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Supplementary Materials

Structural, Electronic and Acid/Base Properties of $[Ru(bpy(OH)_2)_3]^{2+}$ ($bpy(OH)_2$ = 4,4'-dihydroxy-2,2'-bipyridine)

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IR Spectroscopy

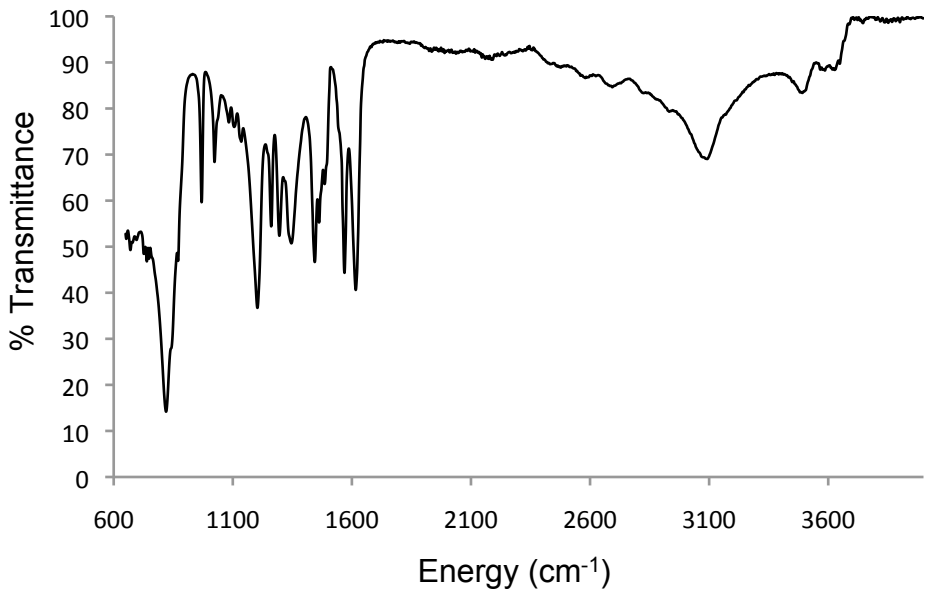


Figure S1 - FT-IR Spectrum of $[Ru(bpy(OH)_2)_3][PF_6]_2$.

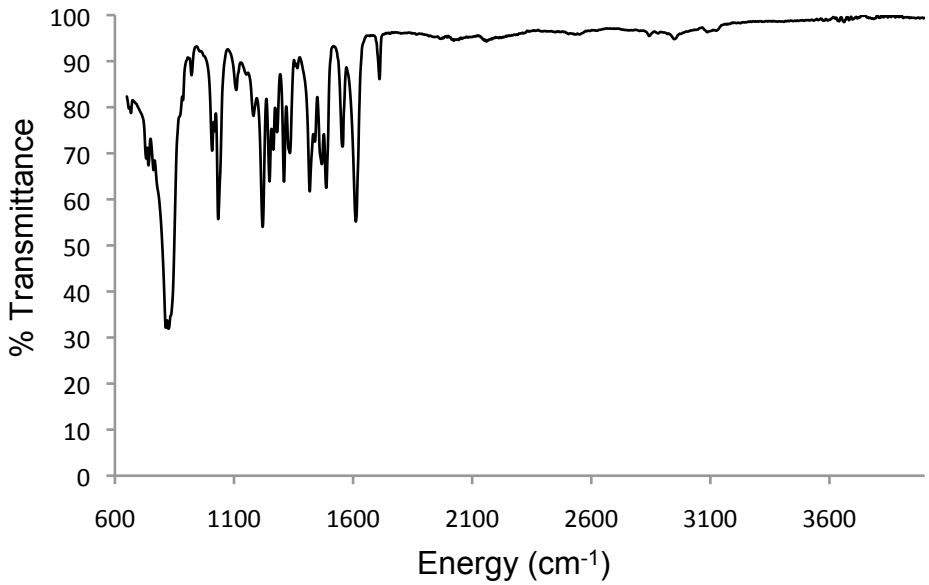


Figure S2 - FT-IR Spectrum of $[Ru(bpy(OMe)_2)_3][PF_6]_2$.

NMR Spectroscopy

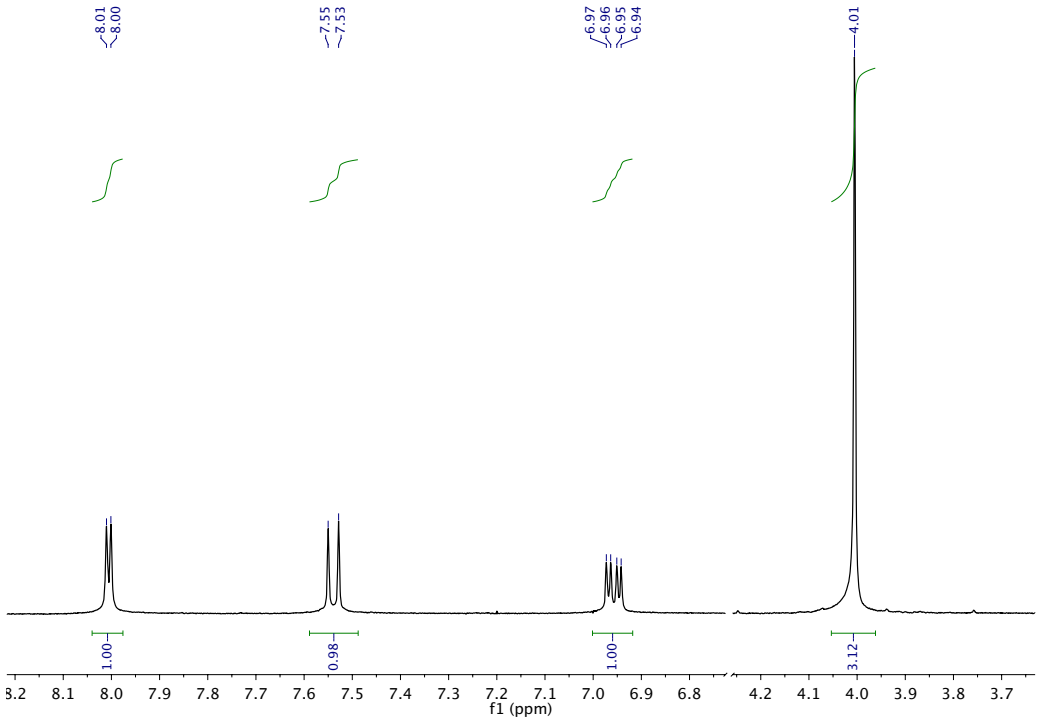


Figure S3 – ^{1}H-NMR Spectrum of $[Ru(bpy(OMe)_2)_3][PF_6]_2$ in CD_3CN.

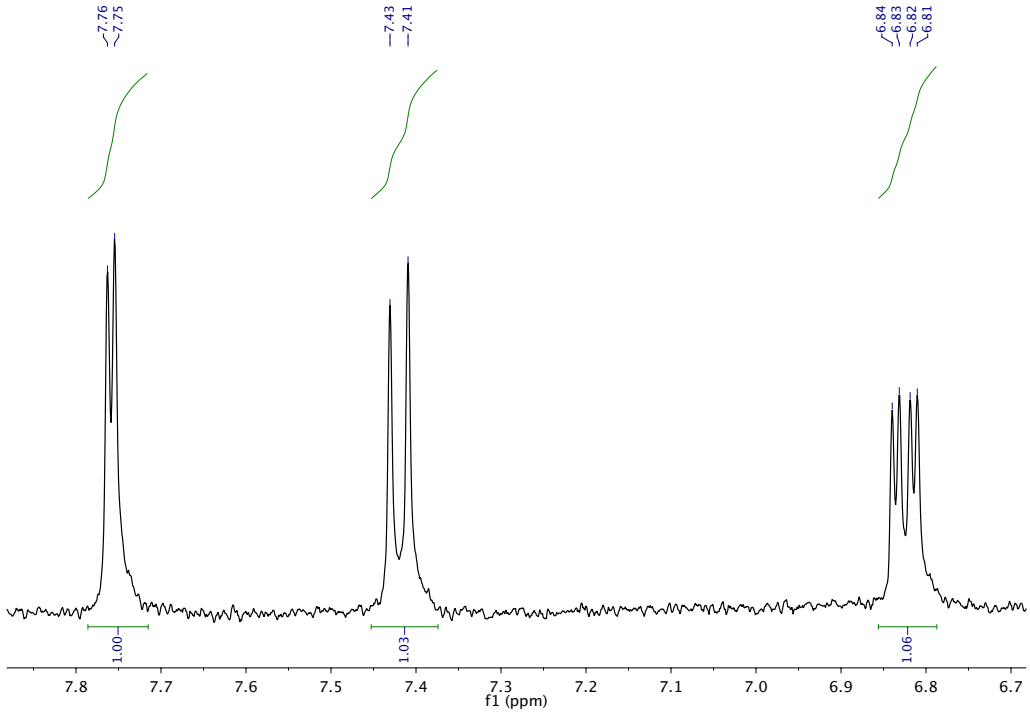


Figure S4 – ^{1}H-NMR Spectrum of $[Ru(bpy(OH)_2)_3][PF_6]_2$ in CD_3CN.

Electrochemistry

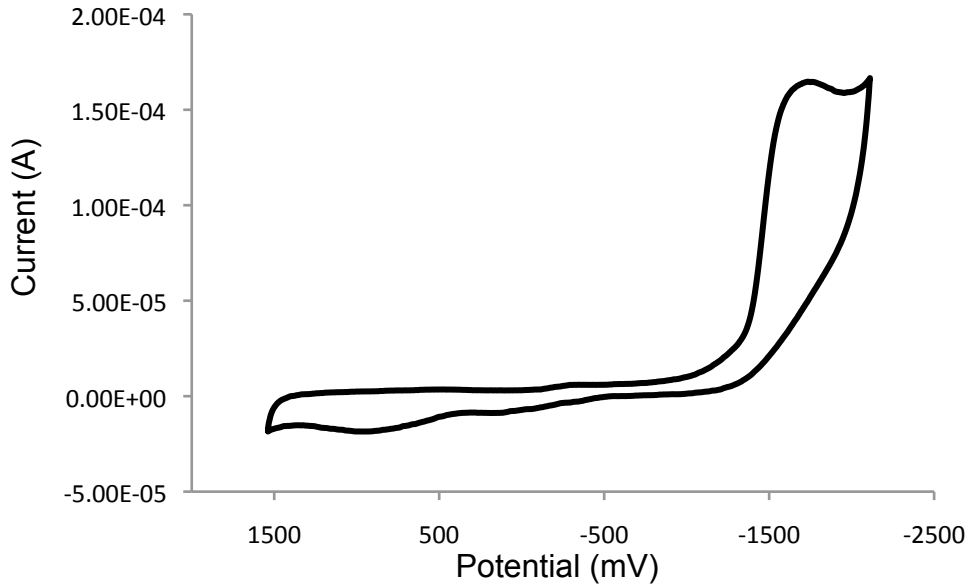


Figure S5 - Cyclic Voltammogram of 10 mM HPF_6 in acetonitrile with 0.1M tetrabutylammonium hexafluorophosphate and glassy carbon working electrode. Potentials corrected vs. SCE.

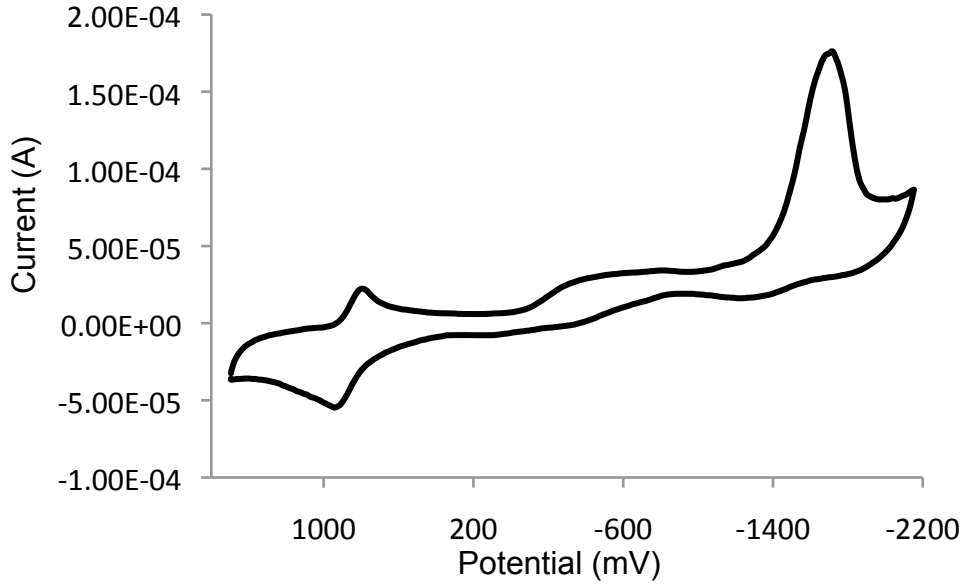


Figure S6 - Cyclic Voltammogram of 0.7 mM $[Ru(bpy(OH)_2)_3][PF_6]_2$ in 10 mM HPF_6 in acetonitrile with 0.1M tetrabutylammonium hexafluorophosphate and glassy carbon working electrode. Potentials corrected vs. SCE.

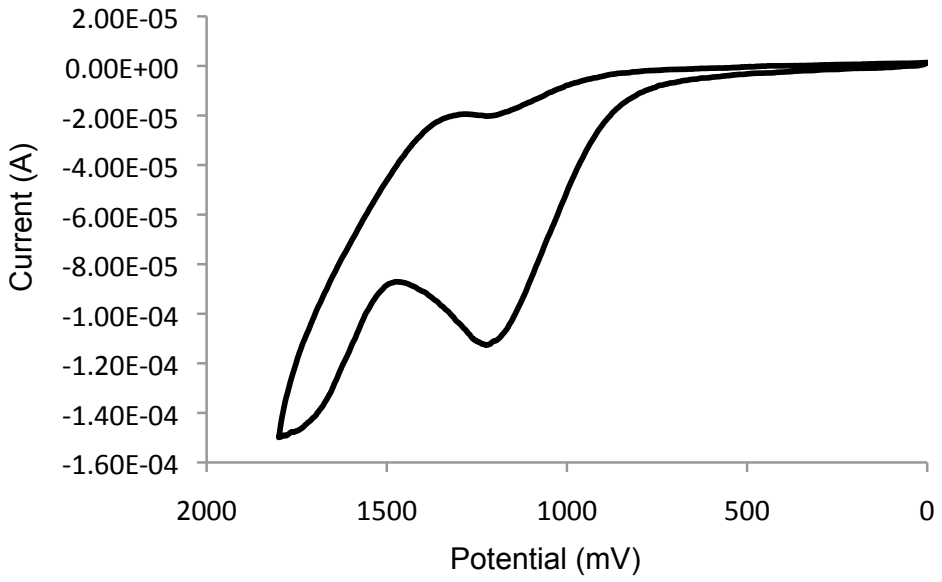


Figure S7 - Cyclic Voltammogram (oxidative scan) of 12.5 mM TBAOH in acetonitrile with 0.1M tetrabutylammonium hexafluorophosphate and glassy carbon working electrode. Potentials are uncorrected.

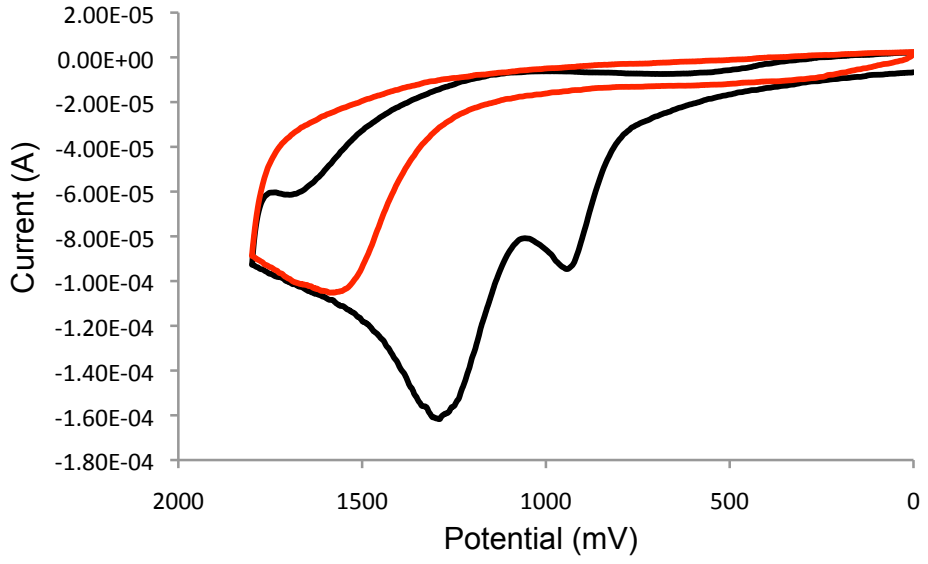


Figure S8 - Cyclic Voltammogram (oxidative scan) of 0.9 mM $[Ru(bpy(OH)_2)_3][PF_6]_2$ in 12.5 mM TBAOH in acetonitrile with 0.1M tetrabutylammonium hexafluorophosphate and glassy carbon working electrode. Initial scan (black line), second scan (red line). Potentials are uncorrected.

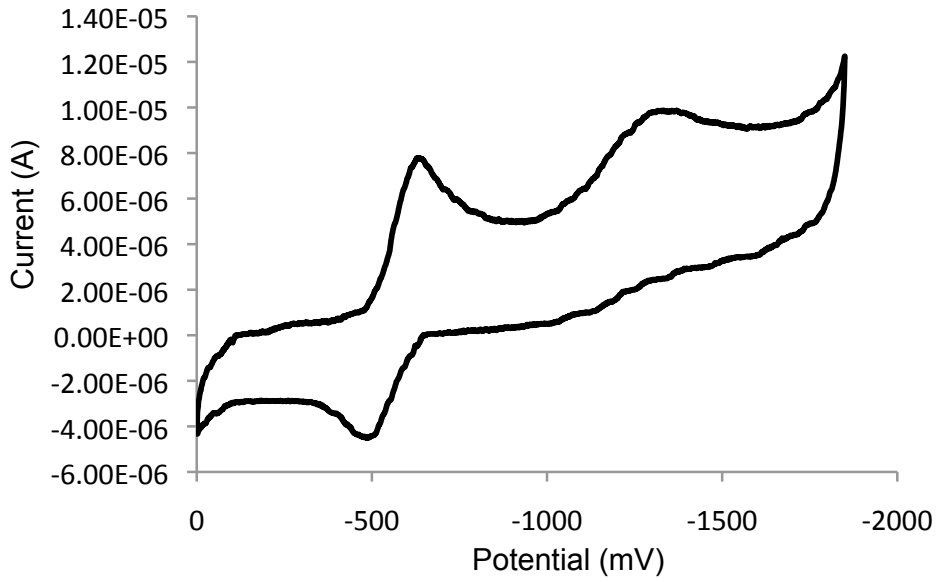


Figure S9 - Cyclic Voltammogram (reductive scan) of 12.5 mM TBAOH in acetonitrile with 0.1M tetrabutylammonium hexafluorophosphate and glassy carbon working electrode. Potentials are uncorrected.

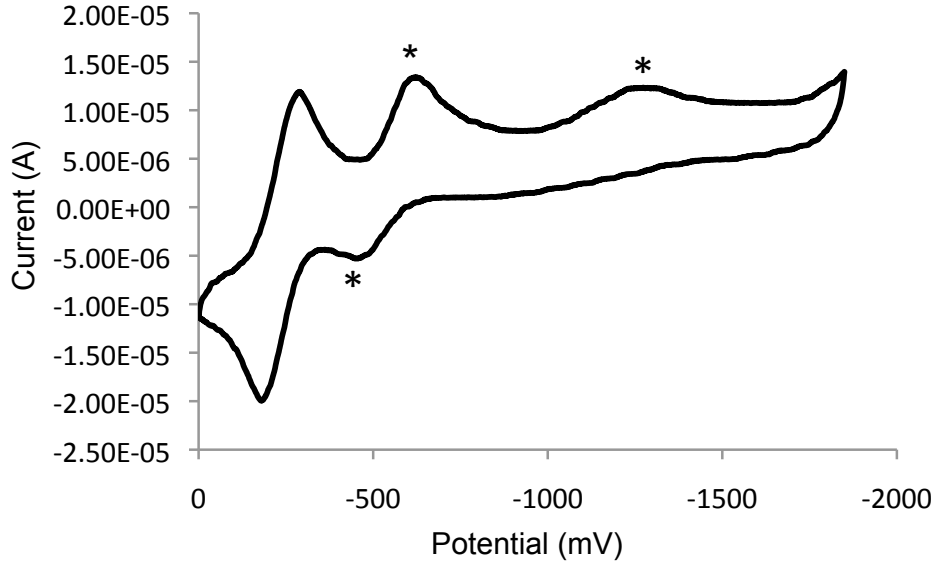


Figure S10 - Cyclic Voltammogram (reductive scan) of 0.9 mM $[Ru(bpy(OH)_2)_3][PF_6]_2$ in 12.5 mM TBAOH in acetonitrile with 0.1M tetrabutylammonium hexafluorophosphate and glassy carbon working electrode. (* = Potentials associated with TBAOH base.) Potentials are uncorrected.

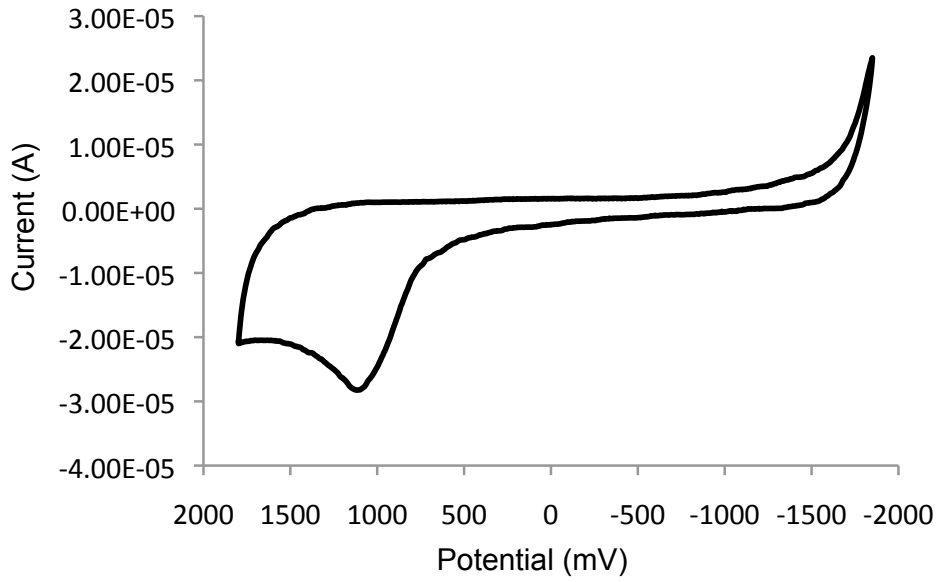


Figure S11 - Cyclic Voltammogram of 2.1 mM $bpy(O)_2^{2-}$ ligand in 5.1 mM TBAOH in acetonitrile with 0.1M tetrabutylammonium hexafluorophosphate and glassy carbon working electrode. Potentials are uncorrected.

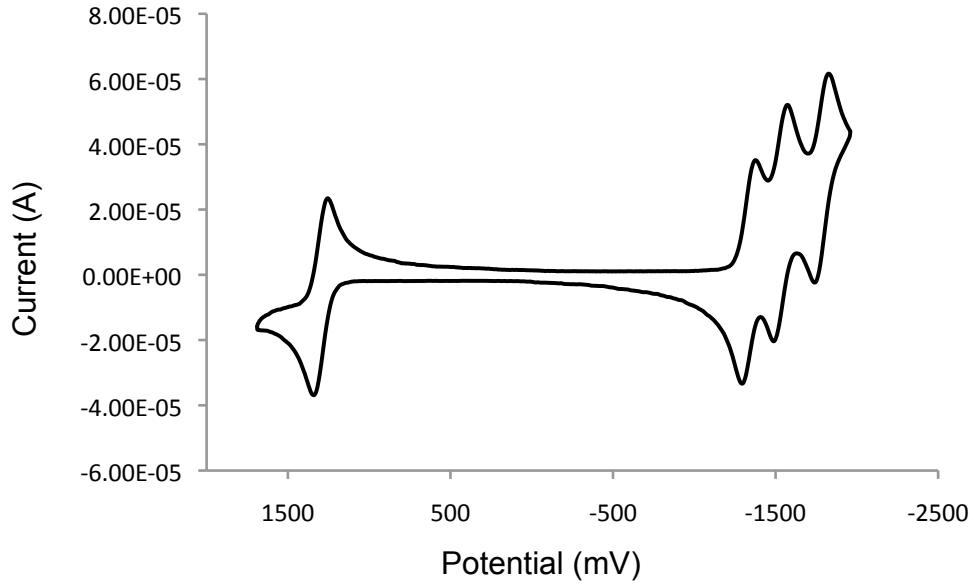


Figure S12 - Cyclic Voltammogram of $[Ru(bpy)_3][PF_6]_2$ in acetonitrile with 0.1M tetrabutylammonium hexafluorophosphate and glassy carbon working electrode. Potentials corrected vs. SCE.

pH Titration

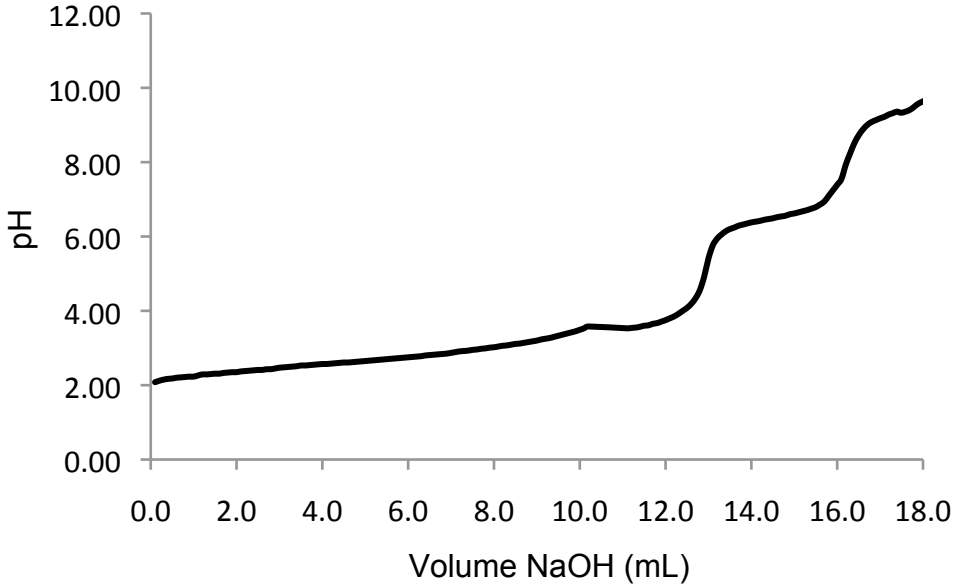


Figure S13 - pH Titration of $[Ru(bpy(OH)_2)_3]^{2+}$ in 0.01 M HCl with 9.2 mM NaOH. The first equivalence point is due to neutralization of the excess HCl used to ensure full protonation of the metal complex.

Absorbance Spectroscopy

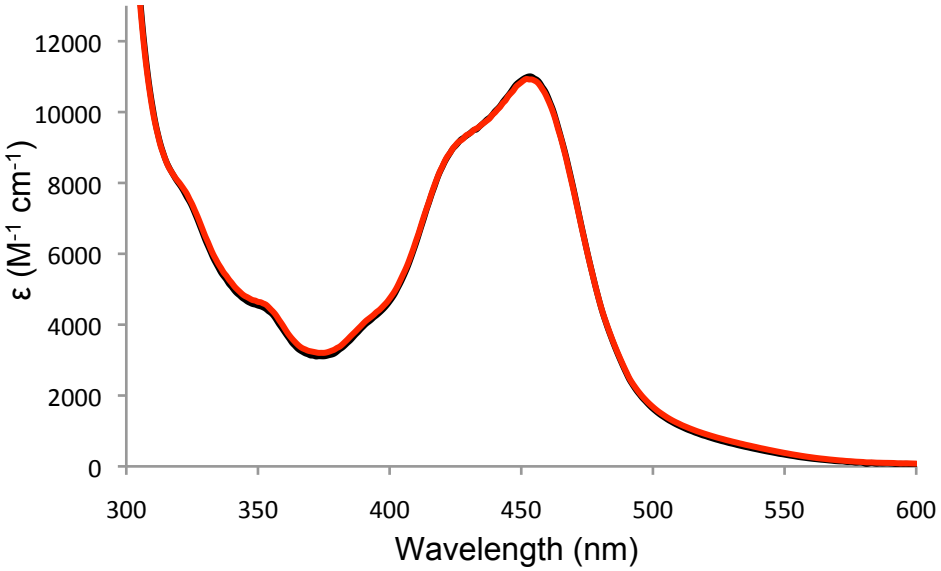
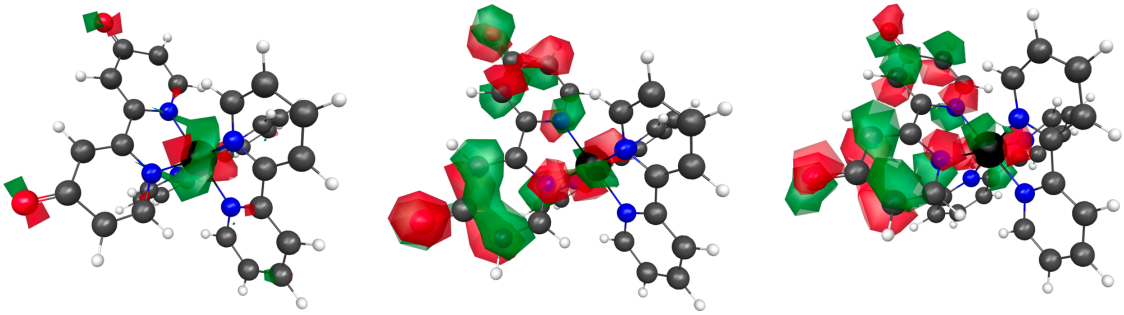


Figure S14 – UV/Visible spectrum of $[Ru(bpy)_3]^{2+}$ in water and (—) HCl; (—) NaOH.

Molecular Orbitals



HOMO-2
-5.361 eV

HOMO-1
-4.653 eV

HOMO
-4.653 eV

Figure S15 – Selected molecular orbitals from the PCM calculation for $[Ru(bpy)_2(bpy(O)_2)]$. Molecular orbital energies are reported in eV using the converstion factor 1 Hartree = 27.2116 eV.

Crystallographic Data

$[Ru(bpy(OH)_2)_3]^{2+}$ (paul003s)

Table S1. Crystal data and structure refinement for paul003s.

Identification code	paul003s	
Empirical formula	C5 H4 Cl0.33 N O Ru0.17	
Formula weight	122.75	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	P-31c	
Unit cell dimensions	a = 12.7647(13) Å	⟨= 90°.
	b = 12.7647(13) Å	®= 90°.
	c = 16.2308(17) Å	© = 120°.
Volume	2290.3(4) $Å^3$	
Z	12	
Density (calculated)	1.068 Mg/m^3	
Absorption coefficient	0.495 mm^{-1}	
F(000)	744	
Crystal size	0.22 x 0.20 x 0.20 mm^3	
Theta range for data collection	1.84 to 33.15°.	
Index ranges	-19<=h<=18, -19<=k<=19, -24<=l<=24	
Reflections collected	28899	
Independent reflections	2922 [R(int) = 0.0600]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9075 and 0.8989	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2922 / 0 / 73	
Goodness-of-fit on F^2	1.074	
Final R indices [I>2sigma(I)]	R1 = 0.0480, wR2 = 0.1386	
R indices (all data)	R1 = 0.0644, wR2 = 0.1451	
Largest diff. peak and hole	2.153 and -1.168 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for paul003s. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	3333	6667	7500	19(1)
Cl(1)	6667	3333	6064(1)	30(1)
N(1)	4628(2)	6517(2)	6830(1)	20(1)
O(1)	6793(2)	5630(2)	5436(1)	37(1)
C(1)	4893(2)	5665(2)	7102(1)	21(1)
C(2)	5615(2)	5337(2)	6658(1)	25(1)
C(3)	6107(2)	5915(2)	5909(1)	27(1)
C(4)	5873(2)	6807(2)	5646(1)	29(1)
C(5)	5140(2)	7084(2)	6117(1)	26(1)

Table S3. Bond lengths [Å] and angles [°] for paul003s.

Ru(1)-N(1)#1	2.0651(18)
Ru(1)-N(1)#2	2.0651(18)
Ru(1)-N(1)#3	2.0651(18)
Ru(1)-N(1)#4	2.0651(18)
Ru(1)-N(1)#5	2.0651(18)
Ru(1)-N(1)	2.0651(18)
N(1)-C(5)	1.348(2)
N(1)-C(1)	1.364(3)
O(1)-C(3)	1.343(3)
C(1)-C(2)	1.390(3)
C(1)-C(1)#5	1.475(4)
C(2)-C(3)	1.398(3)
C(3)-C(4)	1.382(3)
C(4)-C(5)	1.385(3)
N(1)#1-Ru(1)-N(1)#2	92.28(10)
N(1)#1-Ru(1)-N(1)#3	94.84(6)
N(1)#2-Ru(1)-N(1)#3	78.72(9)
N(1)#1-Ru(1)-N(1)#4	78.72(9)
N(1)#2-Ru(1)-N(1)#4	94.84(6)
N(1)#3-Ru(1)-N(1)#4	170.79(10)
N(1)#1-Ru(1)-N(1)#5	94.84(6)
N(1)#2-Ru(1)-N(1)#5	170.79(10)
N(1)#3-Ru(1)-N(1)#5	94.84(6)
N(1)#4-Ru(1)-N(1)#5	92.28(10)
N(1)#1-Ru(1)-N(1)	170.79(10)
N(1)#2-Ru(1)-N(1)	94.84(6)
N(1)#3-Ru(1)-N(1)	92.28(10)
N(1)#4-Ru(1)-N(1)	94.84(6)
N(1)#5-Ru(1)-N(1)	78.72(9)
C(5)-N(1)-C(1)	117.34(18)
C(5)-N(1)-Ru(1)	126.67(15)
C(1)-N(1)-Ru(1)	115.64(12)
N(1)-C(1)-C(2)	122.64(17)

N(1)-C(1)-C(1)#5	114.57(10)
C(2)-C(1)-C(1)#5	122.78(12)
C(1)-C(2)-C(3)	118.8(2)
O(1)-C(3)-C(4)	118.99(18)
O(1)-C(3)-C(2)	122.4(2)
C(4)-C(3)-C(2)	118.6(2)
C(5)-C(4)-C(3)	119.49(19)
N(1)-C(5)-C(4)	123.0(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+y,y,-z+3/2 #2 -y+1,x-y+1,z #3 x,x-y+1,-z+3/2

#4 -x+y,-x+1,z #5 -y+1,-x+1,-z+3/2

Table S4. Anisotropic displacement parameters ($Å^2 x 10^3$) for paul003s. The anisotropic displacement factor exponent takes the form: $-2\partial^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	23(1)	23(1)	10(1)	0	0	11(1)
Cl(1)	27(1)	27(1)	37(1)	0	0	13(1)
N(1)	25(1)	26(1)	12(1)	3(1)	2(1)	15(1)
O(1)	53(1)	47(1)	27(1)	13(1)	22(1)	37(1)
C(1)	26(1)	26(1)	14(1)	4(1)	4(1)	15(1)
C(2)	33(1)	31(1)	18(1)	7(1)	8(1)	22(1)
C(3)	31(1)	34(1)	19(1)	5(1)	10(1)	19(1)
C(4)	37(1)	38(1)	19(1)	11(1)	13(1)	24(1)
C(5)	36(1)	30(1)	19(1)	9(1)	6(1)	21(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^{-3}) for paul003s.

	x	y	z	U(eq)
H(1A)	6880(30)	5070(30)	5750(20)	35(8)
H(2A)	5772	4730	6860	30
H(4A)	6212	7227	5145	35
H(5A)	4990	7703	5929	31

Table S6. Hydrogen bonds for paul003s [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1A)...Cl(1)	0.93(3)	2.15(3)	3.031(2)	156(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+y,y,-z+3/2 #2 -y+1,x-y+1,z #3 x,x-y+1,-z+3/2

#4 -x+y,-x+1,z #5 -y+1,-x+1,-z+3/2

$[Ru(bpy(OMe)_2)_3]^{2+}$ (paul009)

Table S7. Crystal data and structure refinement for paul009.

Identification code	paul009	
Empirical formula	C39 H42 F12 N6 O7 P2 Ru	
Formula weight	1097.80	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.6201(10) Å	α= 76.681(3)°.
	b = 13.0428(11) Å	β= 83.234(3)°.
	c = 14.8647(12) Å	γ = 78.748(3)°.
Volume	2143.9(3) $Å^3$	
Z	2	
Density (calculated)	1.701 Mg/m^3	
Absorption coefficient	0.550 mm^{-1}	
F(000)	1112	
Crystal size	0.15 x 0.06 x 0.06 mm^3	
Theta range for data collection	1.41 to 33.21°.	
Index ranges	-17<=h<=17, -20<=k<=20, -22<=l<=22	
Reflections collected	72892	
Independent reflections	16295 [R(int) = 0.0511]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9677 and 0.9220	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16295 / 180 / 676	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0423, wR2 = 0.0940	
R indices (all data)	R1 = 0.0642, wR2 = 0.1041	
Largest diff. peak and hole	1.047 and -0.825 e.$Å^{-3}$	

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for paul009. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	2613(1)	1786(1)	1988(1)	11(1)
P(1)	6655(2)	3213(2)	3321(1)	21(1)
F(1)	5905(3)	2301(3)	3472(3)	72(1)
F(2)	5517(2)	4010(2)	3573(3)	84(1)
F(3)	6930(2)	2888(2)	4393(1)	44(1)
F(4)	7802(2)	2429(3)	3099(3)	83(1)
F(5)	6430(4)	3524(3)	2257(2)	73(1)
F(6)	7384(3)	4153(3)	3191(2)	47(1)
P(1')	6568(11)	3222(10)	3236(8)	44(2)
F(1')	5850(13)	2429(11)	2996(12)	66(3)
F(2')	5691(12)	3229(11)	4110(8)	81(3)
F(3')	7396(11)	2276(12)	3787(12)	95(4)
F(4')	7383(13)	3184(10)	2327(9)	67(3)
F(5')	5688(11)	4137(9)	2630(11)	75(3)
F(6')	7010(18)	4190(14)	3392(12)	85(4)
P(2)	9427(1)	7834(1)	2104(1)	19(1)
F(7)	8178(2)	7676(2)	1875(2)	58(1)
F(8)	9226(2)	7219(1)	3150(1)	46(1)
F(9)	8825(2)	8934(1)	2372(1)	57(1)
F(10)	9635(2)	8432(1)	1044(1)	37(1)
F(11)	10011(2)	6726(1)	1828(1)	50(1)
F(12)	10666(2)	8004(2)	2313(1)	59(1)
N(1)	2732(1)	780(1)	1082(1)	13(1)
N(2)	3831(1)	2371(1)	983(1)	13(1)
N(3)	1232(1)	2865(1)	1388(1)	13(1)
N(4)	2389(1)	2956(1)	2749(1)	13(1)
N(5)	3849(1)	712(1)	2765(1)	12(1)
N(6)	1567(1)	935(1)	2986(1)	13(1)
O(1)	2823(1)	-711(1)	-1104(1)	20(1)
O(2)	6446(1)	3099(1)	-1078(1)	22(1)
O(3)	-1814(1)	4888(1)	505(1)	21(1)

O(4)	1326(1)	5160(1)	4410(1)	22(1)
O(5)	6035(1)	-1331(1)	4651(1)	20(1)
O(6)	-289(1)	-1303(1)	4611(1)	21(1)
C(1)	2087(2)	14(2)	1152(1)	16(1)
C(2)	2066(2)	-518(2)	455(1)	17(1)
C(3)	2762(2)	-259(2)	-365(1)	15(1)
C(4)	3467(2)	512(2)	-443(1)	15(1)
C(5)	3431(2)	1013(1)	285(1)	13(1)
C(6)	4115(2)	1858(1)	263(1)	12(1)
C(7)	4987(2)	2108(2)	-420(1)	15(1)
C(8)	5599(2)	2917(2)	-388(1)	15(1)
C(9)	5322(2)	3437(2)	345(1)	17(1)
C(10)	4442(2)	3134(2)	1009(1)	16(1)
C(11)	1975(2)	-1374(2)	-1100(2)	26(1)
C(12)	6987(2)	4009(2)	-1159(2)	28(1)
C(13)	709(2)	2796(2)	647(1)	15(1)
C(14)	-296(2)	3474(2)	343(1)	17(1)
C(15)	-818(2)	4268(2)	824(1)	16(1)
C(16)	-276(2)	4372(2)	1576(1)	15(1)
C(17)	747(2)	3666(1)	1831(1)	13(1)
C(18)	1406(2)	3721(2)	2606(1)	13(1)
C(19)	1069(2)	4474(2)	3148(1)	16(1)
C(20)	1746(2)	4456(2)	3868(1)	17(1)
C(21)	2790(2)	3721(2)	3976(1)	17(1)
C(22)	3067(2)	2994(2)	3407(1)	16(1)
C(23)	-2419(2)	5667(2)	1024(2)	22(1)
C(24)	1882(2)	5013(2)	5257(2)	26(1)
C(25)	5020(2)	653(2)	2626(1)	16(1)
C(26)	5810(2)	-27(2)	3208(1)	17(1)
C(27)	5368(2)	-678(2)	4001(1)	15(1)
C(28)	4154(2)	-658(2)	4141(1)	15(1)
C(29)	3430(2)	19(2)	3508(1)	13(1)
C(30)	2141(2)	84(2)	3565(1)	13(1)
C(31)	1572(2)	-696(2)	4133(1)	15(1)
C(32)	364(2)	-592(2)	4120(1)	16(1)
C(33)	-245(2)	325(2)	3576(1)	17(1)

C(34)	381(2)	1056(2)	3022(1)	16(1)
C(35)	7267(2)	-1259(2)	4532(2)	22(1)
C(36)	317(2)	-2349(2)	5000(2)	26(1)
O(7)	4371(2)	-1742(2)	2407(1)	50(1)
C(37)	5657(3)	-3145(3)	3287(4)	70(1)
C(38)	4492(3)	-2599(2)	2944(2)	36(1)
C(39)	3464(3)	-3142(3)	3318(2)	44(1)

Table S9. Bond lengths [Å] and angles [°] for paul009.

Ru(1)-N(2)	2.0534(15)
Ru(1)-N(5)	2.0540(16)
Ru(1)-N(3)	2.0560(16)
Ru(1)-N(4)	2.0613(16)
Ru(1)-N(1)	2.0623(16)
Ru(1)-N(6)	2.0624(15)
P(1)-F(4)	1.566(3)
P(1)-F(1)	1.569(3)
P(1)-F(2)	1.579(3)
P(1)-F(5)	1.580(3)
P(1)-F(6)	1.586(3)
P(1)-F(3)	1.605(3)
P(1')-F(6')	1.525(13)
P(1')-F(3')	1.541(13)
P(1')-F(2')	1.554(13)
P(1')-F(4')	1.562(13)
P(1')-F(1')	1.571(13)
P(1')-F(5')	1.589(13)
P(2)-F(12)	1.5744(18)
P(2)-F(9)	1.5843(18)
P(2)-F(8)	1.5900(16)
P(2)-F(7)	1.5910(18)
P(2)-F(11)	1.5950(17)
P(2)-F(10)	1.6029(15)
N(1)-C(1)	1.341(2)
N(1)-C(5)	1.364(2)
N(2)-C(10)	1.339(2)
N(2)-C(6)	1.365(2)
N(3)-C(13)	1.349(2)
N(3)-C(17)	1.357(2)
N(4)-C(22)	1.341(2)
N(4)-C(18)	1.364(2)
N(5)-C(25)	1.342(2)
N(5)-C(29)	1.363(2)

N(6)-C(30)	1.351(2)
N(6)-C(34)	1.352(2)
O(1)-C(3)	1.351(2)
O(1)-C(11)	1.431(2)
O(2)-C(8)	1.348(2)
O(2)-C(12)	1.423(2)
O(3)-C(15)	1.344(2)
O(3)-C(23)	1.441(3)
O(4)-C(20)	1.342(2)
O(4)-C(24)	1.439(3)
O(5)-C(27)	1.341(2)
O(5)-C(35)	1.440(2)
O(6)-C(32)	1.342(2)
O(6)-C(36)	1.430(3)
C(1)-C(2)	1.377(3)
C(1)-H(1A)	0.9500
C(2)-C(3)	1.392(3)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.393(3)
C(4)-C(5)	1.380(3)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.472(2)
C(6)-C(7)	1.377(2)
C(7)-C(8)	1.395(3)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.387(3)
C(9)-C(10)	1.384(3)
C(9)-H(9A)	0.9500
C(10)-H(10A)	0.9500
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.373(3)

C(13)-H(13A)	0.9500
C(14)-C(15)	1.396(3)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.390(3)
C(16)-C(17)	1.386(3)
C(16)-H(16A)	0.9500
C(17)-C(18)	1.479(3)
C(18)-C(19)	1.380(3)
C(19)-C(20)	1.395(3)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.393(3)
C(21)-C(22)	1.380(3)
C(21)-H(21A)	0.9500
C(22)-H(22A)	0.9500
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(26)	1.375(3)
C(25)-H(25A)	0.9500
C(26)-C(27)	1.394(3)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.398(3)
C(28)-C(29)	1.374(3)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.477(3)
C(30)-C(31)	1.386(2)
C(31)-C(32)	1.386(3)
C(31)-H(31A)	0.9500
C(32)-C(33)	1.394(3)
C(33)-C(34)	1.372(3)
C(33)-H(33A)	0.9500
C(34)-H(34A)	0.9500
C(35)-H(35A)	0.9800

C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
O(7)-C(38)	1.208(3)
C(37)-C(38)	1.489(5)
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-C(39)	1.494(4)
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800

N(2)-Ru(1)-N(5)	94.20(6)
N(2)-Ru(1)-N(3)	93.02(6)
N(5)-Ru(1)-N(3)	171.74(6)
N(2)-Ru(1)-N(4)	98.15(6)
N(5)-Ru(1)-N(4)	96.92(6)
N(3)-Ru(1)-N(4)	78.08(6)
N(2)-Ru(1)-N(1)	78.70(6)
N(5)-Ru(1)-N(1)	90.67(6)
N(3)-Ru(1)-N(1)	94.66(6)
N(4)-Ru(1)-N(1)	172.00(6)
N(2)-Ru(1)-N(6)	169.80(6)
N(5)-Ru(1)-N(6)	78.37(6)
N(3)-Ru(1)-N(6)	94.93(6)
N(4)-Ru(1)-N(6)	89.74(6)
N(1)-Ru(1)-N(6)	94.28(6)
F(4)-P(1)-F(1)	91.1(2)
F(4)-P(1)-F(2)	178.1(2)
F(1)-P(1)-F(2)	89.8(2)
F(4)-P(1)-F(5)	89.5(2)
F(1)-P(1)-F(5)	90.20(19)
F(2)-P(1)-F(5)	92.1(2)

F(4)-P(1)-F(6)	90.5(2)
F(1)-P(1)-F(6)	178.2(2)
F(2)-P(1)-F(6)	88.53(19)
F(5)-P(1)-F(6)	90.70(17)
F(4)-P(1)-F(3)	88.79(18)
F(1)-P(1)-F(3)	90.73(17)
F(2)-P(1)-F(3)	89.6(2)
F(5)-P(1)-F(3)	178.1(2)
F(6)-P(1)-F(3)	88.41(15)
F(6')-P(1')-F(3')	102.6(12)
F(6')-P(1')-F(2')	90.8(10)
F(3')-P(1')-F(2')	90.0(10)
F(6')-P(1')-F(4')	92.7(10)
F(3')-P(1')-F(4')	91.4(10)
F(2')-P(1')-F(4')	175.9(12)
F(6')-P(1')-F(1')	166.3(13)
F(3')-P(1')-F(1')	90.6(10)
F(2')-P(1')-F(1')	85.6(10)
F(4')-P(1')-F(1')	90.5(10)
F(6')-P(1')-F(5')	81.5(11)
F(3')-P(1')-F(5')	175.7(12)
F(2')-P(1')-F(5')	91.1(9)
F(4')-P(1')-F(5')	87.2(9)
F(1')-P(1')-F(5')	85.4(9)
F(12)-P(2)-F(9)	90.65(12)
F(12)-P(2)-F(8)	89.79(11)
F(9)-P(2)-F(8)	90.53(10)
F(12)-P(2)-F(7)	178.94(11)
F(9)-P(2)-F(7)	89.24(12)
F(8)-P(2)-F(7)	91.27(11)
F(12)-P(2)-F(11)	90.40(12)
F(9)-P(2)-F(11)	178.93(12)
F(8)-P(2)-F(11)	89.65(9)
F(7)-P(2)-F(11)	89.71(12)
F(12)-P(2)-F(10)	90.52(10)
F(9)-P(2)-F(10)	90.58(10)

F(8)-P(2)-F(10)	178.85(10)
F(7)-P(2)-F(10)	88.43(10)
F(11)-P(2)-F(10)	89.24(9)
C(1)-N(1)-C(5)	117.45(16)
C(1)-N(1)-Ru(1)	126.18(13)
C(5)-N(1)-Ru(1)	115.85(12)
C(10)-N(2)-C(6)	117.35(16)
C(10)-N(2)-Ru(1)	126.45(13)
C(6)-N(2)-Ru(1)	115.91(12)
C(13)-N(3)-C(17)	117.43(17)
C(13)-N(3)-Ru(1)	125.93(13)
C(17)-N(3)-Ru(1)	116.38(12)
C(22)-N(4)-C(18)	117.51(17)
C(22)-N(4)-Ru(1)	126.40(13)
C(18)-N(4)-Ru(1)	115.92(12)
C(25)-N(5)-C(29)	117.40(16)
C(25)-N(5)-Ru(1)	126.17(12)
C(29)-N(5)-Ru(1)	116.39(12)
C(30)-N(6)-C(34)	117.69(16)
C(30)-N(6)-Ru(1)	115.74(12)
C(34)-N(6)-Ru(1)	125.80(13)
C(3)-O(1)-C(11)	117.13(16)
C(8)-O(2)-C(12)	118.15(17)
C(15)-O(3)-C(23)	117.52(16)
C(20)-O(4)-C(24)	116.99(17)
C(27)-O(5)-C(35)	115.72(15)
C(32)-O(6)-C(36)	117.41(16)
N(1)-C(1)-C(2)	123.64(17)
N(1)-C(1)-H(1A)	118.2
C(2)-C(1)-H(1A)	118.2
C(1)-C(2)-C(3)	118.53(17)
C(1)-C(2)-H(2A)	120.7
C(3)-C(2)-H(2A)	120.7
O(1)-C(3)-C(2)	124.81(17)
O(1)-C(3)-C(4)	116.26(17)
C(2)-C(3)-C(4)	118.93(18)

C(5)-C(4)-C(3)	118.90(17)
C(5)-C(4)-H(4A)	120.5
C(3)-C(4)-H(4A)	120.5
N(1)-C(5)-C(4)	122.50(17)
N(1)-C(5)-C(6)	114.22(16)
C(4)-C(5)-C(6)	123.25(16)
N(2)-C(6)-C(7)	122.15(17)
N(2)-C(6)-C(5)	114.76(15)
C(7)-C(6)-C(5)	123.08(17)
C(6)-C(7)-C(8)	119.52(18)
C(6)-C(7)-H(7A)	120.2
C(8)-C(7)-H(7A)	120.2
O(2)-C(8)-C(9)	125.73(17)
O(2)-C(8)-C(7)	115.52(17)
C(9)-C(8)-C(7)	118.72(17)
C(10)-C(9)-C(8)	118.32(18)
C(10)-C(9)-H(9A)	120.8
C(8)-C(9)-H(9A)	120.8
N(2)-C(10)-C(9)	123.92(18)
N(2)-C(10)-H(10A)	118.0
C(9)-C(10)-H(10A)	118.0
O(1)-C(11)-H(11A)	109.5
O(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
O(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(2)-C(12)-H(12A)	109.5
O(2)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
O(2)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N(3)-C(13)-C(14)	123.15(18)
N(3)-C(13)-H(13A)	118.4
C(14)-C(13)-H(13A)	118.4

C(13)-C(14)-C(15)	119.15(18)
C(13)-C(14)-H(14A)	120.4
C(15)-C(14)-H(14A)	120.4
O(3)-C(15)-C(16)	125.18(19)
O(3)-C(15)-C(14)	116.19(18)
C(16)-C(15)-C(14)	118.62(18)
C(17)-C(16)-C(15)	118.73(18)
C(17)-C(16)-H(16A)	120.6
C(15)-C(16)-H(16A)	120.6
N(3)-C(17)-C(16)	122.83(17)
N(3)-C(17)-C(18)	114.15(17)
C(16)-C(17)-C(18)	123.02(17)
N(4)-C(18)-C(19)	122.06(17)
N(4)-C(18)-C(17)	114.22(16)
C(19)-C(18)-C(17)	123.72(18)
C(18)-C(19)-C(20)	119.46(19)
C(18)-C(19)-H(19A)	120.3
C(20)-C(19)-H(19A)	120.3
O(4)-C(20)-C(21)	124.99(18)
O(4)-C(20)-C(19)	116.50(18)
C(21)-C(20)-C(19)	118.51(18)
C(22)-C(21)-C(20)	118.42(18)
C(22)-C(21)-H(21A)	120.8
C(20)-C(21)-H(21A)	120.8
N(4)-C(22)-C(21)	123.78(19)
N(4)-C(22)-H(22A)	118.1
C(21)-C(22)-H(22A)	118.1
O(3)-C(23)-H(23A)	109.5
O(3)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
O(3)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
O(4)-C(24)-H(24A)	109.5
O(4)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5

O(4)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
N(5)-C(25)-C(26)	123.99(17)
N(5)-C(25)-H(25A)	118.0
C(26)-C(25)-H(25A)	118.0
C(25)-C(26)-C(27)	118.14(18)
C(25)-C(26)-H(26A)	120.9
C(27)-C(26)-H(26A)	120.9
O(5)-C(27)-C(26)	124.18(18)
O(5)-C(27)-C(28)	117.10(16)
C(26)-C(27)-C(28)	118.72(18)
C(29)-C(28)-C(27)	119.31(17)
C(29)-C(28)-H(28A)	120.3
C(27)-C(28)-H(28A)	120.3
N(5)-C(29)-C(28)	122.19(17)
N(5)-C(29)-C(30)	113.64(16)
C(28)-C(29)-C(30)	124.16(16)
N(6)-C(30)-C(31)	122.50(17)
N(6)-C(30)-C(29)	114.75(15)
C(31)-C(30)-C(29)	122.66(17)
C(32)-C(31)-C(30)	118.91(18)
C(32)-C(31)-H(31A)	120.5
C(30)-C(31)-H(31A)	120.5
O(6)-C(32)-C(31)	124.96(18)
O(6)-C(32)-C(33)	116.27(17)
C(31)-C(32)-C(33)	118.76(17)
C(34)-C(33)-C(32)	118.93(18)
C(34)-C(33)-H(33A)	120.5
C(32)-C(33)-H(33A)	120.5
N(6)-C(34)-C(33)	122.92(18)
N(6)-C(34)-H(34A)	118.5
C(33)-C(34)-H(34A)	118.5
O(5)-C(35)-H(35A)	109.5
O(5)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5

O(5)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
O(6)-C(36)-H(36A)	109.5
O(6)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
O(6)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(38)-C(37)-H(37A)	109.5
C(38)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(38)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
O(7)-C(38)-C(37)	122.0(3)
O(7)-C(38)-C(39)	121.1(3)
C(37)-C(38)-C(39)	116.9(3)
C(38)-C(39)-H(39A)	109.5
C(38)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(38)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters ($Å^2 x 10^3$) for paul009. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	11(1)	11(1)	11(1)	-2(1)	0(1)	-2(1)
P(1)	19(1)	20(1)	28(1)	-8(1)	-5(1)	-6(1)
F(1)	70(2)	47(2)	109(3)	-2(2)	-34(2)	-38(2)
F(2)	43(2)	56(2)	151(3)	-43(2)	-8(2)	18(1)
F(3)	66(2)	42(1)	25(1)	2(1)	-3(1)	-22(1)
F(4)	48(2)	115(3)	87(2)	-65(2)	-11(2)	38(2)
F(5)	115(3)	74(2)	46(1)	-6(1)	-51(2)	-31(2)
F(6)	64(2)	62(2)	27(1)	1(1)	-9(1)	-46(1)
P(1')	36(4)	45(3)	53(4)	-17(3)	-4(3)	-7(3)
F(1')	45(6)	40(5)	120(10)	-27(6)	-1(6)	-11(4)
F(2')	82(6)	66(6)	69(5)	-2(4)	31(5)	12(5)
F(3')	47(6)	98(6)	105(7)	21(7)	-13(5)	26(5)
F(4')	77(6)	67(6)	70(5)	-41(4)	28(5)	-31(5)
F(5')	75(6)	41(5)	90(7)	18(5)	-13(5)	0(4)
F(6')	132(10)	78(6)	69(8)	-48(6)	13(6)	-51(6)
P(2)	21(1)	19(1)	19(1)	-5(1)	-1(1)	-5(1)
F(7)	37(1)	68(1)	68(1)	3(1)	-12(1)	-27(1)
F(8)	66(1)	40(1)	22(1)	2(1)	7(1)	-4(1)
F(9)	88(2)	32(1)	46(1)	-16(1)	-5(1)	11(1)
F(10)	43(1)	41(1)	22(1)	4(1)	0(1)	-9(1)
F(11)	81(1)	29(1)	35(1)	-11(1)	-3(1)	10(1)
F(12)	41(1)	78(1)	63(1)	2(1)	-23(1)	-29(1)
N(1)	13(1)	11(1)	14(1)	-2(1)	0(1)	-2(1)
N(2)	14(1)	12(1)	12(1)	-2(1)	0(1)	-2(1)
N(3)	13(1)	12(1)	12(1)	-1(1)	-2(1)	-2(1)
N(4)	13(1)	13(1)	12(1)	-3(1)	-1(1)	-2(1)
N(5)	11(1)	12(1)	14(1)	-3(1)	0(1)	-2(1)
N(6)	12(1)	14(1)	13(1)	-3(1)	0(1)	-2(1)
O(1)	23(1)	23(1)	20(1)	-12(1)	4(1)	-11(1)
O(2)	23(1)	22(1)	24(1)	-8(1)	9(1)	-13(1)
O(3)	18(1)	21(1)	22(1)	-5(1)	-9(1)	4(1)

O(4)	30(1)	19(1)	18(1)	-10(1)	-8(1)	3(1)
O(5)	11(1)	22(1)	21(1)	5(1)	-4(1)	-3(1)
O(6)	12(1)	18(1)	29(1)	3(1)	0(1)	-5(1)
C(1)	16(1)	13(1)	17(1)	-2(1)	2(1)	-4(1)
C(2)	17(1)	15(1)	20(1)	-5(1)	1(1)	-6(1)
C(3)	15(1)	14(1)	18(1)	-6(1)	0(1)	-2(1)
C(4)	14(1)	15(1)	16(1)	-5(1)	1(1)	-4(1)
C(5)	12(1)	11(1)	15(1)	-2(1)	0(1)	-2(1)
C(6)	12(1)	12(1)	13(1)	-2(1)	-1(1)	-3(1)
C(7)	16(1)	15(1)	15(1)	-4(1)	2(1)	-5(1)
C(8)	15(1)	15(1)	16(1)	-2(1)	1(1)	-5(1)
C(9)	18(1)	15(1)	19(1)	-3(1)	0(1)	-7(1)
C(10)	19(1)	15(1)	16(1)	-4(1)	0(1)	-5(1)
C(11)	28(1)	29(1)	29(1)	-13(1)	0(1)	-16(1)
C(12)	28(1)	28(1)	32(1)	-8(1)	8(1)	-18(1)
C(13)	17(1)	15(1)	14(1)	-4(1)	-1(1)	-3(1)
C(14)	18(1)	18(1)	15(1)	-4(1)	-4(1)	-4(1)
C(15)	13(1)	16(1)	17(1)	-1(1)	-3(1)	-2(1)
C(16)	16(1)	14(1)	15(1)	-3(1)	-1(1)	-2(1)
C(17)	16(1)	11(1)	12(1)	-1(1)	-2(1)	-3(1)
C(18)	13(1)	13(1)	13(1)	-1(1)	-2(1)	-3(1)
C(19)	17(1)	14(1)	15(1)	-4(1)	-2(1)	0(1)
C(20)	21(1)	14(1)	15(1)	-4(1)	-2(1)	-4(1)
C(21)	18(1)	19(1)	16(1)	-5(1)	-5(1)	-4(1)
C(22)	15(1)	18(1)	15(1)	-3(1)	-3(1)	-1(1)
C(23)	18(1)	22(1)	25(1)	-6(1)	-4(1)	4(1)
C(24)	37(1)	26(1)	16(1)	-9(1)	-8(1)	-1(1)
C(25)	13(1)	16(1)	16(1)	-1(1)	2(1)	-4(1)
C(26)	11(1)	19(1)	18(1)	-2(1)	0(1)	-3(1)
C(27)	12(1)	15(1)	17(1)	-3(1)	-2(1)	-2(1)
C(28)	13(1)	15(1)	15(1)	-2(1)	0(1)	-4(1)
C(29)	12(1)	12(1)	15(1)	-4(1)	1(1)	-3(1)
C(30)	10(1)	15(1)	13(1)	-4(1)	0(1)	-2(1)
C(31)	13(1)	13(1)	16(1)	-2(1)	-1(1)	-3(1)
C(32)	13(1)	16(1)	18(1)	-2(1)	1(1)	-4(1)
C(33)	11(1)	20(1)	19(1)	-2(1)	0(1)	-3(1)

C(34)	12(1)	15(1)	18(1)	-3(1)	-1(1)	-1(1)
C(35)	10(1)	28(1)	24(1)	2(1)	-3(1)	-2(1)
C(36)	18(1)	18(1)	36(1)	6(1)	-2(1)	-5(1)
O(7)	101(2)	32(1)	23(1)	-12(1)	-1(1)	-22(1)
C(37)	45(2)	47(2)	122(4)	-31(2)	-1(2)	-2(2)
C(38)	53(2)	32(1)	25(1)	-16(1)	6(1)	-9(1)
C(39)	49(2)	48(2)	35(1)	-12(1)	6(1)	-15(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for paul009.

	x	y	z	U(eq)
H(1A)	1618	-173	1713	19
H(2A)	1588	-1050	532	20
H(4A)	3965	691	-990	18
H(7A)	5171	1731	-909	18
H(9A)	5727	3987	391	20
H(10A)	4260	3488	1512	20
H(11A)	2073	-1612	-1688	39
H(11B)	1180	-965	-1024	39
H(11C)	2091	-1998	-586	39
H(12A)	7630	4007	-1649	42
H(12B)	7301	3983	-569	42
H(12C)	6403	4662	-1315	42
H(13A)	1052	2253	318	18
H(14A)	-631	3402	-187	20
H(16A)	-600	4915	1909	18
H(19A)	381	4999	3032	19
H(21A)	3301	3720	4431	21
H(22A)	3778	2492	3486	19
H(23A)	-3138	6050	731	33
H(23B)	-1906	6176	1036	33
H(23C)	-2626	5303	1660	33
H(24A)	1449	5522	5622	39
H(24B)	2695	5135	5110	39
H(24C)	1879	4281	5615	39
H(25A)	5323	1109	2094	19
H(26A)	6633	-52	3073	20
H(28A)	3833	-1109	4668	18
H(31A)	2002	-1293	4524	17
H(33A)	-1079	442	3589	20
H(34A)	-38	1675	2647	19

H(35A)	7659	-1701	5075	33
H(35B)	7356	-513	4467	33
H(35C)	7624	-1513	3975	33
H(36A)	-257	-2820	5257	39
H(36B)	784	-2306	5493	39
H(36C)	839	-2636	4515	39
H(37A)	6269	-2748	2956	106
H(37B)	5828	-3874	3179	106
H(37C)	5639	-3171	3953	106
H(39A)	2772	-2759	2988	65
H(39B)	3302	-3143	3980	65
H(39C)	3643	-3881	3232	65

Computational Information

Table S12. Selected molecular orbital energies from the PCM calculation for ruthenium polypyridyl complexes studies in this work.

$[Ru(bpy(OH)_2)_3]^{2+}$		$[Ru(bpy(O)_2)_3]^{4-}$		$[Ru(bpy)_2(bpy(O)_2)]$	
orbital	energy (eV)	orbital	energy (eV)	orbital	energy (eV)
HOMO-2	-5.633	HOMO-2	-3.456	HOMO-2	-5.361
HOMO-1	-5.633	HOMO-1	-3.456	HOMO-1	-4.653
HOMO	-5.578	HOMO	-3.456	HOMO	-4.653
LUMO	-2.068	LUMO	-0.190	LUMO	-2.041

Molecular orbital energies calculated using the converstion factor: 1 Hartree = 27.2116 eV.

$[Ru(bpy(OH)_2)_3]^{2+}$

Nuclear Repulsion Energy (a.u.) = 5488.8946051

Total Energy (a.u.) = -2006.267166

Max. Gradient = 0.000872 hartree/bohr RMS Gradient = 0.000255 hartree/bohr

C_1 symmetry

Nuclear Coordinates (Ångstroms)

RU	44.0	-0.0044062314	0.0000611706	-0.0003437227
N	7.0	1.7719121932	0.3486631518	1.0685723348
N	7.0	1.3965348379	-1.1441375191	-1.0705513052
N	7.0	-0.5828631221	-1.7120528820	1.0713731401
N	7.0	-1.6926684213	-0.6398672418	-1.0693605510
N	7.0	0.2919971087	1.7859248959	-1.0712611097
N	7.0	-1.1935205806	1.3631835006	1.0633900822
O	8.0	5.3734057051	0.8666616311	3.0462285949
O	8.0	4.3284011375	-3.2995911588	-3.0489353235
O	8.0	-1.9330163094	-5.0926303291	3.0457833308
O	8.0	-5.0245566209	-2.1059358867	-3.0436502076
O	8.0	0.7020092085	5.4039565968	-3.0447679069
O	8.0	-3.4387701174	4.2229866527	3.0457194827
C	6.0	1.8898637536	1.1195519949	2.1714136432
H	1.0	0.9792522029	1.5977610149	2.5119970064
C	6.0	3.0776862896	1.3045987045	2.8529328605
H	1.0	3.1282137882	1.9294937334	3.7377398889
C	6.0	4.2321929663	0.6647671898	2.3751917655
C	6.0	4.1232060019	-0.1373637263	1.2313146359
H	1.0	5.0024356367	-0.6418465615	0.8450223143
C	6.0	2.8863403761	-0.2785554873	0.6002511578
C	6.0	2.6748418135	-1.1195873487	-0.6008623502
C	6.0	3.6978953467	-1.8308264984	-1.2293098227
H	1.0	4.7118463233	-1.7980648200	-0.8448651626
C	6.0	3.4161902257	-2.5876107063	-2.3747374595
C	6.0	2.0977854553	-2.6016862459	-2.8563465859
H	1.0	1.8489779670	-3.1722189042	-3.7442784295
C	6.0	1.1378693668	-1.8784874588	-2.1742277857
H	1.0	0.1097932155	-1.8690347954	-2.5161628976
C	6.0	0.0242023731	-2.1969574337	2.1754487382
H	1.0	0.8948776746	-1.6491619288	2.5172664228
C	6.0	-0.4092123689	-3.3194398802	2.8557035051
H	1.0	0.1069229548	-3.6769898630	3.7399680660
C	6.0	-1.5379313117	-4.0030100382	2.3751673688
C	6.0	-2.1774163315	-3.5065445580	1.2311550191

H	1.0	-3.0534668377	-4.0159047972	0.8436314032
C	6.0	-1.6830657717	-2.3630497246	0.6028277918
C	6.0	-2.3066939104	-1.7603505044	-0.5992173326
C	6.0	-3.4352133944	-2.2916088362	-1.2249005560
H	1.0	-3.9088000561	-3.1888762874	-0.8410444833
C	6.0	-3.9528120309	-1.6700799594	-2.3691654278
C	6.0	-3.3078561872	-0.5197800227	-2.8518862379
H	1.0	-3.6812764628	-0.0201917143	-3.7389722855
C	6.0	-2.1997606097	-0.0492095314	-2.1730852074
H	1.0	-1.6815752806	0.8401256296	-2.5129319015
C	6.0	1.0590711928	1.9287406601	-2.1736861630
H	1.0	1.5666397474	1.0339823152	-2.5139740763
C	6.0	1.2115359389	3.1229538276	-2.8520190896
H	1.0	1.8333229851	3.1925802654	-3.7375347538
C	6.0	0.5411167482	4.2581204317	-2.3703078701
C	6.0	-0.2604847089	4.1233498618	-1.2287181388
H	1.0	-0.7953934269	4.9853450947	-0.8443424800
C	6.0	-0.3696609255	2.8805847080	-0.6030097634
C	6.0	-1.2025482883	2.6435548961	0.5989284010
C	6.0	-1.9449975608	3.6429684350	1.2293738628
H	1.0	-1.9467837216	4.6570389835	0.8441131838
C	6.0	-2.6954906059	3.3355523731	2.3723283319
C	6.0	-2.6717099267	2.0157408947	2.8498680234
H	1.0	-3.2373427905	1.7473633851	3.7353123303
C	6.0	-1.9185236760	1.0796695949	2.1671976387
H	1.0	-1.8777497063	0.0516390099	2.5065573709
H	1.0	-3.4017549909	5.1076725314	2.6444935624
H	1.0	0.2070915906	6.1365919430	-2.6411695273
H	1.0	6.1208029967	0.3924456454	2.6444965619
H	1.0	5.2102402962	-3.2368703887	-2.6449573583
H	1.0	-5.4101332006	-2.9005336110	-2.6379875054
H	1.0	-2.7170199331	-5.5015740732	2.6418029580

Below are a list of frequencies (in cm-1) determined at the DFT level. The frequencies were projected (PROJCT=.T. in $FORCE) in order to make the six translational and rotational modes have a frequency of zero.

0.00	0.00	0.00	0.00	0.00
0.00	16.95	20.16	20.83	23.89
30.34	38.84	78.78	80.40	87.81
92.87	96.12	100.33	119.71	124.00
128.94	130.36	142.26	144.38	176.92
180.38	198.28	217.44	219.12	219.32
246.50	259.57	259.79	306.79	311.83
321.40	324.32	328.84	332.84	338.15

339.06	352.88	354.74	362.53	367.21
438.17	438.32	440.21	445.24	445.68
447.99	452.98	454.00	454.84	455.67
457.13	458.84	470.10	472.04	479.86
511.16	523.71	527.07	563.73	565.30
565.99	574.30	574.96	577.48	585.57
588.33	588.89	666.15	666.82	667.71
680.26	685.69	686.58	737.30	741.29
742.19	760.55	765.38	766.15	767.74
770.61	772.35	850.93	853.43	853.84
858.47	861.75	862.25	863.25	864.14
864.79	865.90	867.16	868.57	891.01
893.63	894.61	982.04	985.72	986.36
986.68	990.01	990.53	991.10	992.17
993.52	1030.15	1033.66	1034.42	1036.75
1037.74	1048.53	1081.04	1088.14	1089.43
1121.16	1133.39	1134.65	1144.73	1153.89
1155.20	1195.50	1195.91	1197.49	1204.02
1205.56	1210.22	1258.96	1268.06	1268.94
1299.47	1304.41	1305.56	1308.59	1309.21
1310.58	1344.81	1346.48	1346.95	1347.48
1348.30	1348.62	1376.94	1379.04	1379.97
1394.15	1398.58	1399.69	1479.20	1488.57
1488.94	1489.84	1491.91	1494.56	1536.88
1539.85	1541.42	1542.35	1542.83	1543.29
1610.70	1616.03	1617.27	1617.43	1621.97
1622.50	1663.86	1669.19	1671.25	1671.50
1676.00	1676.75	3214.43	3214.64	3217.28
3226.96	3227.13	3227.70	3234.27	3234.72
3238.00	3238.17	3238.21	3238.48	3247.92
3248.00	3251.30	3251.37	3251.65	3252.29
3729.65	3730.39	3730.64	3731.62	3732.84
3734.76				

$[Ru(bpy(O)_2)_3]^{4-}$

Nuclear Repulsion Energy (a.u.) = 5278.2644955

Total Energy (a.u.) = -2002.923716

C_1 symmetry

Max. Gradient = 0.000993 hartree/bohr RMS Gradient = 0.000309 hartree/bohr

Nuclear Coordinates (Ångstroms)

RU	44.0	-0.0047230398	0.0010502400	-0.0017552378
N	7.0	1.7945522421	0.3463442617	1.0632003189
N	7.0	1.4174566387	-1.1532528328	-1.0667590730
N	7.0	-0.6026045616	-1.7297868014	1.0659845169
N	7.0	-1.7141475535	-0.6597847451	-1.0609055586
N	7.0	0.2909771433	1.8109845798	-1.0663190820
N	7.0	-1.2011621966	1.3863269788	1.0599446831
O	8.0	5.4520008242	0.7818709496	3.0287314082
O	8.0	4.4366426060	-3.2629711770	-3.0325300714
O	8.0	-2.0382807352	-5.1211762417	3.0331491314
O	8.0	-5.0509317726	-2.2189193948	-3.0266267997
O	8.0	0.6264824687	5.4849684730	-3.0206877203
O	8.0	-3.4056556764	4.3361732843	3.0262726820
C	6.0	1.9331046151	1.1188056364	2.1646471032
H	1.0	1.0184682065	1.6114218713	2.4859092853
C	6.0	3.1150849758	1.2945208210	2.8553393585
H	1.0	3.1378861489	1.9360537090	3.7361552159
C	6.0	4.3403385570	0.6539210457	2.4324620109
C	6.0	4.1476046972	-0.1558543141	1.2484092770
H	1.0	5.0216094082	-0.6769262848	0.8672629726
C	6.0	2.9212174248	-0.2904114140	0.6092935359
C	6.0	2.7105290549	-1.1280770870	-0.6100157970
C	6.0	3.7279324434	-1.8258373385	-1.2488023309
H	1.0	4.7432921778	-1.7833270545	-0.8643220657
C	6.0	3.5171004373	-2.6243961456	-2.4374812940
C	6.0	2.1346090017	-2.6101672448	-2.8606314914
H	1.0	1.8535209328	-3.1819034468	-3.7450248138
C	6.0	1.1759298119	-1.8953497387	-2.1711884961
H	1.0	0.1378858789	-1.8940354109	-2.4952572772
C	6.0	0.0019750105	-2.2346299030	2.1646867733
H	1.0	0.8820698221	-1.6835746098	2.4885570322
C	6.0	-0.4337360344	-3.3456955598	2.8586168375
H	1.0	0.1138069804	-3.6823047825	3.7389415046
C	6.0	-1.5984978287	-4.0926316921	2.4368417123
C	6.0	-2.2058924124	-3.5238744891	1.2522955406

H	1.0	-3.0901948683	-4.0257219935	0.8687131501
C	6.0	-1.7116090515	-2.3953442086	0.6107188474
C	6.0	-2.3371174618	-1.7928246701	-0.6053648415
C	6.0	-3.4452427675	-2.3302034054	-1.2487019263
H	1.0	-3.9155723752	-3.2296754591	-0.8613597631
C	6.0	-4.0383646294	-1.7426582331	-2.4308567777
C	6.0	-3.3367134993	-0.5496735450	-2.8520844563
H	1.0	-3.6926304646	-0.0182803622	-3.7347689934
C	6.0	-2.2417536652	-0.0737484165	-2.1594908964
H	1.0	-1.7196859622	0.8243308070	-2.4813769907
C	6.0	1.0601379235	1.9739263874	-2.1665909006
H	1.0	1.5785356700	1.0744386460	-2.4899411169
C	6.0	1.2052414104	3.1628693998	-2.8525293809
H	1.0	1.8473414998	3.2054200716	-3.7321970034
C	6.0	0.5283881974	4.3681235371	-2.4286925399
C	6.0	-0.2795801860	4.1486570055	-1.2479601412
H	1.0	-0.8200929790	5.0079704406	-0.8607366108
C	6.0	-0.3804943914	2.9173821933	-0.6121893724
C	6.0	-1.2133564844	2.6804017991	0.6056183831
C	6.0	-1.9451504268	3.6743863852	1.2433385266
H	1.0	-1.9302694757	4.6920334441	0.8626963064
C	6.0	-2.7406893374	3.4368869482	2.4290892819
C	6.0	-2.6832815254	2.0554034951	2.8516506186
H	1.0	-3.2525372042	1.7541914692	3.7309933502
C	6.0	-1.9414000907	1.1193744983	2.1597978416
H	1.0	-1.9095803112	0.0810475783	2.4811529225

Below are a list of frequencies (in cm-1) determined at the DFT level. The frequencies were projected (PROJCT=.T. in $FORCE) in order to make the six translational and rotational modes have a frequency of zero.

0.00	0.00	0.00	0.00	0.00
0.00	20.27	23.30	25.79	26.01
33.04	38.11	81.83	82.47	86.67
92.42	94.80	98.01	117.70	121.68
127.41	127.82	140.96	143.97	175.34
179.36	197.19	211.04	211.10	211.87
231.88	245.24	245.74	291.15	298.35
306.49	316.79	320.12	326.03	344.04
349.00	351.55	356.95	358.28	361.59
445.93	447.56	450.46	459.90	461.89
468.51	479.57	485.34	486.44	522.56
533.17	536.12	561.59	563.42	564.07
569.85	570.28	576.04	590.61	594.12
594.94	671.39	675.17	675.95	695.91
696.68	697.48	746.76	747.07	749.85

750.91	751.23	752.12	768.63	771.60
772.88	827.96	829.46	830.47	831.25
834.67	834.96	854.15	856.79	857.09
863.96	869.12	869.92	871.01	873.11
873.87	954.68	956.10	958.35	958.96
961.23	962.47	963.68	968.22	968.86
1009.15	1016.99	1017.07	1023.33	1025.69
1036.03	1043.84	1051.22	1052.81	1092.72
1107.44	1109.25	1109.79	1124.03	1125.45
1220.11	1236.06	1236.53	1239.17	1245.11
1245.44	1261.61	1266.06	1266.57	1288.84
1295.87	1299.55	1304.75	1307.39	1309.38
1388.18	1396.33	1397.01	1405.91	1414.87
1417.40	1484.31	1489.57	1493.12	1493.26
1495.38	1495.76	1502.06	1504.55	1505.81
1517.01	1524.68	1524.82	1577.16	1581.75
1582.30	1587.88	1590.68	1591.65	1667.19
1669.73	1672.23	1675.76	1676.68	1678.13
3143.61	3144.11	3146.40	3146.57	3147.68
3147.95	3179.33	3179.45	3182.10	3190.55
3191.01	3193.01	3193.30	3193.74	3194.34
3196.34	3196.57	3197.05		

Below is an example of some of the input parameters used in calculating vertical excitation eneriges using PCM solvent, as well as information about the basis set used for Ru:

```
$CONTRL SCFTYP=RHF RUNTYP=ENERGY DFTTYP=B3LYP ISPHER=1
        TDDFT=EXCITE PP=MCP $END
$TDDFT NSTATE=18 MAXVEC=20 $END
$PCM SOLVNT=WATER $END
$PCMCAV RADII=SUAHF $END
```

30 core electrons in Ru were represented using a core potential.

Valence orbital exponents and coefficients used for Ru (IMCP-SR1 in GAMESS):

1	S	1	442.6962890	0.052813789055
1	S	2	38.3630417	-0.203722695476
1	S	3	6.0526510	0.531838494497
1	S	4	0.8285946	-1.176794012390
2	S	5	0.0727248	1.000000000000
3	S	6	0.0276180	1.000000000000
4	P	7	304.5768150	0.044730616206
4	P	8	82.3870215	0.116431825015
4	P	9	8.7689927	-0.461838988061
4	P	10	1.2002376	0.793091568105
4	P	11	0.4261142	0.304858861040
5	D	12	54.6234866	-0.068434929283
5	D	13	13.5251253	-0.238070155898
5	D	14	1.4952419	0.521203001235
5	D	15	0.5655327	0.559777423783
6	D	16	0.2183392	1.000000000000
7	D	17	0.0822551	1.000000000000
8	P	18	0.0836973	1.000000000000