metal-organic compounds

Dichloridotripyridine(triphenylphosphine)ruthenium(II)

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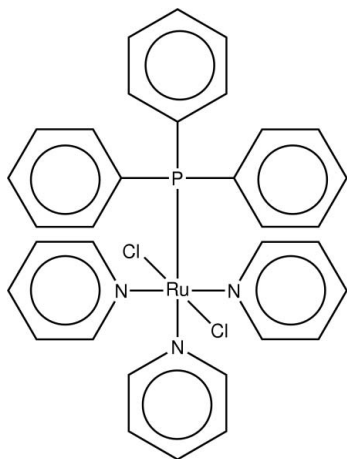Correspondence e-mail: rafal.kruszynski@p.lodz.pl

All interatomic distances and angles in the title compound, $[RuCl_2(C_5H_5N)_3(C_{18}H_{15}P)]$, are normal. The Ru atom is octahedrally and the P atom tetrahedrally coordinated. The structure is stabilized by several weak C—H···Cl intramolecular hydrogen bonds.

Related literature

For related literature, see: Wong & Lau (1994). See also: Allen (2002); Desiraju & Steiner (1999).

Experimental

Crystal data

$[RuCl_2(C_5H_5N)_3(C_{18}H_{15}P)]$	γ = 89.174 (1)°
M_r = 671.54	V = 1446.46 (3) Å^3
Triclinic, $P\bar{1}$	Z = 2
a = 8.5807 (1) Å	Mo $K\alpha$ radiation
b = 10.1447 (1) Å	μ = 0.81 mm^{-1}
c = 16.9834 (2) Å	T = 291.0 (3) K
α = 78.927 (1)°	0.37 × 0.37 × 0.37 mm
β = 85.539 (1)°	

Data collection

Kuma KM4 CCD diffractometer	14401 measured reflections
Absorption correction: numerical (*X-RED*; Stoe & Cie, 1999)	5119 independent reflections
T_{min} = 0.720, T_{max} = 0.740	4735 reflections with $I > 2\sigma(I)$
	R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019	361 parameters
$wR(F^2)$ = 0.052	H-atom parameters constrained
S = 1.07	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
5119 reflections	$\Delta\rho_{min}$ = −0.61 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2···Cl2	0.93	2.55	3.3456 (18)	144
C19—H19···Cl1	0.93	2.69	3.1771 (19)	113
C23—H23···Cl2	0.93	2.72	3.1681 (19)	110
C24—H24···Cl2	0.93	2.76	3.2128 (19)	111
C28—H28···Cl1	0.93	2.81	3.254 (2)	111
C29—H29···Cl2	0.93	2.57	3.257 (2)	131
C33—H33···Cl1	0.93	2.53	3.203 (2)	129

Data collection: *CrysAlis CCD* (Kuma, 2000); cell refinement: *CrysAlis RED* (Kuma, 2000); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL/PC* (Sheldrick, 1990b); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

References

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supplementary materials

Dichloridotripyridine(triphenylphosphine)ruthenium(II)

R. Kruszynski and J. G. Malecki

Comment

In the Cambridge Structural Database (Version 5.28 + 3 updates, 01–2007, 05–2007, 08–2007; Allen, 2002) can be found 213 ruthenium complexes containing pyridine (py) in inner coordination sphere (1 compound containing 6 py molecules, 30 compounds containing 5 py molecules, 14 compounds containing 3 py molecules, 55 compounds containing 2 py molecules and 113 compounds containing 1 py molecule), but title compound (I) is the first reported structure containing 3 py molecules and PPh$_3$ subsituent bonded to Ru cation. Additionally, (I) is the first known structure of compound having 3 py molecules and *trans* arranged halogen atoms.

All intramolecular distances and angles in (I) (Fig. 1) can be considered normal. All atoms lie in general positions. The planes of the phenyl rings of the triphenylphosphine substituent are inclined at 67.93 (6), 67.28 (6) and 59.54 (7)° respectively for pairs of rings indicated by C1/C7, C7/C13 and C1/C13 atoms. The close to planarity pyridine rings are inclined at 66.04 (5), 81.63 (7) and 45.23 (8)° respectively for pairs of rings containing N1/N2, N2/N3 and N1/N3 atoms. The Ru1 atom deviates by 0.098 (3), 0.092 (3) and 0.005 (3)Å from weighted lest squares planes of pyridine rings indicated respectively by N1, N2 and N3 atoms. In the structure can be found several intramolecular C—H···O short contacts (Table 1) which, according to Desiraju & Steiner (1999), can be classified as weak hydrogen bonds. In the structure can not be found any unusual intermolecular interactions.

Experimental

The complex was prepared by adding the pyridine salt of 8-hydroxy-2-methyl-quinoline-7-carbodithioic acid to the solution of [RuCl$_2$(PPh$_3$)$_3$] in methanol (100 ml). The reaction mixture was refluxed by 3 h. The crystals of (I) were obtained by slow evaporation of the methanol solution of the complex.

Usage of pyridine instead of its salt leads to [RuCl$_2$(pyridine)$_4$] (Wong and Lau, 1994), thus usage of salt is important.

Refinement

All hydrogen atoms were placed in calculated positions and were refined as riding on their parent atom with fixed U values [U_{iso}(H) = 1.2U_{eq}(C)].
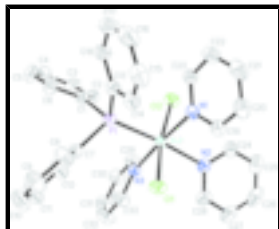
supplementary materials

Figures

Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity.

Dichloridotripyridine(triphenylphosphine)ruthenium(II)

Crystal data

$[RuCl_2(C_5H_5N)_3(C_{18}H_{15}P)]$	$Z = 2$
$M_r = 671.54$	$F_{000} = 684$
	$D_x = 1.542$ Mg m^{-3}
Triclinic, $P\bar{1}$	$D_m = 1.54$ Mg m^{-3}
	D_m measured by Berman density torsion balance
Hall symbol: -P 1	Mo $K\alpha$ radiation
	$\lambda = 0.71073$ Å
$a = 8.5807$ (1) Å	Cell parameters from 7117 reflections
$b = 10.1447$ (1) Å	$\theta = 3$–20º
$c = 16.9834$ (2) Å	$\mu = 0.81$ mm^{-1}
$\alpha = 78.927$ (1)º	$T = 291.0$ (3) K
$\beta = 85.539$ (1)º	Prism, yellow
$\gamma = 89.174$ (1)º	$0.37 \times 0.37 \times 0.37$ mm
$V = 1446.46$ (3) Å^3	

Data collection

Kuma KM4 CCD diffractometer	5119 independent reflections
Radiation source: fine-focus sealed tube	4735 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.019$
Detector resolution: 1048576 pixels mm^{-1}	$\theta_{max} = 25.1$º
$T = 291.0(3)$ K	$\theta_{min} = 2.1$º
ω scans	$h = -10 \rightarrow 10$
Absorption correction: numerical (X-RED; Stoe & Cie,1999)	$k = -9 \rightarrow 12$
$T_{min} = 0.720$, $T_{max} = 0.740$	$l = -20 \rightarrow 20$
14401 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.019$

$wR(F^2) = 0.052$

$S = 1.07$

5119 reflections

361 parameters

Primary atom site location: structure-invariant direct methods

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.028P)^2 + 0.5954P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.28$ e Å^{-3}

$\Delta\rho_{min} = -0.61$ e Å^{-3}

Extinction correction: none

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 > 2sigma(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 (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
Ru1	0.616943 (15)	0.517519 (12)	0.720182 (8)	0.02183 (5)
Cl1	0.78369 (5)	0.48535 (5)	0.82957 (3)	0.03334 (10)
Cl2	0.44394 (5)	0.58568 (4)	0.61271 (3)	0.03378 (10)
P1	0.50574 (5)	0.31054 (4)	0.77488 (3)	0.02394 (10)
C1	0.4244 (2)	0.20909 (17)	0.70880 (11)	0.0278 (4)
C2	0.4343 (2)	0.25245 (18)	0.62632 (11)	0.0317 (4)
H2	0.4719	0.3382	0.6044	0.038*
C3	0.3892 (2)	0.1701 (2)	0.57575 (12)	0.0374 (4)
H3	0.3985	0.2000	0.5203	0.045*
C4	0.3307 (2)	0.0442 (2)	0.60780 (13)	0.0412 (5)
H4	0.2993	−0.0109	0.5741	0.049*
C5	0.3188 (3)	−0.0001 (2)	0.68980 (13)	0.0427 (5)
H5	0.2783	−0.0851	0.7115	0.051*
C6	0.3664 (2)	0.08047 (18)	0.73990 (12)	0.0373 (4)
H6	0.3597	0.0488	0.7952	0.045*
C7	0.6369 (2)	0.17868 (17)	0.82475 (11)	0.0289 (4)
C8	0.6343 (3)	0.1353 (2)	0.90699 (12)	0.0426 (5)
H8	0.5659	0.1751	0.9406	0.051*
C9	0.7321 (3)	0.0333 (2)	0.94012 (14)	0.0535 (6)
H9	0.7277	0.0046	0.9957	0.064*
C10	0.8345 (3)	−0.0252 (2)	0.89218 (16)	0.0571 (6)
H10	0.9018	−0.0921	0.9147	0.069*
C11	0.8376 (3)	0.0153 (3)	0.81022 (16)	0.0623 (7)
H11	0.9063	−0.0251	0.7770	0.075*

C12	0.7388 (3)	0.1161 (2)	0.77697 (13)	0.0469 (5)
H12	0.7411	0.1421	0.7213	0.056*
C13	0.3515 (2)	0.31553 (17)	0.85465 (10)	0.0288 (4)
C14	0.3886 (2)	0.37404 (18)	0.91916 (11)	0.0351 (4)
H14	0.4906	0.4016	0.9218	0.042*
C15	0.2764 (3)	0.3912 (2)	0.97845 (12)	0.0457 (5)
H15	0.3030	0.4286	1.0215	0.055*
C16	0.1246 (3)	0.3530 (2)	0.97428 (14)	0.0539 (6)
H16	0.0482	0.3667	1.0138	0.065*
C17	0.0857 (3)	0.2945 (2)	0.91187 (15)	0.0507 (6)
H17	−0.0166	0.2671	0.9099	0.061*
C18	0.1980 (2)	0.2761 (2)	0.85205 (12)	0.0380 (4)
H18	0.1705	0.2370	0.8098	0.046*
N1	0.46188 (17)	0.62309 (14)	0.78690 (9)	0.0270 (3)
C19	0.5158 (2)	0.70417 (18)	0.83268 (11)	0.0326 (4)
H19	0.6233	0.7149	0.8323	0.039*
C20	0.4199 (3)	0.7718 (2)	0.87986 (12)	0.0425 (5)
H20	0.4622	0.8272	0.9104	0.051*
C21	0.2598 (3)	0.7566 (2)	0.88150 (13)	0.0477 (5)
H21	0.1926	0.7992	0.9143	0.057*
C22	0.2026 (2)	0.6768 (2)	0.83332 (12)	0.0401 (5)
H22	0.0954	0.6661	0.8321	0.048*
C23	0.3050 (2)	0.61331 (18)	0.78716 (11)	0.0312 (4)
H23	0.2646	0.5608	0.7543	0.037*
N2	0.73976 (17)	0.70292 (14)	0.67324 (9)	0.0283 (3)
C24	0.6679 (2)	0.81775 (18)	0.64484 (11)	0.0359 (4)
H24	0.5593	0.8190	0.6471	0.043*
C25	0.7482 (3)	0.9347 (2)	0.61224 (13)	0.0479 (5)
H25	0.6943	1.0132	0.5934	0.057*
C26	0.9085 (3)	0.9341 (2)	0.60793 (14)	0.0535 (6)
H26	0.9651	1.0116	0.5856	0.064*
C27	0.9833 (3)	0.8172 (2)	0.63714 (14)	0.0477 (5)
H27	1.0919	0.8140	0.6349	0.057*
C28	0.8966 (2)	0.7047 (2)	0.66977 (12)	0.0364 (4)
H28	0.9487	0.6261	0.6904	0.044*
N3	0.78249 (16)	0.42674 (13)	0.64618 (8)	0.0252 (3)
C29	0.7641 (2)	0.4297 (2)	0.56892 (11)	0.0345 (4)
H29	0.6772	0.4737	0.5469	0.041*
C30	0.8668 (2)	0.3711 (2)	0.51992 (13)	0.0441 (5)
H30	0.8473	0.3731	0.4666	0.053*
C31	0.9988 (3)	0.3094 (2)	0.55034 (13)	0.0462 (5)
H31	1.0703	0.2691	0.5184	0.055*
C32	1.0214 (3)	0.3092 (2)	0.62922 (14)	0.0490 (5)
H32	1.1105	0.2700	0.6515	0.059*
C33	0.9122 (2)	0.3669 (2)	0.67520 (13)	0.0420 (5)
H33	0.9286	0.3644	0.7289	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.02144 (8)	0.02457 (8)	0.02026 (8)	0.00073 (5)	−0.00374 (5)	−0.00545 (5)
Cl1	0.0321 (2)	0.0429 (2)	0.0281 (2)	0.00523 (19)	−0.01118 (18)	−0.01125 (18)
Cl2	0.0348 (2)	0.0379 (2)	0.0301 (2)	0.00577 (18)	−0.01235 (19)	−0.00677 (18)
P1	0.0261 (2)	0.0258 (2)	0.0202 (2)	−0.00026 (17)	−0.00340 (17)	−0.00459 (16)
C1	0.0280 (9)	0.0282 (9)	0.0281 (9)	−0.0015 (7)	−0.0052 (7)	−0.0064 (7)
C2	0.0344 (10)	0.0316 (9)	0.0287 (10)	−0.0058 (8)	−0.0021 (8)	−0.0042 (7)
C3	0.0419 (11)	0.0454 (11)	0.0265 (10)	−0.0058 (9)	−0.0037 (8)	−0.0095 (8)
C4	0.0449 (12)	0.0423 (11)	0.0414 (12)	−0.0088 (9)	−0.0085 (9)	−0.0180 (9)
C5	0.0531 (13)	0.0302 (10)	0.0451 (12)	−0.0126 (9)	−0.0085 (10)	−0.0054 (8)
C6	0.0488 (12)	0.0318 (10)	0.0304 (10)	−0.0068 (8)	−0.0080 (9)	−0.0012 (8)
C7	0.0309 (9)	0.0259 (9)	0.0305 (9)	0.0001 (7)	−0.0073 (7)	−0.0051 (7)
C8	0.0480 (12)	0.0472 (12)	0.0313 (11)	0.0115 (10)	−0.0067 (9)	−0.0039 (9)
C9	0.0639 (15)	0.0539 (13)	0.0392 (13)	0.0129 (12)	−0.0143 (11)	0.0035 (10)
C10	0.0589 (15)	0.0454 (13)	0.0642 (16)	0.0213 (11)	−0.0177 (12)	0.0004 (11)
C11	0.0671 (16)	0.0594 (15)	0.0599 (16)	0.0329 (13)	−0.0034 (13)	−0.0131 (12)
C12	0.0564 (13)	0.0479 (12)	0.0354 (11)	0.0176 (10)	−0.0030 (10)	−0.0071 (9)
C13	0.0311 (9)	0.0290 (9)	0.0234 (9)	0.0040 (7)	0.0006 (7)	0.0009 (7)
C14	0.0438 (11)	0.0333 (10)	0.0269 (10)	0.0037 (8)	−0.0010 (8)	−0.0033 (7)
C15	0.0650 (15)	0.0422 (11)	0.0264 (10)	0.0116 (10)	0.0066 (10)	−0.0028 (8)
C16	0.0561 (14)	0.0520 (13)	0.0424 (13)	0.0174 (11)	0.0208 (11)	0.0076 (10)
C17	0.0323 (11)	0.0548 (13)	0.0547 (14)	0.0050 (10)	0.0076 (10)	0.0101 (11)
C18	0.0322 (10)	0.0407 (11)	0.0380 (11)	0.0022 (8)	−0.0028 (8)	0.0001 (8)
N1	0.0302 (8)	0.0258 (7)	0.0245 (7)	0.0019 (6)	−0.0021 (6)	−0.0037 (6)
C19	0.0369 (10)	0.0318 (9)	0.0294 (10)	0.0015 (8)	−0.0035 (8)	−0.0062 (7)
C20	0.0576 (13)	0.0388 (11)	0.0329 (11)	0.0056 (9)	−0.0019 (9)	−0.0127 (8)
C21	0.0517 (13)	0.0481 (12)	0.0414 (12)	0.0135 (10)	0.0112 (10)	−0.0104 (10)
C22	0.0327 (10)	0.0430 (11)	0.0396 (11)	0.0058 (8)	0.0049 (9)	0.0012 (9)
C23	0.0299 (9)	0.0293 (9)	0.0323 (10)	0.0017 (7)	−0.0023 (8)	−0.0007 (7)
N2	0.0303 (8)	0.0310 (8)	0.0249 (8)	−0.0040 (6)	0.0002 (6)	−0.0087 (6)
C24	0.0439 (11)	0.0320 (10)	0.0331 (10)	−0.0004 (8)	−0.0043 (8)	−0.0087 (8)
C25	0.0719 (16)	0.0304 (10)	0.0417 (12)	−0.0037 (10)	−0.0066 (11)	−0.0068 (9)
C26	0.0670 (16)	0.0441 (13)	0.0489 (13)	−0.0274 (11)	0.0072 (11)	−0.0104 (10)
C27	0.0430 (12)	0.0523 (13)	0.0506 (13)	−0.0184 (10)	0.0042 (10)	−0.0186 (10)
C28	0.0339 (10)	0.0405 (10)	0.0372 (11)	−0.0057 (8)	−0.0007 (8)	−0.0138 (8)
N3	0.0240 (7)	0.0259 (7)	0.0262 (8)	−0.0011 (6)	−0.0034 (6)	−0.0055 (6)
C29	0.0296 (9)	0.0437 (11)	0.0305 (10)	0.0011 (8)	−0.0028 (8)	−0.0075 (8)
C30	0.0421 (12)	0.0614 (13)	0.0307 (11)	0.0039 (10)	−0.0018 (9)	−0.0144 (10)
C31	0.0420 (12)	0.0554 (13)	0.0435 (13)	0.0097 (10)	0.0042 (10)	−0.0192 (10)
C32	0.0413 (12)	0.0644 (14)	0.0443 (13)	0.0227 (11)	−0.0097 (10)	−0.0174 (11)
C33	0.0396 (11)	0.0546 (12)	0.0347 (11)	0.0144 (9)	−0.0094 (9)	−0.0144 (9)

Geometric parameters (Å, °)

Ru1—N1	2.0956 (14)	C16—H16	0.9300
Ru1—N3	2.1389 (14)	C17—C18	1.382 (3)

Ru1—N2	2.1527 (14)	C17—H17	0.9300
Ru1—P1	2.3137 (4)	C18—H18	0.9300
Ru1—Cl1	2.4026 (4)	N1—C19	1.345 (2)
Ru1—Cl2	2.4331 (4)	N1—C23	1.350 (2)
P1—C13	1.8260 (18)	C19—C20	1.372 (3)
P1—C1	1.8419 (17)	C19—H19	0.9300
P1—C7	1.8557 (18)	C20—C21	1.382 (3)
C1—C2	1.381 (3)	C20—H20	0.9300
C1—C6	1.394 (3)	C21—C22	1.377 (3)
C2—C3	1.387 (3)	C21—H21	0.9300
C2—H2	0.9300	C22—C23	1.368 (3)
C3—C4	1.374 (3)	C22—H22	0.9300
C3—H3	0.9300	C23—H23	0.9300
C4—C5	1.375 (3)	N2—C24	1.334 (2)
C4—H4	0.9300	N2—C28	1.343 (2)
C5—C6	1.375 (3)	C24—C25	1.379 (3)
C5—H5	0.9300	C24—H24	0.9300
C6—H6	0.9300	C25—C26	1.372 (3)
C7—C12	1.377 (3)	C25—H25	0.9300
C7—C8	1.380 (3)	C26—C27	1.366 (3)
C8—C9	1.384 (3)	C26—H26	0.9300
C8—H8	0.9300	C27—C28	1.372 (3)
C9—C10	1.358 (3)	C27—H27	0.9300
C9—H9	0.9300	C28—H28	0.9300
C10—C11	1.372 (4)	N3—C29	1.328 (2)
C10—H10	0.9300	N3—C33	1.342 (2)
C11—C12	1.382 (3)	C29—C30	1.373 (3)
C11—H11	0.9300	C29—H29	0.9300
C12—H12	0.9300	C30—C31	1.373 (3)
C13—C18	1.389 (3)	C30—H30	0.9300
C13—C14	1.401 (3)	C31—C32	1.368 (3)
C14—C15	1.372 (3)	C31—H31	0.9300
C14—H14	0.9300	C32—C33	1.370 (3)
C15—C16	1.375 (3)	C32—H32	0.9300
C15—H15	0.9300	C33—H33	0.9300
C16—C17	1.375 (4)		
N1—Ru1—N3	174.89 (5)	C16—C15—H15	120.0
N1—Ru1—N2	88.61 (5)	C17—C16—C15	120.1 (2)
N3—Ru1—N2	86.42 (5)	C17—C16—H16	119.9
N1—Ru1—P1	94.11 (4)	C15—C16—H16	119.9
N3—Ru1—P1	90.94 (4)	C16—C17—C18	120.3 (2)
N2—Ru1—P1	174.89 (4)	C16—C17—H17	119.8
N1—Ru1—Cl1	88.58 (4)	C18—C17—H17	119.8
N3—Ru1—Cl1	92.37 (4)	C17—C18—C13	120.4 (2)
N2—Ru1—Cl1	87.44 (4)	C17—C18—H18	119.8
P1—Ru1—Cl1	88.298 (16)	C13—C18—H18	119.8
N1—Ru1—Cl2	85.00 (4)	C19—N1—C23	116.58 (15)
N3—Ru1—Cl2	93.51 (4)	C19—N1—Ru1	120.66 (12)
N2—Ru1—Cl2	86.29 (4)	C23—N1—Ru1	122.75 (12)

P1—Ru1—Cl2	98.252 (16)	N1—C19—C20	123.20 (18)
Cl1—Ru1—Cl2	171.122 (16)	N1—C19—H19	118.4
C13—P1—C1	104.93 (8)	C20—C19—H19	118.4
C13—P1—C7	101.78 (8)	C19—C20—C21	119.29 (19)
C1—P1—C7	96.49 (8)	C19—C20—H20	120.4
C13—P1—Ru1	114.03 (6)	C21—C20—H20	120.4
C1—P1—Ru1	119.86 (6)	C22—C21—C20	118.23 (19)
C7—P1—Ru1	116.92 (6)	C22—C21—H21	120.9
C2—C1—C6	118.14 (16)	C20—C21—H21	120.9
C2—C1—P1	120.84 (13)	C23—C22—C21	119.32 (19)
C6—C1—P1	120.67 (14)	C23—C22—H22	120.3
C1—C2—C3	121.03 (17)	C21—C22—H22	120.3
C1—C2—H2	119.5	N1—C23—C22	123.31 (18)
C3—C2—H2	119.5	N1—C23—H23	118.3
C4—C3—C2	119.82 (18)	C22—C23—H23	118.3
C4—C3—H3	120.1	C24—N2—C28	117.26 (16)
C2—C3—H3	120.1	C24—N2—Ru1	123.23 (13)
C3—C4—C5	119.91 (17)	C28—N2—Ru1	119.49 (12)
C3—C4—H4	120.0	N2—C24—C25	122.68 (19)
C5—C4—H4	120.0	N2—C24—H24	118.7
C6—C5—C4	120.30 (18)	C25—C24—H24	118.7
C6—C5—H5	119.8	C26—C25—C24	119.3 (2)
C4—C5—H5	119.8	C26—C25—H25	120.4
C5—C6—C1	120.78 (18)	C24—C25—H25	120.4
C5—C6—H6	119.6	C27—C26—C25	118.5 (2)
C1—C6—H6	119.6	C27—C26—H26	120.7
C12—C7—C8	117.71 (17)	C25—C26—H26	120.7
C12—C7—P1	118.27 (14)	C26—C27—C28	119.4 (2)
C8—C7—P1	123.96 (15)	C26—C27—H27	120.3
C7—C8—C9	121.0 (2)	C28—C27—H27	120.3
C7—C8—H8	119.5	N2—C28—C27	122.9 (2)
C9—C8—H8	119.5	N2—C28—H28	118.6
C10—C9—C8	120.5 (2)	C27—C28—H28	118.6
C10—C9—H9	119.7	C29—N3—C33	116.77 (16)
C8—C9—H9	119.7	C29—N3—Ru1	121.74 (12)
C9—C10—C11	119.4 (2)	C33—N3—Ru1	121.47 (12)
C9—C10—H10	120.3	N3—C29—C30	123.32 (18)
C11—C10—H10	120.3	N3—C29—H29	118.3
C10—C11—C12	120.1 (2)	C30—C29—H29	118.3
C10—C11—H11	119.9	C29—C30—C31	119.41 (19)
C12—C11—H11	119.9	C29—C30—H30	120.3
C7—C12—C11	121.2 (2)	C31—C30—H30	120.3
C7—C12—H12	119.4	C32—C31—C30	117.79 (19)
C11—C12—H12	119.4	C32—C31—H31	121.1
C18—C13—C14	118.24 (18)	C30—C31—H31	121.1
C18—C13—P1	124.34 (14)	C31—C32—C33	119.72 (19)
C14—C13—P1	117.18 (14)	C31—C32—H32	120.1
C15—C14—C13	120.9 (2)	C33—C32—H32	120.1
C15—C14—H14	119.6	N3—C33—C32	122.95 (19)

C13—C14—H14	119.6	N3—C33—H33	118.5
C14—C15—C16	120.0 (2)	C32—C33—H33	118.5
C14—C15—H15	120.0		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Cl2	0.93	2.55	3.3456 (18)	144
C19—H19···Cl1	0.93	2.69	3.1771 (19)	113
C23—H23···Cl2	0.93	2.72	3.1681 (19)	110
C24—H24···Cl2	0.93	2.76	3.2128 (19)	111
C28—H28···Cl1	0.93	2.81	3.254 (2)	111
C29—H29···Cl2	0.93	2.57	3.257 (2)	131
C33—H33···Cl1	0.93	2.53	3.203 (2)	129

Fig. 1