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Table SI. Table of Data Collection and Refinement Parameters for $Ru(tpy)(CO)_2Cl^+$ $(BPh_4)^-$ (1a)

Empirical Formula	$C_{41}H_{31}BClN_3O_2Ru$
Formula Weight	745.05
Crystal Color, Habit	yellow, prism
Crystal Dimensions	0.60 x 0.30 x 0.26 mm
Crystal System	triclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	25 (30.0 - 36.0°)
Omega Scan Peak Width at Half Height	0.50°
Lattice Parameters	a = 13.233(4) Å b = 13.374(6) Å c = 10.918(3) Å α = 113.00(3)° β = 98.96(2)° γ = 78.97(3)° V = 1738(1) Å^3
Space Group	P $\bar{1}$ (#2)
Z value	2
D_{calc}	1.423 g/cm^3
F_{000}	760.00
μ(MoKα)	5.68 cm^{-1}
Diffractometer	CAD4

Table SI. (cont.)

Radiation	MoKα (λ = 0.71073 Å) graphite monochromated
Attenuator	Zr foil (factor = 22.37)
Take-off Angle	2.8°
Detector Aperture	2.0 - 2.5 mm horizontal 2.0 mm vertical
Crystal to Detector Distance	21 mm
Temperature	23(3)°C
Scan Type	ω-2θ
Scan Rate	1.0°/min (in ω) (up to 2 scans)
Scan Width	(0.80 + 0.35 tanθ)°
$2\theta_{max}$	50.0°
No. of Reflections Measured	Total: 6366 Unique: 6079 (R_{int} = 0.007)
Corrections	Lorentz-polarizartion Absorption Ψ (trans. factors: 0.967 - 1.0000) Secondary Extinction (coefficient: 7.29958 e^{-7})
Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
FunctionMinimized	$\Sigma\omega(\|Fo\| - \|Fc\|)^2$

Table SI. (cont.)

Least Squares Weights	$[\sigma^2(F_o)]^{-1}$
p-factor	0.0080
Anomalous Dispersion	all non-hydrogen atoms
No. Observations (I>3.00σ(I))	5571
No. Variables	443
Reflection/Parameter Ratio	12.58
Residuals:[a] R; R_w	0.027; 0.034
GOF	2.93
Max. Shift/Error in Final Cycle	0.02
Maximum Peak in Final Diff. Map	0.39 $e^-/Å^3$
Minimum Peak in Final Diff. Map	-0.44 $e^-/Å^3$
Computer Hardware	Silicon Graphics Iris Indigo
Computer Software	teXsan

a) $R = \Sigma ||F_o|-|F_c||/\Sigma |F_o|$; $R_w = [\Sigma w(|Fo|-|Fc|)^2]/\Sigma wF_o^2]^{1/2}$

Table SII. Positional parameters and B(eq) for 1a

atom	x	y	z	B_{eq}[a](Å^2)
Ru	-0.290772(8)	0.206472(9)	0.51405(1)	2.896(3)
O(2)	-0.3611(1)	0.3365(1)	0.3381(2)	6.95(4)
N(1)	-0.15758(9)	0.28110(9)	0.5946(1)	3.13(3)
N(2)	-0.18523(8)	0.09719(9)	0.3957(1)	2.70(2)
N(3)	-0.37911(8)	0.08325(9)	0.3917(1)	2.99(2)
C(1)	-0.3842(1)	0.3012(1)	0.6425(2)	4.58(4)
C(2)	-0.3333(1)	0.2873(1)	0.4035(2)	4.25(4)
C(3)	-0.1466(1)	0.3750(1)	0.7005(2)	4.08(4)
C(4)	-0.0524(1)	0.4119(1)	0.7468(2)	4.85(4)
C(5)	0.0335(1)	0.3522(1)	0.6836(2)	4.83(4)
C(6)	0.0233(1)	0.2570(1)	0.5747(2)	4.03(4)
C(7)	-0.0721(1)	0.2218(1)	0.5318(1)	3.04(3)
C(8)	-0.0874(1)	0.1178(1)	0.4200(1)	2.96(3)
C(9)	-0.0117(1)	0.0408(1)	0.3476(2)	3.93(3)
C(10)	-0.0398(1)	-0.0571(1)	0.2534(2)	4.31(4)
C(11)	-0.1404(1)	-0.0781(1)	0.2328(1)	3.57(3)
C(12)	-0.2136(1)	0.0019(1)	0.3069(1)	2.80(3)
C(13)	-0.3240(1)	-0.0057(1)	0.3032(1)	2.74(3)
C(14)	-0.3695(1)	-0.0960(1)	0.2189(1)	3.28(3)
C(15)	-0.4727(1)	-0.0972(1)	0.2235(2)	3.92(3)
C(16)	-0.5287(1)	-0.0071(1)	0.3115(2)	4.20(4)
C(17)	-0.4800(1)	0.0817(1)	0.3935(2)	3.78(3)
C(18)	0.2551(1)	0.2705(1)	0.3419(1)	3.30(3)
C(19)	0.2915(1)	0.3670(1)	0.4317(2)	4.86(4)
C(20)	0.3251(2)	0.3819(2)	0.5648(2)	5.40(4)
C(21)	0.3233(1)	0.3007(2)	0.6115(2)	4.58(4)

Table SII. (cont.)

atom	x	y	z	B_{eq}[a](Å^2)
C(22)	0.2876(1)	0.2054(1)	0.5258(2)	4.07(4)
C(23)	0.2546(1)	0.1906(1)	0.3934(1)	3.32(3)
C(24)	0.0822(1)	0.3030(1)	0.1940(1)	3.32(3)
C(25)	0.0348(1)	0.3559(1)	0.3137(2)	4.25(4)
C(26)	-0.0706(1)	0.3933(1)	0.3161(2)	5.14(4)
C(27)	-0.1339(1)	0.3816(1)	0.2007(2)	4.88(4)
C(28)	-0.0902(1)	0.3295(1)	0.0792(2)	4.51(4)
C(29)	0.0148(1)	0.2914(1)	0.0782(2)	3.86(3)
C(30)	0.2218(1)	0.1215(1)	0.0980(1)	3.12(3)
C(31)	0.1438(1)	0.0566(1)	0.0746(2)	4.03(4)
C(32)	0.1587(1)	-0.0571(1)	0.0051(2)	4.97(4)
C(33)	0.2521(2)	-0.1094(1)	-0.0428(2)	5.00(4)
C(34)	0.3321(1)	-0.0489(1)	-0.0210(2)	4.46(4)
C(35)	0.3160(1)	0.0645(1)	0.0489(1)	3.62(3)
C(36)	0.2682(1)	0.3166(1)	0.1246(1)	3.33(3)
C(37)	0.2216(1)	0.3678(1)	0.0355(1)	3.67(3)
C(38)	0.2769(2)	0.4145(1)	-0.0216(2)	4.57(4)
C(39)	0.3820(2)	0.4118(2)	0.0070(2)	5.46(5)
C(40)	0.4319(1)	0.3617(2)	0.0934(2)	5.61(5)
C(41)	0.3751(1)	0.3161(1)	0.1506(2)	4.71(4)
B	0.2064(1)	0.2547(1)	0.1887(2)	3.21(3)

a) $B_{eq} = 8/3\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos\gamma + 2U_{13}aa^*cc^* \cos\beta + 2U_{23}bb^*cc^* \cos\alpha)$

Table SIII. Table of general displacement parameter expressions-U's

atom	U11	U22	U33	U12	U13	U23
Ru	0.03014(7)	0.03239(7)	0.04166(8)	-0.00112(5)	0.00631(5)	0.00780(5)
Cl	0.0444(2)	0.0595(2)	0.0526(2)	-0.0100(2)	0.0043(2)	0.0263(2)
O(1)	0.0602(8)	0.096(1)	0.092(1)	-0.0010(8)	0.0332(7)	-0.0261(9)
O(2)	0.098(1)	0.0764(9)	0.101(1)	-0.0033(8)	-0.0127(9)	0.0572(9)
N(1)	0.0377(6)	0.0328(6)	0.0460(7)	-0.0060(5)	0.0058(5)	0.0108(5)
N(2)	0.0316(6)	0.0351(6)	0.0354(6)	-0.0020(5)	0.0070(5)	0.0122(5)
N(3)	0.0323(6)	0.0394(7)	0.0395(7)	-0.0048(5)	0.0028(5)	0.0123(5)
C(1)	0.0373(9)	0.052(1)	0.064(1)	-0.0047(7)	0.0079(7)	-0.0020(8)
C(2)	0.0473(9)	0.0432(9)	0.065(1)	-0.0043(7)	-0.0001(8)	0.0161(8)
C(3)	0.0514(9)	0.0359(8)	0.058(1)	-0.0069(7)	0.0068(8)	0.0063(7)
C(4)	0.0594(9)	0.0424(9)	0.071(1)	-0.0172(7)	0.0023(8)	0.0053(9)
C(5)	0.0517(9)	0.0534(10)	0.076(1)	-0.0236(8)	-0.0013(8)	0.0163(8)
C(6)	0.0402(8)	0.0534(9)	0.062(1)	-0.0127(7)	0.0058(7)	0.0204(7)
C(7)	0.0362(7)	0.0401(8)	0.0421(8)	-0.0074(6)	0.0053(6)	0.0169(6)
C(8)	0.0327(7)	0.0439(8)	0.0377(8)	-0.0040(6)	0.0068(6)	0.0162(6)
C(9)	0.0329(8)	0.0597(10)	0.0484(9)	-0.0028(7)	0.0110(7)	0.0103(7)
C(10)	0.0431(8)	0.0591(10)	0.0449(9)	0.0030(7)	0.0127(7)	0.0026(7)
C(11)	0.0446(8)	0.0438(9)	0.0369(8)	0.0003(6)	0.0080(6)	0.0051(7)
C(12)	0.0371(7)	0.0375(7)	0.0301(7)	-0.0027(6)	0.0032(6)	0.0119(6)
C(13)	0.0363(7)	0.0369(7)	0.0314(7)	-0.0029(6)	0.0034(6)	0.0140(6)
C(14)	0.0482(8)	0.0401(8)	0.0354(8)	-0.0078(7)	0.0012(6)	0.0133(6)
C(15)	0.0504(8)	0.0496(9)	0.0486(9)	-0.0176(7)	-0.0058(7)	0.0166(7)
C(16)	0.0365(8)	0.0610(10)	0.061(1)	-0.0136(7)	-0.0003(7)	0.0202(7)
C(17)	0.0319(7)	0.0521(9)	0.0547(10)	-0.0039(6)	0.0063(7)	0.0146(7)
C(18)	0.0450(8)	0.0416(8)	0.0344(7)	0.0011(7)	0.0066(6)	0.0114(6)
C(19)	0.090(1)	0.0463(9)	0.0430(8)	-0.0110(9)	-0.0034(9)	0.0135(8)
C(20)	0.084(1)	0.060(1)	0.0416(9)	-0.0057(10)	-0.0029(9)	0.0021(8)

Table SIII. (cont.)

atom	U11	U22	U33	U12	U13	U23
C(21)	0.0529(10)	0.080(1)	0.0344(9)	0.0072(8)	0.0070(7)	0.0207(8)
C(23)	0.0343(8)	0.0523(9)	0.0436(7)	-0.0001(7)	0.0081(6)	0.0232(7)
C(24)	0.0525(8)	0.0317(8)	0.0430(8)	-0.0033(6)	0.0073(6)	0.0150(7)
C(25)	0.0628(9)	0.0529(10)	0.0466(9)	-0.0009(8)	0.0119(8)	0.0201(8)
C(26)	0.069(1)	0.061(1)	0.067(1)	0.0074(9)	0.0286(8)	0.0248(10)
C(27)	0.052(1)	0.052(1)	0.085(1)	0.0026(8)	0.0132(8)	0.0307(9)
C(28)	0.0548(8)	0.0447(9)	0.068(1)	-0.0050(7)	-0.0030(8)	0.0207(8)
C(29)	0.0563(8)	0.0386(8)	0.0458(9)	-0.0048(7)	0.0037(7)	0.0103(7)
C(30)	0.0514(8)	0.0375(8)	0.0301(7)	-0.0043(6)	0.0031(6)	0.0141(6)
C(31)	0.0551(10)	0.0419(8)	0.058(1)	-0.0078(7)	0.0075(8)	0.0191(7)
C(32)	0.075(1)	0.0432(8)	0.072(1)	-0.0181(8)	0.0029(9)	0.0203(8)
C(33)	0.089(1)	0.0358(9)	0.057(1)	-0.0021(8)	0.0073(9)	0.0115(8)
C(34)	0.068(1)	0.0474(8)	0.0474(10)	0.0070(7)	0.0118(8)	0.0147(7)
C(35)	0.0535(9)	0.0451(8)	0.0397(8)	-0.0060(7)	0.0035(7)	0.0172(7)
C(36)	0.0569(9)	0.0324(8)	0.0324(8)	-0.0078(7)	0.0040(7)	0.0062(6)
C(37)	0.063(1)	0.0368(8)	0.0350(8)	0.0003(7)	0.0105(7)	0.0096(6)
C(38)	0.093(1)	0.0435(9)	0.0413(9)	-0.0113(9)	0.0145(9)	0.0160(8)
C(39)	0.099(1)	0.066(1)	0.052(1)	-0.041(1)	0.0117(10)	0.0165(9)
C(40)	0.075(1)	0.087(1)	0.062(1)	-0.044(1)	-0.0087(9)	0.0305(10)
C(41)	0.066(1)	0.066(1)	0.053(1)	-0.0237(9)	-0.0088(8)	0.0273(9)
B	0.0506(9)	0.0362(8)	0.0334(8)	-0.0050(7)	0.0025(7)	0.0121(7)

The general temperature factor expression:
$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table SIV. Table of bond distances

atom	atom	distance	atom	atom	distance
Ru	Cl	2.3917(7)	C(15)	C(16)	1.379(4)
Ru	N(1)	2.092(2)	C(16)	C(17)	1.382(4)
Ru	N(2)	2.016(2)	C(18)	C(19)	1.401(4)
Ru	N(3)	2.097(2)	C(18)	C(23)	1.389(3)
Ru	C(1)	1.912(3)	C(18)	B	1.642(4)
Ru	C(2)	1.873(3)	C(19)	C(20)	1.398(4)
O(1)	C(1)	1.122(3)	C(20)	C(21)	1.372(4)
O(2)	C(2)	1.126(3)	C(21)	C(22)	1.373(4)
N(1)	C(3)	1.349(3)	C(22)	C(23)	1.389(4)
N(1)	C(7)	1.361(3)	C(24)	C(25)	1.401(4)
N(2)	C(8)	1.339(3)	C(24)	C(29)	1.402(3)
N(2)	C(12)	1.345(3)	C(24)	B	1.647(4)
N(3)	C(13)	1.367(3)	C(25)	C(26)	1.388(4)
N(3)	C(17)	1.341(3)	C(26)	C(27)	1.371(4)
C(3)	C(4)	1.376(4)	C(27)	C(28)	1.393(4)
C(4)	C(5)	1.369(4)	C(28)	C(29)	1.385(4)
C(5)	C(6)	1.374(4)	C(30)	C(31)	1.402(4)
C(6)	C(7)	1.379(3)	C(30)	C(35)	1.395(3)
C(7)	C(8)	1.474(3)	C(30)	B	1.657(4)
C(8)	C(9)	1.380(3)	C(31)	C(32)	1.400(4)
C(9)	C(10)	1.388(4)	C(32)	C(33)	1.370(4)
C(10)	C(11)	1.378(4)	C(33)	C(34)	1.388(4)
C(11)	C(12)	1.383(3)	C(34)	C(35)	1.397(4)
C(12)	C(13)	1.476(3)	C(36)	C(37)	1.402(3)
C(13)	C(14)	1.381(3)	C(36)	C(41)	1.397(4)
C(14)	C(15)	1.376(4)	C(36)	B	1.650(4)
C(37)	C(38)	1.388(4)	C(38)	C(39)	1.373(4)
C(39)	C(40)	1.380(4)	C(40)	C(41)	1.392(4)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table SV. Table of bond angles

atom	atom	atom	angle	atom	atom	atom	angle
Cl	Ru	N(1)	86.97(6)	N(1)	C(3)	C(4)	122.3(2)
Cl	Ru	N(2)	86.21(5)	C(3)	C(4)	C(5)	119.4(3)
Cl	Ru	N(3)	88.77(5)	C(4)	C(5)	C(6)	119.0(3)
Cl	Ru	C(1)	86.4(1)	C(5)	C(6)	C(7)	120.1(3)
Cl	Ru	C(2)	178.39(9)	N(1)	C(7)	C(6)	121.0(2)
N(1)	Ru	N(2)	79.01(7)	N(1)	C(7)	C(8)	116.2(2)
N(1)	Ru	N(3)	157.14(7)	C(6)	C(7)	C(8)	122.8(2)
N(1)	Ru	C(1)	99.8(1)	N(2)	C(8)	C(7)	113.7(2)
N(1)	Ru	C(2)	93.1(1)	N(2)	C(8)	C(9)	119.4(2)
N(2)	Ru	N(3)	78.31(7)	C(7)	C(8)	C(9)	126.7(2)
N(2)	Ru	C(1)	172.6(1)	C(8)	C(9)	C(10)	118.4(2)
N(2)	Ru	C(2)	95.4(1)	C(9)	C(10)	C(11)	121.2(2)
N(3)	Ru	C(1)	102.30(9)	C(10)	C(11)	C(12)	118.2(2)
N(3)	Ru	C(2)	91.8(1)	N(2)	C(12)	C(11)	119.6(2)
C(1)	Ru	C(2)	92.0(1)	N(2)	C(12)	C(13)	113.7(2)
Ru	N(1)	C(3)	128.5(2)	C(11)	C(12)	C(13)	126.7(2)
Ru	N(1)	C(7)	113.1(2)	N(3)	C(13)	C(12)	115.1(2)
C(3)	N(1)	C(7)	118.3(2)	N(3)	C(13)	C(14)	121.6(2)
Ru	N(2)	C(8)	117.9(2)	C(12)	C(13)	C(14)	123.3(2)
Ru	N(2)	C(12)	118.6(1)	C(13)	C(14)	C(15)	119.5(2)
C(8)	N(2)	C(12)	123.0(2)	C(14)	C(15)	C(16)	119.0(2)
Ru	N(3)	C(13)	114.1(1)	C(15)	C(16)	C(17)	119.4(2)
Ru	N(3)	C(17)	127.7(2)	N(3)	C(17)	C(16)	122.3(2)
C(13)	N(3)	C(17)	118.2(2)	C(19)	C(18)	C(23)	115.8(2)
Ru	C(1)	O(1)	175.8(3)	C(19)	C(18)	B	123.1(2)
Ru	C(2)	O(2)	178.3(3)	C(23)	C(18)	B	120.9(2)
C(18)	C(19)	C(20)	122.1(3)	C(38)	C(39)	C(40)	118.8(3)

Table SV. (cont.)

atom	atom	atom	angle	atom	atom	atom	angle
C(19)	C(20)	C(21)	120.2(3)	C(39)	C(40)	C(41)	119.7(3)
C(20)	C(21)	C(22)	119.0(3)	C(36)	C(41)	C(40)	123.7(3)
C(21)	C(22)	C(23)	120.8(3)	C(18)	B	C(24)	107.5(2)
C(18)	C(23)	C(22)	122.2(3)	C(18)	B	C(30)	107.6(2)
C(25)	C(24)	C(29)	114.6(2)	C(18)	B	C(36)	110.6(2)
C(25)	C(24)	B	123.0(2)	C(24)	B	C(30)	109.8(2)
C(29)	C(24)	B	122.3(2)	C(24)	B	C(36)	112.4(2)
C(24)	C(25)	C(26)	122.2(3)	C(30)	B	C(36)	108.7(2)
C(25)	C(26)	C(27)	121.4(3)	C(26)	C(27)	C(28)	118.4(3)
C(27)	C(28)	C(29)	119.5(3)	C(24)	C(29)	C(28)	123.7(3)
C(31)	C(30)	C(35)	115.3(2)	C(31)	C(30)	B	122.3(2)
C(35)	C(30)	B	122.2(2)	C(30)	C(31)	C(32)	122.5(3)
C(31)	C(32)	C(33)	120.2(3)	C(32)	C(33)	C(34)	119.5(3)
C(33)	C(34)	C(35)	119.6(3)	C(30)	C(35)	C(34)	122.9(3)
C(37)	C(36)	C(41)	114.2(2)	C(37)	C(36)	B	124.4(2)
C(41)	C(36)	B	121.3(2)	C(36)	C(37)	C(38)	122.9(3)
C(37)	C(38)	C(39)	120.7(3)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table SVI. H-atom positional and thermal parameters

atoms	x	y	z	B_{eq}[a](Å^2)
H(4)	-0.0468	0.4866	0.8358	5.8
H(5)	0.1115	0.3777	0.7211	5.8
H(6)	0.0876	0.2071	0.5278	4.8
H(9)	0.0618	0.0545	0.3635	4.7
H(10)	0.0155	-0.1205	0.1992	5.2
H(11)	-0.1583	-0.1559	0.1653	4.3
H(14)	-0.3206	-0.1625	0.1567	3.9
H(15)	-0.5059	-0.1681	0.1599	4.7
H(16)	-0.6129	0.0062	0.3060	5.0
H(17)	-0.5244	0.1518	0.4515	4.5
H(19)	0.2994	0.4287	0.3912	5.8
H(20)	0.3517	0.4606	0.6326	6.5
H(21)	0.3487	0.3158	0.7170	5.5
H(22)	0.2925	0.1315	0.5540	4.9
H(23)	0.2201	0.1106	0.3271	4.0
H(25)	0.0826	0.3725	0.4091	5.1
H(26)	-0.1016	0.4346	0.4067	6.2
H(27)	-0.2146	0.4096	0.1944	5.9
H(28)	-0.1475	0.3199	-0.0119	5.4
H(29)	0.0436	0.2491	-0.0173	4.6
H(31)	0.0651	0.1019	0.1096	4.8
H(32)	0.0915	-0.1073	0.8000	6.0
H(33)	0.2686	-0.1961	-0.0888	6.0
H(34)	0.4051	-0.0940	-0.0626	5.4
H(35)	0.3740	0.1167	0.0587	4.4
H(37)	0.1392	0.3720	0.0061	4.4
H(38)	0.2429	0.4597	-0.0949	5.5

Table SVI. (cont.)

atoms	x	y	z	B_{eq}[a](Å2)
H(39)	0.4251	0.4511	-0.0352	6.5
H(40)	0.5109	0.3751	0.1368	6.7
H(41)	0.4159	0.2787	0.2137	5.6

a) $B_{eq} = 8/3\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos\gamma + 2U_{13}aa^*cc^* \cos\beta + 2U_{23}bb^*cc^* \cos\alpha)$

Table SVII. Table of data collection and refinement parameters for 7.

Empirical Formula	$C_{40.5}H_{30}F_{12}N_{7.75}O_5P_2Ru_2$
Formula Weight	1197.30
Crystal Color, Habit	orange, block
Crystal Dimensions	0.60 x 0.49 x 0.49 mm
Crystal System	triclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	25 (30.0 - 36.0°)
Omega Scan Peak Width at Half Height	0.50°
Lattice Parameters	a = 14.362(4) Å b = 14.596(3) Å c = 12.895(4) Å α = 93.54(2)° β = 114.80(2)° γ = 71.69(2)° V = 2321(1) Å^3
Space Group	P $\bar{1}$ (#2)
Z value	2
D_{calc}	1.712 g/cm^3
F_{000}	1186.50
μ(MoKα)	8.20 cm^{-1}
Diffractometer	CAD4

Table SVII. (cont.)

Radiation	MoKα (λ = 0.71073 Å) graphite monochromated
Attenuator	Zr foil (factor = 22.37)
Take-off Angle	2.8°
Detector Aperture	2.0 - 2.5 mm horizontal 2.0 mm vertical
Crystal to Detector Distance	21 mm
Temperature	23.(3)°C
Scan Type	ω-2θ
Scan Rate	1.0°-5.0°/min (in ω) (up to 2 scans)
Scan Width	(0.85 + 0.35 tanθ)°
$2\theta_{max}$	50.0°
No. of Reflections Measured	Total: 8488 Unique: 8139 (R_{int} = 0.016)
Corrections	Lorentz-polarization Absorption difabs (trans. factors: 0.5384 - 1.0000) Decay (5.9% decrease) Secondary Extinction (coefficient: 5.28688e-07)
Structure Solution	Direct Methods (SIR 92)
Refinement	Full-matrix least-squares
FunctionMinimized	$\Sigma\omega(\|Fo\| - \|Fc\|)^2$

Table SVII. (cont.)

Least Squares Weights	$[\sigma^2(F_o)]^{-1}$
p-factor	0.0230
Anomalous Dispersion	all non-hydrogen atoms
No. Observations (I>3.00σ(I))	6973
No. Variables	636
Reflection/Parameter Ratio	10.96
Residuals: R; R_w	0.040; 0.054
GOF	2.95
Max. Shift/Error in Final Cycle	0.01
Maximum Peak in Final Diff. Map	0.50 $e^-/Å^3$
Minimum Peak in Final Diff. Map	-0.77 $e^-/Å^3$
Computer Hardware	Silicon Graphics Iris Indigo
Computer Software	teXsan

Table SVIII. Positional and isotropic thermal parameters for non-H atoms

atom	x	y	z	B_{eq}[a](Å^2)	occ.
Ru(1)	0.18620(3)	0.17283(2)	0.62489(3)	3.526(8)	
Ru(2)	0.15060(2)	0.48520(2)	0.78557(3)	3.431(8)	
P(1)	0.7235(1)	0.4104(2)	0.7643(1)	7.31(5)	
P(2)	0.7011(1)	-0.0421(1)	0.7341(2)	7.05(4)	
F(1)	0.6634(3)	0.3612(4)	0.8084(4)	10.9(1)	
F(2)	0.7795(4)	0.4625(4)	0.7173(4)	13.1(2)	
F(3)	0.6312(3)	0.5104(4)	0.7457(5)	12.9(2)	
F(4)	0.8146(4)	0.3169(4)	0.7859(7)	12.2(2)	
F(5)	0.7862(4)	0.4411(3)	0.8837(3)	11.9(1)	
F(6)	0.6545(5)	0.3913(6)	0.6446(4)	12.2(2)	
F(7)	0.7313(4)	0.0510(3)	0.7227(5)	12.0(2)	
F(8)	0.6703(3)	-0.1350(3)	0.7453(4)	10.5(1)	
F(9a)	0.5923(4)	-0.0036(4)	0.6171(4)	9.8(2)	0.75
F(9b)	0.6663	-0.0498	0.6149	12(1)	0.25
F(10a)	0.8018(4)	-0.0778(3)	0.8504(4)	10.6(1)	0.75
F(10b)	0.7102	-0.0173	0.8479	11(1)	0.25
F(11a)	0.6332(6)	0.0193(4)	0.8003(6)	12.4(2)	0.75
F(11b)	0.5996	-0.0159	0.7272	13(1)	0.25
F(12a)	0.7638(4)	-0.0959(4)	0.6620(5)	9.2(2)	0.75
F(12b)	0.8181	-0.1131	0.7642	15.2(8)	0.25
O(1)	0.0227(2)	0.3531(2)	0.6285(3)	5.11(7)	
O(2)	0.1915(2)	0.3510(2)	0.7263(2)	3.89(6)	
O(3)	0.0223(3)	0.2384(2)	0.3844(3)	6.34(9)	
O(4)	-0.0841(3)	0.5611(2)	0.6099(3)	6.66(9)	
O(5)	0.1051(3)	0.6825(2)	0.8729(3)	6.54(10)	
N(1)	0.2288(3)	0.5212(2)	0.6980(3)	3.71(7)	

Table SVIII. (cont.)

atom	x	y	z	B_{eq}[a](Å^2)	occ.
N(2)	0.3062(3)	0.4325(2)	0.8999(3)	3.73(7)	
N(3)	0.1361(3)	0.4158(2)	0.9122(3)	4.12(8)	
N(4)	0.3066(3)	0.2145(2)	0.6146(3)	3.93(8)	
N(5)	0.3036(3)	0.1463(2)	0.7971(3)	3.99(8)	
N(6)	0.0856(3)	0.1094(2)	0.6534(3)	4.37(8)	
N(7)	0.2580(3)	0.0191(2)	0.6121(3)	4.26(8)	
N(100)	0.7383(6)	0.1620(6)	0.0800(8)	9.6(2)	0.75
C(1)	0.1204(3)	0.3111(3)	0.6610(3)	3.73(9)	
C(3)	0.0874(4)	0.2101(3)	0.4756(4)	4.3(1)	
C(4)	0.0033(4)	0.5268(3)	0.6722(4)	4.4(1)	
C(5)	0.1240(3)	0.6082(3)	0.8430(4)	4.3(1)	
C(6)	0.1841(4)	0.5677(3)	0.5936(4)	4.8(1)	
C(7)	0.2462(4)	0.5816(4)	0.5423(4)	5.7(1)	
C(8)	0.3549(5)	0.5490(4)	0.5982(5)	6.0(1)	
C(9)	0.4037(4)	0.5020(3)	0.7077(4)	5.0(1)	
C(10)	0.3393(3)	0.4886(3)	0.7557(4)	3.95(9)	
C(11)	0.3827(3)	0.4386(3)	0.8695(3)	3.93(9)	
C(12)	0.4904(3)	0.3972(3)	0.9446(4)	4.9(1)	
C(13)	0.5148(4)	0.3529(3)	1.0471(4)	5.4(1)	
C(14)	0.4349(4)	0.3464(3)	1.0749(4)	5.0(1)	
C(15)	0.3288(3)	0.3848(3)	0.9981(4)	4.18(10)	
C(16)	0.2313(4)	0.3754(3)	1.0042(4)	4.5(1)	
C(17)	0.2354(4)	0.3242(4)	1.0918(5)	6.1(1)	
C(18)	0.1399(5)	0.3146(4)	1.0859(5)	6.9(2)	
C(19)	0.0469(5)	0.3527(4)	0.9946(6)	6.6(2)	
C(20)	0.0450(4)	0.4040(3)	0.9073(5)	5.4(1)	

Table SVIII. (cont.)

atom	x	y	z	B_{eq}[a](Å^2)	occ.
C(21)	0.3012(4)	0.2522(3)	0.5190(4)	5.0(1)	
C(22)	0.3833(5)	0.2801(4)	0.5172(6)	6.6(2)	
C(23)	0.4755(5)	0.2670(4)	0.6163(6)	6.9(2)	
C(24)	0.4834(4)	0.2287(4)	0.7142(5)	5.6(1)	
C(25)	0.3967(3)	0.2027(3)	0.7126(4)	4.29(10)	
C(26)	0.3960(3)	0.1645(3)	0.8145(4)	4.4(1)	
C(27)	0.4796(4)	0.1489(3)	0.9211(5)	5.8(1)	
C(28)	0.4684(5)	0.1187(4)	1.0125(5)	6.9(1)	
C(29)	0.3756(5)	0.1038(4)	0.9987(5)	6.4(1)	
C(30)	0.2934(4)	0.1176(3)	0.8864(4)	5.3(1)	
C(31)	-0.0033(4)	0.1573(3)	0.6688(5)	5.5(1)	
C(32)	-0.0678(4)	0.1114(4)	0.6839(5)	6.4(2)	
C(33)	-0.0416(5)	0.0143(4)	0.6807(5)	6.7(2)	
C(34)	0.0490(4)	-0.0365(3)	0.6664(5)	5.7(1)	
C(35)	0.1123(4)	0.0112(3)	0.6524(4)	4.6(1)	
C(36)	0.2098(4)	-0.0387(3)	0.6328(4)	4.6(1)	
C(37)	0.2498(5)	-0.1368(3)	0.6335(5)	6.7(2)	
C(38)	0.3397(6)	-0.1767(4)	0.6109(6)	8.4(2)	
C(39)	0.3903(5)	-0.1180(4)	0.5922(6)	7.0(2)	
C(40)	0.3448(4)	-0.0205(3)	0.5929(4)	5.4(1)	
C(100)	0.8703(8)	0.1189(7)	-0.0072(8)	8.8(3)	0.75
C(101)	0.7956(7)	0.1433(6)	0.0405(8)	7.4(2)	0.75

a) $B_{eq} = 8/3\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos\gamma + 2U_{13}aa^*cc^* \cos\beta + 2U_{23}bb^*cc^* \cos\alpha)$

Table SIX. Table of general displacement parameter expressions-U's

atom	U11	U22	U33	U12	U13	U23
Ru(1)	0.0487(2)	0.0421(2)	0.0482(2)	-0.0153(1)	0.0226(2)	-0.0026(1)
Ru(2)	0.0404(2)	0.0457(2)	0.0449(2)	-0.0128(1)	0.0175(2)	-0.0048(1)
P(1)	0.0664(9)	0.160(2)	0.0712(10)	-0.047(1)	0.0390(8)	-0.0283(10)
P(2)	0.102(1)	0.088(1)	0.093(1)	-0.0202(9)	0.058(1)	-0.0033(9)
F(1)	0.102(3)	0.206(5)	0.122(3)	-0.039(3)	0.058(3)	0.038(3)
F(2)	0.157(4)	0.275(6)	0.161(4)	-0.145(4)	0.102(4)	-0.061(4)
F(3)	0.087(3)	0.199(5)	0.194(5)	-0.032(3)	0.045(3)	0.035(4)
F(4)	0.140(4)	0.165(5)	0.398(10)	-0.056(4)	0.156(6)	-0.153(6)
F(5)	0.154(4)	0.159(4)	0.094(3)	-0.027(3)	0.027(3)	-0.038(3)
F(6)	0.255(6)	0.423(9)	0.087(3)	-0.271(7)	0.062(4)	-0.060(4)
F(7)	0.196(5)	0.116(3)	0.189(5)	-0.071(3)	0.102(4)	-0.012(3)
F(8)	0.133(3)	0.114(3)	0.149(4)	-0.049(3)	0.040(3)	0.031(3)
F(9a)	0.080(3)	0.180(5)	0.093(4)	-0.031(3)	0.014(3)	0.057(3)
F(10a)	0.125(4)	0.084(3)	0.106(4)	-0.007(3)	-0.018(3)	-0.013(3)
F(11a)	0.217(6)	0.113(4)	0.151(5)	0.047(4)	0.147(5)	0.039(4)
F(12a)	0.112(4)	0.133(4)	0.139(5)	-0.041(3)	0.084(4)	-0.063(3)
O(1)	0.043(2)	0.052(2)	0.085(2)	-0.011(1)	0.014(2)	-0.010(2)
O(2)	0.040(1)	0.050(1)	0.055(2)	-0.015(1)	0.016(1)	-0.012(1)
O(3)	0.090(3)	0.073(2)	0.061(2)	-0.031(2)	0.009(2)	0.003(2)
O(4)	0.048(2)	0.061(2)	0.108(3)	-0.008(2)	-0.001(2)	0.004(2)
O(5)	0.121(3)	0.055(2)	0.078(2)	-0.022(2)	0.050(2)	-0.017(2)
N(1)	0.047(2)	0.054(2)	0.042(2)	-0.016(1)	0.019(2)	-0.006(1)
N(2)	0.045(2)	0.054(2)	0.042(2)	-0.017(2)	0.016(2)	-0.006(1)
N(3)	0.050(2)	0.055(2)	0.056(2)	-0.013(2)	0.026(2)	-0.002(2)
N(4)	0.053(2)	0.046(2)	0.061(2)	-0.014(2)	0.032(2)	-0.005(2)
N(5)	0.051(2)	0.048(2)	0.048(2)	-0.008(2)	0.020(2)	0.000(1)

Table SIX. (cont.)

atom	U11	U22	U33	U12	U13	U23
N(6)	0.055(2)	0.058(2)	0.061(2)	-0.023(2)	0.025(2)	0.000(2)
N(7)	0.063(2)	0.046(2)	0.057(2)	-0.014(2)	0.030(2)	-0.004(2)
N(100)	0.051(4)	0.155(7)	0.119(7)	-0.012(4)	0.005(4)	0.005(5)
C(1)	0.048(2)	0.045(2)	0.048(2)	-0.010(2)	0.020(2)	0.003(2)
C(3)	0.065(3)	0.044(2)	0.061(3)	-0.021(2)	0.027(2)	-0.004(2)
C(4)	0.053(3)	0.052(2)	0.065(3)	-0.017(2)	0.023(2)	-0.007(2)
C(5)	0.061(3)	0.059(3)	0.047(2)	-0.021(2)	0.025(2)	-0.009(2)
C(6)	0.061(3)	0.067(3)	0.049(3)	-0.015(2)	0.021(2)	-0.001(2)
C(7)	0.084(4)	0.083(3)	0.059(3)	-0.024(3)	0.038(3)	0.003(2)
C(8)	0.086(4)	0.086(3)	0.080(4)	-0.030(3)	0.054(3)	-0.007(3)
C(9)	0.054(3)	0.078(3)	0.069(3)	-0.025(2)	0.033(2)	-0.008(2)
C(10)	0.052(2)	0.052(2)	0.049(2)	-0.019(2)	0.021(2)	-0.006(2)
C(11)	0.044(2)	0.054(2)	0.053(3)	-0.019(2)	0.019(2)	-0.011(2)
C(12)	0.043(2)	0.068(3)	0.067(3)	-0.017(2)	0.016(2)	-0.008(2)
C(13)	0.047(3)	0.070(3)	0.067(3)	-0.012(2)	0.006(2)	-0.001(2)
C(14)	0.062(3)	0.070(3)	0.045(3)	-0.016(2)	0.010(2)	0.002(2)
C(15)	0.054(3)	0.055(2)	0.048(2)	-0.017(2)	0.018(2)	-0.004(2)
C(16)	0.062(3)	0.059(2)	0.055(3)	-0.018(2)	0.030(2)	-0.004(2)
C(17)	0.084(4)	0.078(3)	0.073(3)	-0.012(3)	0.038(3)	0.015(3)
C(18)	0.100(4)	0.092(4)	0.096(4)	-0.027(3)	0.063(4)	0.012(3)
C(19)	0.070(3)	0.088(4)	0.107(5)	-0.018(3)	0.050(4)	0.015(3)
C(20)	0.062(3)	0.068(3)	0.090(4)	-0.018(2)	0.044(3)	0.001(3)
C(21)	0.075(3)	0.062(3)	0.068(3)	-0.024(2)	0.040(3)	-0.005(2)
C(22)	0.105(5)	0.085(4)	0.101(5)	-0.040(3)	0.073(4)	-0.012(3)
C(23)	0.090(4)	0.091(4)	0.131(6)	-0.048(3)	0.076(4)	-0.031(4)
C(24)	0.056(3)	0.078(3)	0.092(4)	-0.026(2)	0.038(3)	-0.020(3)

Table SIX. (cont.)

atom	U11	U22	U33	U12	U13	U23
C(25)	0.050(2)	0.048(2)	0.068(3)	-0.012(2)	0.028(2)	-0.009(2)
C(26)	0.048(2)	0.047(2)	0.066(3)	-0.007(2)	0.020(2)	-0.009(2)
C(27)	0.058(3)	0.067(3)	0.074(4)	-0.009(2)	0.013(3)	-0.005(3)
C(28)	0.088(4)	0.075(3)	0.058(3)	-0.004(3)	0.006(3)	-0.001(3)
C(29)	0.105(4)	0.066(3)	0.059(3)	-0.002(3)	0.035(3)	0.011(2)
C(30)	0.080(3)	0.056(3)	0.070(3)	-0.011(2)	0.040(3)	0.004(2)
C(31)	0.066(3)	0.068(3)	0.092(4)	-0.024(2)	0.042(3)	-0.007(3)
C(32)	0.065(3)	0.093(4)	0.105(4)	-0.032(3)	0.044(3)	-0.001(3)
C(33)	0.084(4)	0.099(4)	0.096(4)	-0.051(3)	0.040(3)	0.004(3)
C(34)	0.071(3)	0.071(3)	0.084(4)	-0.038(3)	0.026(3)	0.002(3)
C(35)	0.062(3)	0.057(2)	0.057(3)	-0.027(2)	0.019(2)	0.001(2)
C(36)	0.067(3)	0.049(2)	0.057(3)	-0.022(2)	0.020(2)	0.000(2)
C(37)	0.103(4)	0.052(3)	0.115(5)	-0.025(3)	0.053(4)	0.001(3)
C(38)	0.138(6)	0.051(3)	0.150(6)	-0.018(3)	0.084(5)	-0.018(3)
C(39)	0.103(4)	0.062(3)	0.120(5)	-0.013(3)	0.072(4)	-0.011(3)
C(40)	0.085(3)	0.054(3)	0.081(3)	-0.016(2)	0.050(3)	-0.005(2)
C(100)	0.105(7)	0.113(7)	0.116(8)	-0.038(6)	0.044(6)	-0.039(6)
C(101)	0.060(5)	0.093(6)	0.097(7)	-0.018(4)	0.006(5)	-0.016(5)

The general temperature factor expression:
$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table SX. Table of bond distances

atom	atom	distance	atom	atom	distance
Ru(1)	N(4)	2.060(3)	P(2)	F(12a)	1.569(4)
Ru(1)	N(5)	2.116(3)	P(2)	F(12b)	1.568(2)
Ru(1)	N(6)	2.099(3)	O(1)	C(1)	1.232(4)
Ru(1)	N(7)	2.183(3)	O(2)	C(1)	1.297(5)
Ru(1)	C(1)	2.059(4)	O(3)	C(3)	1.151(5)
Ru(1)	C(3)	1.835(5)	O(4)	C(4)	1.132(5)
Ru(2)	O(2)	2.058(3)	O(5)	C(5)	1.118(5)
Ru(2)	N(1)	2.078(3)	N(1)	C(6)	1.341(5)
Ru(2)	N(2)	2.014(3)	N(1)	C(10)	1.370(5)
Ru(2)	N(3)	2.087(3)	N(2)	C(11)	1.339(5)
Ru(2)	C(4)	1.921(5)	N(2)	C(15)	1.348(5)
Ru(2)	C(5)	1.886(4)	N(3)	C(16)	1.358(5)
P(1)	F(1)	1.560(4)	N(3)	C(20)	1.348(5)
P(1)	F(2)	1.564(4)	N(4)	C(21)	1.344(6)
P(1)	F(3)	1.583(5)	N(4)	C(25)	1.348(5)
P(1)	F(4)	1.508(5)	N(5)	C(26)	1.358(6)
P(1)	F(5)	1.545(4)	N(5)	C(30)	1.328(6)
P(1)	F(6)	1.510(4)	N(6)	C(31)	1.340(5)
P(2)	F(7)	1.583(4)	N(6)	C(35)	1.364(5)
P(2)	F(8)	1.583(4)	N(7)	C(36)	1.347(5)
P(2)	F(9a)	1.615(5)	N(7)	C(40)	1.319(5)
P(2)	F(9b)	1.412(2)	N(100)	C(101)	1.10(1)
P(2)	F(10a)	1.554(5)	C(6)	C(7)	1.380(6)
P(2)	F(10b)	1.451(2)	C(7)	C(8)	1.347(7)
P(2)	F(11a)	1.593(5)	C(8)	C(9)	1.394(7)
P(2)	F(11b)	1.350(2)	C(9)	C(10)	1.374(6)

Table SX. (cont.)

atom	atom	distance	atom	atom	distance
C(10)	C(11)	1.469(6)	C(38)	C(39)	1.374(8)
C(11)	C(12)	1.387(6)	C(39)	C(40)	1.368(6)
C(12)	C(13)	1.365(7)	C(100)	C(101)	1.39(1)
C(13)	C(14)	1.368(7)	C(14)	C(15)	1.373(6)
C(15)	C(16)	1.483(6)	C(16)	C(17)	1.364(6)
C(17)	C(18)	1.392(7)	C(18)	C(19)	1.333(8)
C(19)	C(20)	1.376(7)	C(21)	C(22)	1.371(7)
C(22)	C(23)	1.368(8)	C(23)	C(24)	1.359(8)
C(24)	C(25)	1.404(6)	C(25)	C(26)	1.463(6)
C(26)	C(27)	1.366(7)	C(27)	C(28)	1.371(8)
C(28)	C(29)	1.354(8)	C(29)	C(30)	1.408(7)
C(31)	C(32)	1.379(6)	C(32)	C(33)	1.350(7)
C(33)	C(34)	1.362(7)	C(34)	C(35)	1.376(6)
C(35)	C(36)	1.480(6)	C(36)	C(37)	1.364(6)
C(37)	C(38)	1.382(8)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table SXI. Table of bond angles

atom	atom	atom	angle	atom	atom	atom	angle
N(4)	Ru(1)	N(5)	78.2(1)	N(2)	Ru(2)	C(5)	95.7(2)
N(4)	Ru(1)	N(6)	170.0(1)	N(3)	Ru(2)	C(4)	100.9(2)
N(4)	Ru(1)	N(7)	95.3(1)	N(3)	Ru(2)	C(5)	94.9(2)
N(4)	Ru(1)	C(1)	89.3(1)	C(4)	Ru(2)	C(5)	88.3(2)
N(4)	Ru(1)	C(3)	96.8(2)	F(1)	P(1)	F(2)	177.8(3)
N(5)	Ru(1)	N(6)	94.6(1)	F(1)	P(1)	F(3)	89.3(2)
N(5)	Ru(1)	N(7)	85.2(1)	F(1)	P(1)	F(4)	91.6(3)
N(5)	Ru(1)	C(1)	88.3(1)	F(1)	P(1)	F(5)	93.7(3)
N(5)	Ru(1)	C(3)	172.9(1)	F(1)	P(1)	F(6)	87.7(2)
N(6)	Ru(1)	N(7)	77.1(1)	F(2)	P(1)	F(3)	88.8(3)
N(6)	Ru(1)	C(1)	97.5(1)	F(2)	P(1)	F(4)	90.3(3)
N(6)	Ru(1)	C(3)	91.0(2)	F(2)	P(1)	F(5)	87.3(3)
N(7)	Ru(1)	C(1)	171.1(1)	F(2)	P(1)	F(6)	91.2(3)
N(7)	Ru(1)	C(3)	100.3(2)	F(3)	P(1)	F(4)	177.6(3)
C(1)	Ru(1)	C(3)	86.6(2)	F(3)	P(1)	F(5)	86.9(3)
O(2)	Ru(2)	N(1)	84.3(1)	F(3)	P(1)	F(6)	87.2(4)
O(2)	Ru(2)	N(2)	80.7(1)	F(4)	P(1)	F(5)	90.8(3)
O(2)	Ru(2)	N(3)	86.8(1)	F(4)	P(1)	F(6)	95.0(4)
O(2)	Ru(2)	C(4)	95.3(1)	F(5)	P(1)	F(6)	174.0(4)
O(2)	Ru(2)	C(5)	175.6(1)	F(7)	P(2)	F(8)	179.8(3)
N(1)	Ru(2)	N(2)	79.0(1)	F(7)	P(2)	F(9a)	89.3(3)
N(1)	Ru(2)	N(3)	157.0(1)	F(7)	P(2)	F(9b)	89.8(2)
N(1)	Ru(2)	C(4)	101.1(2)	F(7)	P(2)	F(10a)	91.6(3)
N(1)	Ru(2)	C(5)	92.6(2)	F(7)	P(2)	F(10b)	88.5(2)
N(2)	Ru(2)	N(3)	78.6(1)	F(7)	P(2)	F(11a)	87.8(3)
N(2)	Ru(2)	C(4)	176.0(1)	F(7)	P(2)	F(11b)	110.1(2)
F(7)	P(2)	F(12a)	89.2(3)	F(10a)	P(2)	F(12a)	93.4(3)

Table SXI. (cont.)

atom	atom	atom	angle	atom	atom	atom	angle
F(7)	P(2)	F(12b)	93.9(2)				
F(8)	P(2)	F(9a)	90.5(3)				
F(8)	P(2)	F(9b)	90.1(2)	F(10b)	P(2)	F(11b)	74.13(7)
F(8)	P(2)	F(10a)	88.6(3)				
F(8)	P(2)	F(10b)	91.5(2)	F(10b)	P(2)	F(12b)	100.3(1)
F(8)	P(2)	F(11a)	92.1(3)				
F(8)	P(2)	F(11b)	69.7(2)	F(11a)	P(2)	F(12a)	175.7(3)
F(8)	P(2)	F(12a)	90.9(3)				
F(8)	P(2)	F(12b)	86.4(2)				
				F(11b)	P(2)	F(12b)	155.0(1)
F(9a)	P(2)	F(10a)	176.9(3)				
				Ru(2)	O(2)	C(1)	123.1(2)
F(9a)	P(2)	F(11a)	87.3(4)	Ru(2)	N(1)	C(6)	127.8(3)
				Ru(2)	N(1)	C(10)	113.4(3)
F(9a)	P(2)	F(12a)	89.6(3)	C(6)	N(1)	C(10)	118.7(3)
				Ru(2)	N(2)	C(11)	118.0(3)
				Ru(2)	N(2)	C(15)	118.5(3)
F(9b)	P(2)	F(10b)	165.9(1)	C(11)	N(2)	C(15)	123.1(4)
				Ru(2)	N(3)	C(16)	114.1(3)
F(9b)	P(2)	F(11b)	93.3(1)	Ru(2)	N(3)	C(20)	126.6(3)
				C(16)	N(3)	C(20)	119.3(4)
F(9b)	P(2)	F(12b)	93.82(8)	Ru(1)	N(4)	C(21)	125.0(3)
				Ru(1)	N(4)	C(25)	116.1(3)
F(10a)	P(2)	F(11a)	89.8(4)	C(21)	N(4)	C(25)	118.8(4)
				Ru(1)	N(5)	C(26)	114.4(3)
Ru(1)	N(5)	C(30)	126.6(3)	C(13)	C(14)	C(15)	119.3(4)
C(26)	N(5)	C(30)	119.0(4)	N(2)	C(15)	C(14)	118.8(4)

Table SXI. (cont.)

atom	atom	atom	angle	atom	atom	atom	angle
Ru(1)	N(6)	C(31)	125.7(3)	N(2)	C(15)	C(16)	113.0(4)
Ru(1)	N(6)	C(35)	116.4(3)	C(14)	C(15)	C(16)	128.1(4)
C(31)	N(6)	C(35)	117.9(4)	N(3)	C(16)	C(15)	115.7(4)
Ru(1)	N(7)	C(36)	114.4(3)	N(3)	C(16)	C(17)	120.8(4)
Ru(1)	N(7)	C(40)	126.5(3)	C(15)	C(16)	C(17)	123.3(4)
C(36)	N(7)	C(40)	119.0(4)	C(16)	C(17)	C(18)	118.9(5)
Ru(1)	C(1)	O(1)	124.6(3)	C(17)	C(18)	C(19)	120.3(5)
Ru(1)	C(1)	O(2)	114.1(3)	C(18)	C(19)	C(20)	119.7(5)
O(1)	C(1)	O(2)	121.3(4)	N(3)	C(20)	C(19)	121.1(5)
Ru(1)	C(3)	O(3)	175.9(4)	N(4)	C(21)	C(22)	122.6(5)
Ru(2)	C(4)	O(4)	172.5(4)	C(21)	C(22)	C(23)	118.7(5)
Ru(2)	C(5)	O(5)	177.2(4)	C(22)	C(23)	C(24)	120.0(5)
N(1)	C(6)	C(7)	121.8(4)	C(23)	C(24)	C(25)	119.5(5)
C(6)	C(7)	C(8)	119.7(5)	N(4)	C(25)	C(24)	120.4(4)
C(7)	C(8)	C(9)	119.8(4)	N(4)	C(25)	C(26)	116.1(4)
C(8)	C(9)	C(10)	118.9(4)	C(24)	C(25)	C(26)	123.5(4)
N(1)	C(10)	C(9)	121.1(4)	N(5)	C(26)	C(25)	115.1(4)
N(1)	C(10)	C(11)	115.8(3)	N(5)	C(26)	C(27)	120.8(5)
C(9)	C(10)	C(11)	123.1(4)	C(25)	C(26)	C(27)	124.1(4)
N(2)	C(11)	C(10)	113.7(3)	C(26)	C(27)	C(28)	119.6(5)
N(2)	C(11)	C(12)	118.6(4)	C(27)	C(28)	C(29)	120.9(5)
C(10)	C(11)	C(12)	127.7(4)	C(28)	C(29)	C(30)	117.1(5)
C(11)	C(12)	C(13)	119.0(4)	N(5)	C(30)	C(29)	122.4(5)
C(12)	C(13)	C(14)	121.0(4)	N(6)	C(31)	C(32)	122.8(4)
C(31)	C(32)	C(33)	118.6(5)	C(32)	C(33)	C(34)	119.9(4)
C(33)	C(34)	C(35)	120.2(5)	N(6)	C(35)	C(34)	120.5(4)
N(6)	C(35)	C(36)	116.2(3)	C(34)	C(35)	C(36)	123.2(4)

Table SXI. (cont.)

atom	atom	atom	angle	atom	atom	atom	angle
N(7)	C(36)	C(35)	115.8(4)	N(7)	C(36)	C(37)	120.6(4)
C(35)	C(36)	C(37)	123.6(4)	C(36)	C(37)	C(38)	119.4(5)
C(37)	C(38)	C(39)	120.0(5)	C(38)	C(39)	C(40)	116.8(5)
N(7)	C(40)	C(39)	124.2(5)	N(100)	C(101)	C(100)	179(1)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table SXII. H-atom positional and thermal parameters

atom	x	y	z	B_{eq}(Å^2)
H(6)	0.1061	0.5906	0.5522	5.5
H(7)	0.2112	0.6145	0.4672	6.7
H(8)	0.3995	0.5575	0.5640	7.2
H(9)	0.4816	0.4791	0.7493	5.9
H(12)	0.5462	0.3992	0.9239	5.8
H(13)	0.5879	0.3263	1.0996	6.5
H(14)	0.4533	0.3154	1.1473	6.0
H(17)	0.3048	0.2955	1.1576	7.4
H(18)	0.1424	0.2815	1.1501	8.4
H(19)	-0.0180	0.3438	0.9894	7.9
H(20)	-0.0235	0.4316	0.8411	6.4
H(21)	0.2356	0.2619	0.4494	5.9
H(22)	0.3743	0.3077	0.4468	7.6
H(23)	0.5321	0.2847	0.6138	8.4
H(24)	0.5471	0.2200	0.7841	6.7
H(27)	0.5454	0.1596	0.9323	7.1
H(28)	0.5270	0.1092	1.0868	8.0
H(29)	0.3659	0.0841	1.0614	7.7
H(30)	0.2278	0.1065	0.8750	6.4
H(31)	-0.0238	0.2272	0.6677	6.6
H(32)	-0.1297	0.1498	0.6956	7.4
H(33)	-0.0875	-0.0149	0.6907	8.0
H(34)	0.0659	-0.1040	0.6622	7.1
H(37)	0.2152	-0.1778	0.6477	8.0
H(38)	0.3662	-0.2453	0.6086	9.7
H(39)	0.4525	-0.1446	0.5779	8.4

Table SXII. (cont.)

atom	x	y	z	B_{eq}(Å^2)
H(40)	0.3791	0.0216	0.5797	6.2
H(100c)	0.9406	0.1221	0.0440	10.1
H(100a)	0.8840	0.0511	-0.0305	10.1
H(100b)	0.8484	0.1577	-0.0777	10.1

a) $B_{eq} = 8/3\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos\gamma + 2U_{13}aa^*cc^* \cos\beta + 2U_{23}bb^*cc^* \cos\alpha)$