Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dichloro(η^6-*p*-cymene)(triphenylphosphine)-ruthenium(II)

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Received 26 September 2006
Accepted 28 September 2006

The title compound, $[Ru(C_{10}H_{14})Cl_2(C_{18}H_{15}P)]$, crystallizes with two molecules in the asymmetric unit. It adopts the classic pseudo-tetrahedral piano-stool structure. A comparison of the Ru—P, Ru—Cl, Ru—C(av) bond lengths and the sum of the P—Ru—Cl1, P—Ru—Cl2 and Cl1—Ru—Cl2 angles (for both independent molecules) with those of previously determined compounds $[(\eta^6\text{-arene})Ru(PPh_3)Cl_2]$ reveals that the nature of the η^6-arene ligand has a marginal effect on these structural parameters.

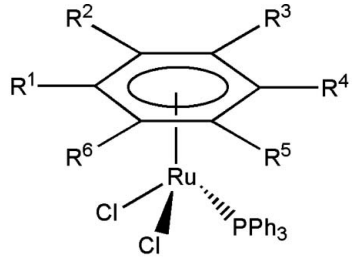
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.028
wR factor = 0.067
Data-to-parameter ratio = 20.1

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

Comment

Organometallic arene ruthenium(II) complexes have attracted much interest for a range of uses, including DNA-binding studies, chemosensors, highly selective receptors, catalysis and for the development of chiral half-sandwich compounds (Dorcier *et al.*, 2005; Buryak & Severin, 2005; Ion *et al.*, 2006; Morris *et al.*, 2006; Ganter, 2003). Tertiary phosphines, such as the ubiquitous triphenylphosphine, are known to rapidly cleave Ru—Cl—Ru bridges in dinuclear arene complexes to give achiral (Baldwin *et al.*, 2002; Hansen & Nelson, 2000; Therrien *et al.*, 2004) or chiral (Therrien & Süss-Fink, 2004; Vieille-Petit *et al.* (2003) mononuclear compounds of the type $[(\eta^6\text{-arene})Ru(PPh_3)Cl_2]$. Recently we reported (Dann *et al.*, 2006) the supramolecular chemistry of $[(\eta^6\text{-}p\text{-cymene})Ru(PR_3)Cl_2]$ complexes with highly functionalized *P*-monodentate tertiary phosphines. During efforts to prepare a mixed-metal Cu/Ru complex using pyrazine-2,3-dicarboxylic acid as a bridging ligand, we isolated and crystallographically verified the structure of the title pseudo-tetrahedral ruthenium(II) triphenylphosphine complex, (I).



$R^1 = CH_3$, $R^4 = CH(CH_3)_2$, R^2, R^3, R^5, R^6 = H	I
$R^1 = CH(CH_3)CH_2OH$, $R^2 > R^6$ = H	II
$R^1 > R^6$ = H	III
$R^1 = R^3 = R^4 = CH_3$, R^2, R^5, R^6 = H	IV
$R^1 > R^6 = CH_3$	V
$R^1 > R^6 = CH_2CH_3$	VI

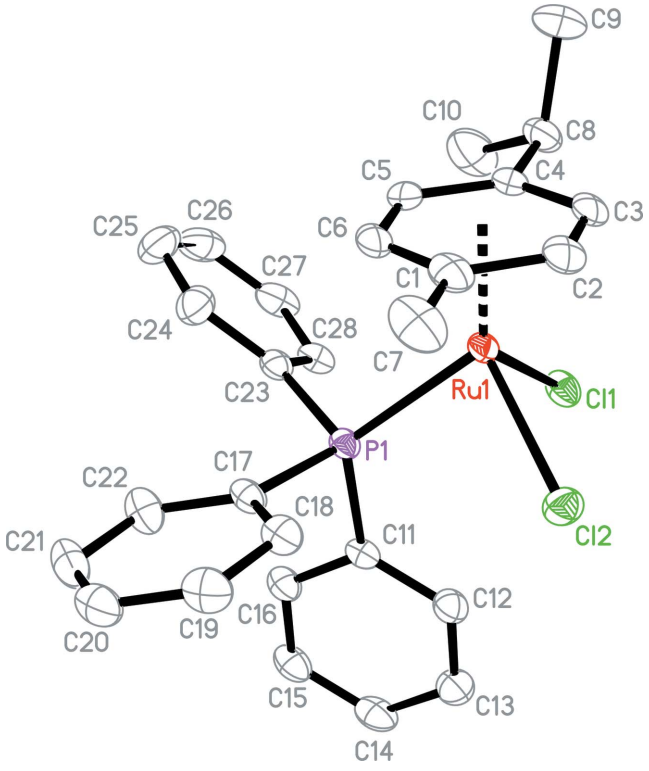


Figure 1
The structure of one of the two independent molecules (I), showing the atom-labelling scheme; the other molecule is very similar. Displacement ellipsoids are drawn at the 50% probability level. All H atoms have been omitted for clarity.

There are two similar molecules in the asymmetric unit, so discussion will primarily focus on one of these independent molecules; see Fig. 1 for a view of one of the two independent molecules. The Ru atom has a typical piano-stool coordination environment, with an η^6-coordinated *p*-cymene ligand, two chlorides and a triphenylphosphine ligand. Both molecules adopt a conformation half way between staggered and eclipsed orientations with regard to the *p*-cymene ring and the other three coordinated atoms. The metric parameters around the Ru core (Table 1) compare well with those of similar three-legged piano-stool [(η^6-arene)Ru(PPh_3)Cl_2] complexes (II)–(VI) (Table 2). The two *p*-cymene alkyl substituents bend very slightly away from the metal by 0.03 Å at the methyl group and 0.05 Å at the isopropyl group (for molecule 1) and by 0.02 Å at the methyl group and 0.01 Å at the isopropyl group (for molecule 2). The average Ru—C distances are 2.218 (2) and 2.215 (2) Å for the two independent molecules, in the range found in compounds (II)–(VI) [2.202 (3)–2.249 (4) Å]. There is very little difference in the Ru—$C_{centroid}$ parameters (1.709 and 1.705 Å) for the two independent molecules in (I). We also find some evidence for bond-length alternation around the *p*-cymene ring: average long = 1.426; average short = 1.403 Å (molecule 1), (1.426 and 1.401 Å for molecule 2). In previous structures (Elsegood & Tocher, 1995; Therrien & Süss-Fink, 2004; Vieille-Petit *et al.* (2003), a *trans* bond lengthening has been observed in the Ru—C bonds *trans* to P donors such as PPh_3. In the case of (I), the Ru1—C3, Ru1—C4, Ru2—C31 and Ru2—C32 bonds are longer than the other Ru—C bonds, with C2/C3 *trans* to P1 and C30/C31 *trans* to P2. A comparison of the sum of the P—Ru—Cl1, P—Ru—Cl2 and Cl1—Ru—Cl2 angles for (I) with (II) reveals that both (η^6-arene) groups have similar steric hindrance. The sum of these angles is *ca* 4–8° larger than found in (III)–(VI) (Table 2).

In summary, we have shown that triphenylphosphine affords a classic pseudo-tetrahedral (η^6-*p*-cymene)ruthenium(II) chloro complex with typical Ru—P/Ru—Cl bond lengths and angles.

Experimental

To a CH_3OH (10 ml) solution of [(η^6-*p*-cymene)$RuCl_2$]$_2$ (0.043 g, 0.057 mmol) was added a CH_3OH (10 ml) solution of Cu[2,3-pz(CO_2)(CO_2H)](PPh_3)$_2$ (0.018 g, 0.028 mmol) (pz = pyrazine). The dark-orange solution was stirred at room temperature for 2 h. The mixture was evaporated to dryness under reduced pressure, affording a dark-orange solid which was redissolved in the minimum volume of CH_2Cl_2 (*ca* 2 ml) and precipitated with diethyl ether (10 ml). The green solid was collected by suction filtration and dried *in vacuo*. Suitable X-ray quality crystals of (I) were obtained by slow evaporation of the CH_2Cl_2/diethyl ether filtrate.

Crystal data

[Ru($C_{10}H_{14}$)Cl_2($C_{18}H_{15}P$)]
M_r = 568.45
Monoclinic, $P2_1/n$
a = 15.4858 (8) Å
b = 9.1887 (5) Å
c = 35.0089 (19) Å
β = 96.568 (2)°
V = 4948.9 (5) Å^3
Z = 8
D_x = 1.526 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.93 mm^{-1}
T = 150 (2) K
Plate, red
0.71 × 0.28 × 0.10 mm

Data collection

Bruker SMART 1000 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.558, T_{max} = 0.913
42058 measured reflections
11719 independent reflections
9288 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 29.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.067
S = 1.06
11719 reflections
583 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0233P)^2 + 4.6393P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ru1—C1	2.213 (2)	Ru2—C29	2.210 (2)
Ru1—C2	2.216 (2)	Ru2—C30	2.212 (2)
Ru1—C3	2.245 (2)	Ru2—C31	2.247 (2)
Ru1—C4	2.247 (2)	Ru2—C32	2.239 (2)
Ru1—C5	2.213 (2)	Ru2—C33	2.207 (2)
Ru1—C6	2.176 (2)	Ru2—C34	2.173 (2)

Table 2
Selected geometric parameters (Å, °) for (I) and comparison with reported compounds (II)–(VI).

	(I)	(II)	(III)	(IV)	(V)	(VI)
Ru—P	2.3438 (6) [2.3442 (6)]	2.3530 (10)	2.3637 (12)	2.3533 (14)	2.3607 (10)	2.388 (1)
Ru—Cl1	2.4154 (6) [2.4154 (6)]	2.4134 (9)	2.406 (2)	2.4008 (18)	2.4117 (10)	2.423 (1)
Ru—Cl2	2.4151 (6) [2.4131 (6)]	2.3995 (10)	2.4118 (10)	2.4299 (15)	2.4118 (10)	2.412 (1)
Ru—C(av)	2.218 (2) [2.215 (2)]	2.215 (4)	2.202 (3)	2.230 (7)	2.249 (4)	2.231 (5)
P—Ru—Cl1	87.094 (19) [89.78 (2)]	91.81 (3)	86.15 (4)	85.82 (5)	84.99 (3)	86.83 (5)
P—Ru—Cl2	90.27 (2) [87.518 (19)]	86.34 (4)	86.15 (4)	91.46 (5)	88.22 (4)	82.63 (4)
Cl1—Ru—Cl2	88.41 (2) [88.91 (2)]	86.62 (4)	88.18 (3)	86.40 (6)	88.16 (4)	87.99 (4)
Σ angles	265.77 [266.21]	264.77	260.48	263.68	261.37	257.45

References: (II): Vieille-Petit *et al.* (2003); (III) Elsegood & Tocher (1995); (IV): Therrien & Süss-Fink (2004); (V): Hansen & Nelson (2000); (VI): Baldwin *et al.* (2002). Value in square brackets is for the second independent molecule. Σ angles = the sum of the P—Ru—Cl1, P—Ru—Cl2 and Cl1—Ru—Cl2 angles.

H atoms were positioned geometrically (C—H = 0.95 Å for aryl, 0.98 Å for methine and 1.00 Å for methyl H atoms) and refined using a riding model; U_{iso} values were set at $1.2U_{eq}$(C) ($1.5U_{eq}$ for methyl H atoms).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

We acknowledge Loughborough University for the provision of a studentship (NMSB).

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supporting information

Acta Cryst. (2006). E**62**, m2838–m2840 [https://doi.org/10.1107/S1600536806039869]

Dichloro(η^6-*p*-cymene)(triphenylphosphine)ruthenium(II)

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(η^6-*p*-Cymene)(triphenylphosphine)ruthenium(II) dichloride

Crystal data

$[Ru(C_{10}H_{14})(C_{18}H_{15}P)]Cl_2$
$M_r = 568.45$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 15.4858$ (8) Å
$b = 9.1887$ (5) Å
$c = 35.0089$ (19) Å
$\beta = 96.568$ (2)°
$V = 4948.9$ (5) Å^3
$Z = 8$
$F(000) = 2320$
$D_x = 1.526$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 20183 reflections
$\theta = 2.3$–$28.7°$
$\mu = 0.93$ mm^{-1}
$T = 150$ K
Plate, red
0.71 × 0.28 × 0.10 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
ω rotation with narrow frames scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.558$, $T_{max} = 0.913$
42058 measured reflections
11719 independent reflections
9288 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 29.0°$, $\theta_{min} = 1.5°$
$h = -20 \rightarrow 20$
$k = -12 \rightarrow 11$
$l = -46 \rightarrow 46$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.067$
$S = 1.06$
11719 reflections
583 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
$w = 1/[\sigma^2(F_o^2) + (0.0233P)^2 + 4.6393P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru1	0.457155 (11)	0.290762 (18)	0.176533 (5)	0.01739 (4)
Cl1	0.51009 (4)	0.53631 (6)	0.171123 (15)	0.02427 (11)
Cl2	0.60601 (3)	0.21219 (6)	0.191479 (16)	0.02706 (12)
C1	0.40512 (16)	0.0910 (3)	0.20082 (7)	0.0281 (5)
C2	0.43240 (15)	0.1895 (3)	0.23170 (6)	0.0259 (5)
H2	0.4727	0.1568	0.2524	0.031*
C3	0.40151 (14)	0.3311 (3)	0.23205 (6)	0.0236 (5)
H3	0.4204	0.3930	0.2531	0.028*
C4	0.34170 (14)	0.3851 (3)	0.20120 (6)	0.0239 (5)
C5	0.31333 (14)	0.2897 (3)	0.17078 (6)	0.0271 (5)
H5	0.2725	0.3224	0.1502	0.033*
C6	0.34538 (15)	0.1456 (3)	0.17073 (7)	0.0283 (5)
H6	0.3261	0.0836	0.1498	0.034*
C7	0.4374 (2)	−0.0629 (3)	0.20136 (8)	0.0399 (6)
H7A	0.4090	−0.1193	0.2202	0.060*
H7B	0.5004	−0.0639	0.2085	0.060*
H7C	0.4238	−0.1060	0.1758	0.060*
C8	0.30820 (15)	0.5379 (3)	0.20388 (7)	0.0299 (5)
H8	0.3557	0.5981	0.2177	0.036*
C9	0.23285 (18)	0.5328 (4)	0.22879 (9)	0.0482 (7)
H9A	0.1860	0.4720	0.2162	0.072*
H9B	0.2110	0.6315	0.2321	0.072*
H9C	0.2534	0.4914	0.2540	0.072*
C10	0.2799 (2)	0.6109 (3)	0.16526 (8)	0.0480 (7)
H10A	0.3293	0.6148	0.1501	0.072*
H10B	0.2597	0.7099	0.1696	0.072*
H10C	0.2326	0.5547	0.1513	0.072*
P1	0.46883 (3)	0.26578 (6)	0.110695 (15)	0.01762 (11)
C11	0.55591 (13)	0.3523 (2)	0.08712 (6)	0.0194 (4)
C12	0.63292 (14)	0.4011 (2)	0.10733 (6)	0.0246 (5)
H12	0.6412	0.3951	0.1346	0.030*
C13	0.69818 (15)	0.4592 (3)	0.08733 (7)	0.0298 (5)
H13	0.7507	0.4932	0.1011	0.036*
C14	0.68677 (16)	0.4675 (3)	0.04765 (7)	0.0303 (5)
H14	0.7318	0.5056	0.0343	0.036*
C15	0.61012 (16)	0.4204 (2)	0.02745 (7)	0.0278 (5)
H15	0.6022	0.4268	0.0002	0.033*
C16	0.54484 (15)	0.3639 (2)	0.04698 (6)	0.0246 (5)
H16	0.4919	0.3327	0.0330	0.030*
C17	0.47598 (14)	0.0800 (2)	0.09213 (6)	0.0211 (4)

C18	0.52235 (15)	−0.0233 (2)	0.11549 (7)	0.0256 (5)
H18	0.5444	0.0012	0.1411	0.031*
C19	0.53643 (16)	−0.1620 (3)	0.10142 (7)	0.0316 (5)
H19	0.5672	−0.2322	0.1176	0.038*
C20	0.50572 (16)	−0.1976 (3)	0.06404 (8)	0.0329 (6)
H20	0.5164	−0.2917	0.0544	0.039*
C21	0.45952 (17)	−0.0972 (3)	0.04058 (7)	0.0334 (6)
H21	0.4380	−0.1226	0.0150	0.040*
C22	0.44450 (16)	0.0413 (3)	0.05447 (7)	0.0300 (5)
H22	0.4126	0.1101	0.0382	0.036*
C23	0.37291 (13)	0.3476 (2)	0.08398 (6)	0.0208 (4)
C24	0.29661 (15)	0.2725 (3)	0.07179 (7)	0.0309 (5)
H24	0.2940	0.1700	0.0750	0.037*
C25	0.22398 (16)	0.3485 (4)	0.05485 (8)	0.0414 (7)
H25	0.1720	0.2971	0.0465	0.050*
C26	0.22702 (16)	0.4972 (3)	0.05011 (7)	0.0390 (6)
H26	0.1775	0.5480	0.0384	0.047*
C27	0.30252 (16)	0.5722 (3)	0.06255 (7)	0.0325 (6)
H27	0.3049	0.6747	0.0593	0.039*
C28	0.37450 (15)	0.4983 (3)	0.07975 (6)	0.0249 (5)
H28	0.4256	0.5509	0.0888	0.030*
Ru2	0.952432 (11)	0.071276 (18)	0.175744 (5)	0.01814 (5)
Cl3	1.10149 (3)	0.14538 (6)	0.192860 (16)	0.02753 (12)
Cl4	1.00234 (4)	−0.17523 (6)	0.169096 (15)	0.02601 (12)
C29	0.90022 (16)	0.2689 (3)	0.20079 (7)	0.0287 (5)
C30	0.92535 (15)	0.1671 (3)	0.23109 (6)	0.0269 (5)
H30	0.9649	0.1973	0.2524	0.032*
C31	0.89361 (14)	0.0255 (3)	0.23027 (6)	0.0246 (5)
H31	0.9107	−0.0386	0.2510	0.030*
C32	0.83523 (14)	−0.0241 (3)	0.19829 (6)	0.0252 (5)
C33	0.80898 (14)	0.0752 (3)	0.16861 (6)	0.0273 (5)
H33	0.7687	0.0455	0.1475	0.033*
C34	0.84189 (15)	0.2186 (3)	0.16985 (7)	0.0287 (5)
H34	0.8242	0.2829	0.1492	0.034*
C35	0.9337 (2)	0.4224 (3)	0.20274 (8)	0.0398 (6)
H35A	0.9209	0.4687	0.1775	0.060*
H35B	0.9967	0.4216	0.2101	0.060*
H35C	0.9055	0.4771	0.2219	0.060*
C36	0.80193 (16)	−0.1783 (3)	0.19884 (7)	0.0318 (5)
H36	0.8499	−0.2408	0.2114	0.038*
C37	0.72736 (19)	−0.1806 (4)	0.22437 (9)	0.0508 (8)
H37A	0.7489	−0.1462	0.2502	0.076*
H37B	0.7054	−0.2802	0.2259	0.076*
H37C	0.6803	−0.1169	0.2132	0.076*
C38	0.7725 (2)	−0.2426 (4)	0.15925 (8)	0.0502 (8)
H38A	0.7245	−0.1845	0.1465	0.075*
H38B	0.7530	−0.3430	0.1622	0.075*
H38C	0.8211	−0.2415	0.1436	0.075*

P2	0.96908 (3)	0.10460 (6)	0.110605 (15)	0.01856 (11)
C39	1.05999 (13)	0.0239 (2)	0.08843 (6)	0.0198 (4)
C40	1.13137 (14)	−0.0396 (2)	0.10987 (6)	0.0234 (5)
H40	1.1334	−0.0463	0.1370	0.028*
C41	1.20001 (15)	−0.0934 (3)	0.09141 (7)	0.0267 (5)
H41	1.2482	−0.1381	0.1061	0.032*
C42	1.19835 (15)	−0.0821 (3)	0.05189 (7)	0.0273 (5)
H42	1.2457	−0.1175	0.0396	0.033*
C43	1.12781 (15)	−0.0193 (3)	0.03043 (7)	0.0282 (5)
H43	1.1264	−0.0119	0.0033	0.034*
C44	1.05886 (14)	0.0331 (3)	0.04856 (6)	0.0260 (5)
H44	1.0103	0.0759	0.0336	0.031*
C45	0.87456 (13)	0.0282 (2)	0.08155 (6)	0.0216 (4)
C46	0.87620 (15)	−0.1185 (3)	0.07250 (7)	0.0283 (5)
H46	0.9277	−0.1733	0.0794	0.034*
C47	0.80346 (18)	−0.1863 (3)	0.05347 (8)	0.0395 (6)
H47	0.8059	−0.2865	0.0469	0.047*
C48	0.72790 (17)	−0.1091 (4)	0.04406 (8)	0.0449 (7)
H48	0.6782	−0.1556	0.0310	0.054*
C49	0.72461 (16)	0.0356 (4)	0.05363 (8)	0.0425 (7)
H49	0.6721	0.0884	0.0475	0.051*
C50	0.79758 (15)	0.1062 (3)	0.07219 (7)	0.0322 (6)
H50	0.7949	0.2066	0.0784	0.039*
C51	0.97691 (14)	0.2932 (2)	0.09428 (6)	0.0238 (5)
C52	0.94276 (17)	0.3409 (3)	0.05769 (7)	0.0332 (5)
H52	0.9079	0.2772	0.0410	0.040*
C53	0.95951 (19)	0.4810 (3)	0.04555 (8)	0.0419 (7)
H53	0.9356	0.5129	0.0208	0.050*
C54	1.01053 (18)	0.5737 (3)	0.06923 (9)	0.0411 (7)
H54	1.0230	0.6685	0.0605	0.049*
C55	1.04391 (17)	0.5296 (3)	0.10582 (8)	0.0373 (6)
H55	1.0780	0.5947	0.1224	0.045*
C56	1.02741 (15)	0.3895 (3)	0.11824 (7)	0.0287 (5)
H56	1.0507	0.3592	0.1432	0.034*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.01844 (8)	0.02018 (9)	0.01417 (8)	−0.00149 (7)	0.00458 (6)	−0.00022 (6)
Cl1	0.0313 (3)	0.0216 (3)	0.0211 (3)	−0.0039 (2)	0.0081 (2)	−0.0015 (2)
Cl2	0.0224 (3)	0.0327 (3)	0.0258 (3)	0.0036 (2)	0.0015 (2)	0.0022 (2)
C1	0.0341 (12)	0.0273 (12)	0.0255 (12)	−0.0069 (10)	0.0148 (10)	0.0024 (9)
C2	0.0296 (12)	0.0298 (12)	0.0199 (11)	−0.0039 (10)	0.0099 (9)	0.0057 (9)
C3	0.0267 (11)	0.0297 (12)	0.0164 (10)	−0.0053 (9)	0.0104 (9)	0.0000 (9)
C4	0.0194 (10)	0.0342 (13)	0.0196 (11)	−0.0022 (9)	0.0089 (8)	−0.0027 (9)
C5	0.0164 (10)	0.0449 (14)	0.0210 (11)	−0.0043 (10)	0.0062 (8)	−0.0044 (10)
C6	0.0269 (11)	0.0367 (13)	0.0236 (12)	−0.0135 (10)	0.0129 (9)	−0.0087 (10)
C7	0.0621 (18)	0.0262 (13)	0.0346 (14)	−0.0065 (12)	0.0200 (13)	0.0067 (11)

C8	0.0283 (12)	0.0379 (14)	0.0245 (12)	0.0070 (10)	0.0077 (10)	−0.0048 (10)
C9	0.0350 (14)	0.063 (2)	0.0507 (18)	0.0082 (14)	0.0218 (13)	−0.0113 (15)
C10	0.0525 (18)	0.0525 (18)	0.0391 (16)	0.0257 (15)	0.0056 (13)	0.0005 (14)
P1	0.0199 (3)	0.0188 (3)	0.0147 (2)	−0.0009 (2)	0.0043 (2)	−0.0002 (2)
C11	0.0229 (10)	0.0165 (10)	0.0202 (10)	0.0013 (8)	0.0077 (8)	0.0001 (8)
C12	0.0261 (11)	0.0269 (12)	0.0216 (11)	−0.0032 (9)	0.0064 (9)	−0.0014 (9)
C13	0.0271 (12)	0.0301 (13)	0.0334 (13)	−0.0074 (10)	0.0086 (10)	−0.0044 (10)
C14	0.0354 (13)	0.0248 (12)	0.0346 (13)	−0.0071 (10)	0.0204 (11)	−0.0017 (10)
C15	0.0376 (13)	0.0255 (12)	0.0224 (11)	−0.0022 (10)	0.0125 (10)	0.0000 (9)
C16	0.0286 (11)	0.0264 (12)	0.0195 (11)	−0.0005 (9)	0.0059 (9)	−0.0011 (9)
C17	0.0263 (11)	0.0182 (10)	0.0205 (11)	−0.0019 (9)	0.0093 (9)	−0.0012 (8)
C18	0.0283 (11)	0.0232 (11)	0.0262 (12)	−0.0005 (9)	0.0061 (9)	−0.0001 (9)
C19	0.0351 (13)	0.0203 (11)	0.0405 (14)	0.0015 (10)	0.0093 (11)	0.0024 (10)
C20	0.0374 (14)	0.0205 (12)	0.0441 (15)	−0.0074 (10)	0.0189 (12)	−0.0076 (10)
C21	0.0462 (15)	0.0294 (13)	0.0258 (12)	−0.0073 (11)	0.0094 (11)	−0.0075 (10)
C22	0.0414 (14)	0.0257 (12)	0.0232 (12)	−0.0015 (10)	0.0053 (10)	−0.0009 (9)
C23	0.0217 (10)	0.0272 (11)	0.0142 (10)	0.0009 (9)	0.0052 (8)	0.0012 (8)
C24	0.0277 (12)	0.0371 (14)	0.0278 (12)	−0.0057 (11)	0.0027 (10)	0.0010 (11)
C25	0.0219 (12)	0.066 (2)	0.0349 (14)	−0.0056 (12)	−0.0005 (10)	−0.0006 (14)
C26	0.0290 (13)	0.0597 (18)	0.0290 (13)	0.0174 (12)	0.0062 (10)	0.0069 (13)
C27	0.0368 (13)	0.0355 (14)	0.0270 (13)	0.0131 (11)	0.0115 (10)	0.0041 (10)
C28	0.0269 (11)	0.0272 (12)	0.0221 (11)	0.0031 (9)	0.0093 (9)	−0.0010 (9)
Ru2	0.01867 (8)	0.02237 (9)	0.01395 (8)	0.00185 (7)	0.00433 (6)	−0.00069 (6)
Cl3	0.0225 (2)	0.0352 (3)	0.0246 (3)	−0.0033 (2)	0.0012 (2)	−0.0021 (2)
Cl4	0.0321 (3)	0.0230 (3)	0.0243 (3)	0.0028 (2)	0.0095 (2)	−0.0003 (2)
C29	0.0325 (12)	0.0296 (12)	0.0263 (12)	0.0083 (10)	0.0138 (10)	−0.0020 (10)
C30	0.0286 (12)	0.0357 (13)	0.0181 (11)	0.0041 (10)	0.0094 (9)	−0.0071 (9)
C31	0.0258 (11)	0.0338 (13)	0.0159 (10)	0.0060 (10)	0.0097 (9)	0.0023 (9)
C32	0.0205 (10)	0.0361 (13)	0.0209 (11)	0.0010 (9)	0.0108 (9)	0.0017 (9)
C33	0.0177 (10)	0.0437 (14)	0.0212 (11)	0.0040 (10)	0.0054 (9)	0.0019 (10)
C34	0.0274 (12)	0.0354 (13)	0.0252 (12)	0.0136 (10)	0.0111 (9)	0.0065 (10)
C35	0.0609 (18)	0.0271 (13)	0.0348 (14)	0.0076 (12)	0.0201 (13)	−0.0025 (11)
C36	0.0286 (12)	0.0413 (14)	0.0270 (12)	−0.0101 (11)	0.0100 (10)	0.0024 (11)
C37	0.0400 (16)	0.064 (2)	0.0535 (19)	−0.0107 (14)	0.0264 (14)	0.0092 (16)
C38	0.0548 (18)	0.0579 (19)	0.0384 (16)	−0.0300 (16)	0.0077 (14)	−0.0062 (14)
P2	0.0194 (3)	0.0221 (3)	0.0146 (3)	0.0022 (2)	0.0041 (2)	−0.0006 (2)
C39	0.0212 (10)	0.0210 (10)	0.0180 (10)	−0.0004 (8)	0.0064 (8)	−0.0011 (8)
C40	0.0262 (11)	0.0266 (12)	0.0180 (10)	0.0022 (9)	0.0057 (9)	0.0018 (9)
C41	0.0244 (11)	0.0289 (12)	0.0272 (12)	0.0058 (9)	0.0050 (9)	0.0042 (9)
C42	0.0278 (11)	0.0269 (12)	0.0292 (12)	0.0037 (10)	0.0124 (10)	−0.0012 (10)
C43	0.0307 (12)	0.0360 (13)	0.0192 (11)	0.0021 (10)	0.0085 (9)	−0.0003 (9)
C44	0.0243 (11)	0.0339 (13)	0.0199 (11)	0.0037 (10)	0.0031 (9)	−0.0001 (9)
C45	0.0195 (10)	0.0304 (12)	0.0155 (10)	0.0004 (9)	0.0049 (8)	0.0004 (9)
C46	0.0284 (12)	0.0310 (13)	0.0256 (12)	−0.0034 (10)	0.0041 (10)	0.0013 (10)
C47	0.0425 (15)	0.0407 (15)	0.0350 (14)	−0.0170 (12)	0.0031 (12)	−0.0027 (12)
C48	0.0314 (14)	0.073 (2)	0.0294 (14)	−0.0198 (14)	−0.0001 (11)	−0.0026 (14)
C49	0.0214 (12)	0.075 (2)	0.0297 (14)	0.0062 (13)	−0.0015 (10)	0.0020 (14)
C50	0.0265 (12)	0.0463 (15)	0.0235 (12)	0.0090 (11)	0.0015 (10)	−0.0036 (11)

C51	0.0272 (11)	0.0237 (11)	0.0223 (11)	0.0050 (9)	0.0107 (9)	0.0023 (9)
C52	0.0405 (14)	0.0322 (13)	0.0279 (13)	0.0051 (11)	0.0086 (11)	0.0030 (10)
C53	0.0526 (17)	0.0387 (15)	0.0379 (15)	0.0152 (13)	0.0202 (13)	0.0151 (12)
C54	0.0461 (16)	0.0266 (13)	0.0559 (18)	0.0100 (12)	0.0280 (14)	0.0113 (12)
C55	0.0382 (14)	0.0236 (12)	0.0533 (17)	0.0006 (11)	0.0184 (12)	−0.0051 (12)
C56	0.0303 (12)	0.0264 (12)	0.0312 (13)	0.0040 (10)	0.0118 (10)	−0.0026 (10)

Geometric parameters (Å, º)

Ru1—C1	2.213 (2)	Ru2—C29	2.210 (2)
Ru1—C2	2.216 (2)	Ru2—C30	2.212 (2)
Ru1—C3	2.245 (2)	Ru2—C31	2.247 (2)
Ru1—C4	2.247 (2)	Ru2—C32	2.239 (2)
Ru1—C5	2.213 (2)	Ru2—C33	2.207 (2)
Ru1—C6	2.176 (2)	Ru2—C34	2.173 (2)
Ru1—P1	2.3438 (6)	Ru2—P2	2.3442 (6)
Ru1—Cl1	2.4154 (6)	Ru2—Cl3	2.4154 (6)
Ru1—Cl2	2.4151 (6)	Ru2—Cl4	2.4131 (6)
C1—C6	1.412 (3)	C29—C34	1.407 (3)
C1—C2	1.436 (3)	C29—C30	1.435 (3)
C1—C7	1.499 (3)	C29—C35	1.502 (3)
C2—C3	1.387 (3)	C30—C31	1.389 (3)
C2—H2	0.9500	C30—H30	0.9500
C3—C4	1.429 (3)	C31—C32	1.431 (3)
C3—H3	0.9500	C31—H31	0.9500
C4—C5	1.410 (3)	C32—C33	1.408 (3)
C4—C8	1.504 (3)	C32—C36	1.509 (3)
C5—C6	1.414 (3)	C33—C34	1.411 (3)
C5—H5	0.9500	C33—H33	0.9500
C6—H6	0.9500	C34—H34	0.9500
C7—H7A	0.9800	C35—H35A	0.9800
C7—H7B	0.9800	C35—H35B	0.9800
C7—H7C	0.9800	C35—H35C	0.9800
C8—C10	1.528 (4)	C36—C38	1.527 (4)
C8—C9	1.535 (3)	C36—C37	1.539 (3)
C8—H8	1.0000	C36—H36	1.0000
C9—H9A	0.9800	C37—H37A	0.9800
C9—H9B	0.9800	C37—H37B	0.9800
C9—H9C	0.9800	C37—H37C	0.9800
C10—H10A	0.9800	C38—H38A	0.9800
C10—H10B	0.9800	C38—H38B	0.9800
C10—H10C	0.9800	C38—H38C	0.9800
P1—C23	1.824 (2)	P2—C45	1.825 (2)
P1—C17	1.835 (2)	P2—C51	1.833 (2)
P1—C11	1.840 (2)	P2—C39	1.840 (2)
C11—C12	1.390 (3)	C39—C40	1.391 (3)
C11—C16	1.400 (3)	C39—C44	1.397 (3)
C12—C13	1.399 (3)	C40—C41	1.396 (3)

C12—H12	0.9500	C40—H40	0.9500
C13—C14	1.382 (3)	C41—C42	1.385 (3)
C13—H13	0.9500	C41—H41	0.9500
C14—C15	1.380 (3)	C42—C43	1.379 (3)
C14—H14	0.9500	C42—H42	0.9500
C15—C16	1.385 (3)	C43—C44	1.389 (3)
C15—H15	0.9500	C43—H43	0.9500
C16—H16	0.9500	C44—H44	0.9500
C17—C18	1.396 (3)	C45—C46	1.385 (3)
C17—C22	1.398 (3)	C45—C50	1.398 (3)
C18—C19	1.393 (3)	C46—C47	1.389 (3)
C18—H18	0.9500	C46—H46	0.9500
C19—C20	1.380 (4)	C47—C48	1.376 (4)
C19—H19	0.9500	C47—H47	0.9500
C20—C21	1.379 (4)	C48—C49	1.373 (4)
C20—H20	0.9500	C48—H48	0.9500
C21—C22	1.391 (3)	C49—C50	1.397 (4)
C21—H21	0.9500	C49—H49	0.9500
C22—H22	0.9500	C50—H50	0.9500
C23—C24	1.392 (3)	C51—C56	1.396 (3)
C23—C28	1.394 (3)	C51—C52	1.399 (3)
C24—C25	1.397 (4)	C52—C53	1.389 (4)
C24—H24	0.9500	C52—H52	0.9500
C25—C26	1.378 (4)	C53—C54	1.374 (4)
C25—H25	0.9500	C53—H53	0.9500
C26—C27	1.384 (4)	C54—C55	1.386 (4)
C26—H26	0.9500	C54—H54	0.9500
C27—C28	1.383 (3)	C55—C56	1.391 (3)
C27—H27	0.9500	C55—H55	0.9500
C28—H28	0.9500	C56—H56	0.9500

C6—Ru1—C1	37.53 (9)	C34—Ru2—C33	37.58 (9)
C6—Ru1—C5	37.57 (9)	C34—Ru2—C29	37.44 (9)
C1—Ru1—C5	67.95 (9)	C33—Ru2—C29	67.81 (9)
C6—Ru1—C2	66.99 (9)	C34—Ru2—C30	66.99 (9)
C1—Ru1—C2	37.83 (8)	C33—Ru2—C30	78.66 (9)
C5—Ru1—C2	78.75 (9)	C29—Ru2—C30	37.87 (9)
C6—Ru1—C3	78.58 (8)	C34—Ru2—C32	67.42 (9)
C1—Ru1—C3	67.14 (8)	C33—Ru2—C32	36.91 (8)
C5—Ru1—C3	66.27 (8)	C29—Ru2—C32	80.44 (9)
C2—Ru1—C3	36.21 (8)	C30—Ru2—C32	66.70 (9)
C6—Ru1—C4	67.23 (9)	C34—Ru2—C31	78.80 (8)
C1—Ru1—C4	80.31 (9)	C33—Ru2—C31	66.33 (8)
C5—Ru1—C4	36.86 (8)	C29—Ru2—C31	67.31 (9)
C2—Ru1—C4	66.58 (8)	C30—Ru2—C31	36.31 (9)
C3—Ru1—C4	37.10 (8)	C32—Ru2—C31	37.21 (8)
C6—Ru1—P1	89.90 (6)	C34—Ru2—P2	89.96 (6)
C1—Ru1—P1	111.66 (6)	C33—Ru2—P2	96.26 (6)

C5—Ru1—P1	95.75 (6)	C29—Ru2—P2	111.38 (6)
C2—Ru1—P1	148.91 (6)	C30—Ru2—P2	148.57 (7)
C3—Ru1—P1	161.43 (6)	C32—Ru2—P2	125.30 (6)
C4—Ru1—P1	124.76 (6)	C31—Ru2—P2	162.05 (6)
C6—Ru1—Cl2	124.50 (7)	C34—Ru2—Cl4	146.39 (7)
C1—Ru1—Cl2	92.83 (7)	C33—Ru2—Cl4	109.50 (7)
C5—Ru1—Cl2	160.74 (7)	C29—Ru2—Cl4	160.99 (6)
C2—Ru1—Cl2	86.65 (6)	C30—Ru2—Cl4	123.57 (6)
C3—Ru1—Cl2	108.25 (6)	C32—Ru2—Cl4	87.02 (6)
C4—Ru1—Cl2	144.48 (6)	C31—Ru2—Cl4	94.12 (6)
C6—Ru1—Cl1	146.99 (7)	P2—Ru2—Cl4	87.518 (19)
C1—Ru1—Cl1	161.19 (6)	C34—Ru2—Cl3	124.61 (7)
C5—Ru1—Cl1	110.11 (7)	C33—Ru2—Cl3	160.79 (7)
C2—Ru1—Cl1	123.68 (6)	C29—Ru2—Cl3	93.01 (7)
C3—Ru1—Cl1	94.65 (6)	C30—Ru2—Cl3	86.68 (6)
C4—Ru1—Cl1	87.81 (6)	C32—Ru2—Cl3	144.40 (6)
P1—Ru1—Cl1	87.094 (19)	C31—Ru2—Cl3	108.11 (6)
P1—Ru1—Cl2	90.27 (2)	P2—Ru2—Cl3	89.78 (2)
Cl2—Ru1—Cl1	88.41 (2)	Cl4—Ru2—Cl3	88.91 (2)
C6—C1—C2	116.7 (2)	C34—C29—C30	116.8 (2)
C6—C1—C7	122.2 (2)	C34—C29—C35	122.1 (2)
C2—C1—C7	121.1 (2)	C30—C29—C35	121.1 (2)
C6—C1—Ru1	69.81 (13)	C34—C29—Ru2	69.87 (13)
C2—C1—Ru1	71.20 (12)	C30—C29—Ru2	71.13 (13)
C7—C1—Ru1	130.66 (17)	C35—C29—Ru2	130.51 (17)
C3—C2—C1	121.7 (2)	C31—C30—C29	122.0 (2)
C3—C2—Ru1	73.03 (13)	C31—C30—Ru2	73.23 (13)
C1—C2—Ru1	70.97 (12)	C29—C30—Ru2	71.00 (12)
C3—C2—H2	119.1	C31—C30—H30	119.0
C1—C2—H2	119.1	C29—C30—H30	119.0
Ru1—C2—H2	129.4	Ru2—C30—H30	129.3
C2—C3—C4	120.9 (2)	C30—C31—C32	120.3 (2)
C2—C3—Ru1	70.76 (13)	C30—C31—Ru2	70.47 (12)
C4—C3—Ru1	71.51 (12)	C32—C31—Ru2	71.10 (12)
C2—C3—H3	119.5	C30—C31—H31	119.8
C4—C3—H3	119.5	C32—C31—H31	119.8
Ru1—C3—H3	131.0	Ru2—C31—H31	131.4
C5—C4—C3	118.3 (2)	C33—C32—C31	118.3 (2)
C5—C4—C8	123.2 (2)	C33—C32—C36	123.2 (2)
C3—C4—C8	118.4 (2)	C31—C32—C36	118.4 (2)
C5—C4—Ru1	70.29 (12)	C33—C32—Ru2	70.32 (12)
C3—C4—Ru1	71.39 (12)	C31—C32—Ru2	71.70 (12)
C8—C4—Ru1	132.83 (16)	C36—C32—Ru2	131.63 (16)
C4—C5—C6	120.3 (2)	C32—C33—C34	120.7 (2)
C4—C5—Ru1	72.86 (12)	C32—C33—Ru2	72.77 (12)
C6—C5—Ru1	69.78 (12)	C34—C33—Ru2	69.91 (13)
C4—C5—H5	119.9	C32—C33—H33	119.7
C6—C5—H5	119.9	C34—C33—H33	119.7

Ru1—C5—H5	130.0	Ru2—C33—H33	130.2
C1—C6—C5	122.1 (2)	C29—C34—C33	121.9 (2)
C1—C6—Ru1	72.66 (13)	C29—C34—Ru2	72.69 (13)
C5—C6—Ru1	72.64 (13)	C33—C34—Ru2	72.51 (13)
C1—C6—H6	118.9	C29—C34—H34	119.1
C5—C6—H6	118.9	C33—C34—H34	119.1
Ru1—C6—H6	128.0	Ru2—C34—H34	128.0
C1—C7—H7A	109.5	C29—C35—H35A	109.5
C1—C7—H7B	109.5	C29—C35—H35B	109.5
H7A—C7—H7B	109.5	H35A—C35—H35B	109.5
C1—C7—H7C	109.5	C29—C35—H35C	109.5
H7A—C7—H7C	109.5	H35A—C35—H35C	109.5
H7B—C7—H7C	109.5	H35B—C35—H35C	109.5
C4—C8—C10	114.9 (2)	C32—C36—C38	114.7 (2)
C4—C8—C9	107.3 (2)	C32—C36—C37	107.5 (2)
C10—C8—C9	110.9 (2)	C38—C36—C37	110.8 (2)
C4—C8—H8	107.9	C32—C36—H36	107.9
C10—C8—H8	107.9	C38—C36—H36	107.9
C9—C8—H8	107.9	C37—C36—H36	107.9
C8—C9—H9A	109.5	C36—C37—H37A	109.5
C8—C9—H9B	109.5	C36—C37—H37B	109.5
H9A—C9—H9B	109.5	H37A—C37—H37B	109.5
C8—C9—H9C	109.5	C36—C37—H37C	109.5
H9A—C9—H9C	109.5	H37A—C37—H37C	109.5
H9B—C9—H9C	109.5	H37B—C37—H37C	109.5
C8—C10—H10A	109.5	C36—C38—H38A	109.5
C8—C10—H10B	109.5	C36—C38—H38B	109.5
H10A—C10—H10B	109.5	H38A—C38—H38B	109.5
C8—C10—H10C	109.5	C36—C38—H38C	109.5
H10A—C10—H10C	109.5	H38A—C38—H38C	109.5
H10B—C10—H10C	109.5	H38B—C38—H38C	109.5
C23—P1—C17	106.28 (10)	C45—P2—C51	105.52 (10)
C23—P1—C11	100.81 (10)	C45—P2—C39	102.32 (10)
C17—P1—C11	99.57 (9)	C51—P2—C39	99.69 (10)
C23—P1—Ru1	108.29 (7)	C45—P2—Ru2	108.75 (7)
C17—P1—Ru1	117.00 (7)	C51—P2—Ru2	116.45 (7)
C11—P1—Ru1	122.80 (7)	C39—P2—Ru2	122.17 (7)
C12—C11—C16	119.1 (2)	C40—C39—C44	118.89 (19)
C12—C11—P1	122.77 (16)	C40—C39—P2	122.71 (16)
C16—C11—P1	118.12 (16)	C44—C39—P2	118.32 (16)
C11—C12—C13	119.7 (2)	C39—C40—C41	119.9 (2)
C11—C12—H12	120.2	C39—C40—H40	120.0
C13—C12—H12	120.2	C41—C40—H40	120.0
C14—C13—C12	120.5 (2)	C42—C41—C40	120.5 (2)
C14—C13—H13	119.8	C42—C41—H41	119.7
C12—C13—H13	119.8	C40—C41—H41	119.7
C15—C14—C13	120.1 (2)	C43—C42—C41	119.9 (2)
C15—C14—H14	120.0	C43—C42—H42	120.0

C13—C14—H14	120.0	C41—C42—H42	120.0
C14—C15—C16	119.9 (2)	C42—C43—C44	119.9 (2)
C14—C15—H15	120.1	C42—C43—H43	120.1
C16—C15—H15	120.1	C44—C43—H43	120.1
C15—C16—C11	120.8 (2)	C43—C44—C39	120.9 (2)
C15—C16—H16	119.6	C43—C44—H44	119.6
C11—C16—H16	119.6	C39—C44—H44	119.6
C18—C17—C22	118.7 (2)	C46—C45—C50	118.9 (2)
C18—C17—P1	118.21 (16)	C46—C45—P2	117.87 (17)
C22—C17—P1	122.81 (17)	C50—C45—P2	122.78 (18)
C19—C18—C17	120.4 (2)	C45—C46—C47	120.7 (2)
C19—C18—H18	119.8	C45—C46—H46	119.6
C17—C18—H18	119.8	C47—C46—H46	119.6
C20—C19—C18	120.1 (2)	C48—C47—C46	120.3 (3)
C20—C19—H19	120.0	C48—C47—H47	119.9
C18—C19—H19	120.0	C46—C47—H47	119.9
C21—C20—C19	120.4 (2)	C49—C48—C47	119.7 (2)
C21—C20—H20	119.8	C49—C48—H48	120.2
C19—C20—H20	119.8	C47—C48—H48	120.2
C20—C21—C22	120.0 (2)	C48—C49—C50	120.8 (2)
C20—C21—H21	120.0	C48—C49—H49	119.6
C22—C21—H21	120.0	C50—C49—H49	119.6
C21—C22—C17	120.5 (2)	C49—C50—C45	119.6 (3)
C21—C22—H22	119.7	C49—C50—H50	120.2
C17—C22—H22	119.7	C45—C50—H50	120.2
C24—C23—C28	119.0 (2)	C56—C51—C52	118.6 (2)
C24—C23—P1	124.45 (18)	C56—C51—P2	117.69 (17)
C28—C23—P1	116.14 (16)	C52—C51—P2	123.40 (19)
C23—C24—C25	119.7 (2)	C53—C52—C51	120.4 (3)
C23—C24—H24	120.1	C53—C52—H52	119.8
C25—C24—H24	120.1	C51—C52—H52	119.8
C26—C25—C24	120.7 (2)	C54—C53—C52	120.3 (3)
C26—C25—H25	119.7	C54—C53—H53	119.9
C24—C25—H25	119.7	C52—C53—H53	119.9
C25—C26—C27	119.7 (2)	C53—C54—C55	120.3 (2)
C25—C26—H26	120.2	C53—C54—H54	119.9
C27—C26—H26	120.2	C55—C54—H54	119.9
C28—C27—C26	120.2 (2)	C54—C55—C56	119.8 (3)
C28—C27—H27	119.9	C54—C55—H55	120.1
C26—C27—H27	119.9	C56—C55—H55	120.1
C27—C28—C23	120.7 (2)	C55—C56—C51	120.6 (2)
C27—C28—H28	119.6	C55—C56—H56	119.7
C23—C28—H28	119.6	C51—C56—H56	119.7

C5—Ru1—C1—C6	28.79 (13)	C33—Ru2—C29—C34	−28.94 (14)
C2—Ru1—C1—C6	129.1 (2)	C30—Ru2—C29—C34	−129.2 (2)
C3—Ru1—C1—C6	101.30 (15)	C32—Ru2—C29—C34	−65.13 (14)
C4—Ru1—C1—C6	65.02 (14)	C31—Ru2—C29—C34	−101.52 (15)

P1—Ru1—C1—C6	−58.66 (14)	P2—Ru2—C29—C34	59.16 (14)
Cl2—Ru1—C1—C6	−150.07 (13)	Cl4—Ru2—C29—C34	−114.5 (2)
Cl1—Ru1—C1—C6	116.6 (2)	Cl3—Ru2—C29—C34	150.10 (13)
C6—Ru1—C1—C2	−129.1 (2)	C34—Ru2—C29—C30	129.2 (2)
C5—Ru1—C1—C2	−100.29 (15)	C33—Ru2—C29—C30	100.29 (15)
C3—Ru1—C1—C2	−27.77 (13)	C32—Ru2—C29—C30	64.10 (14)
C4—Ru1—C1—C2	−64.05 (14)	C31—Ru2—C29—C30	27.71 (13)
P1—Ru1—C1—C2	172.27 (12)	P2—Ru2—C29—C30	−171.62 (12)
Cl2—Ru1—C1—C2	80.86 (13)	Cl4—Ru2—C29—C30	14.7 (3)
Cl1—Ru1—C1—C2	−12.5 (3)	Cl3—Ru2—C29—C30	−80.67 (13)
C6—Ru1—C1—C7	115.7 (3)	C34—Ru2—C29—C35	−115.6 (3)
C5—Ru1—C1—C7	144.5 (3)	C33—Ru2—C29—C35	−144.5 (3)
C2—Ru1—C1—C7	−115.2 (3)	C30—Ru2—C29—C35	115.2 (3)
C3—Ru1—C1—C7	−143.0 (3)	C32—Ru2—C29—C35	179.3 (2)
C4—Ru1—C1—C7	−179.3 (3)	C31—Ru2—C29—C35	142.9 (3)
P1—Ru1—C1—C7	57.0 (2)	P2—Ru2—C29—C35	−56.4 (2)
Cl2—Ru1—C1—C7	−34.4 (2)	Cl4—Ru2—C29—C35	129.9 (2)
Cl1—Ru1—C1—C7	−127.7 (2)	Cl3—Ru2—C29—C35	34.5 (2)
C6—C1—C2—C3	0.2 (3)	C34—C29—C30—C31	−0.3 (3)
C7—C1—C2—C3	−178.4 (2)	C35—C29—C30—C31	178.6 (2)
Ru1—C1—C2—C3	54.81 (19)	Ru2—C29—C30—C31	−54.89 (19)
C6—C1—C2—Ru1	−54.62 (17)	C34—C29—C30—Ru2	54.56 (18)
C7—C1—C2—Ru1	126.8 (2)	C35—C29—C30—Ru2	−126.5 (2)
C6—Ru1—C2—C3	−102.47 (15)	C34—Ru2—C30—C31	102.80 (15)
C1—Ru1—C2—C3	−133.4 (2)	C33—Ru2—C30—C31	65.27 (14)
C5—Ru1—C2—C3	−64.98 (14)	C29—Ru2—C30—C31	133.6 (2)
C4—Ru1—C2—C3	−28.39 (13)	C32—Ru2—C30—C31	28.55 (13)
P1—Ru1—C2—C3	−147.39 (11)	P2—Ru2—C30—C31	148.66 (11)
Cl2—Ru1—C2—C3	127.65 (13)	Cl4—Ru2—C30—C31	−40.72 (15)
Cl1—Ru1—C2—C3	41.80 (15)	Cl3—Ru2—C30—C31	−127.21 (13)
C6—Ru1—C2—C1	30.92 (14)	C34—Ru2—C30—C29	−30.77 (14)
C5—Ru1—C2—C1	68.40 (14)	C33—Ru2—C30—C29	−68.30 (15)
C3—Ru1—C2—C1	133.4 (2)	C32—Ru2—C30—C29	−105.02 (15)
C4—Ru1—C2—C1	105.00 (15)	C31—Ru2—C30—C29	−133.6 (2)
P1—Ru1—C2—C1	−14.0 (2)	P2—Ru2—C30—C29	15.1 (2)
Cl2—Ru1—C2—C1	−98.96 (13)	Cl4—Ru2—C30—C29	−174.30 (11)
Cl1—Ru1—C2—C1	175.19 (11)	Cl3—Ru2—C30—C29	99.22 (13)
C1—C2—C3—C4	−0.8 (3)	C29—C30—C31—C32	1.2 (3)
Ru1—C2—C3—C4	53.09 (18)	Ru2—C30—C31—C32	−52.71 (18)
C1—C2—C3—Ru1	−53.87 (19)	C29—C30—C31—Ru2	53.89 (19)
C6—Ru1—C3—C2	66.47 (14)	C34—Ru2—C31—C30	−66.21 (14)
C1—Ru1—C3—C2	28.92 (14)	C33—Ru2—C31—C30	−103.52 (15)
C5—Ru1—C3—C2	103.86 (15)	C29—Ru2—C31—C30	−28.82 (14)
C4—Ru1—C3—C2	133.7 (2)	C32—Ru2—C31—C30	−133.5 (2)
P1—Ru1—C3—C2	119.10 (19)	P2—Ru2—C31—C30	−118.4 (2)
Cl2—Ru1—C3—C2	−56.34 (14)	Cl4—Ru2—C31—C30	146.98 (13)
Cl1—Ru1—C3—C2	−146.19 (13)	Cl3—Ru2—C31—C30	56.78 (14)
C6—Ru1—C3—C4	−67.20 (14)	C34—Ru2—C31—C32	67.25 (14)

C1—Ru1—C3—C4	−104.74 (15)	C33—Ru2—C31—C32	29.94 (13)
C5—Ru1—C3—C4	−29.80 (13)	C29—Ru2—C31—C32	104.64 (15)
C2—Ru1—C3—C4	−133.7 (2)	C30—Ru2—C31—C32	133.5 (2)
P1—Ru1—C3—C4	−14.6 (3)	P2—Ru2—C31—C32	15.1 (3)
Cl2—Ru1—C3—C4	170.00 (11)	Cl4—Ru2—C31—C32	−79.57 (13)
Cl1—Ru1—C3—C4	80.15 (13)	Cl3—Ru2—C31—C32	−169.77 (12)
C2—C3—C4—C5	1.4 (3)	C30—C31—C32—C33	−2.1 (3)
Ru1—C3—C4—C5	54.18 (17)	Ru2—C31—C32—C33	−54.49 (17)
C2—C3—C4—C8	177.9 (2)	C30—C31—C32—C36	−179.5 (2)
Ru1—C3—C4—C8	−129.31 (19)	Ru2—C31—C32—C36	128.07 (19)
C2—C3—C4—Ru1	−52.75 (18)	C30—C31—C32—Ru2	52.43 (18)
C6—Ru1—C4—C5	−29.18 (14)	C34—Ru2—C32—C33	28.89 (14)
C1—Ru1—C4—C5	−65.97 (15)	C29—Ru2—C32—C33	65.57 (15)
C2—Ru1—C4—C5	−102.91 (15)	C30—Ru2—C32—C33	102.53 (15)
C3—Ru1—C4—C5	−130.7 (2)	C31—Ru2—C32—C33	130.4 (2)
P1—Ru1—C4—C5	43.74 (16)	P2—Ru2—C32—C33	−43.92 (16)
Cl2—Ru1—C4—C5	−147.16 (12)	Cl4—Ru2—C32—C33	−128.76 (13)
Cl1—Ru1—C4—C5	128.67 (14)	Cl3—Ru2—C32—C33	147.30 (12)
C6—Ru1—C4—C3	101.48 (15)	C34—Ru2—C32—C31	−101.54 (15)
C1—Ru1—C4—C3	64.70 (14)	C33—Ru2—C32—C31	−130.4 (2)
C5—Ru1—C4—C3	130.7 (2)	C29—Ru2—C32—C31	−64.86 (14)
C2—Ru1—C4—C3	27.76 (13)	C30—Ru2—C32—C31	−27.90 (13)
P1—Ru1—C4—C3	174.40 (10)	P2—Ru2—C32—C31	−174.36 (11)
Cl2—Ru1—C4—C3	−16.49 (19)	Cl4—Ru2—C32—C31	100.81 (13)
Cl1—Ru1—C4—C3	−100.66 (12)	Cl3—Ru2—C32—C31	16.87 (19)
C6—Ru1—C4—C8	−146.6 (2)	C34—Ru2—C32—C36	146.4 (2)
C1—Ru1—C4—C8	176.6 (2)	C33—Ru2—C32—C36	117.5 (3)
C5—Ru1—C4—C8	−117.5 (3)	C29—Ru2—C32—C36	−177.0 (2)
C2—Ru1—C4—C8	139.6 (2)	C30—Ru2—C32—C36	−140.0 (2)
C3—Ru1—C4—C8	111.9 (3)	C31—Ru2—C32—C36	−112.1 (3)
P1—Ru1—C4—C8	−73.7 (2)	P2—Ru2—C32—C36	73.5 (2)
Cl2—Ru1—C4—C8	95.4 (2)	Cl4—Ru2—C32—C36	−11.3 (2)
Cl1—Ru1—C4—C8	11.2 (2)	Cl3—Ru2—C32—C36	−95.2 (2)
C3—C4—C5—C6	−1.5 (3)	C31—C32—C33—C34	2.2 (3)
C8—C4—C5—C6	−177.8 (2)	C36—C32—C33—C34	179.5 (2)
Ru1—C4—C5—C6	53.23 (18)	Ru2—C32—C33—C34	−53.00 (18)
C3—C4—C5—Ru1	−54.71 (17)	C31—C32—C33—Ru2	55.16 (17)
C8—C4—C5—Ru1	128.9 (2)	C36—C32—C33—Ru2	−127.5 (2)
C6—Ru1—C5—C4	132.5 (2)	C34—Ru2—C33—C32	−133.0 (2)
C1—Ru1—C5—C4	103.74 (15)	C29—Ru2—C33—C32	−104.15 (15)
C2—Ru1—C5—C4	65.77 (14)	C30—Ru2—C33—C32	−66.12 (14)
C3—Ru1—C5—C4	29.99 (13)	C31—Ru2—C33—C32	−30.17 (13)
P1—Ru1—C5—C4	−145.19 (13)	P2—Ru2—C33—C32	145.28 (13)
Cl2—Ru1—C5—C4	107.2 (2)	Cl4—Ru2—C33—C32	55.70 (14)
Cl1—Ru1—C5—C4	−56.19 (14)	Cl3—Ru2—C33—C32	−107.1 (2)
C1—Ru1—C5—C6	−28.75 (13)	C29—Ru2—C33—C34	28.84 (13)
C2—Ru1—C5—C6	−66.72 (14)	C30—Ru2—C33—C34	66.86 (14)
C3—Ru1—C5—C6	−102.51 (15)	C32—Ru2—C33—C34	133.0 (2)

C4—Ru1—C5—C6	−132.5 (2)	C31—Ru2—C33—C34	102.82 (15)
P1—Ru1—C5—C6	82.31 (13)	P2—Ru2—C33—C34	−81.74 (13)
Cl2—Ru1—C5—C6	−25.3 (3)	Cl4—Ru2—C33—C34	−171.32 (12)
Cl1—Ru1—C5—C6	171.32 (11)	Cl3—Ru2—C33—C34	25.9 (3)
C2—C1—C6—C5	−0.3 (3)	C30—C29—C34—C33	0.4 (3)
C7—C1—C6—C5	178.3 (2)	C35—C29—C34—C33	−178.5 (2)
Ru1—C1—C6—C5	−55.59 (19)	Ru2—C29—C34—C33	55.62 (19)
C2—C1—C6—Ru1	55.33 (17)	C30—C29—C34—Ru2	−55.19 (18)
C7—C1—C6—Ru1	−126.1 (2)	C35—C29—C34—Ru2	125.9 (2)
C4—C5—C6—C1	0.9 (3)	C32—C33—C34—C29	−1.4 (3)
Ru1—C5—C6—C1	55.60 (19)	Ru2—C33—C34—C29	−55.70 (19)
C4—C5—C6—Ru1	−54.65 (19)	C32—C33—C34—Ru2	54.31 (19)
C5—Ru1—C6—C1	−133.0 (2)	C33—Ru2—C34—C29	132.7 (2)
C2—Ru1—C6—C1	−31.15 (13)	C30—Ru2—C34—C29	31.10 (14)
C3—Ru1—C6—C1	−67.20 (14)	C32—Ru2—C34—C29	104.31 (15)
C4—Ru1—C6—C1	−104.29 (15)	C31—Ru2—C34—C29	67.16 (14)
P1—Ru1—C6—C1	127.46 (13)	P2—Ru2—C34—C29	−126.92 (13)
Cl2—Ru1—C6—C1	37.21 (15)	Cl4—Ru2—C34—C29	147.62 (12)
Cl1—Ru1—C6—C1	−148.04 (12)	Cl3—Ru2—C34—C29	−37.22 (16)
C1—Ru1—C6—C5	133.0 (2)	C29—Ru2—C34—C33	−132.7 (2)
C2—Ru1—C6—C5	101.80 (15)	C30—Ru2—C34—C33	−101.62 (15)
C3—Ru1—C6—C5	65.75 (14)	C32—Ru2—C34—C33	−28.41 (13)
C4—Ru1—C6—C5	28.66 (13)	C31—Ru2—C34—C33	−65.56 (14)
P1—Ru1—C6—C5	−99.59 (13)	P2—Ru2—C34—C33	100.35 (13)
Cl2—Ru1—C6—C5	170.16 (11)	Cl4—Ru2—C34—C33	14.9 (2)
Cl1—Ru1—C6—C5	−15.1 (2)	Cl3—Ru2—C34—C33	−169.94 (11)
C5—C4—C8—C10	−29.7 (3)	C33—C32—C36—C38	26.6 (3)
C3—C4—C8—C10	153.9 (2)	C31—C32—C36—C38	−156.1 (2)
Ru1—C4—C8—C10	63.5 (3)	Ru2—C32—C36—C38	−66.0 (3)
C5—C4—C8—C9	94.0 (3)	C33—C32—C36—C37	−97.2 (3)
C3—C4—C8—C9	−82.3 (3)	C31—C32—C36—C37	80.1 (3)
Ru1—C4—C8—C9	−172.71 (18)	Ru2—C32—C36—C37	170.28 (19)
C6—Ru1—P1—C23	65.93 (10)	C34—Ru2—P2—C45	−65.95 (10)
C1—Ru1—P1—C23	97.28 (10)	C33—Ru2—P2—C45	−28.83 (10)
C5—Ru1—P1—C23	28.75 (10)	C29—Ru2—P2—C45	−97.41 (10)
C2—Ru1—P1—C23	106.47 (14)	C30—Ru2—P2—C45	−107.30 (14)
C3—Ru1—P1—C23	14.8 (2)	C32—Ru2—P2—C45	−4.06 (11)
C4—Ru1—P1—C23	4.12 (11)	C31—Ru2—P2—C45	−15.2 (2)
Cl2—Ru1—P1—C23	−169.58 (8)	Cl4—Ru2—P2—C45	80.52 (8)
Cl1—Ru1—P1—C23	−81.19 (8)	Cl3—Ru2—P2—C45	169.44 (8)
C6—Ru1—P1—C17	−54.06 (10)	C34—Ru2—P2—C51	53.02 (11)
C1—Ru1—P1—C17	−22.71 (11)	C33—Ru2—P2—C51	90.15 (11)
C5—Ru1—P1—C17	−91.24 (10)	C29—Ru2—P2—C51	21.56 (11)
C2—Ru1—P1—C17	−13.52 (15)	C30—Ru2—P2—C51	11.68 (15)
C3—Ru1—P1—C17	−105.2 (2)	C32—Ru2—P2—C51	114.92 (11)
C4—Ru1—P1—C17	−115.87 (11)	C31—Ru2—P2—C51	103.8 (2)
Cl2—Ru1—P1—C17	70.44 (8)	Cl4—Ru2—P2—C51	−160.50 (8)
Cl1—Ru1—P1—C17	158.83 (8)	Cl3—Ru2—P2—C51	−71.58 (8)

C6—Ru1—P1—C11	−177.45 (11)	C34—Ru2—P2—C39	175.37 (11)
C1—Ru1—P1—C11	−146.10 (11)	C33—Ru2—P2—C39	−147.50 (11)
C5—Ru1—P1—C11	145.38 (10)	C29—Ru2—P2—C39	143.91 (11)
C2—Ru1—P1—C11	−136.91 (14)	C30—Ru2—P2—C39	134.03 (14)
C3—Ru1—P1—C11	131.4 (2)	C32—Ru2—P2—C39	−122.73 (11)
C4—Ru1—P1—C11	120.74 (11)	C31—Ru2—P2—C39	−133.9 (2)
Cl2—Ru1—P1—C11	−52.95 (8)	Cl4—Ru2—P2—C39	−38.15 (8)
Cl1—Ru1—P1—C11	35.44 (8)	Cl3—Ru2—P2—C39	50.77 (8)
C23—P1—C11—C12	139.46 (19)	C45—P2—C39—C40	−133.06 (19)
C17—P1—C11—C12	−111.78 (19)	C51—P2—C39—C40	118.58 (19)
Ru1—P1—C11—C12	19.2 (2)	Ru2—P2—C39—C40	−11.3 (2)
C23—P1—C11—C16	−43.02 (19)	C45—P2—C39—C44	50.0 (2)
C17—P1—C11—C16	65.74 (19)	C51—P2—C39—C44	−58.34 (19)
Ru1—P1—C11—C16	−163.24 (14)	Ru2—P2—C39—C44	171.77 (15)
C16—C11—C12—C13	−0.7 (3)	C44—C39—C40—C41	−0.4 (3)
P1—C11—C12—C13	176.77 (17)	P2—C39—C40—C41	−177.25 (17)
C11—C12—C13—C14	−0.4 (4)	C39—C40—C41—C42	1.0 (3)
C12—C13—C14—C15	1.0 (4)	C40—C41—C42—C43	−1.0 (4)
C13—C14—C15—C16	−0.4 (4)	C41—C42—C43—C44	0.4 (4)
C14—C15—C16—C11	−0.7 (4)	C42—C43—C44—C39	0.3 (4)
C12—C11—C16—C15	1.3 (3)	C40—C39—C44—C43	−0.3 (3)
P1—C11—C16—C15	−176.31 (17)	P2—C39—C44—C43	176.74 (18)
C23—P1—C17—C18	−157.50 (17)	C51—P2—C45—C46	147.66 (17)
C11—P1—C17—C18	98.17 (18)	C39—P2—C45—C46	43.80 (19)
Ru1—P1—C17—C18	−36.45 (19)	Ru2—P2—C45—C46	−86.72 (17)
C23—P1—C17—C22	28.9 (2)	C51—P2—C45—C50	−40.3 (2)
C11—P1—C17—C22	−75.4 (2)	C39—P2—C45—C50	−144.15 (19)
Ru1—P1—C17—C22	149.97 (17)	Ru2—P2—C45—C50	85.33 (19)
C22—C17—C18—C19	−0.2 (3)	C50—C45—C46—C47	1.8 (3)
P1—C17—C18—C19	−174.09 (18)	P2—C45—C46—C47	174.17 (19)
C17—C18—C19—C20	1.0 (4)	C45—C46—C47—C48	−1.4 (4)
C18—C19—C20—C21	−1.2 (4)	C46—C47—C48—C49	−0.1 (4)
C19—C20—C21—C22	0.7 (4)	C47—C48—C49—C50	1.2 (4)
C20—C21—C22—C17	0.1 (4)	C48—C49—C50—C45	−0.8 (4)
C18—C17—C22—C21	−0.3 (3)	C46—C45—C50—C49	−0.7 (3)
P1—C17—C22—C21	173.26 (18)	P2—C45—C50—C49	−172.70 (19)
C17—P1—C23—C24	35.5 (2)	C45—P2—C51—C56	162.38 (17)
C11—P1—C23—C24	138.87 (19)	C39—P2—C51—C56	−91.83 (18)
Ru1—P1—C23—C24	−91.04 (19)	Ru2—P2—C51—C56	41.66 (19)
C17—P1—C23—C28	−152.07 (16)	C45—P2—C51—C52	−24.5 (2)
C11—P1—C23—C28	−48.65 (18)	C39—P2—C51—C52	81.3 (2)
Ru1—P1—C23—C28	81.44 (17)	Ru2—P2—C51—C52	−145.25 (18)
C28—C23—C24—C25	1.4 (3)	C56—C51—C52—C53	0.5 (3)
P1—C23—C24—C25	173.70 (19)	P2—C51—C52—C53	−172.58 (19)
C23—C24—C25—C26	−0.1 (4)	C51—C52—C53—C54	0.6 (4)
C24—C25—C26—C27	−0.6 (4)	C52—C53—C54—C55	−1.7 (4)
C25—C26—C27—C28	−0.2 (4)	C53—C54—C55—C56	1.6 (4)
C26—C27—C28—C23	1.6 (3)	C54—C55—C56—C51	−0.5 (4)

C24—C23—C28—C27	−2.2 (3)	C52—C51—C56—C55	−0.5 (3)
P1—C23—C28—C27	−175.08 (17)	P2—C51—C56—C55	172.92 (18)