CRYSTAL DATA for $\{Ru(CN^tBu)_2[(PPh_2)_2C(CN)]_2\}, 2\ CH_2Cl_2$

Fw =	1254.00
a (Å) =	12.011(3)
b (Å) =	23.027(6)
c (Å) =	12.60(1)
β (°) =	116.93(5)
V (Å^3) =	3107(5)
Z =	2
Space group	C 2/m
Systematic absences	none
Crystal shape	parallelepiped
Crystal colour	orange
Linear absorption coefficient μ (cm^{-1})	5.62
Density ρ(g cm^3)	1.34
Diffractometer	CAD4 - Enraf-Nonius
Radiation	MoKα (λ = 0.71069 Å)
Scan type	ω /2θ
Scan range (°)	0.8 + 0.345 tgθ
θ Limits (°)	1 - 25
Temperature of measurement	Room temperature
Octants collected	-14,12; 0,27; 0,14
Nb of data collected	2948
Nb of unique data collected	2815
Nb of unique data used for refinement	2049 $(Fo)^2 > 3\sigma(Fo)^2$
R (int)	.030
Decay of standards reflections %	69%
$R = \Sigma\|\|Fo\| - \|Fc\|\| / \Sigma\|Fo\|$	0.044
$Rw = [\Sigma w(\|Fo\| - \|Fc\|)^2 / \Sigma wFo^2]^{1/2}$	0.049
Absorption correction	DIFABS (min = 0. 93 , max = 1.10)
Exctinction parameter (x 10^{-6})	116
Nb of variables	350
Δρmin (e/ Å^3)	-0.39
Δρmax (e/ Å^3)	0.39

Crystal data : A selected crystal mounted in a glass capillary tube, with inert oil,was set up on an automatic diffractometer. Unit cell dimensions with estimated standard deviations were obtained from least-squares refinements of the setting angles of 25 well centered reflections. Two standard reflections were monitored periodically, their intensities showed a regular decay of 69% over the period of the experiment; a correction was applied. Crystallographic data and other pertinent informations are summarized in Table I. Corrections were made for Lorentz and polarization effects. Empirical absorption correction (Difabs)[1] and a secondary extinction correction were applied.

Computations were performed by using CRYSTALS[2] adapted on a MicroVax II. Atomic form factors for neutral Ru, P, N, Cl, C and H were taken from ref.3., anomalous dispersion was taken in account.The symmetry is monoclinic, with a C lattice and without systematic extinctions, the unit cell contains two formula units. Interpretation of the Patterson function shows that the ruthenium atom lies in special position, this atom being introduced in the position (0,0,0), attemps to solve the structure in the C2 or Cm group failed. So, we supposed that the group was C 2/m with a disorder. The octaedric complex lies on an inversion center, but it can occupy two possible orientations symmetrically related through a binary axis; so, refinements were carried out in the C 2/m group with occupancy factors of 0.5 for all atoms (except ruthenium on the inversion center, which has an occupancy factor of 0.25). In the first stage of the refinements phenyl rings were introduced as rigid groups with an overall thermal parameter, then , when all other atoms had been located they were individually refined. Hydrogen atoms were not introduced in the calculations. All atoms were anisotropically refined. The unit cell also contains 8 CH_2Cl_2 molecules with an occupancy factor of 0.5, so there are two solvent molecules for one complex molecule.

Full matrix least-squares refinements were carried out by minimizing the function $\Sigma w(|F_o|-|F_c|)^2$, where F_o and F_c are the observed and calculated structure factors. Models reached convergence with $R=\Sigma(||F_o|-|F_c||)/\Sigma|F_o|$ and $R_w= [\Sigma w(|F_o|-|F_c|)^2/\Sigma w(F_o)^2]^{1/2}$ having values listed in Table I. The weighting scheme was unity. Criteria for a satisfactory complete analysis were the ratios of rms shift to standard deviation being less than 0.1 and no significant features in final difference map (the residual maxima and minima in the last difference map were 0.39 and -0.39 eÅ-3).

Atomic coordinates are given in Table II.

Table III. contains interatomic distances and bond angles.

The view of the molecule is done using Cameron.[4] Ellipsoids represent 30% of probability.

Supplementary Material available: table of anisotropic thermal parameters, list of observed and calculated structure factors.

References

1 N.Walker and D. Stuart, *Acta Crystallogr.*, **39** (1983) 158.

2 D.J. Watkin, J. R. Carruthers and P.W. Betteridge, *CRYSTALS*, An Advanced Crystallographic Program System ; Chemical Crystallography Laboratory, University of Oxford : Oxford, England, 1988.

3 *International Tables for X-ray Crystallography* ; Vol. IV, Kynoch Press, Birmingham, England, 1974

4 L.J.Pearce and D.J.Watkin. Chemical Crystallography Laboratory. Oxford.

Table II: Fractional atomic coordinates.

Atom	x/a	y/b	z/c	U(eqv)
Ru(1)	0.0000	0.0000	0.0000	0.0318
P(1)	0.0664(2)	-0.003(4)	-0.1516(2)	0.0437
P(2)	0.1120(2)	0.0847(1)	-0.0012(2)	0.0408
C(1)	0.147(1)	0.0591(6)	-0.115(1)	0.0367
C(2)	0.226(1)	0.0814(6)	-0.158(1)	0.0514
N(1)	0.2940(9)	0.1005(5)	-0.1904(9)	0.0708
C(3)	-0.1543(8)	0.0382(4)	-0.1183(7)	0.0382
N(2)	-0.2423(7)	0.0615(3)	-0.1896(7)	0.0467
C(4)	-0.3448(9)	0.0919(5)	-0.2863(9)	0.0544
C(5)	-0.409(1)	0.0484(5)	-0.390(1)	0.0698
C(6)	-0.446(4)	0.107(2)	-0.244(5)	0.0901
C(7)	-0.287(2)	0.1417(7)	-0.323(1)	0.0948
C(10)	0.172(1)	-0.0645(7)	-0.152(1)	0.0349
C(11)	0.128(1)	-0.1121(5)	-0.230(1)	0.0633
C(12)	0.214(1)	-0.1567(6)	-0.220(1)	0.0800
C(13)	0.337(1)	-0.1539(7)	-0.139(1)	0.0780
C(14)	0.379(1)	-0.1058(7)	-0.065(1)	0.0811
C(15)	0.298(1)	-0.0611(6)	-0.072(1)	0.0668
C(20)	-0.0521(7)	0.0079(8)	-0.3069(7)	0.0381
C(21)	-0.047(1)	-0.0369(6)	-0.3832(9)	0.0651
C(22)	-0.137(1)	-0.0337(8)	-0.508(1)	0.0841
C(23)	-0.222(1)	0.012(1)	-0.548(1)	0.0685
C(24)	-0.228(1)	0.0513(6)	-0.470(1)	0.0736
C(25)	-0.1436(9)	0.0491(5)	-0.3470(9)	0.0603
C(30)	0.2581(9)	0.1084(4)	0.1274(8)	0.0451
C(31)	0.365(1)	0.0755(6)	0.157(1)	0.0677
C(32)	0.472(3)	0.092(2)	0.249(4)	0.0840
C(33)	0.483(1)	0.1387(7)	0.318(1)	0.0706
C(34)	0.376(2)	0.1707(8)	0.293(2)	0.1071
C(35)	0.263(1)	0.1568(6)	0.195(1)	0.0742
C(40)	0.030(2)	0.1538(8)	-0.048(1)	0.0455
C(41)	0.046(1)	0.1909(5)	-0.121(1)	0.0672
C(42)	-0.018(1)	0.2461(6)	-0.146(1)	0.0831
C(43)	-0.095(1)	0.2614(6)	-0.094(1)	0.0853
C(44)	-0.110(1)	0.2236(6)	-0.018(1)	0.0849
C(45)	-0.047(2)	0.1674(8)	0.007(1)	0.0500
Cl(1)	0.9916(6)	0.2054(3)	0.4428(5)	0.1564
Cl(2)	0.8123(7)	0.2161(3)	0.5288(7)	0.1865
C(50)	0.844(2)	0.187(1)	0.419(2)	0.1362

Table III: Interatomic distances (A) and bond angles (deg.)

Ru(1) - P(1)	2.379(3)	Ru(1) - P(2)	2.374(2)
Ru(1) - C(3)	1.983(9)	P(1) - C(1)	1.68(7)
P(1) - C(10)	1.90(7)	P(1) - C(20)	1.85(1)
P(2) - C(1)	1.77(1)	P(2) - C(30)	1.852(9)
P(2) - C(40)	1.82(2)	C(1) - C(2)	1.38(1)
C(2) - N(1)	1.16(2)	C(3) - N(2)	1.16(1)
N(2) - C(4)	1.46(1)	C(4) - C(5)	1.54(1)
C(4) - C(6)	1.56(4)	C(4) - C(7)	1.52(2)
C(10) - C(11)	1.41(2)	C(10) - C(15)	1.39(2)
C(11) - C(12)	1.42(2)	C(12) - C(13)	1.37(2)
C(13) - C(14)	1.39(2)	C(14) - C(15)	1.39(2)
C(20) - C(21)	1.43(2)	C(20) - C(25)	1.36(2)
C(21) - C(22)	1.45(2)	C(22) - C(23)	1.39(3)
C(23) - C(24)	1.36(3)	C(24) - C(25)	1.42(2)
C(30) - C(31)	1.39(1)	C(30) - C(35)	1.39(1)
C(31) - C(32)	1.34(5)	C(32) - C(33)	1.36(6)
C(33) - C(34)	1.39(2)	C(34) - C(35)	1.40(2)
C(40) - C(41)	1.33(2)	C(40) - C(45)	1.42(2)
C(41) - C(42)	1.45(2)	C(42) - C(43)	1.40(2)
C(43) - C(44)	1.37(2)	C(44) - C(45)	1.46(2)
Cl(1) - C(50)	1.71(2)	Cl(2) - C(50)	1.74(2)

P(1) - Ru(1) - P(1)'	180.00	P(1) - Ru(1) - P(2)	68.0(19)
P(1) - Ru(1) - P(2)'	112.0(19)	P(2) - Ru(1) - P(2)	180.00
P(1) - Ru(1) - C(3)	87.1(9)	P(1) - Ru(1) - C(3)'	92.9(9)
P(2) - Ru(1) - C(3)	88.3(2)	P(2) - Ru(1) - C(3)'	91.7(2)
C(3) - Ru(1) - C(3)'	180.0	Ru(1) - P(1) - C(1)	96.4(22)
Ru(1) - P(1) - C(10)	119.8(27)	C(1) - P(1) - C(10)	109.3(6)
Ru(1) - P(1) - C(20)	118.0(7)	C(1) - P(1) - C(20)	104.2(36)
C(10) - P(1) - C(20)	107.2(23)	Ru(1) - P(2) - C(1)	94.3(4)
Ru(1) - P(2) - C(30)	123.4(3)	C(1) - P(2) - C(30)	109.1(5)
Ru(1) - P(2) - C(40)	119.6(6)	C(1) - P(2) - C(40)	108.8(6)
C(30) - P(2) - C(40)	100.7(5)	P(1) - C(1) - P(2)	100.9(9)
P(1) - C(1) - C(2)	128.3(12)	P(2) - C(1) - C(2)	130.7(10)
C(1) - C(2) - N(1)	177.5(14)	Ru(1) - C(3) - N(2)	177.5(7)
C(3) - N(2) - C(4)	173.7(9)	N(2) - C(4) - C(5)	107.6(8)
N(2) - C(4) - C(6)	108.4(21)	C(5) - C(4) - C(6)	105.4(18)
N(2) - C(4) - C(7)	106.7(10)	C(5) - C(4) - C(7)	110.9(12)
C(6) - C(4) - C(7)	117.5(23)	P(1) - C(10) - C(11)	122.6(15)
P(1) - C(10) - C(15)	117.7(16)	C(11) - C(10) - C(15)	119.7(14)
C(10) - C(11) - C(12)	118.1(13)	C(11) - C(12) - C(13)	122.0(13)
C(12) - C(13) - C(14)	118.8(12)	C(13) - C(14) - C(15)	120.9(12)
C(10) - C(15) - C(14)	120.4(14)	P(1) - C(20) - C(21)	111.4(24)
P(1) - C(20) - C(25)	126.6(22)	C(21) - C(20) - C(25)	121.6(9)
C(20) - C(21) - C(22)	117.0(12)	C(21) - C(22) - C(23)	119.8(14)
C(22) - C(23) - C(24)	120.8(11)	C(23) - C(24) - C(25)	121.1(13)
C(20) - C(25) - C(24)	119.1(12)	P(2) - C(30) - C(31)	117.9(8)
P(2) - C(30) - C(35)	122.3(8)	C(31) - C(30) - C(35)	119.8(10)
C(30) - C(31) - C(32)	119.3(22)	C(31) - C(32) - C(33)	123.4(28)
C(32) - C(33) - C(34)	118.0(18)	C(33) - C(34) - C(35)	120.4(16)
C(30) - C(35) - C(34)	118.9(14)	P(2) - C(40) - C(41)	123.9(14)
P(2) - C(40) - C(45)	114.3(15)	C(41) - C(40) - C(45)	121.6(19)
C(40) - C(41) - C(42)	119.1(14)	C(41) - C(42) - C(43)	121.3(13)
C(42) - C(43) - C(44)	119.6(13)	C(43) - C(44) - C(45)	119.3(14)
C(40) - C(45) - C(44)	119.0(16)	Cl(1) - C(50) - Cl(2)	110.1(10)

Symmetry code : ' -x, -y, -z

Anisotropic thermal parameters.

Atom	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Ru(1)	0.0320(4)	0.0310(5)	0.0315(4)	0.0000	0.0136(3)	0.0000
P(1)	0.037(1)	0.06(2)	0.037(1)	0.001(3)	0.0172(8)	-0.011(7)
P(2)	0.043(1)	0.040(1)	0.040(1)	0.000(1)	0.018(1)	-0.004(1)
C(1)	0.037(6)	0.049(6)	0.040(7)	0.001(5)	0.026(5)	-0.004(5)
C(2)	0.057(9)	0.062(8)	0.058(8)	0.003(6)	0.038(8)	-0.012(7)
N(1)	0.071(6)	0.094(8)	0.079(7)	-0.008(6)	0.047(6)	-0.026(6)
C(3)	0.043(5)	0.039(5)	0.041(5)	-0.006(4)	0.024(4)	-0.009(4)
N(2)	0.038(4)	0.055(5)	0.046(4)	0.006(4)	0.015(4)	0.009(4)
C(4)	0.059(6)	0.052(7)	0.056(6)	0.004(5)	0.017(5)	0.024(5)
C(5)	0.062(7)	0.088(9)	0.054(6)	-0.014(6)	0.006(5)	0.009(6)
C(6)	0.16(3)	0.23(5)	0.09(2)	0.04(3)	0.06(3)	0.16(3)
C(7)	0.13(1)	0.08(1)	0.10(1)	0.05(1)	-0.02(1)	-0.03(1)
C(10)	0.049(8)	0.07(1)	0.041(7)	0.006(7)	0.039(6)	0.005(7)
C(11)	0.083(8)	0.048(6)	0.074(7)	-0.003(6)	0.042(7)	0.011(6)
C(12)	0.09(1)	0.069(9)	0.10(1)	0.003(8)	0.054(8)	0.025(8)
C(13)	0.089(9)	0.10(1)	0.073(8)	0.007(8)	0.044(7)	0.034(8)
C(14)	0.068(8)	0.13(1)	0.081(9)	0.006(9)	0.041(7)	0.031(8)
C(15)	0.044(6)	0.10(1)	0.066(7)	-0.005(7)	0.022(6)	0.012(6)
C(20)	0.038(3)	0.04(1)	0.038(4)	0.003(4)	0.016(3)	-0.006(4)
C(21)	0.060(6)	0.107(9)	0.048(6)	-0.017(6)	0.025(5)	-0.018(6)
C(22)	0.072(8)	0.14(1)	0.056(7)	-0.017(8)	0.023(7)	-0.019(9)
C(23)	0.065(7)	0.10(3)	0.052(6)	0.009(9)	0.019(5)	-0.03(1)
C(24)	0.058(7)	0.10(1)	0.080(9)	0.042(8)	0.004(7)	-0.012(7)
C(25)	0.052(6)	0.064(7)	0.059(6)	0.012(5)	0.011(5)	-0.007(5)
C(30)	0.049(5)	0.049(6)	0.039(5)	0.005(4)	0.014(4)	-0.015(5)
C(31)	0.054(6)	0.078(8)	0.064(7)	0.008(6)	0.015(5)	-0.004(6)
C(32)	0.07(1)	0.11(2)	0.07(1)	0.01(1)	0.024(9)	-0.01(1)
C(33)	0.078(8)	0.079(9)	0.054(7)	0.002(7)	0.009(7)	-0.029(8)
C(34)	0.13(2)	0.10(1)	0.10(1)	-0.02(1)	0.02(1)	-0.04(1)
C(35)	0.091(9)	0.073(9)	0.061(7)	-0.027(6)	0.012(6)	-0.016(7)
C(40)	0.071(8)	0.049(9)	0.026(8)	-0.011(6)	0.010(7)	-0.015(6)
C(41)	0.072(7)	0.048(7)	0.082(8)	0.009(6)	0.020(6)	-0.013(6)
C(42)	0.11(1)	0.049(8)	0.10(1)	0.019(8)	0.015(9)	-0.017(8)
C(43)	0.09(1)	0.061(9)	0.11(1)	-0.016(8)	0.017(8)	0.009(7)
C(44)	0.081(9)	0.08(1)	0.089(9)	-0.004(8)	0.025(7)	0.015(8)
C(45)	0.07(1)	0.05(1)	0.036(8)	0.005(7)	0.020(9)	-0.003(7)
Cl(1)	0.178(5)	0.168(5)	0.146(5)	-0.025(4)	0.086(5)	-0.021(5)
Cl(2)	0.283(9)	0.141(5)	0.271(9)	-0.029(6)	0.197(8)	-0.019(5)
C(50)	0.16(2)	0.18(2)	0.14(2)	-0.07(1)	0.08(1)	-0.07(2)

Table 1. Crystal data and structure refinement for 3.

Identification code	3
Empirical formula	$C_{100}H_{92}Au_2Cl_4F_{12}N_4P_8Ru$
Formula weight	2462.34
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 13.329(5) Å alpha = 86.12(7)°. b = 13.899(5) Å beta = 81.26(4)°. c = 13.969(6) Å gamma = 86.62(7)°.
Volume	2548.9(17) $Å^3$
Z	1
Density (calculated)	1.604 Mg/m^3
Absorption coefficient	3.317 mm^{-1}
F(000)	1218
Crystal size	0.20 x 0.13 x 0.10 mm
Theta range for data collection	1.47 to 24.98°
Index ranges	$-15 \le h \le 15$ $0 \le k \le 16$ $-16 \le l \le 16$
Reflections collected	9377
Independent reflections	8971 [R(int) = 0.0683]
Absorption correction	Empirical
Max. and min. transmission	0.727 and 0.615
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8971 / 20 / 599
Goodness-of-fit on F^2	1.027
Final R indices [I>2sigma(I)]	R_1 = 0.0601, wR_2 = 0.1655
R indices (all data)	R_1 = 0.1755, wR_2 = 0.2062
Largest diff. peak and hole	2.350 and -1.445 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 3. Ueq is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	Ueq	
Au(1)	-4161(1)	3666(1)	-1094(1)	42(1)	
Ru(1)	0	0	0	21(1)	
C(1)	-2482(10)	2135(10)	-528(10)	35(3)	
N(1)	-3139(9)	2703(10)	-616(10)	54(4)	
C(3)	579(10)	165(9)	-1444(10)	29(3)	
N(2)	835(9)	262(8)	-2240(8)	35(3)	
C(2)	-1715(10)	1468(9)	-398(9)	29(3)	
C(4)	1118(12)	455(12)	-3267(10)	47(4)	
C(5)	2047(16)	1031(15)	-3433(12)	77(6)	
C(6)	1293(19)	-492(14)	-3714(13)	87(7)	
C(7)	239(15)	1014(16)	-3605(13)	80(6)	
P(1)	-5359(3)	4627(3)	-1672(3)	37(1)	
C(11)	-5623(11)	4209(12)	-2797(12)	51(4)	
C(12)	-5936(14)	4828(15)	-3526(13)	66(5)	
C(13)	-6160(2)	4460(2)	-4360(15)	109(10)	
C(14)	-6055(18)	3530(2)	-4483(16)	98(9)	
C(15)	-5717(16)	2884(18)	-3803(17)	86(7)	
C(16)	-5519(12)	3228(13)	-2911(12)	56(5)	
C(21)	-5007(11)	5864(9)	-1969(11)	37(4)	
C(22)	-5582(12)	6618(11)	-1565(11)	49(4)	
C(23)	-5296(13)	7573(12)	-1775(13)	60(5)	
C(24)	-4481(15)	7761(13)	-2422(16)	75(6)	
C(25)	-3816(16)	6992(14)	-2825(15)	76(6)	
C(26)	-4134(12)	6042(13)	-2594(14)	58(5)	
C(31)	-6543(10)	4664(9)	-838(11)	35(3)	
C(32)	-6567(11)	4274(11)	88(12)	48(4)	
C(33)	-7450(15)	4342(13)	750(14)	65(5)	
C(34)	-8323(13)	4803(11)	460(14)	59(5)	
C(35)	-8270(13)	5156(11)	-470(16)	63(5)	
C(36)	-7393(12)	5101(12)	-1126(13)	52(4)	
P(2)	-513(2)	1664(2)	-51(2)	25(1)	
C(41)	-714(10)	2374(9)	1013(10)	32(3)	
C(42)	-1640(12)	2311(10)	1642(10)	44(4)	
C(43)	-1837(16)	2814(13)	2498(13)	60(5)	
C(44)	-1088(17)	3328(12)	2741(12)	62(5)	
C(45)	-146(17)	3353(12)	2132(13)	67(5)	
C(46)	7(13)	2891(9)	1265(10)	42(4)	
C(51)	221(10)	2480(9)	-949(10)	31(3)	
C(52)	-249(12)	3090(10)	-1572(10)	43(4)	
C(53)	353(15)	3653(12)	-2283(12)	58(5)	
C(54)	1361(16)	3604(13)	-2341(13)	64(5)	
C(55)	1836(13)	2984(12)	-1712(14)	63(5)	
C(56)	1274(10)	2411(10)	-1027(11)	40(4)	
P(3)	-1648(2)	208(2)	-487(2)	26(1)	
C(61)	-1832(9)	-59(9)	-1697(9)	27(3)	
C(62)	-2462(11)	498(12)	-2213(10)	44(4)	
C(63)	-2677(13)	208(14)	-3082(12)	60(5)	
C(64)	-2223(15)	-669(15)	-3456(11)	61(5)	
C(65)	-1618(14)	-1193(13)	-2946(13)	62(5)	
C(66)	-1405(13)	-910(11)	-2074(11)	49(4)	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 3. Ueq is defined as one third of the trace of the orthogonalized Uij tensor. (Cont.)

Atom	x	y	z	Ueq	
C(71)	-2821(10)	-252(9)	215(10)	31(3)	
C(72)	-3098(12)	20(11)	1153(11)	46(4)	
C(73)	-4011(12)	-323(11)	1685(13)	52(4)	
C(74)	-4563(12)	-897(13)	1338(15)	60(5)	
C(75)	-4301(15)	-1226(14)	419(17)	79(6)	
C(76)	-3384(12)	-887(13)	-138(13)	56(5)	
P(4)	5000	0	5000	69(2)	
F(1)	5878(12)	595(15)	4487(16)	185(8)	
F(2)	4234(10)	868(12)	4779(10)	126(5)	
F(3)	5102(11)	445(12)	5966(9)	136(6)	
P(5)	1086(8)	4024(8)	4559(7)	68(3)	
F(4)	1020(2)	4742(16)	5398(15)	126(10)	
F(5)	326(17)	4810(2)	3950(19)	176(15)	
F(6)	1657(14)	3133(12)	5038(13)	73(6)	
F(7)	1761(13)	4562(13)	3724(12)	68(5)	
F(8)	10(2)	3750(3)	5340(2)	230(2)	
F(9)	810(3)	3150(2)	3820(2)	430(5)	
C(8)	1930(3)	7110(3)	4350(3)	250(3)	
Cl(1)	2515(8)	6886(7)	3096(6)	165(4)	
Cl(2)	2953(10)	7290(11)	4914(8)	231(6)	

Table 3. Bond lengths (Å) and angles (º), with esd´s in parentheses, for 3.

Au(1)-N(1)	2.009(12)	Au(1)-P(1)	2.230(4)
Ru(1)-C(3)	2.050(15)	Ru(1)-C(3)#1	2.050(15)
Ru(1)-P(2)#1	2.372(3)	Ru(1)-P(2)	2.372(3)
Ru(1)-P(3)#1	2.393(3)	Ru(1)-P(3)	2.393(3)
C(1)-N(1)	1.159(17)	C(1)-C(2)	1.364(18)
C(3)-N(2)	1.113(15)	N(2)-C(4)	1.438(18)
C(2)-P(3)	1.760(13)	C(2)-P(2)	1.783(13)
C(4)-C(7)	1.49(2)	C(4)-C(6)	1.49(2)
C(4)-C(5)	1.49(2)	P(1)-C(11)	1.801(17)
P(1)-C(21)	1.813(14)	P(1)-C(31)	1.814(14)
C(11)-C(16)	1.38(2)	C(11)-C(12)	1.39(2)
C(12)-C(13)	1.38(3)	C(13)-C(14)	1.32(3)
C(14)-C(15)	1.37(3)	C(15)-C(16)	1.43(3)
C(21)-C(22)	1.36(2)	C(21)-C(26)	1.37(2)
C(22)-C(23)	1.40(2)	C(23)-C(24)	1.33(2)
C(24)-C(25)	1.44(3)	C(25)-C(26)	1.41(2)
C(31)-C(36)	1.356(19)	C(31)-C(32)	1.37(2)
C(32)-C(33)	1.38(2)	C(33)-C(34)	1.40(2)
C(34)-C(35)	1.35(2)	C(35)-C(36)	1.37(2)
P(2)-C(41)	1.816(14)	P(2)-C(51)	1.840(14)
C(41)-C(46)	1.34(2)	C(41)-C(42)	1.41(2)
C(42)-C(43)	1.41(2)	C(43)-C(44)	1.36(3)
C(44)-C(45)	1.41(3)	C(45)-C(46)	1.39(2)
C(51)-C(52)	1.369(19)	C(51)-C(56)	1.389(18)
C(52)-C(53)	1.40(2)	C(53)-C(54)	1.33(2)
C(54)-C(55)	1.38(3)	C(55)-C(56)	1.36(2)
P(3)-C(61)	1.811(13)	P(3)-C(71)	1.838(13)
C(61)-C(62)	1.362(18)	C(61)-C(66)	1.383(19)
C(62)-C(63)	1.38(2)	C(63)-C(64)	1.42(2)
C(64)-C(65)	1.31(2)	C(65)-C(66)	1.38(2)
C(71)-C(76)	1.35(2)	C(71)-C(72)	1.38(2)
C(72)-C(73)	1.42(2)	C(73)-C(74)	1.28(2)
C(74)-C(75)	1.38(3)	C(75)-C(76)	1.43(2)
P(4)-F(1)#2	1.532(17)	P(4)-F(1)	1.532(17)
P(4)-F(3)#2	1.550(11)	P(4)-F(3)	1.550(11)
P(4)-F(2)#2	1.580(13)	P(4)-F(2)	1.580(13)
P(5)-F(7)	1.541(18)	P(5)-F(6)	1.578(16)
P(5)-F(4)	1.579(17)	P(5)-F(8)	1.71(2)
P(5)-F(5)	1.719(18)	P(5)-F(9)	1.74(2)
C(8)-Cl(2)	1.72(4)	C(8)-Cl(1)	1.84(5)
N(1)-Au(1)-P(1)	174.9(4)	C(3)-Ru(1)-C(3)#1	180.0
C(3)-Ru(1)-P(2)#1	91.5(4)	C(3)#1-Ru(1)-P(2)#1	88.5(4)
C(3)-Ru(1)-P(2)	88.5(4)	C(3)#1-Ru(1)-P(2)	91.5(4)
P(2)#1-Ru(1)-P(2)	180.0	C(3)-Ru(1)-P(3)#1	93.2(4)
C(3)#1-Ru(1)-P(3)#1	86.8(4)	P(2)#1-Ru(1)-P(3)#1	70.50(13)
P(2)-Ru(1)-P(3)#1	109.49(13)	C(3)-Ru(1)-P(3)	86.8(4)
C(3)#1-Ru(1)-P(3)	93.2(4)	P(2)#1-Ru(1)-P(3)	109.50(13)
P(2)-Ru(1)-P(3)	70.50(13)	P(3)#1-Ru(1)-P(3)	180.0
N(1)-C(1)-C(2)	178.5(16)	C(1)-N(1)-Au(1)	166.8(13)
N(2)-C(3)-Ru(1)	175.8(12)	C(3)-N(2)-C(4)	175.6(13)
C(1)-C(2)-P(3)	130.2(11)	C(1)-C(2)-P(2)	127.9(10)
P(3)-C(2)-P(2)	101.8(6)	N(2)-C(4)-C(7)	105.9(12)
N(2)-C(4)-C(6)	107.3(13)	C(7)-C(4)-C(6)	111.1(17)
N(2)-C(4)-C(5)	108.7(13)	C(7)-C(4)-C(5)	111.2(16)
C(6)-C(4)-C(5)	112.3(15)	C(11)-P(1)-C(21)	104.5(7)

Table 3. Angles (º), with esd´s in parentheses, for 3. (Cont.)

C(11)-P(1)-C(31)	107.6(7)	C(21)-P(1)-C(31)	107.3(7)
C(11)-P(1)-Au(1)	110.4(5)	C(21)-P(1)-Au(1)	114.4(5)
C(31)-P(1)-Au(1)	112.3(5)	C(16)-C(11)-C(12)	119.9(16)
C(16)-C(11)-P(1)	117.4(14)	C(12)-C(11)-P(1)	122.7(13)
C(13)-C(12)-C(11)	120(2)	C(14)-C(13)-C(12)	121(2)
C(13)-C(14)-C(15)	122(2)	C(14)-C(15)-C(16)	119(2)
C(11)-C(16)-C(15)	118.2(18)	C(22)-C(21)-C(26)	119.3(14)
C(22)-C(21)-P(1)	1121.3(12)	C(26)-C(21)-P(1)	119.3(11)
C(21)-C(22)-C(23)	121.3(15)	C(24)-C(23)-C(22)	119.9(16)
C(23)-C(24)-C(25)	120.8(17)	C(26)-C(25)-C(24)	116.9(17)
C(21)-C(26)-C(25)	121.3(16)	C(36)-C(31)-C(32)	120.2(14)
C(36)-C(31)-P(1)	120.2(12)	C(32)-C(31)-P(1)	119.7(10)
C(31)-C(32)-C(33)	120.5(14)	C(32)-C(33)-C(34)	119.4(17)
C(35)-C(34)-C(33)	117.9(16)	C(34)-C(35)-C(36)	122.8(16)
C(31)-C(36)-C(35)	119.1(16)	C(2)-P(2)-C(41)	108.9(6)
C(2)-P(2)-C(51)	110.9(6)	C(41)-P(2)-C(51)	101.5(6)
C(2)-P(2)-Ru(1)	93.9(4)	C(41)-P(2)-Ru(1)	123.2(4)
C(51)-P(2)-Ru(1)	118.0(4)	C(46)-C(41)-C(42)	118.4(14)
C(46)-C(41)-P(2)	122.9(11)	C(42)-C(41)-P(2)	118.4(11)
C(41)-C(42)-C(43)	121.7(16)	C(44)-C(43)-C(42)	118.6(17)
C(43)-C(44)-C(45)	119.4(17)	C(46)-C(45)-C(44)	120.5(18)
C(41)-C(46)-C(45)	121.1(16)	C(52)-C(51)-C(56)	120.7(13)
C(52)-C(51)-P(2)	121.0(11)	C(56)-C(51)-P(2)	118.1(10)
C(51)-C(52)-C(53)	118.6(15)	C(54)-C(53)-C(52)	120.7(16)
C(53)-C(54)-C(55)	120.6(16)	C(56)-C(55)-C(54)	120.2(16)
C(55)-C(56)-C(51)	119.2(15)	C(2)-P(3)-C(61)	109.2(6)
C(2)-P(3)-C(71)	107.1(6)	C(61)-P(3)-C(71)	100.0(6)
C(2)-P(3)-Ru(1)	93.8(4)	C(61)-P(3)-Ru(1)	120.5(4)
C(71)-P(3)-Ru(1)	125.0(4)	C(62)-C(61)-C(66)	118.3(13)
C(62)-C(61)-P(3)	122.2(10)	C(66)-C(61)-P(3)	119.1(10)
C(61)-C(62)-C(63)	120.5(15)	C(62)-C(63)-C(64)	120.0(15)
C(65)-C(64)-C(63)	118.4(15)	C(64)-C(65)-C(66)	121.8(17)
C(65)-C(66)-C(61)	120.9(14)	C(76)-C(71)-C(72)	119.3(14)
C(76)-C(71)-P(3)	122.4(12)	C(72)-C(71)-P(3)	118.3(11)
C(71)-C(72)-C(73)	118.1(15)	C(74)-C(73)-C(72)	122.5(17)
C(73)-C(74)-C(75)	121.9(17)	C(74)-C(75)-C(76)	116.8(17)
C(71)-C(76)-C(75)	121.3(17)	F(1)#2-P(4)-F(1)	179.999(3)
F(1)#2-P(4)-F(3)#2	89.4(11)	F(1)-P(4)-F(3)#2	90.6(11)
F(1)#2-P(4)-F(3)	90.6(11)	F(1)-P(4)-F(3)	89.4(11)
F(3)#2-P(4)-F(3)	179.997(3)	F(1)#2-P(4)-F(2)#2	89.1(9)
F(1)-P(4)-F(2)#2	90.9(9)	F(3)#2-P(4)-F(2)#2	88.9(7)
F(3)-P(4)-F(2)#2	91.1(7)	F(1)#2-P(4)-F(2)	90.9(9)
F(1)-P(4)-F(2)	89.1(9)	F(3)#2-P(4)-F(2)	91.1(7)
F(3)-P(4)-F(2)	88.9(7)	F(2)#2-P(4)-F(2)	179.999(2)
F(7)-P(5)-F(6)	113.4(10)	F(7)-P(5)-F(4)	101.7(13)
F(6)-P(5)-F(4)	99.2(11)	F(7)-P(5)-F(8)	158.1(13)
F(6)-P(5)-F(8)	88.5(12)	F(4)-P(5)-F(8)	74.5(17)
F(7)-P(5)-F(5)	71.3(9)	F(6)-P(5)-F(5)	168.0(14)
F(4)-P(5)-F(5)	90.3(12)	F(8)-P(5)-F(5)	87.1(12)
F(7)-P(5)-F(9)	93.1(14)	F(6)-P(5)-F(9)	81.9(12)
F(4)-P(5)-F(9)	163.2(18)	F(8)-P(5)-F(9)	88.8(15)
F(5)-P(5)-F(9)	87.0(13)	Cl(2)-C(8)-Cl(1)	103(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x+1,-y,-z+1

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3). The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2a^{*2} U11 + ... + 2hka* b* U12].

Atom	U11	U22	U33	U23	U13	U12
Au(1)	33(1)	31(1)	63(1)	-5(1)	-12(1)	12(1)
Ru(1)	19(1)	21(1)	23(1)	-1(1)	-3(1)	4(1)
C(1)	31(8)	25(7)	45(9)	6(7)	2(7)	-2(6)
N(1)	28(7)	55(9)	77(10)	-4(8)	-15(7)	14(6)
C(3)	29(7)	23(7)	35(9)	-11(6)	-7(6)	10(6)
N(2)	51(8)	38(7)	15(7)	-7(5)	3(6)	1(6)
C(2)	28(7)	24(7)	32(8)	3(6)	-2(6)	4(6)
C(4)	52(10)	58(11)	24(8)	-10(7)	14(7)	5(8)
C(5)	105(17)	90(15)	33(10)	3(10)	5(10)	-19(13)
C(6)	150(2)	66(14)	34(11)	-3(9)	13(11)	0(14)
C(7)	78(14)	113(18)	45(11)	30(11)	-12(10)	-1(12)
P(1)	33(2)	33(2)	45(2)	-6(2)	-11(2)	6(2)
C(11)	40(9)	52(10)	61(11)	-19(9)	-1(8)	-3(8)
C(12)	72(13)	69(13)	63(13)	0(10)	-30(10)	-10(10)
C(13)	150(2)	140(3)	49(14)	16(15)	-54(15)	-60(2)
C(14)	101(18)	140(2)	53(14)	-38(16)	7(12)	-52(18)
C(16)	58(11)	59(12)	58(11)	-28(9)	-21(9)	-1(9)
C(21)	51(9)	18(7)	44(9)	0(6)	-18(8)	1(6)
C(22)	44(9)	48(10)	51(10)	5(8)	1(8)	5(8)
C(23)	53(11)	41(10)	81(13)	6(9)	3(10)	5(8)
C(24)	77(14)	35(10)	114(17)	1(11)	-16(13)	-19(10)
C(25)	76(14)	61(13)	87(15)	-9(11)	8(12)	-22(11)
C(26)	38(9)	51(11)	85(14)	-17(10)	-3(9)	-3(8)
C(31)	36(8)	21(7)	46(9)	0(7)	-6(7)	-2(6)
C(32)	28(8)	55(10)	59(11)	-7(9)	-9(7)	14(7)
C(33)	81(14)	51(11)	61(12)	1(9)	-7(10)	-5(10)
C(34)	54(11)	32(9)	82(14)	-14(9)	19(10)	-4(8)
C(35)	51(11)	28(9)	109(17)	9(10)	-21(11)	8(8)
C(36)	41(9)	50(10)	63(12)	7(9)	-12(9)	7(8)
P(2)	25(2)	22(2)	26(2)	-1(2)	-3(1)	5(1)
C(41)	35(8)	25(7)	37(8)	-6(6)	-6(7)	5(6)
C(42)	67(11)	31(8)	33(9)	6(7)	-11(8)	5(7)
C(43)	80(14)	49(11)	45(11)	-11(9)	12(10)	10(10)
C(44)	105(16)	40(10)	33(10)	-3(8)	-1(11)	31(11)
C(45)	110(17)	48(11)	52(12)	2(9)	-46(12)	-5(11)
C(46)	73(11)	21(7)	35(9)	-5(6)	-17(8)	7(7)
C(51)	29(7)	28(7)	35(8)	-4(6)	-1(6)	5(6)
C(52)	58(10)	34(8)	37(9)	-9(7)	-6(8)	1(7)
C(53)	83(14)	40(10)	52(11)	15(8)	-19(10)	-5(9)
C(54)	84(15)	55(12)	52(12)	-8(9)	15(10)	-45(11)
C(55)	45(10)	46(11)	90(15)	-10(10)	21(10)	-10(8)
C(56)	36(8)	28(8)	54(10)	3(7)	-6(7)	2(6)
P(3)	22(2)	25(2)	30(2)	1(2)	-5(2)	0(1)
C(61)	31(7)	23(7)	29(8)	-2(6)	-11(6)	-2(6)
C(62)	51(9)	58(10)	25(8)	-12(7)	-15(7)	2(8)
C(63)	66(12)	74(13)	45(11)	22(10)	-33(9)	-15(10)
C(64)	82(14)	85(15)	20(9)	-7(9)	-4(9)	-41(12)
C(65)	78(13)	54(11)	54(12)	-17(9)	-3(10)	4(10)
C(66)	83(12)	36(9)	35(9)	-9(7)	-33(8)	9(8)
C(71)	28(7)	19(7)	45(9)	9(6)	-9(6)	0(6)
C(72)	56(10)	31(8)	49(10)	2(7)	-4(8)	-5(7)

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2a^{*2} U11 + ... + 2hka^* b^* U12]$. (Continued)

Atom	U11	U22	U33	U23	U13	U12
C(73)	51(10)	35(9)	60(12)	6(8)	21(9)	-6(8)
C(74)	35(9)	56(12)	83(15)	18(11)	2(9)	-4(8)
C(75)	80(14)	59(13)	106(18)	25(12)	-34(13)	-47(11)
C(76)	46(10)	73(13)	55(11)	-5(9)	-12(8)	-27(9)
P(4)	43(4)	113(6)	50(4)	-25(4)	-4(3)	7(4)
F(1)	95(12)	181(18)	260(2)	7(17)	29(13)	-23(12)
F(2)	104(10)	172(15)	104(10)	-41(10)	-30(8)	60(10)
F(3)	135(12)	192(16)	94(10)	-93(10)	-46(9)	54(11)
P(5)	68(7)	74(7)	66(7)	-17(6)	-24(5)	24(5)
C(8)	210(4)	310(6)	250(5)	190(5)	-110(4)	-140(4)
Cl(1)	206(10)	178(9)	103(6)	24(6)	-3(6)	-19(7)
Cl(2)	223(13)	339(18)	126(8)	-53(9)	29(8)	-58(12)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 3.

Atom	x	y	z	U(eq)
H(501)	1901	1632	-3128	90(2)
H(502)	2250	1155	-4118	90(2)
H(503)	2586	675	-3161	90(2)
H(601)	1860	-840	-3481	90(2)
H(602)	1436	-389	-4407	90(2)
H(603)	697	-858	-3545	90(2)
H(701)	136	1618	-3299	90(2)
H(702)	-360	651	-3437	90(2)
H(703)	373	1134	-4296	90(2)
H(12)	-5993	5491	-3455	71(15)
H(13)	-6395	4879	-4837	71(15)
H(14)	-6213	3296	-5050	71(15)
H(15)	-5617	2231	-3918	71(15)
H(16)	-5326	2802	-2422	71(15)
H(22)	-6176	6497	-1141	71(15)
H(23)	-5676	8074	-1462	71(15)
H(24)	-4340	8398	-2616	71(15)
H(25)	-3204	7114	-3219	71(15)
H(26)	-3744	5528	-2872	71(15)
H(32)	-5986	3961	276	71(15)
H(33)	-7461	4083	1383	71(15)
H(34)	-8923	4864	894	71(15)
H(35)	-8853	5450	-674	71(15)
H(36)	-7383	5360	-1758	71(15)
H(42)	-2135	1927	1489	44(14)
H(43)	-2467	2794	2888	44(14)
H(44)	-1197	3662	3306	44(14)
H(45)	379	3681	2310	44(14)
H(46)	622	2943	855	44(14)
H(52)	-954	3131	-1526	44(14)
H(53)	46	4064	-2718	44(14)
H(54)	1750	3990	-2808	44(14)
H(55)	2540	2959	-1756	44(14)
H(56)	1592	1979	-617	44(14)
H(62)	-2749	1077	-1977	60(16)
H(63)	-3118	586	-3423	60(16)
H(64)	-2352	-865	-4047	60(16)
H(65)	-1325	-1772	-3179	60(16)
H(66)	-968	-1296	-1735	60(16)
H(72)	-2697	418	1428	60(16)
H(73)	-4218	-124	2310	60(16)
H(74)	-5158	-1098	1717	60(16)
H(75)	-4701	-1647	172	60(16)
H(76)	-3170	-1108	-753	60(16)
H(81)	1465	7673	4365	304
H(82)	1563	6556	4650	304

SUPPLEMENTARY MATERIAL (Continued).

Torsion angles (°), with esd´s in parentheses.

				Angle (e.s.d.)					Angle (e.s.d.)
N(1)	-Au(1)	-P(1)	-C(11)	-38.(5)	N(1)	-Au(1)	-P(1)	-C(21)	-155.(5)
N(1)	-Au(1)	-P(1)	-C(31)	82.(5)	P(1)	-Au(1)	-N(1)	-C(1)	71.(8)
P(2)	-Ru(1)	-P(3)	-C(61)	113.7(5)	C(3)	-Ru(1)	-P(3)	-C(61)	24.1(6)
P(2)	-Ru(1)	-P(3)	-C(71)	-115.2(6)	C(3)	-Ru(1)	-P(3)	-C(71)	155.3(7)
P(2)	-Ru(1)	-P(3)	-C(2)	-1.2(4)	C(3)	-Ru(1)	-P(3)	-C(2)	-90.8(6)
C(3)	-Ru(1)	-P(2)	-C(41)	-156.0(7)	C(3)	-Ru(1)	-P(2)	-C(51)	-27.8(6)
P(3)	-Ru(1)	-P(2)	-C(2)	1.2(4)	C(3)	-Ru(1)	-P(2)	-C(2)	88.4(6)
P(2)	-Ru(1)	-C(3)	-N(2)	-69.(16)	P(3)	-Ru(1)	-C(3)	-N(2)	2.(16)
P(3)	-Ru(1)	-P(2)	-C(51)	-115.0(5)	P(3)	-Ru(1)	-P(2)	-C(41)	116.8(6)
C(2)	-C(1)	-N(1)	-Au(1)	175.(53)	N(1)	-C(1)	-C(2)	-P(2)	-73.(58)
N(1)	-C(1)	-C(2)	-P(3)	105.(57)	Ru(1)	-C(3)	-N(2)	-C(4)	52.(30)
C(3)	-N(2)	-C(4)	-C(5)	90.(18)	C(3)	-N(2)	-C(4)	-C(6)	-148.(18)
C(3)	-N(2)	-C(4)	-C(7)	-29.(19)	C(1)	-C(2)	-P(2)	-Ru(1)	177.(1)
C(1)	-C(2)	-P(3)	-Ru(1)	-177.(1)	P(2)	-C(2)	-P(3)	-Ru(1)	1.6(6)
C(1)	-C(2)	-P(3)	-C(61)	59.(1)	C(1)	-C(2)	-P(3)	-C(71)	-48.(1)
C(1)	-C(2)	-P(2)	-C(41)	50.(1)	C(1)	-C(2)	-P(2)	-C(51)	-61.(1)
P(3)	-C(2)	-P(2)	-Ru(1)	-1.6(6)	P(2)	-C(2)	-P(3)	-C(61)	-122.6(6)
P(2)	-C(2)	-P(3)	-C(71)	130.0(6)	P(3)	-C(2)	-P(2)	-C(51)	120.4(7)
P(3)	-C(2)	-P(2)	-C(41)	-128.7(7)	Au(1)	-P(1)	-C(31)	-C(32)	11.(1)
Au(1)	-P(1)	-C(31)	-C(36)	-171.(1)	Au(1)	-P(1)	-C(21)	-C(22)	-123.(1)
Au(1)	-P(1)	-C(21)	-C(26)	55.(1)	Au(1)	-P(1)	-C(11)	-C(12)	-149.(1)
Au(1)	-P(1)	-C(11)	-C(16)	32.(1)	C(21)	-P(1)	-C(31)	-C(32)	-115.(1)
C(11)	-P(1)	-C(31)	-C(32)	133.(1)	C(21)	-P(1)	-C(31)	-C(36)	63.(1)
C(11)	-P(1)	-C(31)	-C(36)	-49.(1)	C(11)	-P(1)	-C(21)	-C(22)	116.(1)
C(11)	-P(1)	-C(21)	-C(26)	-66.(1)	C(21)	-P(1)	-C(11)	-C(16)	155.(1)
C(21)	-P(1)	-C(11)	-C(12)	-26.(2)	C(31)	-P(1)	-C(11)	-C(16)	-91.(1)
C(31)	-P(1)	-C(11)	-C(12)	88.(2)	C(31)	-P(1)	-C(21)	-C(26)	-180.(1)
C(31)	-P(1)	-C(21)	-C(22)	2.(1)	P(1)	-C(11)	-C(16)	-C(15)	-179.(1)
P(1)	-C(11)	-C(12)	-C(13)	-178.(2)	C(12)	-C(11)	-C(16)	-C(15)	2.(3)
C(16)	-C(11)	-C(12)	-C(13)	1.(3)	C(11)	-C(12)	-C(13)	-C(14)	-2.(4)
C(12)	-C(13)	-C(14)	-C(15)	0.(4)	C(13)	-C(14)	-C(15)	-C(16)	3.(4)
C(11)	-C(16)	-C(15)	-C(14)	-4.(3)	P(1)	-C(21)	-C(26)	-C(25)	-178.(1)
P(1)	-C(21)	-C(22)	-C(23)	178.(1)	C(22)	-C(21)	-C(26)	-C(25)	0.(3)
C(26)	-C(21)	-C(22)	-C(23)	0.(2)	C(21)	-C(22)	-C(23)	-C(24)	4.(3)
C(22)	-C(23)	-C(24)	-C(25)	-8.(3)	C(23)	-C(24)	-C(25)	-C(26)	8.(3)
C(24)	-C(25)	-C(26)	-C(21)	-4.(3)	P(1)	-C(31)	-C(36)	-C(35)	-177.(1)
P(1)	-C(31)	-C(32)	-C(33)	176.(1)	C(32)	-C(31)	-C(36)	-C(35)	1.(2)
C(36)	-C(31)	-C(32)	-C(33)	-2.(2)	C(31)	-C(32)	-C(33)	-C(34)	1.(3)
C(32)	-C(33)	-C(34)	-C(35)	1.(3)	C(33)	-C(34)	-C(35)	-C(36)	-2.(3)
C(34)	-C(35)	-C(36)	-C(31)	1.(3)	C(2)	-P(2)	-C(51)	-C(52)	21.(1)
Ru(1)	-P(2)	-C(51)	-C(52)	128.(1)	C(2)	-P(2)	-C(51)	-C(56)	-154.(1)
Ru(1)	-P(2)	-C(51)	-C(56)	-48.(1)	C(2)	-P(2)	-C(41)	-C(42)	27.(1)
Ru(1)	-P(2)	-C(41)	-C(42)	-81.(1)	C(2)	-P(2)	-C(41)	-C(46)	-158.(1)
Ru(1)	-P(2)	-C(41)	-C(46)	94.(1)	C(41)	-P(2)	-C(51)	-C(52)	-94.(1)
C(41)	-P(2)	-C(51)	-C(56)	90.(1)	C(51)	-P(2)	-C(41)	-C(46)	-41.(1)
C(51)	-P(2)	-C(41)	-C(42)	144.(1)	P(2)	-C(41)	-C(46)	-C(45)	-174.(1)
P(2)	-C(41)	-C(42)	-C(43)	178.(1)	C(42)	-C(41)	-C(46)	-C(45)	0.(2)
C(46)	-C(41)	-C(42)	-C(43)	3.(2)	C(41)	-C(42)	-C(43)	-C(44)	-4.(3)
C(42)	-C(43)	-C(44)	-C(45)	1.(3)	C(43)	-C(44)	-C(45)	-C(46)	3.(3)
C(44)	-C(45)	-C(46)	-C(41)	-3.(3)	P(2)	-C(51)	-C(56)	-C(55)	178.(1)
P(2)	-C(51)	-C(52)	-C(53)	-176.(1)	C(52)	-C(51)	-C(56)	-C(55)	2.(2)
C(56)	-C(51)	-C(52)	-C(53)	-1.(2)	C(51)	-C(52)	-C(53)	-C(54)	-1.(3)
C(52)	-C(53)	-C(54)	-C(55)	1.(3)	C(53)	-C(54)	-C(55)	-C(56)	0.(3)
C(54)	-C(55)	-C(56)	-C(51)	-2.(3)	C(2)	-P(3)	-C(71)	-C(72)	-51.(1)

SUPPLEMENTARY MATERIAL (Continued).

Torsion angles (°), with esd's in parentheses.

				Angle (e.s.d.)					Angle (e.s.d.)
Ru(1)	-P(3)	-C(71)	-C(72)	57.(1)	C(2)	-P(3)	-C(71)	-C(76)	133.(1)
Ru(1)	-P(3)	-C(71)	-C(76)	-120.(1)	C(2)	-P(3)	-C(61)	-C(62)	-34.(1)
Ru(1)	-P(3)	-C(61)	-C(62)	-141.(1)	C(2)	-P(3)	-C(61)	-C(66)	153.(1)
Ru(1)	-P(3)	-C(61)	-C(66)	46.(1)	C(61)	-P(3)	-C(71)	-C(72)	-165.(1)
C(61)	-P(3)	-C(71)	-C(76)	19.(1)	C(71)	-P(3)	-C(61)	-C(66)	-95.(1)
C(71)	-P(3)	-C(61)	-C(62)	78.(1)	P(3)	-C(61)	-C(66)	-C(65)	173.(1)
P(3)	-C(61)	-C(62)	-C(63)	-172.(1)	C(62)	-C(61)	-C(66)	-C(65)	-1.(2)
C(66)	-C(61)	-C(62)	-C(63)	1.(2)	C(61)	-C(62)	-C(63)	-C(64)	-1.(2)
C(62)	-C(63)	-C(64)	-C(65)	1.(3)	C(63)	-C(64)	-C(65)	-C(66)	-1.(3)
C(64)	-C(65)	-C(66)	-C(61)	1.(3)	P(3)	-C(71)	-C(76)	-C(75)	-179.(1)
P(3)	-C(71)	-C(72)	-C(73)	179.(1)	C(72)	-C(71)	-C(76)	-C(75)	5.(2)
C(76)	-C(71)	-C(72)	-C(73)	-5.(2)	C(71)	-C(72)	-C(73)	-C(74)	2.(3)
C(72)	-C(73)	-C(74)	-C(75)	0.(3)	C(73)	-C(74)	-C(75)	-C(76)	-1.(3)
C(74)	-C(75)	-C(76)	-C(71)	-2.(3)	F(9)	-P(5)	-F(7)	-F(5)	86.(2)
F(8)	-P(5)	-F(7)	-F(5)	-9.(4)	F(6)	-P(5)	-F(7)	-F(5)	168.(1)
F(4)	-P(5)	-F(7)	-F(5)	-86.(1)	F(4)	-P(5)	-F(5)	-F(7)	102.(1)
F(6)	-P(5)	-F(5)	-F(7)	-115.(6)	F(8)	-P(5)	-F(5)	-F(7)	177.(1)
F(9)	-P(5)	-F(5)	-F(7)	-94.(1)					

SUPPLEMENTARY MATERIAL (Continued).

Torsion angles involving hydrogen atoms.(°), with esd's in parentheses.

				Angle (e.s.d.)
N(2)	-C(4)	-C(7)	-H(701)	63.(2)
N(2)	-C(4)	-C(7)	-H(703)	-177.(2)
N(2)	-C(4)	-C(6)	-H(602)	176.(2)
N(2)	-C(4)	-C(5)	-H(501)	-61.(2)
N(2)	-C(4)	-C(5)	-H(503)	59.(2)
C(5)	-C(4)	-C(7)	-H(701)	-55.(2)
C(5)	-C(4)	-C(7)	-H(702)	-175.(2)
C(5)	-C(4)	-C(7)	-H(703)	65.(2)
C(5)	-C(4)	-C(6)	-H(602)	-65.(2)
C(6)	-C(4)	-C(5)	-H(503)	-60.(2)
C(6)	-C(4)	-C(5)	-H(501)	-180.(2)
C(7)	-C(4)	-C(5)	-H(502)	-65.(2)
C(7)	-C(4)	-C(6)	-H(603)	-59.(2)
C(7)	-C(4)	-C(6)	-H(601)	-180.(2)
P(1)	-C(11)	-C(12)	-H(12)	2.(3)
C(16)	-C(11)	-C(12)	-H(12)	-179.(2)
H(12)	-C(12)	-C(13)	-H(13)	-2.(4)
C(12)	-C(13)	-C(14)	-H(14)	-180.(2)
H(13)	-C(13)	-C(14)	-C(15)	-180.(3)
H(14)	-C(14)	-C(15)	-C(16)	-177.(2)
C(11)	-C(16)	-C(15)	-H(15)	176.(2)
H(16)	-C(16)	-C(15)	-H(15)	-4.(3)
P(1)	-C(21)	-C(22)	-H(22)	-2.(2)
C(26)	-C(21)	-C(22)	-H(22)	180.(2)
H(22)	-C(22)	-C(23)	-H(23)	4.(3)
C(22)	-C(23)	-C(24)	-H(24)	172.(2)
H(23)	-C(23)	-C(24)	-C(25)	172.(2)
H(24)	-C(24)	-C(25)	-H(25)	8.(3)
C(24)	-C(25)	-C(26)	-H(26)	176.(2)
H(25)	-C(25)	-C(26)	-H(26)	-4.(3)
P(1)	-C(31)	-C(32)	-H(32)	-4.(2)
C(36)	-C(31)	-C(32)	-H(32)	178.(2)
H(32)	-C(32)	-C(33)	-H(33)	1.(3)
C(32)	-C(33)	-C(34)	-H(34)	-179.(2)
H(33)	-C(33)	-C(34)	-C(35)	-179.(2)
H(34)	-C(34)	-C(35)	-H(35)	-2.(3)
C(34)	-C(35)	-C(36)	-H(36)	-179.(2)
H(35)	-C(35)	-C(36)	-H(36)	1.(3)
P(2)	-C(41)	-C(42)	-H(42)	-2.(2)
C(46)	-C(41)	-C(42)	-H(42)	-177.(1)
H(42)	-C(42)	-C(43)	-H(43)	-4.(3)
C(42)	-C(43)	-C(44)	-H(44)	-179.(2)
H(43)	-C(43)	-C(44)	-C(45)	-179.(2)
H(44)	-C(44)	-C(45)	-H(45)	3.(3)
C(44)	-C(45)	-C(46)	-H(46)	177.(2)
H(45)	-C(45)	-C(46)	-H(46)	-3.(3)
P(2)	-C(51)	-C(52)	-H(52)	4.(2)
C(56)	-C(51)	-C(52)	-H(52)	179.(1)
H(52)	-C(52)	-C(53)	-H(53)	-1.(3)
C(52)	-C(53)	-C(54)	-H(54)	-179.(2)
H(53)	-C(53)	-C(54)	-C(55)	-179.(2)
H(54)	-C(54)	-C(55)	-H(55)	0.(3)
C(54)	-C(55)	-C(56)	-H(56)	178.(2)
H(55)	-C(55)	-C(56)	-H(56)	-2.(3)
N(2)	-C(4)	-C(7)	-H(702)	-57.(2)
N(2)	-C(4)	-C(6)	-H(601)	-64.(2)
N(2)	-C(4)	-C(6)	-H(603)	56.(2)
N(2)	-C(4)	-C(5)	-H(502)	179.(2)
C(6)	-C(4)	-C(7)	-H(701)	179.(2)
C(6)	-C(4)	-C(7)	-H(702)	59.(2)
C(6)	-C(4)	-C(7)	-H(703)	-61.(2)
C(5)	-C(4)	-C(6)	-H(601)	55.(2)
C(5)	-C(4)	-C(6)	-H(603)	175.(2)
C(6)	-C(4)	-C(5)	-H(502)	61.(2)
C(7)	-C(4)	-C(5)	-H(503)	175.(2)
C(7)	-C(4)	-C(5)	-H(501)	55.(2)
C(7)	-C(4)	-C(6)	-H(602)	61.(2)
P(1)	-C(11)	-C(16)	-H(16)	1.(2)
C(12)	-C(11)	-C(16)	-H(16)	-178.(2)
C(11)	-C(12)	-C(13)	-H(13)	178.(2)
H(12)	-C(12)	-C(13)	-C(14)	178.(2)
H(13)	-C(13)	-C(14)	-H(14)	0.(4)
C(13)	-C(14)	-C(15)	-H(15)	-177.(3)
H(14)	-C(14)	-C(15)	-H(15)	3.(4)
H(16)	-C(16)	-C(15)	-C(14)	176.(2)
P(1)	-C(21)	-C(26)	-H(26)	2.(2)
C(22)	-C(21)	-C(26)	-H(26)	-180.(2)
C(21)	-C(22)	-C(23)	-H(23)	-176.(2)
H(22)	-C(22)	-C(23)	-C(24)	-176.(2)
H(23)	-C(23)	-C(24)	-H(24)	-8.(3)
C(23)	-C(24)	-C(25)	-H(25)	-172.(2)
H(24)	-C(24)	-C(25)	-C(26)	-172.(2)
H(25)	-C(25)	-C(26)	-C(21)	176.(2)
P(1)	-C(31)	-C(36)	-H(36)	3.(2)
C(32)	-C(31)	-C(36)	-H(36)	-179.(2)
C(31)	-C(32)	-C(33)	-H(33)	-179.(2)
H(32)	-C(32)	-C(33)	-C(34)	-179.(2)
H(33)	-C(33)	-C(34)	-H(34)	1.(3)
C(33)	-C(34)	-C(35)	-H(35)	178.(2)
H(34)	-C(34)	-C(35)	-C(36)	178.(2)
H(35)	-C(35)	-C(36)	-C(31)	-179.(2)
P(2)	-C(41)	-C(46)	-H(46)	6.(2)
C(42)	-C(41)	-C(46)	-H(46)	-180.(1)
C(41)	-C(42)	-C(43)	-H(43)	176.(2)
H(42)	-C(42)	-C(43)	-C(44)	176.(2)
H(43)	-C(43)	-C(44)	-H(44)	1.(3)
C(43)	-C(44)	-C(45)	-H(45)	-177.(2)
H(44)	-C(44)	-C(45)	-C(46)	-177.(2)
H(45)	-C(45)	-C(46)	-C(41)	177.(2)
P(2)	-C(51)	-C(56)	-H(56)	-2.(2)
C(52)	-C(51)	-C(56)	-H(56)	-178.(1)
C(51)	-C(52)	-C(53)	-H(53)	179.(2)
H(52)	-C(52)	-C(53)	-C(54)	179.(2)
H(53)	-C(53)	-C(54)	-H(54)	1.(3)
C(53)	-C(54)	-C(55)	-H(55)	-180.(2)
H(54)	-C(54)	-C(55)	-C(56)	-180.(2)
H(55)	-C(55)	-C(56)	-C(51)	178.(2)
P(3)	-C(61)	-C(66)	-H(66)	-7.(2)

SUPPLEMENTARY MATERIAL (Continued).

Torsion angles involving hydrogen atoms.(°), with esd´s in parentheses.

				Angle (e.s.d.)					Angle (e.s.d.)
P(3)	-C(61)	-C(62)	-H(62)	8.(2)	C(62)	-C(61)	-C(66)	-H(66)	179.(1)
C(66)	-C(61)	-C(62)	-H(62)	-179.(1)	C(61)	-C(62)	-C(63)	-H(63)	179.(2)
H(62)	-C(62)	-C(63)	-H(63)	-1.(3)	H(62)	-C(62)	-C(63)	-C(64)	179.(2)
C(62)	-C(63)	-C(64)	-H(64)	-179.(2)	H(63)	-C(63)	-C(64)	-H(64)	1.(3)
H(63)	-C(63)	-C(64)	-C(65)	-179.(2)	C(63)	-C(64)	-C(65)	-H(65)	179.(2)
H(64)	-C(64)	-C(65)	-H(65)	-1.(3)	H(64)	-C(64)	-C(65)	-C(66)	179.(2)
C(64)	-C(65)	-C(66)	-H(66)	-179.(2)	H(65)	-C(65)	-C(66)	-C(61)	-179.(2)
H(65)	-C(65)	-C(66)	-H(66)	1.(3)	P(3)	-C(71)	-C(76)	-H(76)	1.(2)
P(3)	-C(71)	-C(72)	-H(72)	-1.(2)	C(72)	-C(71)	-C(76)	-H(76)	-175.(2)
C(76)	-C(71)	-C(72)	-H(72)	175.(2)	C(71)	-C(72)	-C(73)	-H(73)	-178.(2)
H(72)	-C(72)	-C(73)	-H(73)	2.(3)	H(72)	-C(72)	-C(73)	-C(74)	-178.(2)
C(72)	-C(73)	-C(74)	-H(74)	-180.(2)	H(73)	-C(73)	-C(74)	-H(74)	0.(3)
H(73)	-C(73)	-C(74)	-C(75)	-180.(2)	C(73)	-C(74)	-C(75)	-H(75)	179.(2)
H(74)	-C(74)	-C(75)	-H(75)	-1.(3)	H(74)	-C(74)	-C(75)	-C(76)	179.(2)
C(74)	-C(75)	-C(76)	-H(76)	178.(2)	H(75)	-C(75)	-C(76)	-C(71)	178.(2)
H(75)	-C(75)	-C(76)	-H(76)	-2.(3)					