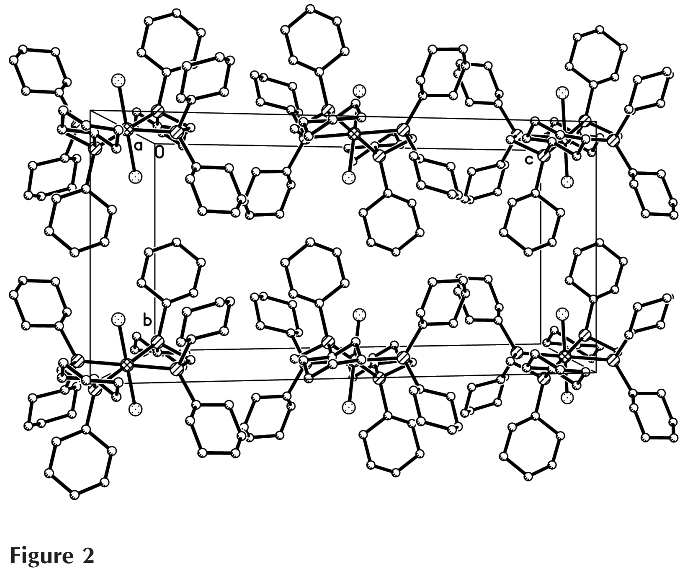

Figure 2
Unit-cell packing in (I), viewed along the *a* axis. H atoms have been omitted for clarity.

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