

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

# ( $\eta^6$ -Benzene)dichlorido(chlorodicyclohexylphosphane- $\kappa P$ )ruthenium(II) chloroform monosolvate

Saravanan Gowrisankar,<sup>a</sup> Helfried Neumann,<sup>b</sup> Anke Spannberg<sup>b</sup> and Matthias Beller<sup>b\*</sup>

<sup>a</sup>Division of Organic Chemistry, Institute of Chemical and Engineering Sciences, 8 Biomedical Grove, Neuros, #07-01, 138665, Singapore, and <sup>b</sup>Leibniz-Institut für Katalyse e. V. an der Universität Rostock, Albert-Einstein-Strasse 29a, 18059 Rostock, Germany

Correspondence e-mail: matthias.beller@catalysis.de

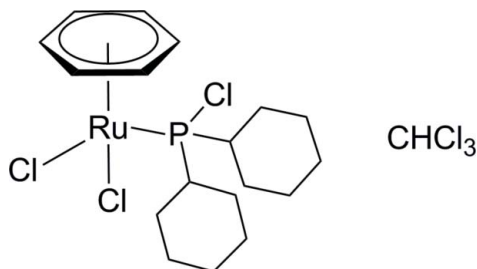
Received 21 May 2014; accepted 4 June 2014

Key indicators: single-crystal X-ray study;  $T = 150$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.019;  $wR$  factor = 0.048; data-to-parameter ratio = 23.0.

The title compound,  $[\text{RuCl}_2(\eta^6\text{-C}_6\text{H}_6)(\text{C}_{12}\text{H}_{22}\text{ClP})]\cdot\text{CHCl}_3$ , was prepared by reaction of  $[\text{RuCl}_2(\eta^6\text{-C}_6\text{H}_6)]_2$  with chlorodicyclohexylphosphane in  $\text{CHCl}_3$  at 323 K under argon. The  $\text{Ru}^{\text{II}}$  atom is surrounded by one arene ligand, two Cl atoms and a phosphane ligand in a piano-stool geometry. The phosphane ligand is linked by the P atom, with an  $\text{Ru}-\text{P}$  bond length of 2.3247 (4) Å. Both cyclohexyl rings at the P atom adopt a chair conformation. In the crystal, the  $\text{Ru}^{\text{II}}$  complex molecule and the chloroform solvent molecule are linked by a bifurcated  $\text{C}-\text{H}\cdots(\text{Cl},\text{Cl})$  hydrogen bond. Intramolecular  $\text{C}-\text{H}\cdots\text{Cl}$  hydrogen bonds are also observed.

## Related literature

For the molecular structure of Ru complexes with the related chlorodiphenylphosphane ligand, see: Jantscher *et al.* (2009); Torres-Lubián *et al.* (1999).



## Experimental

### Crystal data

$[\text{RuCl}_2(\text{C}_6\text{H}_6)(\text{C}_{12}\text{H}_{22}\text{ClP})]\cdot\text{CHCl}_3$   $V = 2346.45$  (6) Å<sup>3</sup>  
 $M_r = 602.16$   $Z = 4$   
 Monoclinic,  $P2_1/n$   $\text{Mo } K\alpha$  radiation  
 $a = 7.9717$  (1) Å  $\mu = 1.42$  mm<sup>-1</sup>  
 $b = 16.3020$  (2) Å  $T = 150$  K  
 $c = 18.0602$  (3) Å  $0.36 \times 0.22 \times 0.11$  mm  
 $\beta = 91.244$  (1)°

### Data collection

Bruker Kappa APEXII DUO diffractometer 37052 measured reflections  
 5619 independent reflections  
 Absorption correction: multi-scan (SADABS; Bruker, 2008) 4963 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$   
 $T_{\text{min}} = 0.630$ ,  $T_{\text{max}} = 0.859$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.019$  244 parameters  
 $wR(F^2) = 0.048$  H-atom parameters constrained  
 $S = 1.05$   $\Delta\rho_{\text{max}} = 0.41$  e Å<sup>-3</sup>  
 5619 reflections  $\Delta\rho_{\text{min}} = -0.37$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C14}-\text{H14B}\cdots\text{Cl1}$	0.99	2.56	3.4080 (17)	144
$\text{C18}-\text{H18A}\cdots\text{Cl1}$	0.99	2.74	3.5366 (17)	138
$\text{C19}-\text{H19}\cdots\text{Cl1}^i$	1.00	2.69	3.5539 (17)	144
$\text{C19}-\text{H19}\cdots\text{Cl2}^i$	1.00	2.77	3.6119 (18)	142

Symmetry code: (i)  $x, y, z + 1$ .

Data collection: APEX2 (Bruker, 2011); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: XP in SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXL97.

Supporting information for this paper is available from the IUCr electronic archives (Reference: IS5363).

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## supporting information

*Acta Cryst.* (2014). E70, m255 [https://doi.org/10.1107/S1600536814012975]

## ( $\eta^6$ -Benzene)dichlorido(chlorodicyclohexylphosphane- $\kappa P$ )ruthenium(II) chloroform monosolvate

Saravanan Gowrisankar, Helfried Neumann, Anke Spannenberg and Matthias Beller

### S1. Comment

The half-sandwich ( $\eta^6$ -C<sub>6</sub>H<sub>6</sub>)-dichlorido(chlorodicyclohexylphosphane)ruthenium(II) complex was formed by reaction of one equivalent of [RuCl<sub>2</sub>( $\eta^6$ -C<sub>6</sub>H<sub>6</sub>)<sub>2</sub>] with two equivalents of (Cy<sub>2</sub>P(1-naphthoyl)) ligand under hydrogenation conditions (CHCl<sub>3</sub>, 60 bar of H<sub>2</sub>, 353 K, 3 hrs) as a side product. The cleavage of the 1-naphthoyl group from [RuCl<sub>2</sub>( $\eta^6$ -C<sub>6</sub>H<sub>6</sub>)(Cy<sub>2</sub>P(1-naphthoyl))] complex forms firstly [RuCl<sub>2</sub>( $\eta^6$ -C<sub>6</sub>H<sub>6</sub>)(Cy<sub>2</sub>PH)] and subsequent chlorination of the dicyclohexylphosphane unit due to CHCl<sub>3</sub> yields the title compound in poor yield. Additionally, we could not observe any trace amount of title compound by using non-chlorinated solvents such as MeOH. The substitution of hydrogen next to phosphane by chlorine coming from solvent molecules is also described for the formation of a Ru-complex with the related chlorodiphenylphosphane ligand by Torres-Lubián *et al.* (1999). More specifically, the title complex was formed by reaction of [RuCl<sub>2</sub>( $\eta^6$ -C<sub>6</sub>H<sub>6</sub>)<sub>2</sub>] with chlorodicyclohexylphosphane in CHCl<sub>3</sub> at 323 K under argon in 41% yield. Crystals suitable for X-ray crystal structure analysis could be obtained by crystallization from a chloroform/heptane mixture. In the <sup>31</sup>P NMR spectrum of the complex the signal for the phosphorus was observed at 156.3 p.p.m., whereas free ligand signal appears at 128.8 p.p.m.. The title compound shows the three legged piano-stool geometry at the ruthenium centre with the arene, chlorodicyclohexylphosphane and two chlorine ligands in the coordination sphere (Fig. 1). The phosphane ligand is linked by the phosphorus with a Ru—P bond length of 2.3247 (4) Å. Both cyclohexyl rings at the phosphorus atom adopt a chair conformation. The Ru complex is co-crystallized with CHCl<sub>3</sub>.

### S2. Experimental

A 50 ml round bottom flask with inert gas valve was charged with 0.05 mmol (25 mg) [RuCl<sub>2</sub>( $\eta^6$ -C<sub>6</sub>H<sub>6</sub>)<sub>2</sub>] and 4 ml CHCl<sub>3</sub> under argon atmosphere. To this suspension 0.105 mmol (21  $\mu$ L) chlorodicyclohexylphosphane was added and the reaction mixture was allowed to react 3 h at 323 K. A clear red brown solution has been formed and the volume was reduced carefully in high vacuum to *ca* 1 ml. Next 20 ml heptane was added to the reaction mixture and cooled for 1 h with ice bath. The precipitate was washed with heptane (3  $\times$  5 ml) to yield the title compound as an orange brown solid (20 mg, 41%). Red single crystals were grown in CHCl<sub>3</sub>/heptane mixture at 245 K for 1 day. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  5.71 (s, 6H, benzene), 2.79 (m, 2H, Cy), 2.06–1.54 (m, 14H, Cy), 1.27 (br s, 6H, Cy). <sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  89.8 (RuPh), 40.4 (d,  $J_{PC}$  = 9.5 Hz, PCH), 27.2, 26.9, 26.7, 26.4, 26.3, 26.0, 26.0, 25.6 (CH<sub>2</sub>). <sup>31</sup>P {<sup>1</sup>H} NMR (121 MHz, CDCl<sub>3</sub>):  $\delta$  156.3.

### S3. Refinement

H atoms were placed in idealized positions with C—H = 0.95–1.00 Å (CH), 0.99 Å (CH<sub>2</sub>) and refined using a riding model with  $U_{iso}(H)$  fixed at 1.2 $U_{eq}(C)$ .

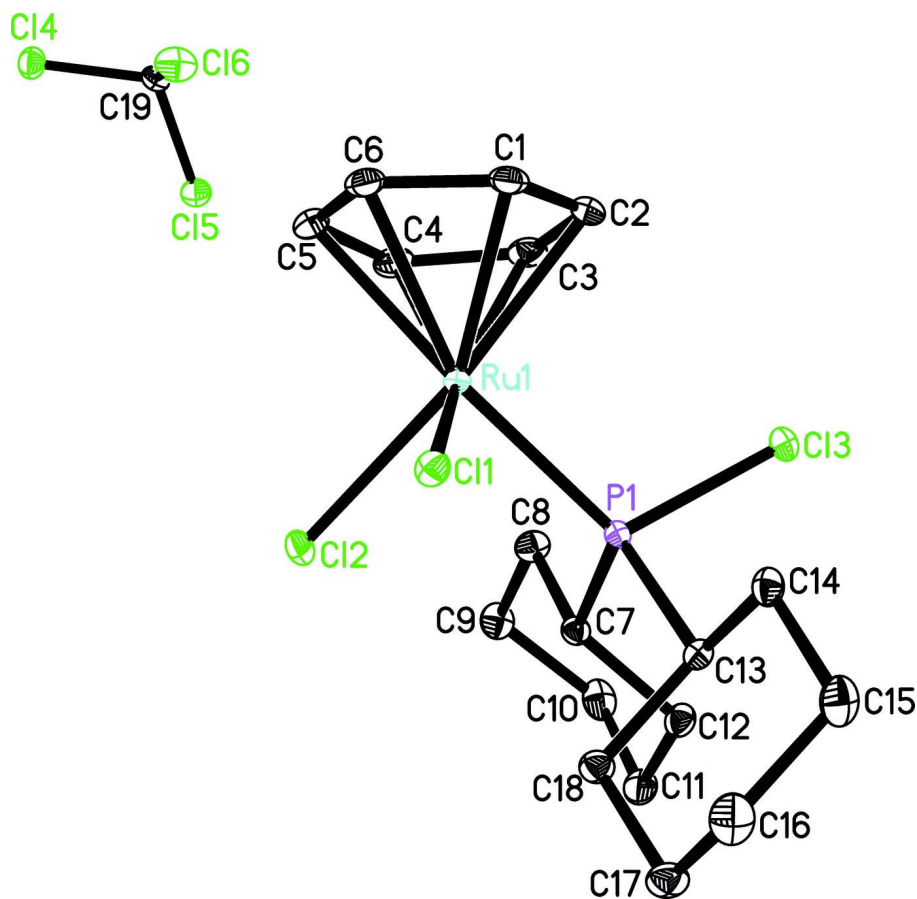


Figure 1

The molecular structure of the title compound with 30% displacement ellipsoids. Hydrogen atoms are omitted for clarity.

**( $\eta^6$ -Benzene)dichlorido(chlorodicyclohexylphosphane- $\kappa P$ )ruthenium(II) chloroform monosolvate**

*Crystal data*

[RuCl<sub>2</sub>(C<sub>6</sub>H<sub>6</sub>)(C<sub>12</sub>H<sub>22</sub>ClP)]·CHCl<sub>3</sub>

$M_r$  = 602.16

Monoclinic,  $P2_1/n$

$a$  = 7.9717 (1) Å

$b$  = 16.3020 (2) Å

$c$  = 18.0602 (3) Å

$\beta$  = 91.244 (1)°

$V$  = 2346.45 (6) Å<sup>3</sup>

$Z$  = 4

$F(000)$  = 1216

$D_x$  = 1.705 Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda$  = 0.71073 Å

Cell parameters from 9877 reflections

$\theta$  = 2.3–27.9°

$\mu$  = 1.42 mm<sup>-1</sup>

$T$  = 150 K

Prism, orange

0.36 × 0.22 × 0.11 mm

*Data collection*

Bruker Kappa APEXII DUO  
diffractometer

Radiation source: fine-focus sealed tube

Curved graphite monochromator

Detector resolution: 8.3333 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2008)

$T_{\min}$  = 0.630,  $T_{\max}$  = 0.859

37052 measured reflections

5619 independent reflections

4963 reflections with  $I > 2\sigma(I)$

$R_{\text{int}}$  = 0.031

$\theta_{\max} = 27.9^\circ$ ,  $\theta_{\min} = 1.7^\circ$   
 $h = -10 \rightarrow 10$

$k = -21 \rightarrow 21$   
 $l = -23 \rightarrow 23$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.019$   
 $wR(F^2) = 0.048$   
 $S = 1.05$   
 5619 reflections  
 244 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0187P)^2 + 1.4791P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.41 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$

*Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	-0.2498 (2)	0.37279 (11)	0.04879 (10)	0.0223 (4)
H1	-0.3279	0.3746	0.0083	0.027*
C2	-0.2406 (2)	0.30292 (11)	0.09373 (10)	0.0227 (4)
H2	-0.3181	0.2592	0.0863	0.027*
C3	-0.1149 (2)	0.29763 (11)	0.15045 (10)	0.0230 (4)
H3	-0.1069	0.2501	0.1808	0.028*
C4	-0.0024 (2)	0.36315 (11)	0.16134 (10)	0.0231 (4)
H4	0.0864	0.3585	0.1970	0.028*
C5	-0.0212 (2)	0.43653 (11)	0.11906 (10)	0.0235 (4)
H5	0.0498	0.4822	0.1291	0.028*
C6	-0.1430 (2)	0.44123 (11)	0.06332 (10)	0.0227 (4)
H6	-0.1552	0.4900	0.0349	0.027*
C7	0.2490 (2)	0.14568 (10)	0.07869 (9)	0.0160 (3)
H7	0.3484	0.1741	0.0577	0.019*
C8	0.2460 (2)	0.16860 (11)	0.16112 (9)	0.0211 (3)
H8A	0.2381	0.2290	0.1661	0.025*
H8B	0.1456	0.1442	0.1837	0.025*
C9	0.4035 (2)	0.13820 (11)	0.20233 (10)	0.0238 (4)
H9A	0.5032	0.1664	0.1828	0.029*
H9B	0.3958	0.1518	0.2556	0.029*
C10	0.4238 (2)	0.04591 (11)	0.19335 (11)	0.0276 (4)
H10A	0.5280	0.0278	0.2193	0.033*
H10B	0.3280	0.0174	0.2160	0.033*

C11	0.4316 (2)	0.02332 (11)	0.11175 (11)	0.0260 (4)
H11A	0.4399	-0.0370	0.1070	0.031*
H11B	0.5337	0.0476	0.0905	0.031*
C12	0.2773 (2)	0.05349 (10)	0.06779 (10)	0.0205 (3)
H12A	0.1771	0.0231	0.0840	0.025*
H12B	0.2924	0.0421	0.0145	0.025*
C13	0.0709 (2)	0.13975 (10)	-0.06377 (9)	0.0161 (3)
H13	0.0799	0.0791	-0.0565	0.019*
C14	-0.0879 (2)	0.15535 (10)	-0.11130 (10)	0.0200 (3)
H14A	-0.1863	0.1318	-0.0865	0.024*
H14B	-0.1060	0.2152	-0.1166	0.024*
C15	-0.0711 (2)	0.11651 (12)	-0.18795 (10)	0.0270 (4)
H15A	-0.0682	0.0561	-0.1828	0.032*
H15B	-0.1705	0.1310	-0.2190	0.032*
C16	0.0864 (3)	0.14489 (13)	-0.22631 (10)	0.0305 (4)
H16A	0.0799	0.2047	-0.2356	0.037*
H16B	0.0953	0.1167	-0.2746	0.037*
C17	0.2405 (2)	0.12592 (12)	-0.17829 (10)	0.0246 (4)
H17A	0.3422	0.1453	-0.2035	0.030*
H17B	0.2503	0.0658	-0.1715	0.030*
C18	0.2299 (2)	0.16729 (10)	-0.10279 (9)	0.0193 (3)
H18A	0.2282	0.2276	-0.1092	0.023*
H18B	0.3298	0.1528	-0.0720	0.023*
C19	0.4349 (2)	0.38768 (11)	0.85956 (10)	0.0222 (4)
H19	0.3475	0.3760	0.8970	0.027*
Cl1	0.01613 (5)	0.35589 (2)	-0.08323 (2)	0.01901 (8)
Cl2	0.30706 (5)	0.34441 (2)	0.04619 (2)	0.02103 (9)
Cl3	-0.12314 (5)	0.11221 (2)	0.07235 (2)	0.02052 (8)
Cl4	0.54297 (6)	0.47752 (3)	0.88609 (3)	0.03089 (10)
Cl5	0.57325 (6)	0.30361 (3)	0.85639 (3)	0.03164 (11)
Cl6	0.33498 (7)	0.40171 (4)	0.77265 (3)	0.03799 (12)
P1	0.06247 (5)	0.18613 (2)	0.02855 (2)	0.01377 (8)
Ru1	0.007356 (16)	0.324634 (7)	0.046687 (7)	0.01356 (4)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0154 (8)	0.0266 (9)	0.0251 (9)	0.0050 (7)	0.0032 (7)	-0.0038 (7)
C2	0.0166 (8)	0.0240 (8)	0.0279 (9)	-0.0015 (7)	0.0095 (7)	-0.0046 (7)
C3	0.0270 (9)	0.0234 (8)	0.0190 (8)	0.0043 (7)	0.0099 (7)	0.0008 (7)
C4	0.0251 (9)	0.0275 (9)	0.0170 (8)	0.0056 (7)	0.0010 (7)	-0.0062 (7)
C5	0.0250 (9)	0.0204 (8)	0.0253 (9)	0.0017 (7)	0.0054 (7)	-0.0085 (7)
C6	0.0232 (9)	0.0191 (8)	0.0260 (9)	0.0067 (7)	0.0067 (7)	-0.0004 (7)
C7	0.0141 (7)	0.0165 (7)	0.0173 (8)	0.0005 (6)	-0.0004 (6)	0.0005 (6)
C8	0.0222 (8)	0.0236 (8)	0.0176 (8)	0.0027 (7)	-0.0016 (7)	-0.0017 (7)
C9	0.0224 (9)	0.0273 (9)	0.0213 (9)	-0.0005 (7)	-0.0066 (7)	0.0002 (7)
C10	0.0218 (9)	0.0260 (9)	0.0344 (10)	-0.0004 (7)	-0.0097 (8)	0.0074 (8)
C11	0.0202 (9)	0.0197 (8)	0.0378 (10)	0.0045 (7)	-0.0052 (8)	-0.0008 (8)

C12	0.0206 (8)	0.0159 (8)	0.0248 (9)	0.0015 (6)	-0.0029 (7)	-0.0004 (7)
C13	0.0174 (8)	0.0145 (7)	0.0165 (8)	-0.0002 (6)	0.0008 (6)	-0.0024 (6)
C14	0.0196 (8)	0.0189 (8)	0.0213 (8)	-0.0024 (6)	-0.0035 (7)	-0.0011 (6)
C15	0.0309 (10)	0.0306 (10)	0.0192 (9)	-0.0067 (8)	-0.0079 (7)	0.0000 (7)
C16	0.0403 (11)	0.0340 (10)	0.0171 (9)	-0.0065 (9)	-0.0011 (8)	0.0025 (8)
C17	0.0279 (9)	0.0283 (9)	0.0178 (8)	0.0010 (8)	0.0057 (7)	-0.0024 (7)
C18	0.0196 (8)	0.0216 (8)	0.0168 (8)	0.0000 (6)	0.0015 (6)	-0.0015 (6)
C19	0.0174 (8)	0.0282 (9)	0.0210 (8)	0.0003 (7)	0.0000 (7)	0.0001 (7)
C11	0.02313 (19)	0.01688 (18)	0.01704 (19)	-0.00012 (15)	0.00118 (15)	0.00162 (14)
C12	0.01470 (18)	0.02085 (19)	0.0275 (2)	-0.00415 (15)	0.00011 (16)	-0.00070 (16)
C13	0.01850 (18)	0.01891 (19)	0.0243 (2)	-0.00493 (15)	0.00428 (15)	0.00082 (15)
C14	0.0287 (2)	0.0250 (2)	0.0388 (3)	-0.00293 (18)	-0.0043 (2)	-0.00117 (19)
C15	0.0251 (2)	0.0273 (2)	0.0425 (3)	0.00382 (18)	0.0000 (2)	-0.0002 (2)
C16	0.0334 (3)	0.0535 (3)	0.0266 (2)	0.0079 (2)	-0.0096 (2)	-0.0028 (2)
P1	0.01298 (18)	0.01378 (18)	0.01459 (19)	-0.00112 (15)	0.00104 (15)	-0.00075 (15)
Ru1	0.01285 (6)	0.01339 (6)	0.01447 (6)	-0.00015 (5)	0.00123 (5)	-0.00095 (5)

*Geometric parameters (Å, °)*

C1—C2	1.400 (3)	C11—C12	1.530 (2)
C1—C6	1.425 (2)	C11—H11A	0.9900
C1—Ru1	2.1966 (17)	C11—H11B	0.9900
C1—H1	0.9500	C12—H12A	0.9900
C2—C3	1.420 (3)	C12—H12B	0.9900
C2—Ru1	2.1970 (17)	C13—C18	1.530 (2)
C2—H2	0.9500	C13—C14	1.535 (2)
C3—C4	1.406 (3)	C13—P1	1.8334 (16)
C3—Ru1	2.1759 (17)	C13—H13	1.0000
C3—H3	0.9500	C14—C15	1.531 (2)
C4—C5	1.425 (3)	C14—H14A	0.9900
C4—Ru1	2.1668 (17)	C14—H14B	0.9900
C4—H4	0.9500	C15—C16	1.519 (3)
C5—C6	1.386 (3)	C15—H15A	0.9900
C5—Ru1	2.2585 (17)	C15—H15B	0.9900
C5—H5	0.9500	C16—C17	1.520 (3)
C6—Ru1	2.2705 (17)	C16—H16A	0.9900
C6—H6	0.9500	C16—H16B	0.9900
C7—C12	1.533 (2)	C17—C18	1.525 (2)
C7—C8	1.536 (2)	C17—H17A	0.9900
C7—P1	1.8457 (16)	C17—H17B	0.9900
C7—H7	1.0000	C18—H18A	0.9900
C8—C9	1.528 (2)	C18—H18B	0.9900
C8—H8A	0.9900	C19—C16	1.7596 (18)
C8—H8B	0.9900	C19—C14	1.7602 (18)
C9—C10	1.522 (3)	C19—C15	1.7609 (18)
C9—H9A	0.9900	C19—H19	1.0000
C9—H9B	0.9900	C11—Ru1	2.4036 (4)
C10—C11	1.522 (3)	C12—Ru1	2.4110 (4)

C10—H10A	0.9900	C13—P1	2.0779 (6)
C10—H10B	0.9900	P1—Ru1	2.3247 (4)
C2—C1—C6	120.45 (17)	C15—C14—C13	110.48 (14)
C2—C1—Ru1	71.44 (10)	C15—C14—H14A	109.6
C6—C1—Ru1	74.25 (10)	C13—C14—H14A	109.6
C2—C1—H1	119.8	C15—C14—H14B	109.6
C6—C1—H1	119.8	C13—C14—H14B	109.6
Ru1—C1—H1	126.4	H14A—C14—H14B	108.1
C1—C2—C3	119.69 (16)	C16—C15—C14	112.07 (15)
C1—C2—Ru1	71.41 (10)	C16—C15—H15A	109.2
C3—C2—Ru1	70.25 (10)	C14—C15—H15A	109.2
C1—C2—H2	120.2	C16—C15—H15B	109.2
C3—C2—H2	120.2	C14—C15—H15B	109.2
Ru1—C2—H2	130.8	H15A—C15—H15B	107.9
C4—C3—C2	119.52 (17)	C15—C16—C17	110.09 (15)
C4—C3—Ru1	70.76 (10)	C15—C16—H16A	109.6
C2—C3—Ru1	71.86 (10)	C17—C16—H16A	109.6
C4—C3—H3	120.2	C15—C16—H16B	109.6
C2—C3—H3	120.2	C17—C16—H16B	109.6
Ru1—C3—H3	129.5	H16A—C16—H16B	108.2
C3—C4—C5	120.24 (17)	C16—C17—C18	111.10 (15)
C3—C4—Ru1	71.47 (10)	C16—C17—H17A	109.4
C5—C4—Ru1	74.74 (10)	C18—C17—H17A	109.4
C3—C4—H4	119.9	C16—C17—H17B	109.4
C5—C4—H4	119.9	C18—C17—H17B	109.4
Ru1—C4—H4	125.7	H17A—C17—H17B	108.0
C6—C5—C4	119.95 (17)	C17—C18—C13	110.17 (14)
C6—C5—Ru1	72.66 (10)	C17—C18—H18A	109.6
C4—C5—Ru1	67.75 (9)	C13—C18—H18A	109.6
C6—C5—H5	120.0	C17—C18—H18B	109.6
C4—C5—H5	120.0	C13—C18—H18B	109.6
Ru1—C5—H5	132.5	H18A—C18—H18B	108.1
C5—C6—C1	119.83 (17)	C16—C19—C14	110.13 (10)
C5—C6—Ru1	71.71 (10)	C16—C19—C15	110.11 (10)
C1—C6—Ru1	68.61 (9)	C14—C19—C15	110.69 (9)
C5—C6—H6	120.1	C16—C19—H19	108.6
C1—C6—H6	120.1	C14—C19—H19	108.6
Ru1—C6—H6	132.6	C15—C19—H19	108.6
C12—C7—C8	111.62 (14)	C13—P1—C7	104.70 (7)
C12—C7—P1	114.00 (11)	C13—P1—C13	98.49 (5)
C8—C7—P1	111.07 (11)	C7—P1—C13	100.29 (6)
C12—C7—H7	106.5	C13—P1—Ru1	122.65 (5)
C8—C7—H7	106.5	C7—P1—Ru1	115.50 (5)
P1—C7—H7	106.5	C13—P1—Ru1	111.79 (2)
C9—C8—C7	111.31 (14)	C4—Ru1—C3	37.77 (7)
C9—C8—H8A	109.4	C4—Ru1—C1	80.04 (7)
C7—C8—H8A	109.4	C3—Ru1—C1	67.77 (7)

C9—C8—H8B	109.4	C4—Ru1—C2	68.03 (7)
C7—C8—H8B	109.4	C3—Ru1—C2	37.89 (7)
H8A—C8—H8B	108.0	C1—Ru1—C2	37.15 (7)
C10—C9—C8	110.91 (15)	C4—Ru1—C5	37.51 (7)
C10—C9—H9A	109.5	C3—Ru1—C5	67.19 (7)
C8—C9—H9A	109.5	C1—Ru1—C5	66.15 (7)
C10—C9—H9B	109.5	C2—Ru1—C5	78.67 (7)
C8—C9—H9B	109.5	C4—Ru1—C6	66.48 (7)
H9A—C9—H9B	108.0	C3—Ru1—C6	78.92 (7)
C11—C10—C9	110.42 (15)	C1—Ru1—C6	37.15 (6)
C11—C10—H10A	109.6	C2—Ru1—C6	66.53 (7)
C9—C10—H10A	109.6	C5—Ru1—C6	35.63 (7)
C11—C10—H10B	109.6	C4—Ru1—P1	115.27 (5)
C9—C10—H10B	109.6	C3—Ru1—P1	90.82 (5)
H10A—C10—H10B	108.1	C1—Ru1—P1	121.93 (5)
C10—C11—C12	112.06 (15)	C2—Ru1—P1	94.15 (5)
C10—C11—H11A	109.2	C5—Ru1—P1	152.59 (5)
C12—C11—H11A	109.2	C6—Ru1—P1	159.01 (5)
C10—C11—H11B	109.2	C4—Ru1—Cl1	150.91 (5)
C12—C11—H11B	109.2	C3—Ru1—Cl1	155.05 (5)
H11A—C11—H11B	107.9	C1—Ru1—Cl1	89.32 (5)
C11—C12—C7	111.57 (14)	C2—Ru1—Cl1	117.20 (5)
C11—C12—H12A	109.3	C5—Ru1—Cl1	113.53 (5)
C7—C12—H12A	109.3	C6—Ru1—Cl1	88.76 (5)
C11—C12—H12B	109.3	P1—Ru1—Cl1	93.366 (15)
C7—C12—H12B	109.3	C4—Ru1—Cl2	91.20 (5)
H12A—C12—H12B	108.0	C3—Ru1—Cl2	119.52 (5)
C18—C13—C14	112.01 (14)	C1—Ru1—Cl2	151.36 (5)
C18—C13—P1	110.18 (11)	C2—Ru1—Cl2	157.35 (5)
C14—C13—P1	113.20 (11)	C5—Ru1—Cl2	90.37 (5)
C18—C13—H13	107.0	C6—Ru1—Cl2	114.49 (5)
C14—C13—H13	107.0	P1—Ru1—Cl2	86.505 (14)
P1—C13—H13	107.0	Cl1—Ru1—Cl2	85.306 (15)

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C14—H14B $\cdots$ C11	0.99	2.56	3.4080 (17)	144
C18—H18A $\cdots$ C11	0.99	2.74	3.5366 (17)	138
C19—H19 $\cdots$ C11 <sup>i</sup>	1.00	2.69	3.5539 (17)	144
C19—H19 $\cdots$ C12 <sup>i</sup>	1.00	2.77	3.6119 (18)	142

Symmetry code: (i) *x*, *y*, *z*+1.