

Figure S1. Quantitative electronic spectrum of Ru(bpy)(trpy)(2,4-Cl₂pcyd)PF₆ (6.17×10^{-5} M in acetonitrile)

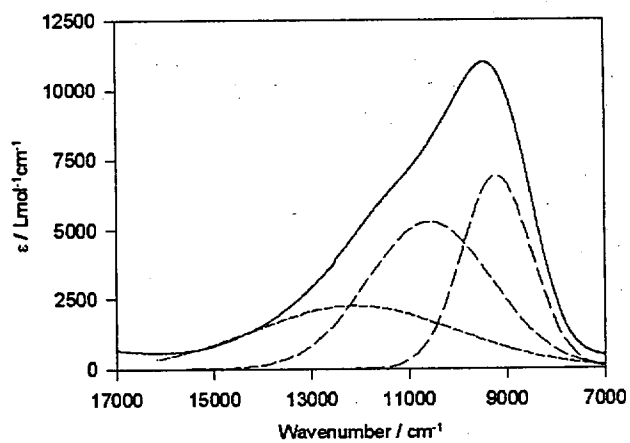


Figure S2. Electronic spectrum of $[\text{Ru}(\text{bpy})(\text{trpy})(2,3,4,5\text{-Cl}_4\text{pcyd})]^{2+}$ showing the best fit of three Gaussian curves used for the calculation of oscillator strength.

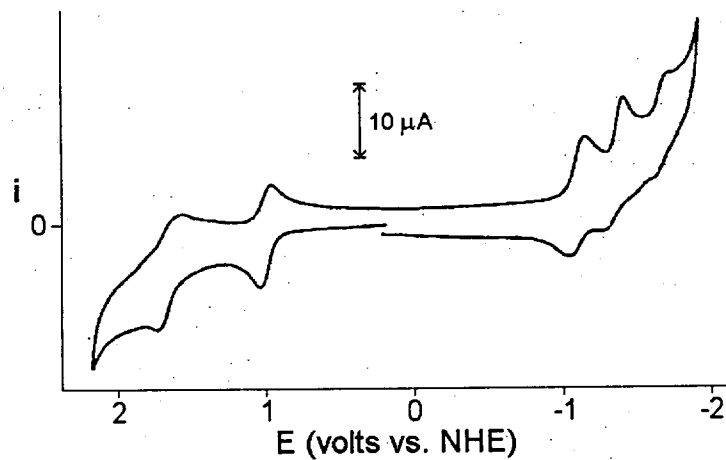


Figure S3. Cyclic voltammogram of $[\text{Ru}(\text{bpy})(\text{trpy})(2,4\text{-Cl}_2\text{pcyd})]\text{PF}_6$ (1 mM in acetonitrile) at a scan rate of 75 mV/s; 0.1M TBAH; ferrocene ($E^\circ = 0.665$ V vs. NHE) was used as an internal reference.

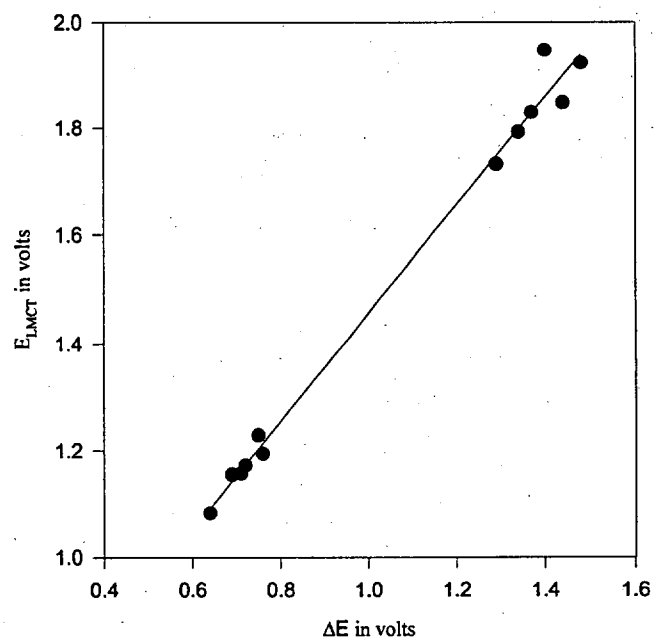


Figure S4. Plot of E_{LMCT} versus $L(0/-)-Ru(III/II)$, using the data in Table 2 and 3, The equation of the line is $y = 1.01x + 0.45$ and the square of the correlation coefficient = 0.99.

Complex Syntheses and Characterization

[Ru(bpy)(trpy)(3-Clpcyd)][PF₆]·H₂O was prepared in the same manner as above. Yield:

0.28g (68%). $\nu(\text{NCN})$: 2174, 2132 cm^{-1} ; $^1\text{H NMR}$ (400 MHz, DMSO- d_6): 9.63(d, 1H), 8.94(d, 1H), 8.88(d, 2H), 8.76(d, 2H), 8.67(d, 1H), 8.39(t, 1H), 8.30(t, 1H), 8.06(m, 3H), 7.84(t, 1H), 7.71(d, 2H), 7.43(m, 3H), 6.79(t, 1H), 6.45(d, 1H), 5.95(d, 1H), 5.83(s, 1H). Anal. Calcd for [Ru(bpy)(trpy)(3-Clpcyd)][PF₆]·H₂O (C₃₂H₂₅N₇OPClF₆Ru): C, 47.74; H, 3.13; N, 12.18. Found: C, 48.33; H, 3.18; N, 12.05.

Multiple $\nu(\text{NCN})$ bands where only one is expected have been seen observed previously and are likely due to crystal packing forces. See Crutchley, R. J.; Hynes, R.; Gabe, E. J. *Inorg. Chem.* **1990**, *29*, 4921

[Ru(bpy)(trpy)(2,4-Cl₂pcyd)][PF₆]·DMF was prepared in the same manner as above.

Yield: 0.38 g (89%). $\nu(\text{NCN})$: 2167 cm^{-1} ; $^1\text{H NMR}$ (400 MHz, DMSO- d_6): 9.63(d, 1H), 8.94(d, 1H), 8.87(d, 2H), 8.75(d, 2H), 8.67(d, 1H), 8.39(t, 1H), 8.31(t, 1H), 8.08(m, 3H), 7.84(t, 1H), 7.71(d, 2H), 7.44(m, 3H), 7.14(t, 1H), 7.08(d, 1H), 6.75(m, 1H), 5.73(d, 1H). Anal. Calcd for [Ru(bpy)(trpy)(2,4-Cl₂pcyd)][PF₆]·DMF (C₃₅H₂₉N₈OPCl₂F₆Ru): C, 46.99; H, 3.27; N, 12.53. Found: C, 46.86; H, 3.34; N, 12.47.

[Ru(bpy)(trpy)(2,4,5-Cl₃pcyd)][PF₆]·DMF was prepared in the same manner as above.

Yield: 0.32g (74%). $\nu(\text{NCN})$: 2181 cm^{-1} ; $^1\text{H NMR}$ (400 MHz, DMSO- d_6): 9.61(d, 1H), 8.94(d, 1H), 8.90(d, 2H), 8.77(d, 2H), 8.68(d, 1H), 8.39(t, 1H), 8.33(t, 1H), 8.08(m, 3H), 7.85(t, 1H), 7.72(d, 2H), 7.45(m, 3H), 7.29(s, 1H), 7.14(t, 1H), 5.80(s, 1H). Anal. Calcd

for $[\text{Ru}(\text{bpy})(\text{trpy})(2,4,5\text{-Cl}_3\text{pcyd})][\text{PF}_6]\cdot\text{DMF}$ ($\text{C}_{35}\text{H}_{28}\text{N}_8\text{OPCl}_3\text{F}_6\text{Ru}$): C, 45.25; H, 3.04; N, 12.06. Found: C, 45.28; H, 3.25; N, 12.09.

$[\text{Ru}(\text{bpy})(\text{trpy})(2,4,6\text{-Cl}_3\text{pcyd})][\text{PF}_6]\cdot 1/5\text{toluene}$ was prepared in the same manner as above, but required further purification. The crude product (0.16 g) was dissolved in 25 mL of 1:1 MeCN/toluene, filtered, and purified by chromatography on a 50 cm x 3 cm diameter column containing ~250 g grade III alumina (Brockmann I, weakly acidic, 150 mesh) using 1:1 MeCN/toluene as the eluent. Three bands separated out on the column. The first band was eluted in ~100 mL and contained the target complex, which crystallized from the solution upon evaporation of the MeCN. Yield: 0.03g (10%).

$\nu(\text{NCN})$: 2169 cm^{-1} ; $^1\text{H NMR}$ (400 MHz, DMSO-d_6): 9.62(d, 1H), 8.93(d, 1H), 8.87(d, 2H), 8.74(d, 2H), 8.67(d, 1H), 8.34(m, 2H), 8.09(m, 3H), 7.83(t, 1H), 7.69(d, 2H), 7.42(t, 2H), 7.34(d, 1H), 7.12(t, 1H), 7.06(s, 2H); Anal. Calcd for $[\text{Ru}(\text{bpy})(\text{trpy})(2,4,6\text{-Cl}_3\text{pcyd})][\text{PF}_6]\cdot 1/5\text{toluene}$ ($\text{C}_{33.4}\text{H}_{22.6}\text{N}_7\text{PCl}_3\text{F}_6\text{Ru}$): C, 45.89; H, 2.61; N, 11.21. Found: C, 45.91; H, 2.68; N, 11.04.

$[\text{Ru}(\text{bpy})(\text{trpy})(2,3,4,5\text{-Cl}_4\text{pcyd})][\text{PF}_6]$ was prepared in the same manner as above.

Yield: 0.35 g (78%). $\nu(\text{NCN})$: 2167 cm^{-1} ; $^1\text{H NMR}$ (400 MHz, DMSO-d_6): 9.60(d, 1H), 8.95(d, 1H), 8.90(d, 2H), 8.78(d, 2H), 8.68(d, 1H), 8.39(t, 1H), 8.34(t, 1H), 8.08(m, 3H), 7.86(t, 1H), 7.72(d, 2H), 7.45(m, 3H), 7.15(t, 1H), 5.81(s, 1H). Anal. Calcd for $[\text{Ru}(\text{bpy})(\text{trpy})(2,3,4,5\text{-Cl}_4\text{pcyd})][\text{PF}_6]$ ($\text{C}_{32}\text{H}_{20}\text{N}_7\text{PCl}_4\text{F}_6\text{Ru}$): C, 43.17; H, 2.26; N, 11.01. Found: C, 42.80; H, 2.45; N, 10.95.

$[\text{Ru}(\text{bpy})(\text{trpy})(2,3,5,6\text{-Cl}_4\text{pcyd})][\text{PF}_6]$ was prepared in the same manner as above, and purified by column chromatography. Yield: 0.04 g (9%). $\nu(\text{NCN})$: 2181 cm^{-1} ; $^1\text{H NMR}$ (400 MHz, DMSO-d_6): 9.60(d, 1H), 8.93(d, 1H), 8.88(d, 2H), 8.75(d, 2H), 8.67(d, 1H),

8.39(t, 1H), 8.32(t, 1H), 8.12(t, 1H); 8.07(t, 2H), 7.83(t, 1H), 7.70(d, 2H), 7.43(t, 2H), 7.35(t, 1H), 7.13(t, 1H), 7.01(s, 1H). Anal. Calcd for [Ru(bpy)(trpy)(2,3,5,6-Cl₄pcyd)][PF₆] (C₃₂H₂₀N₇PCl₄F₆Ru): C, 43.17; H, 2.26; N, 11.01. Found: C, 42.83; H, 2.25; N, 10.70.

[Ru(bpy)(trpy)(Cl₅-pcyd)][PF₆]·1/3toluene was prepared in the same manner as above, and purified by column chromatography. Yield: 0.06 g (20%). $\nu(\text{NCN})$: 2184 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) 9.60(d, 1H), 8.93(d, 1H), 8.88(d, 2H), 8.75(d, 2H), 8.67(d, 1H), 8.39(t, 1H), 8.33(t, 1H), 8.12(t, 1H), 8.07(t, 2H), 7.84(t, 1H), 7.71(d, 2H), 7.44(t, 2H), 7.35(d, 1H), 7.14(t, 1H). Anal. Calcd for [Ru(bpy)(trpy)(Cl₅-pcyd)][PF₆]·1/3toluene (C_{34.3}H_{21.7}N₇PCl₅F₆Ru): C, 43.16; H, 2.29; N, 10.26. Found: C, 43.52; H, 2.41; N, 10.30.

Most of these complexes required the addition of a solvent of crystallization to their molecular formulae. While the crystal structure of [Ru(bpy)(trpy)(2,4-Cl₂pcyd)][PF₆]·DMF clearly established the presence of DMF, the presence of toluene or DMF solvent of crystallization for the other complexes was demonstrated by ¹H-NMR spectroscopy. The cyclic voltammograms of these complexes showed no evidence of redox active impurities.

Table 1. Crystal data and structure refinement for $[\text{Ru}(\text{bpy})(\text{trpy})(2,4\text{-6l}_2\text{pcyd})]\text{PF}_6 \cdot \text{DMF}$

Identification code	rc008
Empirical formula	C ₃₅ H ₂₉ Cl ₂ F ₆ N ₈ O P Ru
Formula weight	894.60
Temperature	238(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 11.681(4) Å alpha = 68.00(2) deg. b = 12.240(5) Å beta = 70.05(3) deg. c = 15.017(5) Å gamma = 78.55(2) deg.
Volume	1865(1) Å ³
Z, Calculated density	2, 1.593 Mg/m ³
Absorption coefficient	0.678 mm ⁻¹
F(000)	900
Crystal size	0.10 x 0.08 x 0.05 mm
Theta range for data collection	1.86 to 26.37 deg.
Limiting indices	-13 ≤ h ≤ 14, -13 ≤ k ≤ 15, 0 ≤ l ≤ 14
Reflections collected / unique	9530 / 4848 [R(int) = 0.0636]
Completeness to theta = 26.37	63.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.928077 and 0.407972
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4848 / 51 / 450
Goodness-of-fit on F ²	1.100
Final R indices [I > 2σ(I)]	R1 = 0.0722, wR2 = 0.2122
R indices (all data)	R1 = 0.0955, wR2 = 0.2397
Largest diff. peak and hole	0.889 and -0.862 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for rc008. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ru	7409(1)	6358(1)	5826(1)	29(1)
P	7504(3)	2367(2)	11384(3)	56(1)
Cl(1)	9354(4)	184(3)	5946(5)	132(2)
Cl(2)	5776(11)	-1462(8)	9283(8)	315(7)
F(1)	7952(7)	3667(6)	10866(7)	94(3)
F(2)	7058(8)	2521(7)	12467(6)	95(3)
F(3)	7062(6)	1068(6)	11906(7)	83(3)
F(4)	7962(8)	2214(8)	10294(7)	105(3)
F(5)	8811(6)	1854(6)	11570(6)	87(3)
F(6)	6180(6)	2889(6)	11246(7)	87(3)
N(1)	5811(6)	6205(6)	5582(8)	25(3)
N(2)	6406(6)	5663(7)	7217(7)	38(3)
N(3)	8584(6)	6344(6)	6609(8)	36(2)
N(4)	6926(6)	8113(6)	5581(7)	38(2)
N(5)	8437(5)	7083(6)	4343(7)	35(2)
N(6)	8024(5)	4612(6)	5900(6)	31(2)
N(7)	8464(6)	2551(6)	6046(7)	47(3)
C(1)	5537(8)	6613(8)	4711(11)	35(4)
C(2)	4394(8)	6521(8)	4649(9)	39(3)
C(3)	3508(8)	6010(9)	5516(12)	52(4)
C(4)	3767(7)	5583(8)	6435(10)	40(4)
C(5)	4942(8)	5713(8)	6447(10)	34(3)
C(6)	5285(8)	5311(8)	7362(11)	34(4)
C(7)	4699(10)	4582(9)	8324(11)	46(4)
C(8)	5183(11)	4269(10)	9120(11)	56(4)
C(9)	6321(10)	4639(9)	8966(10)	51(4)
C(10)	6912(8)	5324(8)	7994(10)	40(3)
C(11)	8129(9)	5788(8)	7657(10)	39(3)
C(12)	8791(10)	5725(10)	8297(11)	55(3)
C(13)	9882(9)	6240(11)	7924(13)	60(4)
C(14)	10319(9)	6790(11)	6908(13)	64(5)
C(15)	9654(7)	6821(8)	6266(9)	45(3)
C(16)	6091(8)	8590(8)	6265(9)	45(3)
C(17)	5826(11)	9800(11)	6014(12)	66(4)
C(18)	6390(12)	10534(10)	5088(13)	76(5)
C(19)	7226(9)	10069(8)	4400(10)	54(3)
C(20)	7483(7)	8855(7)	4634(9)	34(3)
C(21)	8319(7)	8293(7)	3939(9)	41(3)
C(22)	8976(8)	8876(9)	2921(9)	47(3)
C(23)	9712(9)	8242(10)	2311(10)	55(3)
C(24)	9806(8)	7037(10)	2720(10)	51(3)
C(25)	9166(7)	6473(7)	3717(9)	37(3)
C(26)	8169(7)	3629(8)	6025(7)	30(3)
C(27)	8196(8)	480(7)	6844(9)	95(6)
C(28)	7576(12)	-471(5)	7583(11)	127(9)
C(29)	6582(12)	-286(10)	8361(9)	158(12)
C(30)	6207(9)	851(12)	8398(7)	147(9)
C(31)	6827(7)	1803(8)	7659(8)	104(5)
C(32)	7822(7)	1617(5)	6882(7)	59(3)

O	3261 (10)	2794 (11)	7762 (10)	120 (4)
N(8)	1964 (9)	1800 (9)	9255 (9)	70 (3)
C(33)	2903 (12)	1843 (14)	8382 (13)	88 (4)
C(34)	1456 (16)	2870 (16)	9425 (15)	123 (6)
C(35)	1562 (15)	658 (14)	9950 (14)	111 (5)

Table 3. Bond lengths [Å] and angles [deg] for rc008.

Ru-N(2)	1.962 (9)
Ru-N(4)	2.035 (6)
Ru-N(5)	2.076 (8)
Ru-N(1)	2.076 (8)
Ru-N(3)	2.084 (8)
Ru-N(6)	2.088 (7)
P-F(3)	1.588 (7)
P-F(1)	1.593 (7)
P-F(2)	1.601 (8)
P-F(6)	1.603 (7)
P-F(5)	1.607 (7)
P-F(4)	1.610 (9)
Cl(1)-C(27)	1.645 (11)
Cl(2)-C(29)	1.741 (8)
N(1)-C(1)	1.339 (13)
N(1)-C(5)	1.355 (13)
N(2)-C(10)	1.377 (14)
N(2)-C(6)	1.381 (12)
N(3)-C(15)	1.339 (11)
N(3)-C(11)	1.413 (13)
N(4)-C(16)	1.373 (11)
N(4)-C(20)	1.381 (13)
N(5)-C(21)	1.372 (11)
N(5)-C(25)	1.377 (11)
N(6)-C(26)	1.132 (10)
N(7)-C(26)	1.288 (10)
N(7)-C(32)	1.437 (10)
C(1)-C(2)	1.400 (13)
C(2)-C(3)	1.373 (16)
C(3)-C(4)	1.396 (15)
C(4)-C(5)	1.420 (12)
C(5)-C(6)	1.443 (15)
C(6)-C(7)	1.397 (16)
C(7)-C(8)	1.389 (17)
C(8)-C(9)	1.405 (16)
C(9)-C(10)	1.391 (16)
C(10)-C(11)	1.488 (14)
C(11)-C(12)	1.397 (15)
C(12)-C(13)	1.380 (15)
C(13)-C(14)	1.370 (17)
C(14)-C(15)	1.416 (16)
C(16)-C(17)	1.383 (14)
C(17)-C(18)	1.359 (18)
C(18)-C(19)	1.370 (16)
C(19)-C(20)	1.388 (11)
C(20)-C(21)	1.446 (14)
C(21)-C(22)	1.427 (15)
C(22)-C(23)	1.382 (14)
C(23)-C(24)	1.367 (15)
C(24)-C(25)	1.395 (15)
C(27)-C(28)	1.3900
C(27)-C(32)	1.3900
C(28)-C(29)	1.3900
C(29)-C(30)	1.3900
C(30)-C(31)	1.3900
C(31)-C(32)	1.3900

O-C(33)	1.230(17)
N(8)-C(33)	1.383(17)
N(8)-C(34)	1.405(18)
N(8)-C(35)	1.448(18)
N(2)-Ru-N(4)	101.5(3)
N(2)-Ru-N(5)	178.5(3)
N(4)-Ru-N(5)	78.7(3)
N(2)-Ru-N(1)	79.7(4)
N(4)-Ru-N(1)	89.4(3)
N(5)-Ru-N(1)	98.8(3)
N(2)-Ru-N(3)	79.4(3)
N(4)-Ru-N(3)	91.4(3)
N(5)-Ru-N(3)	102.1(3)
N(1)-Ru-N(3)	158.8(4)
N(2)-Ru-N(6)	85.2(3)
N(4)-Ru-N(6)	173.3(3)
N(5)-Ru-N(6)	94.6(3)
N(1)-Ru-N(6)	91.2(2)
N(3)-Ru-N(6)	90.5(3)
F(3)-P-F(1)	179.5(5)
F(3)-P-F(2)	88.8(5)
F(1)-P-F(2)	90.9(5)
F(3)-P-F(6)	90.6(4)
F(1)-P-F(6)	89.8(4)
F(2)-P-F(6)	89.6(5)
F(3)-P-F(5)	89.5(4)
F(1)-P-F(5)	90.1(4)
F(2)-P-F(5)	87.8(5)
F(6)-P-F(5)	177.3(5)
F(3)-P-F(4)	91.4(5)
F(1)-P-F(4)	88.9(5)
F(2)-P-F(4)	179.6(5)
F(6)-P-F(4)	90.8(5)
F(5)-P-F(4)	91.8(5)
C(1)-N(1)-C(5)	119.3(9)
C(1)-N(1)-Ru	127.8(6)
C(5)-N(1)-Ru	112.6(8)
C(10)-N(2)-C(6)	121.1(10)
C(10)-N(2)-Ru	120.1(7)
C(6)-N(2)-Ru	117.5(8)
C(15)-N(3)-C(11)	117.1(9)
C(15)-N(3)-Ru	129.6(9)
C(11)-N(3)-Ru	113.3(6)
C(16)-N(4)-C(20)	119.3(8)
C(16)-N(4)-Ru	125.4(7)
C(20)-N(4)-Ru	115.4(5)
C(21)-N(5)-C(25)	117.3(9)
C(21)-N(5)-Ru	116.0(6)
C(25)-N(5)-Ru	126.6(6)
C(26)-N(6)-Ru	169.0(6)
C(26)-N(7)-C(32)	119.6(8)
N(1)-C(1)-C(2)	122.7(10)
C(3)-C(2)-C(1)	118.8(11)
C(2)-C(3)-C(4)	119.7(9)
C(3)-C(4)-C(5)	118.7(10)
N(1)-C(5)-C(4)	120.8(12)
N(1)-C(5)-C(6)	116.7(9)
C(4)-C(5)-C(6)	122.5(11)
N(2)-C(6)-C(7)	117.3(13)

N(2)-C(6)-C(5)	112.5(9)
C(7)-C(6)-C(5)	130.0(11)
C(8)-C(7)-C(6)	121.9(12)
C(7)-C(8)-C(9)	120.3(13)
C(10)-C(9)-C(8)	116.8(13)
N(2)-C(10)-C(9)	122.5(10)
N(2)-C(10)-C(11)	111.6(10)
C(9)-C(10)-C(11)	125.9(12)
C(12)-C(11)-N(3)	120.7(11)
C(12)-C(11)-C(10)	124.8(12)
N(3)-C(11)-C(10)	114.5(9)
C(13)-C(12)-C(11)	120.9(14)
C(14)-C(13)-C(12)	118.4(13)
C(13)-C(14)-C(15)	120.1(11)
N(3)-C(15)-C(14)	122.8(12)
N(4)-C(16)-C(17)	120.4(11)
C(18)-C(17)-C(16)	120.5(10)
C(17)-C(18)-C(19)	119.7(10)
C(18)-C(19)-C(20)	120.5(12)
N(4)-C(20)-C(19)	119.6(9)
N(4)-C(20)-C(21)	116.5(7)
C(19)-C(20)-C(21)	123.9(10)
N(5)-C(21)-C(22)	120.3(9)
N(5)-C(21)-C(20)	113.4(9)
C(22)-C(21)-C(20)	126.2(8)
C(23)-C(22)-C(21)	121.1(10)
C(24)-C(23)-C(22)	117.9(11)
C(23)-C(24)-C(25)	120.7(9)
N(5)-C(25)-C(24)	122.6(8)
N(6)-C(26)-N(7)	171.5(10)
C(28)-C(27)-C(32)	120.0
C(28)-C(27)-Cl(1)	116.8(6)
C(32)-C(27)-Cl(1)	123.2(6)
C(29)-C(28)-C(27)	120.0
C(28)-C(29)-C(30)	120.0
C(28)-C(29)-Cl(2)	120.8(10)
C(30)-C(29)-Cl(2)	119.2(10)
C(31)-C(30)-C(29)	120.0
C(30)-C(31)-C(32)	120.0
C(31)-C(32)-C(27)	120.0
C(31)-C(32)-N(7)	124.0(6)
C(27)-C(32)-N(7)	115.8(6)
C(33)-N(8)-C(34)	118.1(13)
C(33)-N(8)-C(35)	118.6(12)
C(34)-N(8)-C(35)	123.3(13)
O-C(33)-N(8)	120.9(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for rc008.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ru	30(1)	25(1)	32(1)	-9(1)	-14(1)	5(1)
P	66(2)	46(2)	51(3)	-7(2)	-27(2)	6(1)
Cl(1)	138(4)	71(2)	224(6)	-87(3)	-78(4)	30(2)
Cl(2)	447(14)	221(8)	255(11)	140(8)	-187(10)	-267(10)
F(1)	116(6)	55(4)	104(8)	15(5)	-60(5)	-21(4)
F(2)	156(8)	83(5)	45(8)	-21(5)	-37(5)	4(5)
F(3)	96(5)	47(4)	103(8)	-2(4)	-49(5)	-4(3)
F(4)	140(7)	100(6)	64(8)	-31(6)	-25(5)	9(5)
F(5)	67(4)	76(5)	98(8)	-3(5)	-36(4)	9(3)
F(6)	74(4)	80(5)	98(8)	-10(5)	-45(4)	8(3)
N(1)	36(4)	18(3)	16(9)	0(5)	-14(4)	7(3)
N(2)	41(4)	38(4)	35(9)	-18(5)	-12(4)	6(3)
N(3)	37(4)	36(4)	40(8)	-16(4)	-20(4)	10(3)
N(4)	41(4)	26(4)	47(8)	-9(5)	-22(4)	5(3)
N(5)	29(3)	34(4)	41(8)	-12(4)	-12(3)	-3(3)
N(6)	31(3)	32(4)	23(7)	-1(4)	-9(3)	-3(3)
N(7)	44(4)	28(4)	63(8)	-14(5)	-13(4)	2(3)
C(1)	44(5)	22(4)	33(13)	0(7)	-20(6)	6(3)
C(2)	48(5)	36(5)	40(10)	-11(6)	-31(5)	11(4)
C(3)	41(5)	55(6)	83(14)	-44(8)	-33(7)	12(4)
C(4)	30(4)	35(5)	49(12)	-16(6)	-7(5)	1(3)
C(5)	47(5)	26(4)	34(12)	-8(6)	-26(6)	6(4)
C(6)	40(4)	34(5)	23(13)	-13(7)	0(5)	-2(4)
C(7)	59(6)	44(6)	31(13)	-1(7)	-14(7)	-14(5)
C(8)	73(7)	46(6)	24(14)	13(8)	-11(7)	-9(5)
C(9)	65(6)	51(6)	24(12)	3(7)	-17(6)	1(5)
C(10)	46(5)	37(5)	31(11)	-10(6)	-10(5)	3(4)
C(11)	57(5)	35(5)	32(9)	-12(5)	-31(5)	14(4)
C(12)	72(6)	60(6)	46(10)	-23(7)	-41(6)	19(5)
C(13)	47(6)	82(8)	59(14)	-27(9)	-19(7)	-9(5)
C(14)	39(5)	79(8)	101(16)	-58(10)	-28(7)	7(5)
C(15)	37(4)	50(5)	54(10)	-33(6)	-10(5)	8(4)
C(16)	52(5)	46(5)	46(10)	-27(6)	-19(5)	7(4)
C(17)	70(7)	61(7)	93(15)	-52(9)	-44(8)	27(6)
C(18)	89(9)	37(6)	106(16)	-34(9)	-36(9)	14(6)
C(19)	70(6)	27(5)	63(11)	-11(6)	-28(6)	4(4)
C(20)	43(4)	29(4)	34(10)	-2(6)	-29(5)	3(4)
C(21)	42(4)	21(4)	58(11)	2(6)	-32(5)	2(3)
C(22)	53(5)	41(5)	36(11)	-3(7)	-12(6)	-1(4)
C(23)	50(5)	60(7)	39(11)	-4(7)	-9(5)	-3(5)
C(24)	41(5)	76(8)	45(11)	-34(8)	-15(5)	10(5)
C(25)	38(4)	30(4)	38(10)	-5(6)	-15(5)	2(3)
C(26)	30(4)	39(5)	18(9)	-6(5)	-8(4)	1(3)
C(27)	110(10)	40(6)	175(18)	-31(9)	-107(11)	10(6)
C(28)	190(19)	55(8)	180(20)	15(12)	-140(17)	-54(10)
C(29)	190(20)	107(15)	150(30)	88(16)	-107(19)	-100(16)
C(30)	124(13)	162(17)	104(17)	51(14)	-43(10)	-73(13)
C(31)	75(8)	141(13)	57(13)	38(9)	-30(7)	-44(8)
C(32)	61(5)	27(4)	95(11)	5(6)	-55(5)	-8(4)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for rc008.

	x	y	z	U(eq)
H(1A)	6138	6976	4118	42
H(2A)	4235	6805	4024	47
H(3A)	2730	5949	5491	62
H(4A)	3176	5215	7033	48
H(7A)	3956	4294	8435	56
H(8A)	4748	3809	9765	67
H(9A)	6666	4434	9494	61
H(12A)	8488	5327	8990	66
H(13A)	10316	6215	8357	72
H(14A)	11060	7148	6637	77
H(15A)	9978	7191	5570	54
H(16A)	5698	8091	6908	54
H(17A)	5250	10118	6486	79
H(18A)	6208	11356	4921	91
H(19A)	7629	10576	3765	65
H(22A)	8907	9707	2660	57
H(23A)	10135	8627	1638	66
H(24A)	10307	6584	2324	62
H(25A)	9236	5642	3972	45
H(28A)	7830	-1240	7558	152
H(30A)	5535	976	8924	177
H(31A)	6574	2572	7685	125
H(33A)	3273	1136	8262	105
H(34A)	1900	3516	8892	185
H(34B)	1511	2837	10065	185
H(34C)	605	2997	9437	185
H(35A)	2044	42	9689	166
H(35B)	706	633	10029	166
H(35C)	1664	535	10596	166