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Dichlorotris(triphenylphosphine)ruthenium(II) dichloromethane hemisolvate

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.006 Å
R factor = 0.039
wR factor = 0.041
Data-to-parameter ratio = 10.8

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

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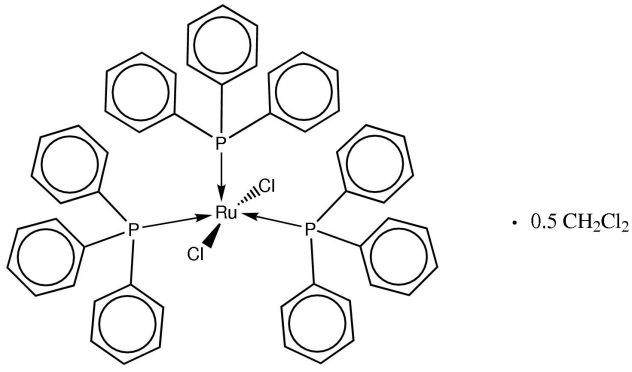
A third modification of $[RuCl_2(PPh_3)_3]$ has been characterized, this time as the title compound, $[RuCl_2(C_{18}H_{15}P)_3]\cdot 0.5CH_2Cl_2$. As seen for the previous modifications, the complex has a distorted square-pyramidal geometry with an *ortho*-H atom 'blocking' the site *trans* to the apical PPh_3 ligand. There is no evidence for a strong C—H···Ru interaction nor any specific directional force in the solid state.

Comment

Two different modifications of $[RuCl_2(PPh_3)_3]$ have been solved in the space groups $P2_1/c$ (La Placa & Ibers, 1965) and $P2_1/n$ (Ernst *et al.*, 2003). Both show a distorted square-pyramidal geometry about Ru, with an *ortho*-H atom approaching the metal and 'blocking' the site *trans* to the apical PPh_3 ligand. As part of our studies on Ru^{II} thioether complexes, we discovered the title compound, (I), (Fig. 1), also containing the $[RuCl_2(PPh_3)_3]$ complex, as the dichloromethane hemisolvate in the space group $C2/c$.



(I)

The metal complex in (I) adopts a distorted square-pyramidal geometry with bond lengths, angles and phenyl ring orientations virtually identical to the $P2_1/c$ modification of $[RuCl_2(PPh_3)_3]$. In fact, most $[Ru^{II}X_2(PPh_3)_3]$ complexes are distorted square-pyramidal (Anillo *et al.*, 1993; MacFarlane *et al.*, 1996), due to electronic (vibrational distortions, Jahn–Teller effects) and/or steric reasons.

The shortest Ru···H distance in (I) is due to an *ortho*-H atom located approximately *trans* to P2 [Ru1···H2 = 2.83 (4) Å and P2—Ru1···H2 = 168 (2)°]. The shortest Ru···C distance in (I) [Ru1···C2 3.445 (4) Å] is average for penta-coordinate $[Ru^{II}(PPh_3)_3]$ complexes (Anillo *et al.*, 1993; MacFarlane *et al.*, 1996) and some 0.2 Å shorter than in $[Ru^{0}(CO)_2(PPh_3)_3]$ (Hiraki *et al.*, 1997). It is 0.1–0.3 Å shorter than the analogous distance in hexa-coordinate $[Ru^{II}(PPh_3)_3]$ complexes (Skapski & Stephens, 1974; Alexander *et al.*, 1988;

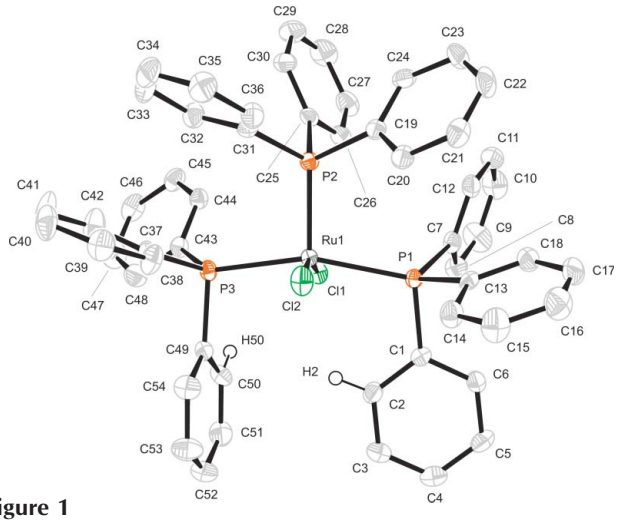


Figure 1
A view of (I), with displacement ellipsoids shown at the 50% probability level. The solvent molecule and most H atoms have been omitted for clarity.

Mizuho *et al.*, 1991; Poulton *et al.*, 1992; Junk & Steed, 1999; Jazzar *et al.*, 2001) and some 0.2 Å longer than in tetra-coordinate $[Ru^{II}(SC_6F_5)_2(PPh_3)_2]$ (Catalá *et al.*, 1987, 1989). There is no elongation of the C2—H2 bond in (I) as observed in the $P2_1/n$ modification of $[RuCl_2(PPh_3)_3]$, so overall there appears to be no strong C2—H2···Ru1 interaction in (I).

$[RuCl_2(PPh_3)_3]$ has been referred to as an agostic complex (Leung *et al.*, 2000; Perera & Shaw, 1994, 1995; Catalá *et al.*, 1987, 1989), but much shorter and stronger agostic C—H···Ru bonds are known (Huang *et al.*, 1999, 2000; Jiménez Tenorio *et al.*, 2000). The close approach of the *ortho*-H atom to Ru and subsequent 'blocking' of the site *trans* to the apical PPh_3 ligand may therefore be due to a weak C—H···Ru interaction, steric crowding of the metal centre and/or crystal packing forces in the solid state.

The crystal packing in (I) is unexceptional and gives no indication of any specific directional force being present. The CH_2Cl_2 solvent molecule lies on a twofold symmetry axis and plays no role in metal coordination.

Experimental

$[RuCl_2(PPh_3)_3]$ was synthesized according to the literature method of Hallman *et al.* (1970) but using only one-quarter the specified volume of methanol. Suitable single crystals of (I) were grown by two-phase dichloromethane–methanol liquid diffusion.

Crystal data

$[RuCl_2(C_{18}H_{15}P)_3]\cdot 0.5CH_2Cl_2$
$M_r = 1001.31$
Monoclinic, $C2/c$
$a = 22.2083\ (2)$ Å
$b = 12.84460\ (10)$ Å
$c = 33.9272\ (5)$ Å
$\beta = 107.5681\ (5)^\circ$
$V = 9226.57\ (18)$ Å^3
$Z = 8$
$D_x = 1.442$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 17441 reflections
$\theta = 5.0$–27.5°
$\mu = 0.66$ mm^{-1}
$T = 150$ K
Block, purple–brown
0.10 × 0.10 × 0.10 mm

Data collection

Nonius KappaCCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*DENZO* and *SCALEPACK*; Otwinowski & Minor, 1997)
$T_{min} = 0.93$, $T_{max} = 0.94$
17441 measured reflections
10441 independent reflections
6083 reflections with $I > 3\sigma(I)$
$R_{int} = 0.05$
$\theta_{max} = 27.5^\circ$
$h = -28 \rightarrow 28$
$k = -14 \rightarrow 16$
$l = -44 \rightarrow 43$

Refinement

Refinement on F
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.041$
$S = 1.11$
6083 reflections
563 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = [1 - (F_o - F_c)^2/36\sigma(F_o)^2]^2/0.437T_0(x) + 0.0688T_1(x) + 0.16T_2(x)]$, where $T_n(x)$ are Chebychev polynomials and $x = F_c/F_{max}$ (Watkin, 1994; Prince, 1982)
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.76$ e Å^{-3}
$\Delta\rho_{min} = -1.04$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ru1—P3	2.3557 (9)	Ru1—Cl1	2.3916 (9)
Ru1—P2	2.2118 (10)	C2—H2	0.94 (4)
Ru1—P1	2.4334 (9)	C50—H50	0.96 (5)
Ru1—Cl2	2.3732 (9)		
P3—Ru1—P2	98.27 (4)	P1—Ru1—Cl2	91.36 (3)
P3—Ru1—P1	160.12 (4)	P3—Ru1—Cl1	86.29 (3)
P2—Ru1—P1	101.08 (4)	P2—Ru1—Cl1	107.46 (4)
P3—Ru1—Cl2	92.05 (3)	P1—Ru1—Cl1	83.63 (3)
P2—Ru1—Cl2	93.27 (4)	Cl2—Ru1—Cl1	159.24 (4)

Atoms H2 and H50 were located in a difference Fourier map and their coordinates and isotropic displacement parameters were subsequently refined. All other H atoms were positioned geometrically with C—H = 1.00 Å. The most positive and negative residual electron densities are located 1.11 and 1.05 Å from Cl61, respectively, possibly indicating disorder in the CH_2Cl_2 solvent molecule. No attempt was made to model this disorder.

Data collection: *COLLECT* (Nonius, 2001); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS*.

References

Alexander, B. D., Gomez-Sal, M. P., Gannon, P. R., Blaine, C. A., Boyle, P. D., Mueting, A. M. & Pignolet, L. H. (1988). *Inorg. Chem.* **27**, 3301–3308.
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Anillo, A., Barrio, C., García-Granda, S. & Obeso-Rosete, R. (1993). *J. Chem. Soc. Dalton Trans.* pp. 1125–1130.
Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, C. K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
Catalá, R.-M., Cruz-Garritz, D., Terreros, P., Torrens, H., Hills, A., Hughes, D. L. & Richards, R. L. (1987). *J. Organomet. Chem.* **328**, C37–C39.
Catalá, R.-M., Cruz-Garritz, D., Sosa, P., Terreros, P., Torrens, H., Hills, A., Hughes, D. L. & Richards, R. L. (1989). *J. Organomet. Chem.* **359**, 219–232.
Ernst, R. D., Basta, R. & Arif, A. M. (2003). *Z. Kristallogr. New Cryst. Struct.* **218**, 49–51.
Hallman, P. S., Stephenson T. A. & Wilkinson, G. (1970). *Inorg. Synth.* **12**, 237–240.
Hiraki, K., Kira, S. & Kawano H. (1997). *Bull. Chem. Soc. Jpn*, **70**, 1583–1592.

Huang, D., Bollinger, J. C., Streib, W. E., Folting, K., Young, V. Jr, Eisenstein, O. & Caulton, K. G. (2000). *Organometallics*, **19**, 2281–2290.
Huang, D., Streib, W. E., Bollinger, J. C., Caulton, K. G., Winter, R. F. & Scheiring T. (1999). *J. Am. Chem. Soc.* **121**, 8087–8097.
Jazzar, R. F. R., Mahon, M. F. & Whittlesey, M. K. (2001). *Organometallics*, **20**, 3745–3751.
Jiménez Tenorio, M., Mereiter, K., Puerta, M. C. & Valerga, P. (2000). *J. Am. Chem. Soc.* **122**, 11230–11231.
Junk, P. C. & Steed, J. W. (1999). *J. Organomet. Chem.* **587**, 191–194.
La Placa, S. J. & Ibers, J. A. (1965). *Inorg. Chem.* **4**, 778–783.
Leung, W.-H., Zheng, H., Chim, J. L. C., Chan, J., Wong, W.-T. & Williams, I. D. (2000). *J. Chem. Soc. Dalton Trans.* pp. 423–430.
MacFarlane, K. S., Joshi, A. M., Rettig, S. J. & James, B. R. (1996). *Inorg. Chem.* **35**, 7304–7310.
Mizuho, Y., Kasuga, N. & Komiya, S. (1991). *Chem. Lett.* pp. 2127–2130.
Nonius (2001). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307-326. New York: Academic Press.
Perera, S. D. & Shaw, B. L. (1994). *J. Chem. Soc. Chem. Commun.* pp. 1201–1202.
Perera, S. D. & Shaw, B. L. (1995). *J. Chem. Soc. Dalton Trans.* pp. 3861–3866.
Poulton, J. T., Folting, K. & Caulton, K. G. (1992). *Organometallics,* **11**, 1364–1372.
Prince, E. (1982). *Mathematical Techniques in Crystallography and Materials Science*. New York: Springer-Verlag.
Skapski, A. C. & Stephens, F. A. (1974). *J. Chem. Soc. Dalton Trans.* pp. 390–395.
Watkin, D. J. (1994). *Acta Cryst.* A**50**, 411–437.
Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.

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$b = 12.8446$ (1) Å
$c = 33.9272$ (5) Å
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$V = 9226.57$ (18) Å^3
$Z = 8$
$F(000) = 4104$
$D_x = 1.442$ Mg m^{-3}
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$\theta_{max} = 27.5°$, $\theta_{min} = 5.1°$
$h = -28\rightarrow 28$
$k = -14\rightarrow 16$
$l = -44\rightarrow 43$

Refinement

Refinement on *F*
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.041$
$S = 1.11$
6083 reflections
563 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 atoms treated by a mixture of independent and constrained refinement
Method, part 1, Chebychev polynomial (Watkin, 1994; *P*rince, 1982). [*w*eight] = 1.0/[A_0*T_0(x) + A_1*T_1(x) ··· + A_{n-1}]*T_{n-1}(x)] where A_i are the Chebychev coefficients 0.437 0.688E-01 0.160 and x = *F* /*F*max. Method, part 2, Robust Weighting (*P*rince, 1982). W = [*w*eight]*[1-(delta*F*/6*sigma*F*)^2]^2
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.76$ e Å^{-3}
$\Delta\rho_{min} = -1.04$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru1	0.775455 (13)	−0.12420 (2)	0.118831 (8)	0.0156
Cl1	0.82062 (4)	−0.18547 (8)	0.18806 (3)	0.0225
Cl2	0.71825 (4)	−0.12677 (9)	0.04738 (3)	0.0286
P1	0.67803 (4)	−0.12197 (8)	0.13763 (3)	0.0170
P2	0.79616 (5)	0.04418 (7)	0.11854 (3)	0.0183
P3	0.86747 (4)	−0.18753 (8)	0.10621 (3)	0.0185
C1	0.65610 (18)	−0.2584 (3)	0.14161 (11)	0.0215
C2	0.6878 (2)	−0.3382 (3)	0.12885 (13)	0.0251
C3	0.6658 (2)	−0.4400 (3)	0.12618 (15)	0.0327
C4	0.6119 (2)	−0.4626 (3)	0.13678 (14)	0.0318
C5	0.57960 (19)	−0.3843 (4)	0.15002 (13)	0.0299
C6	0.60135 (19)	−0.2830 (3)	0.15204 (13)	0.0262
C7	0.68439 (18)	−0.0651 (3)	0.18829 (11)	0.0220
C8	0.69975 (19)	−0.1256 (4)	0.22389 (12)	0.0283
C9	0.7116 (3)	−0.0785 (4)	0.26248 (13)	0.0428
C10	0.7082 (2)	0.0290 (4)	0.26578 (14)	0.0423
C11	0.6924 (2)	0.0890 (4)	0.23038 (14)	0.0328
C12	0.68043 (19)	0.0428 (3)	0.19190 (12)	0.0255
C13	0.59868 (17)	−0.0829 (3)	0.10429 (11)	0.0193
C14	0.57985 (18)	−0.1250 (4)	0.06433 (12)	0.0301
C15	0.5188 (2)	−0.1096 (4)	0.03881 (13)	0.0405
C16	0.4751 (2)	−0.0551 (4)	0.05218 (15)	0.0420
C17	0.4931 (2)	−0.0157 (4)	0.09183 (17)	0.0414
C18	0.5553 (2)	−0.0277 (3)	0.11781 (14)	0.0301
C19	0.72758 (17)	0.1308 (3)	0.10889 (12)	0.0222
C20	0.67111 (19)	0.1063 (3)	0.07843 (13)	0.0270
C21	0.61850 (19)	0.1703 (4)	0.07249 (14)	0.0324
C22	0.6206 (2)	0.2566 (4)	0.09678 (16)	0.0393
C23	0.6755 (2)	0.2819 (3)	0.12672 (16)	0.0363
C24	0.72886 (19)	0.2215 (3)	0.13245 (13)	0.0277
C25	0.84676 (17)	0.1040 (3)	0.16634 (12)	0.0217
C26	0.84022 (18)	0.0704 (3)	0.20377 (12)	0.0250
C27	0.8708 (2)	0.1208 (4)	0.24050 (13)	0.0345
C28	0.9091 (2)	0.2054 (4)	0.24021 (16)	0.0442
C29	0.9165 (2)	0.2397 (4)	0.20337 (16)	0.0416
C30	0.8852 (2)	0.1904 (3)	0.16658 (14)	0.0303
C31	0.83186 (18)	0.0890 (3)	0.07931 (12)	0.0214
C32	0.8972 (2)	0.0854 (3)	0.08688 (13)	0.0295
C33	0.9245 (2)	0.1236 (4)	0.05824 (15)	0.0394
C34	0.8874 (2)	0.1626 (4)	0.02092 (16)	0.0416
C35	0.8222 (2)	0.1631 (4)	0.01210 (14)	0.0376
C36	0.79494 (19)	0.1269 (4)	0.04112 (12)	0.0282
C37	0.89276 (18)	−0.1568 (3)	0.06048 (12)	0.0224
C38	0.8486 (2)	−0.1444 (4)	0.02180 (13)	0.0323
C39	0.8675 (2)	−0.1226 (4)	−0.01271 (13)	0.0359

C40	0.9296 (2)	−0.1117 (4)	−0.00982 (14)	0.0417
C41	0.9740 (2)	−0.1186 (5)	0.02893 (17)	0.0552
C42	0.9561 (2)	−0.1401 (5)	0.06367 (15)	0.0440
C43	0.94259 (17)	−0.1839 (3)	0.14762 (11)	0.0209
C44	0.95713 (18)	−0.0994 (3)	0.17480 (12)	0.0235
C45	1.0165 (2)	−0.0900 (4)	0.20395 (13)	0.0297
C46	1.0612 (2)	−0.1662 (4)	0.20716 (13)	0.0350
C47	1.0473 (2)	−0.2513 (4)	0.18098 (15)	0.0386
C48	0.9888 (2)	−0.2605 (3)	0.15141 (14)	0.0318
C49	0.84951 (18)	−0.3283 (3)	0.10039 (12)	0.0223
C50	0.8574 (2)	−0.3899 (3)	0.13559 (13)	0.0267
C51	0.8413 (2)	−0.4943 (4)	0.13162 (14)	0.0331
C52	0.8165 (2)	−0.5394 (3)	0.09296 (15)	0.0363
C53	0.8078 (2)	−0.4782 (4)	0.05796 (14)	0.0378
C54	0.8242 (2)	−0.3729 (4)	0.06187 (12)	0.0306
Cl61	1.02310 (13)	−0.51128 (15)	0.21487 (8)	0.1049
C62	1.0000	−0.4347 (8)	0.2500	0.0865
H2	0.725 (2)	−0.325 (3)	0.1222 (13)	0.026 (11)*
H50	0.877 (2)	−0.359 (4)	0.1621 (15)	0.032 (12)*
H3	0.6889	−0.4967	0.1166	0.0401*
H4	0.5961	−0.5359	0.1349	0.0375*
H5	0.5409	−0.4011	0.1580	0.0356*
H6	0.5776	−0.2263	0.1611	0.0325*
H8	0.7023	−0.2031	0.2218	0.0345*
H9	0.7227	−0.1224	0.2880	0.0506*
H10	0.7170	0.0626	0.2935	0.0499*
H11	0.6897	0.1664	0.2325	0.0400*
H12	0.6688	0.0871	0.1665	0.0314*
H14	0.6105	−0.1661	0.0542	0.0352*
H15	0.5062	−0.1386	0.0101	0.0469*
H16	0.4312	−0.0444	0.0334	0.0473*
H17	0.4615	0.0219	0.1022	0.0489*
H18	0.5682	0.0036	0.1461	0.0363*
H20	0.6685	0.0429	0.0609	0.0328*
H21	0.5786	0.1531	0.0502	0.0377*
H22	0.5822	0.3009	0.0926	0.0487*
H23	0.6770	0.3445	0.1445	0.0453*
H24	0.7691	0.2425	0.1537	0.0327*
H26	0.8129	0.0087	0.2042	0.0282*
H27	0.8652	0.0960	0.2671	0.0406*
H28	0.9315	0.2417	0.2667	0.0505*
H29	0.9446	0.3004	0.2033	0.0487*
H30	0.8901	0.2168	0.1400	0.0362*
H32	0.9246	0.0548	0.1133	0.0367*
H33	0.9715	0.1229	0.0646	0.0502*
H34	0.9074	0.1904	0.0003	0.0543*
H35	0.7950	0.1896	−0.0152	0.0465*
H36	0.7479	0.1279	0.0346	0.0346*

H38	0.8025	−0.1514	0.0188	0.0400*
H39	0.8348	−0.1146	−0.0402	0.0432*
H40	0.9430	−0.0992	−0.0350	0.0540*
H41	1.0197	−0.1077	0.0317	0.0699*
H42	0.9889	−0.1438	0.0913	0.0537*
H44	0.9244	−0.0448	0.1733	0.0283*
H45	1.0266	−0.0278	0.2225	0.0357*
H46	1.1036	−0.1602	0.2283	0.0397*
H47	1.0798	−0.3068	0.1834	0.0436*
H48	0.9796	−0.3224	0.1326	0.0367*
H51	0.8476	−0.5378	0.1570	0.0407*
H52	0.8051	−0.6149	0.0903	0.0439*
H53	0.7897	−0.5096	0.0299	0.0429*
H54	0.8175	−0.3293	0.0365	0.0353*
H62	1.0362	−0.3898	0.2654	0.1098*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.01569 (13)	0.01675 (13)	0.01414 (13)	0.00115 (14)	0.00420 (10)	0.00035 (13)
Cl1	0.0232 (5)	0.0269 (5)	0.0163 (4)	0.0038 (4)	0.0042 (3)	0.0024 (4)
Cl2	0.0235 (4)	0.0449 (6)	0.0155 (4)	0.0021 (5)	0.0033 (3)	−0.0034 (5)
P1	0.0173 (4)	0.0189 (4)	0.0153 (4)	0.0002 (4)	0.0056 (3)	0.0001 (4)
P2	0.0174 (5)	0.0176 (5)	0.0193 (4)	0.0008 (4)	0.0045 (4)	0.0008 (4)
P3	0.0150 (4)	0.0228 (5)	0.0170 (4)	0.0025 (4)	0.0040 (4)	−0.0012 (4)
C1	0.0212 (19)	0.022 (2)	0.0206 (18)	−0.0025 (15)	0.0051 (15)	0.0011 (15)
C2	0.022 (2)	0.024 (2)	0.031 (2)	0.0003 (16)	0.0103 (17)	0.0049 (16)
C3	0.037 (3)	0.023 (2)	0.041 (3)	−0.0021 (19)	0.015 (2)	−0.0046 (18)
C4	0.037 (3)	0.024 (2)	0.032 (2)	−0.0059 (19)	0.0082 (19)	0.0007 (18)
C5	0.024 (2)	0.029 (2)	0.035 (2)	−0.0067 (18)	0.0078 (17)	0.0079 (19)
C6	0.026 (2)	0.024 (2)	0.031 (2)	0.0011 (17)	0.0129 (17)	−0.0007 (17)
C7	0.0225 (19)	0.030 (2)	0.0161 (17)	−0.0006 (16)	0.0093 (15)	−0.0025 (15)
C8	0.032 (2)	0.031 (2)	0.0241 (19)	−0.003 (2)	0.0104 (16)	−0.0009 (19)
C9	0.059 (3)	0.049 (3)	0.018 (2)	0.012 (3)	0.009 (2)	0.004 (2)
C10	0.041 (3)	0.060 (3)	0.024 (2)	0.001 (2)	0.007 (2)	−0.014 (2)
C11	0.033 (2)	0.033 (2)	0.034 (2)	−0.0033 (19)	0.0125 (19)	−0.0103 (19)
C12	0.021 (2)	0.031 (2)	0.027 (2)	0.0000 (16)	0.0100 (16)	−0.0031 (17)
C13	0.0150 (17)	0.0209 (18)	0.0205 (18)	−0.0040 (15)	0.0028 (14)	0.0006 (15)
C14	0.0226 (19)	0.039 (2)	0.027 (2)	0.000 (2)	0.0037 (15)	−0.004 (2)
C15	0.032 (2)	0.057 (3)	0.028 (2)	0.002 (2)	0.0026 (18)	−0.003 (2)
C16	0.026 (2)	0.051 (3)	0.042 (3)	0.006 (2)	−0.001 (2)	−0.002 (2)
C17	0.020 (2)	0.038 (3)	0.064 (3)	0.0036 (19)	0.010 (2)	−0.012 (2)
C18	0.025 (2)	0.030 (2)	0.035 (2)	−0.0011 (18)	0.0099 (18)	−0.0088 (19)
C19	0.0221 (18)	0.0184 (18)	0.0272 (19)	0.0046 (17)	0.0091 (15)	0.0095 (17)
C20	0.026 (2)	0.026 (2)	0.031 (2)	0.0034 (16)	0.0097 (17)	0.0101 (17)
C21	0.021 (2)	0.039 (3)	0.034 (2)	0.0070 (18)	0.0035 (17)	0.017 (2)
C22	0.027 (2)	0.039 (3)	0.055 (3)	0.018 (2)	0.018 (2)	0.017 (2)
C23	0.035 (2)	0.026 (2)	0.052 (3)	0.0131 (19)	0.020 (2)	0.006 (2)

C24	0.025 (2)	0.0199 (19)	0.037 (2)	−0.0027 (17)	0.0073 (17)	0.0032 (17)
C25	0.0172 (18)	0.018 (2)	0.027 (2)	0.0041 (14)	0.0031 (15)	−0.0028 (15)
C26	0.0187 (19)	0.026 (2)	0.026 (2)	0.0014 (16)	0.0001 (15)	−0.0076 (16)
C27	0.032 (2)	0.037 (2)	0.032 (2)	0.004 (2)	0.0064 (18)	−0.009 (2)
C28	0.036 (3)	0.046 (3)	0.044 (3)	−0.004 (2)	0.003 (2)	−0.020 (2)
C29	0.034 (3)	0.034 (3)	0.054 (3)	−0.012 (2)	0.009 (2)	−0.018 (2)
C30	0.025 (2)	0.022 (2)	0.043 (3)	−0.0013 (17)	0.0100 (19)	−0.0018 (18)
C31	0.026 (2)	0.0142 (17)	0.026 (2)	0.0004 (15)	0.0099 (16)	0.0035 (15)
C32	0.030 (2)	0.031 (2)	0.031 (2)	0.0048 (18)	0.0143 (18)	0.0074 (18)
C33	0.032 (2)	0.046 (3)	0.048 (3)	0.006 (2)	0.023 (2)	0.015 (2)
C34	0.047 (3)	0.044 (3)	0.044 (3)	−0.002 (2)	0.030 (2)	0.010 (2)
C35	0.049 (3)	0.041 (3)	0.027 (2)	0.005 (2)	0.017 (2)	0.0114 (19)
C36	0.029 (2)	0.030 (2)	0.028 (2)	0.004 (2)	0.0115 (16)	0.0039 (19)
C37	0.0200 (19)	0.024 (2)	0.026 (2)	0.0026 (15)	0.0116 (16)	−0.0005 (15)
C38	0.029 (2)	0.046 (3)	0.025 (2)	−0.0026 (19)	0.0129 (17)	0.0041 (19)
C39	0.039 (2)	0.045 (3)	0.023 (2)	0.002 (2)	0.0098 (18)	0.003 (2)
C40	0.044 (3)	0.056 (3)	0.036 (2)	0.009 (2)	0.027 (2)	0.008 (2)
C41	0.031 (2)	0.092 (4)	0.052 (3)	0.009 (3)	0.026 (2)	0.021 (3)
C42	0.027 (2)	0.069 (4)	0.039 (3)	0.014 (2)	0.013 (2)	0.013 (3)
C43	0.0154 (18)	0.026 (2)	0.0197 (18)	0.0023 (15)	0.0027 (14)	0.0026 (16)
C44	0.0223 (19)	0.028 (2)	0.0207 (18)	−0.0007 (15)	0.0069 (15)	−0.0021 (15)
C45	0.025 (2)	0.040 (2)	0.024 (2)	−0.0089 (18)	0.0078 (17)	−0.0039 (18)
C46	0.021 (2)	0.052 (3)	0.026 (2)	−0.003 (2)	−0.0019 (17)	0.006 (2)
C47	0.025 (2)	0.043 (3)	0.041 (3)	0.010 (2)	−0.0002 (19)	0.009 (2)
C48	0.023 (2)	0.032 (2)	0.036 (2)	0.0028 (18)	0.0039 (17)	−0.0039 (19)
C49	0.022 (2)	0.022 (2)	0.024 (2)	0.0010 (16)	0.0087 (16)	−0.0035 (16)
C50	0.033 (2)	0.022 (2)	0.026 (2)	0.0055 (17)	0.0104 (17)	−0.0015 (17)
C51	0.035 (2)	0.031 (2)	0.036 (2)	0.0061 (19)	0.014 (2)	0.0080 (19)
C52	0.044 (3)	0.022 (2)	0.044 (3)	0.0001 (19)	0.015 (2)	−0.0026 (19)
C53	0.044 (3)	0.031 (2)	0.032 (2)	−0.006 (2)	0.002 (2)	−0.0061 (19)
C54	0.034 (2)	0.032 (2)	0.0222 (19)	0.000 (2)	0.0035 (16)	0.001 (2)
Cl61	0.164 (2)	0.0642 (11)	0.1330 (19)	−0.0189 (13)	0.1155 (18)	−0.0077 (11)
C62	0.144 (11)	0.069 (7)	0.061 (6)	0.0000	0.053 (7)	0.0000

Geometric parameters (Å, º)

Ru1—P3	2.3557 (9)	C25—C30	1.399 (5)
Ru1—P2	2.2118 (10)	C25—C26	1.389 (6)
Ru1—P1	2.4334 (9)	C26—H26	1.000
Ru1—Cl2	2.3732 (9)	C26—C27	1.387 (6)
Ru1—Cl1	2.3916 (9)	C27—H27	1.000
P1—C13	1.853 (4)	C27—C28	1.382 (7)
P1—C7	1.834 (4)	C28—H28	1.000
P1—C1	1.835 (4)	C28—C29	1.381 (7)
P2—C31	1.836 (4)	C29—H29	1.000
P2—C25	1.839 (4)	C29—C30	1.385 (6)
P2—C19	1.834 (4)	C30—H30	1.000
P3—C49	1.850 (4)	C31—C36	1.395 (6)

P3—C43	1.829 (4)	C31—C32	1.396 (6)
P3—C37	1.845 (4)	C32—H32	1.000
C1—C6	1.401 (5)	C32—C33	1.381 (6)
C1—C2	1.384 (6)	C33—H33	1.000
C2—H2	0.94 (4)	C33—C34	1.380 (7)
C2—C3	1.389 (6)	C34—H34	1.000
C3—H3	1.000	C34—C35	1.387 (7)
C3—C4	1.379 (6)	C35—H35	1.000
C4—H4	1.000	C35—C36	1.383 (6)
C4—C5	1.387 (6)	C36—H36	1.000
C5—H5	1.000	C37—C42	1.395 (6)
C5—C6	1.383 (6)	C37—C38	1.391 (6)
C6—H6	1.000	C38—H38	1.000
C7—C12	1.396 (6)	C38—C39	1.387 (6)
C7—C8	1.389 (6)	C39—H39	1.000
C8—H8	1.000	C39—C40	1.361 (6)
C8—C9	1.393 (6)	C40—H40	1.000
C9—H9	1.000	C40—C41	1.387 (7)
C9—C10	1.390 (7)	C41—H41	1.000
C10—H10	1.000	C41—C42	1.380 (6)
C10—C11	1.380 (7)	C42—H42	1.000
C11—H11	1.000	C43—C48	1.399 (6)
C11—C12	1.385 (6)	C43—C44	1.398 (5)
C12—H12	1.000	C44—H44	1.000
C13—C18	1.381 (5)	C44—C45	1.395 (5)
C13—C14	1.401 (5)	C45—H45	1.000
C14—H14	1.000	C45—C46	1.375 (6)
C14—C15	1.384 (6)	C46—H46	1.000
C15—H15	1.000	C46—C47	1.383 (7)
C15—C16	1.379 (7)	C47—H47	1.000
C16—H16	1.000	C47—C48	1.386 (6)
C16—C17	1.379 (7)	C48—H48	1.000
C17—H17	1.000	C49—C54	1.382 (6)
C17—C18	1.405 (6)	C49—C50	1.398 (6)
C18—H18	1.000	C50—H50	0.96 (5)
C19—C24	1.409 (6)	C50—C51	1.384 (6)
C19—C20	1.399 (6)	C51—H51	1.000
C20—H20	1.000	C51—C52	1.387 (7)
C20—C21	1.392 (6)	C52—H52	1.000
C21—H21	1.000	C52—C53	1.388 (7)
C21—C22	1.374 (7)	C53—H53	1.000
C22—H22	1.000	C53—C54	1.396 (6)
C22—C23	1.370 (7)	C54—H54	1.000
C23—H23	1.000	Cl61—C62	1.738 (6)
C23—C24	1.380 (6)	C62—H62	1.000
C24—H24	1.000	C62—H62^{i}	1.000
P3—Ru1—P2	98.27 (4)	H24—C24—C19	119.469

P3—Ru1—P1	160.12 (4)	C23—C24—C19	121.1 (4)
P2—Ru1—P1	101.08 (4)	C30—C25—C26	118.2 (4)
P3—Ru1—Cl2	92.05 (3)	C30—C25—P2	123.1 (3)
P2—Ru1—Cl2	93.27 (4)	C26—C25—P2	118.1 (3)
P1—Ru1—Cl2	91.36 (3)	H26—C26—C27	119.394
P3—Ru1—Cl1	86.29 (3)	H26—C26—C25	119.394
P2—Ru1—Cl1	107.46 (4)	C27—C26—C25	121.2 (4)
P1—Ru1—Cl1	83.63 (3)	H27—C27—C28	120.112
Cl2—Ru1—Cl1	159.24 (4)	H27—C27—C26	120.111
C13—P1—C7	104.73 (17)	C28—C27—C26	119.8 (4)
C13—P1—C1	94.51 (17)	H28—C28—C29	120.056
C7—P1—C1	104.97 (18)	H28—C28—C27	120.055
C13—P1—Ru1	126.89 (12)	C29—C28—C27	119.9 (4)
C7—P1—Ru1	115.31 (12)	H29—C29—C30	119.791
C1—P1—Ru1	106.55 (13)	H29—C29—C28	119.791
C31—P2—C25	103.05 (18)	C30—C29—C28	120.4 (4)
C31—P2—C19	101.39 (17)	H30—C30—C29	119.774
C25—P2—C19	99.07 (17)	H30—C30—C25	119.774
C31—P2—Ru1	116.49 (13)	C29—C30—C25	120.5 (4)
C25—P2—Ru1	118.48 (13)	C36—C31—C32	118.0 (4)
C19—P2—Ru1	115.55 (13)	C36—C31—P2	121.4 (3)
C49—P3—C43	102.95 (18)	C32—C31—P2	120.6 (3)
C49—P3—C37	103.29 (17)	H32—C32—C33	119.615
C43—P3—C37	101.65 (17)	H32—C32—C31	119.615
C49—P3—Ru1	100.72 (12)	C33—C32—C31	120.8 (4)
C43—P3—Ru1	119.46 (12)	H33—C33—C34	119.781
C37—P3—Ru1	125.45 (13)	H33—C33—C32	119.781
C6—C1—C2	118.3 (4)	C34—C33—C32	120.4 (4)
C6—C1—P1	120.2 (3)	H34—C34—C35	120.145
C2—C1—P1	120.9 (3)	H34—C34—C33	120.145
H2—C2—C3	118 (3)	C35—C34—C33	119.7 (4)
H2—C2—C1	121 (3)	H35—C35—C36	120.082
C3—C2—C1	121.0 (4)	H35—C35—C34	120.082
H3—C3—C4	120.114	C36—C35—C34	119.8 (4)
H3—C3—C2	120.114	H36—C36—C35	119.419
C4—C3—C2	119.8 (4)	H36—C36—C31	119.419
H4—C4—C5	119.779	C35—C36—C31	121.2 (4)
H4—C4—C3	119.780	C42—C37—C38	117.6 (4)
C5—C4—C3	120.4 (4)	C42—C37—P3	121.6 (3)
H5—C5—C6	120.302	C38—C37—P3	120.7 (3)
H5—C5—C4	120.302	H38—C38—C39	119.586
C6—C5—C4	119.4 (4)	H38—C38—C37	119.586
H6—C6—C5	119.462	C39—C38—C37	120.8 (4)
H6—C6—C1	119.463	H39—C39—C40	119.367
C5—C6—C1	121.1 (4)	H39—C39—C38	119.366
C12—C7—C8	119.0 (4)	C40—C39—C38	121.3 (4)
C12—C7—P1	119.2 (3)	H40—C40—C41	120.771
C8—C7—P1	121.4 (3)	H40—C40—C39	120.770

H8—C8—C9	119.976	C41—C40—C39	118.5 (4)
H8—C8—C7	119.976	H41—C41—C42	119.433
C9—C8—C7	120.0 (4)	H41—C41—C40	119.433
H9—C9—C10	119.728	C42—C41—C40	121.1 (4)
H9—C9—C8	119.727	H42—C42—C41	119.752
C10—C9—C8	120.5 (4)	H42—C42—C37	119.752
H10—C10—C11	120.324	C41—C42—C37	120.5 (4)
H10—C10—C9	120.324	C48—C43—C44	117.9 (3)
C11—C10—C9	119.4 (4)	C48—C43—P3	121.8 (3)
H11—C11—C12	119.757	C44—C43—P3	120.1 (3)
H11—C11—C10	119.757	H44—C44—C45	119.480
C12—C11—C10	120.5 (4)	H44—C44—C43	119.479
H12—C12—C11	119.712	C45—C44—C43	121.0 (4)
H12—C12—C7	119.712	H45—C45—C46	119.991
C11—C12—C7	120.6 (4)	H45—C45—C44	119.991
C18—C13—C14	119.0 (4)	C46—C45—C44	120.0 (4)
C18—C13—P1	124.5 (3)	H46—C46—C47	120.138
C14—C13—P1	116.0 (3)	H46—C46—C45	120.138
H14—C14—C15	119.991	C47—C46—C45	119.7 (4)
H14—C14—C13	119.991	H47—C47—C48	119.636
C15—C14—C13	120.0 (4)	H47—C47—C46	119.637
H15—C15—C16	119.345	C48—C47—C46	120.7 (4)
H15—C15—C14	119.345	H48—C48—C47	119.733
C16—C15—C14	121.3 (4)	H48—C48—C43	119.733
H16—C16—C17	120.599	C47—C48—C43	120.5 (4)
H16—C16—C15	120.599	C54—C49—C50	118.9 (4)
C17—C16—C15	118.8 (4)	C54—C49—P3	121.3 (3)
H17—C17—C18	119.599	C50—C49—P3	119.6 (3)
H17—C17—C16	119.599	H50—C50—C51	121 (3)
C18—C17—C16	120.8 (4)	H50—C50—C49	118 (3)
H18—C18—C13	119.998	C51—C50—C49	120.2 (4)
H18—C18—C17	119.997	H51—C51—C52	119.539
C13—C18—C17	120.0 (4)	H51—C51—C50	119.539
C24—C19—C20	117.7 (4)	C52—C51—C50	120.9 (4)
C24—C19—P2	121.8 (3)	H52—C52—C53	120.460
C20—C19—P2	120.4 (3)	H52—C52—C51	120.460
H20—C20—C21	119.976	C53—C52—C51	119.1 (4)
H20—C20—C19	119.976	H53—C53—C54	119.943
C21—C20—C19	120.0 (4)	H53—C53—C52	119.944
H21—C21—C22	119.544	C54—C53—C52	120.1 (4)
H21—C21—C20	119.544	H54—C54—C49	119.615
C22—C21—C20	120.9 (4)	H54—C54—C53	119.615
H22—C22—C23	120.058	C49—C54—C53	120.8 (4)
H22—C22—C21	120.057	H62—C62—Cl61^{i}	109.069
C23—C22—C21	119.9 (4)	H62—C62—Cl61	109.070
H23—C23—C24	119.833	Cl61^{i}—C62—Cl61	111.1 (6)
H23—C23—C22	119.833	H62—C62—H62^{i}	109.463

C24—C23—C22	120.3 (4)	Cl61^{i}—C62—H62^{i}	109.070
H24—C24—C23	119.469	Cl61—C62—H62^{i}	109.069

Symmetry code: (i) $-x+2, y, -z+1/2$.