Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Data

Spectroelectrochemical studies of ruthenium complexes containing the 4,4'-dihydroxy-2,2'-bipyridine ligand.

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Pourbaix Diagram

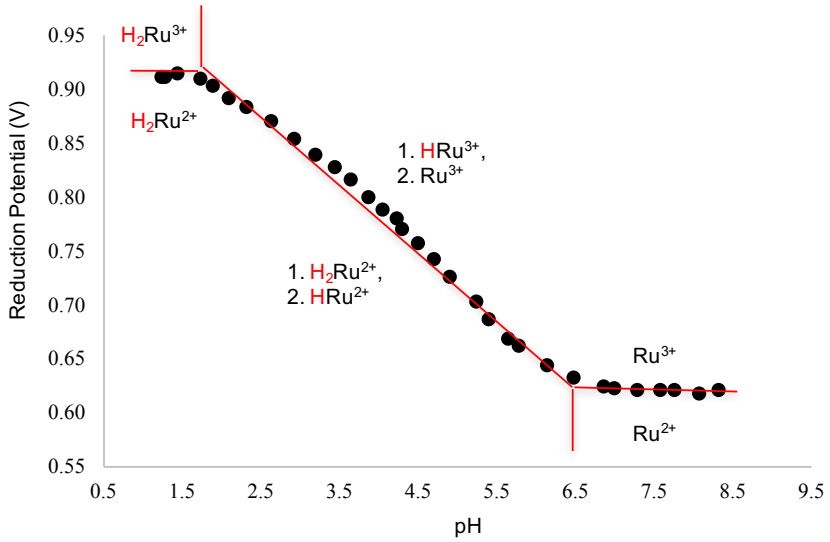

Figure S1 – Potential vs. pH diagram for $[Ru(bpy)_2(44'bpy(OH)_2)][Cl]_2$ in Britton-Robinson Buffer electrolyte solutions. Data reported vs Ag/AgCl. For these solutions, all solutions were kept in the dark and data was collected with protection from light. There is no noticeable difference in reduction potentials between the Pourbaix data collected in the dark vs. the light.

Cyclic Voltammetry

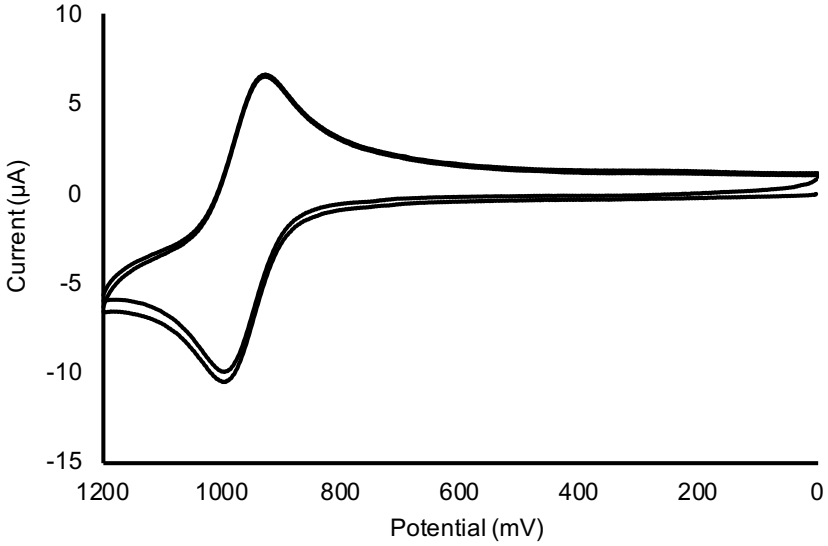

Figure S2 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OMe)_2)][Cl]_2$ in pH 1.85 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.96 V vs. Ag/AgCl.

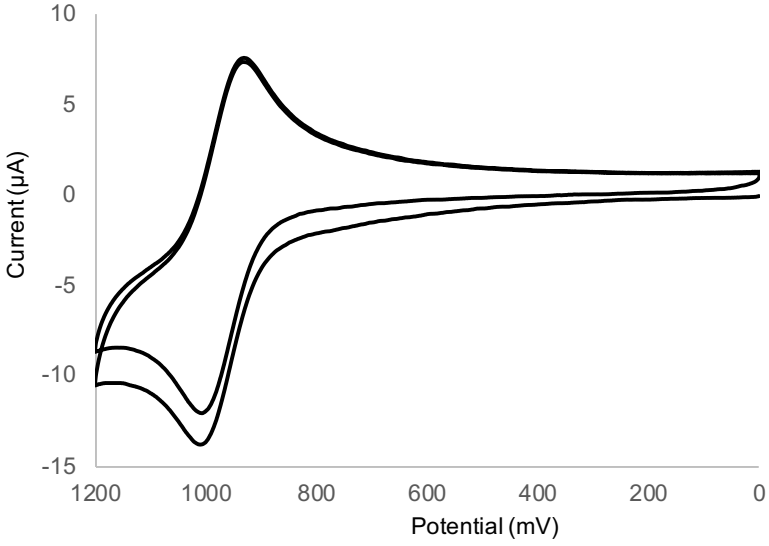

Figure S3 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OMe)_2)][Cl]_2$ in pH 4.84 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.96 V vs. Ag/AgCl.

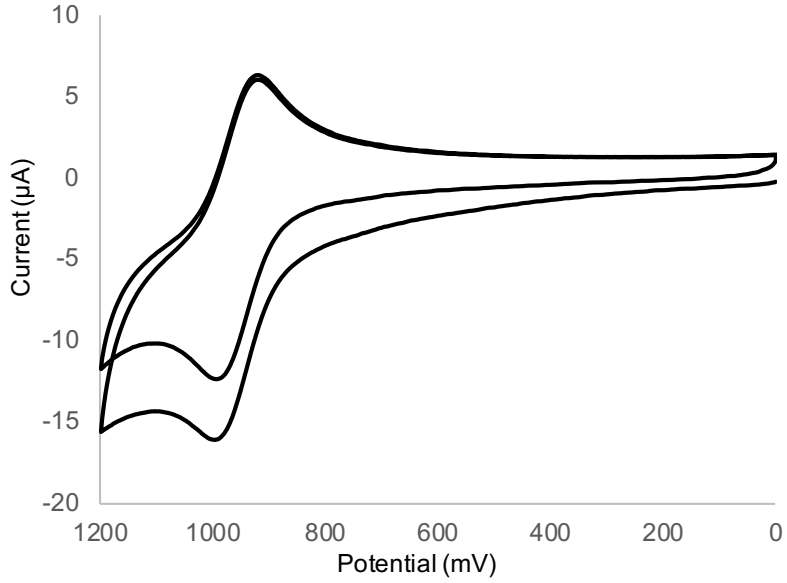

Figure S4 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OMe)_2)][Cl]_2$ in pH 7.35 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.96 V vs. Ag/AgCl.

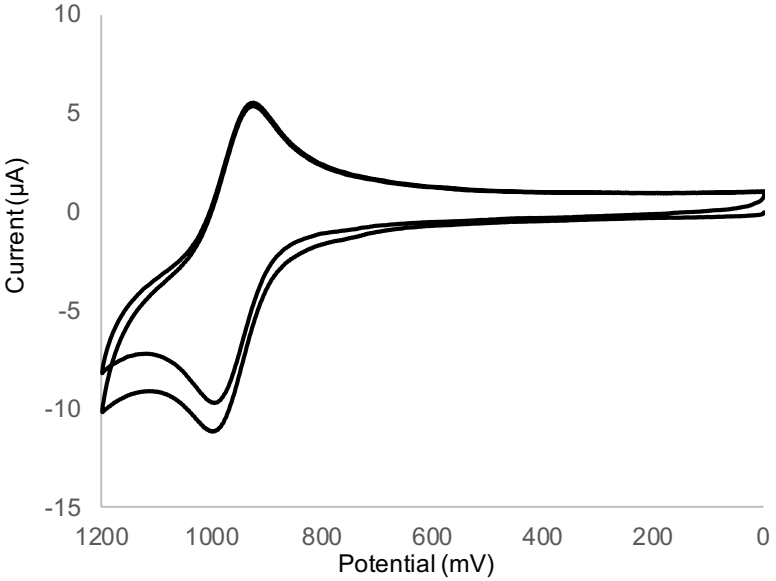

Figure S5 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OMe)_2)][Cl]_2$ in pH 9.04 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.96 V vs. Ag/AgCl.

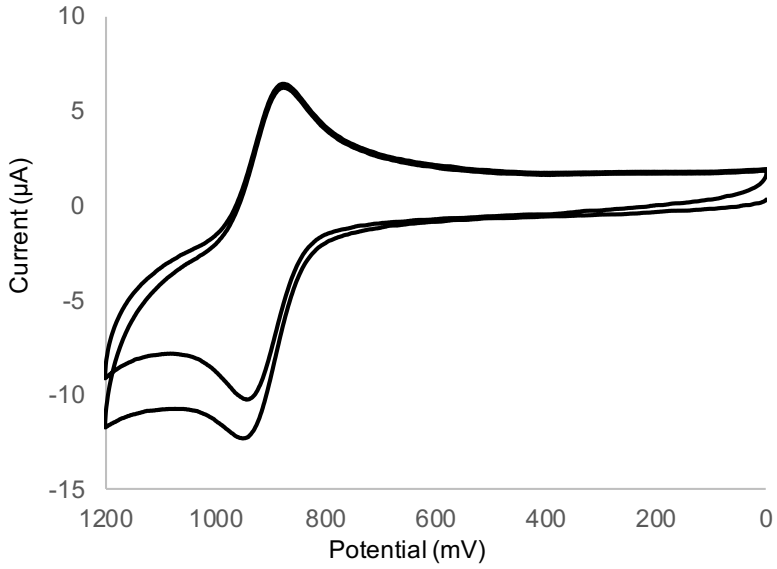

Figure S6 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 1.24 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.91 V vs. Ag/AgCl.

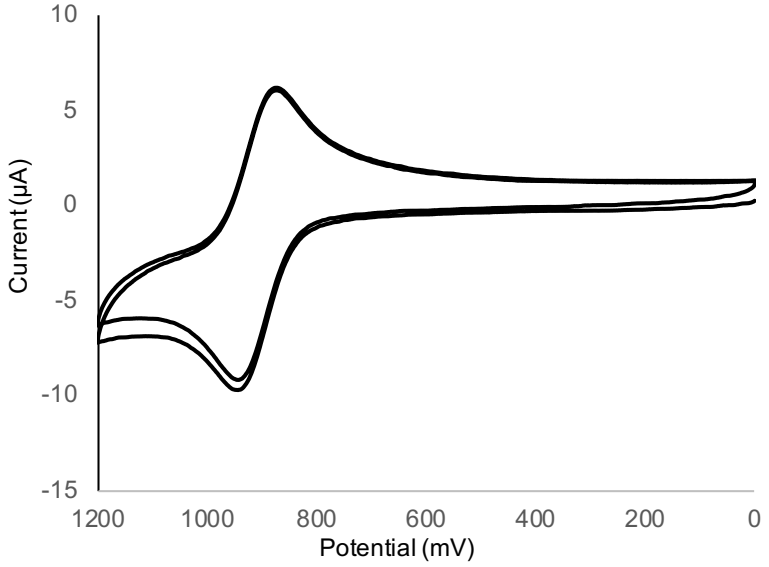

Figure S7 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 1.74 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.91 V vs. Ag/AgCl.

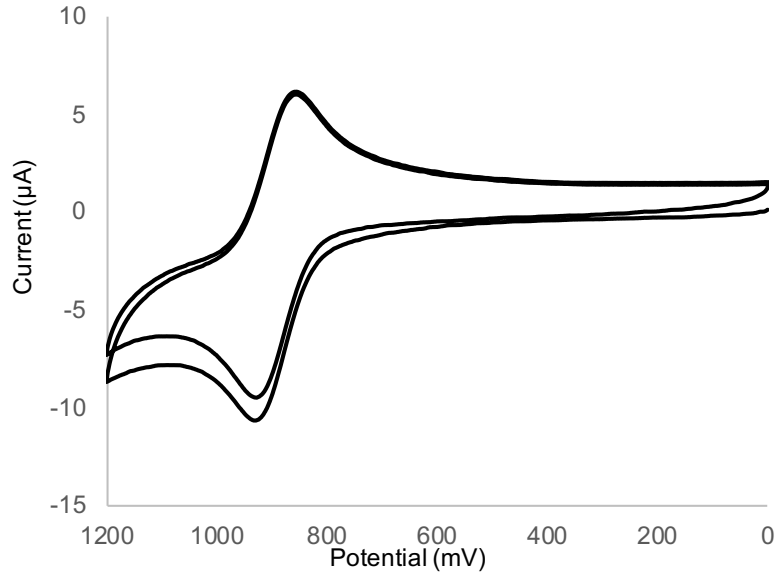

Figure S8 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 2.11 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.89 V vs. Ag/AgCl.

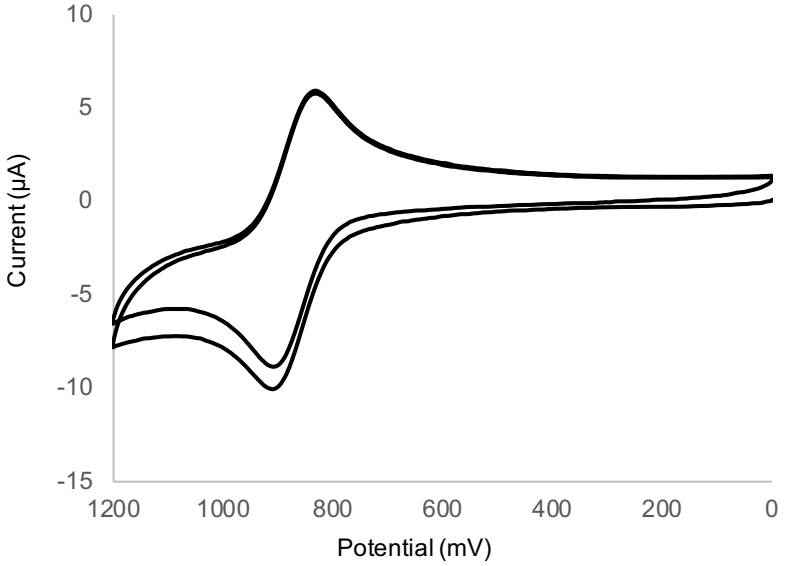

Figure S9 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 2.64 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.87 V vs. Ag/AgCl.

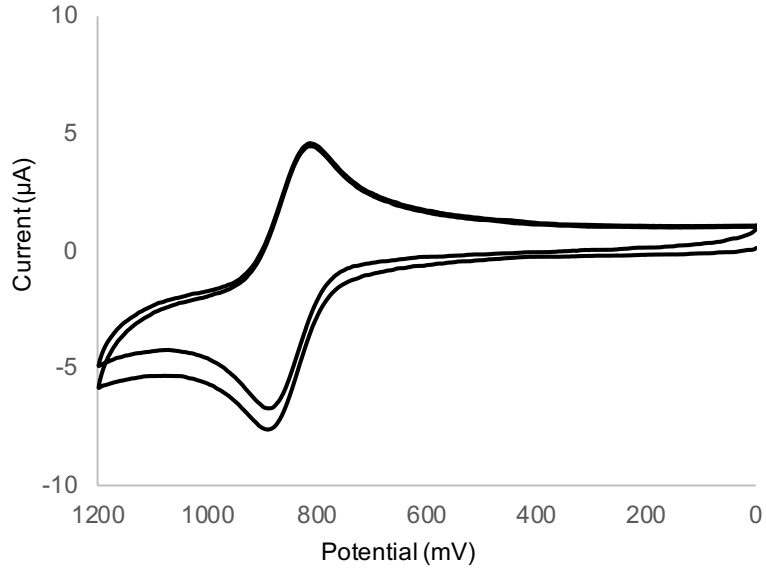

Figure S10 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 2.94 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.85 V vs. Ag/AgCl.

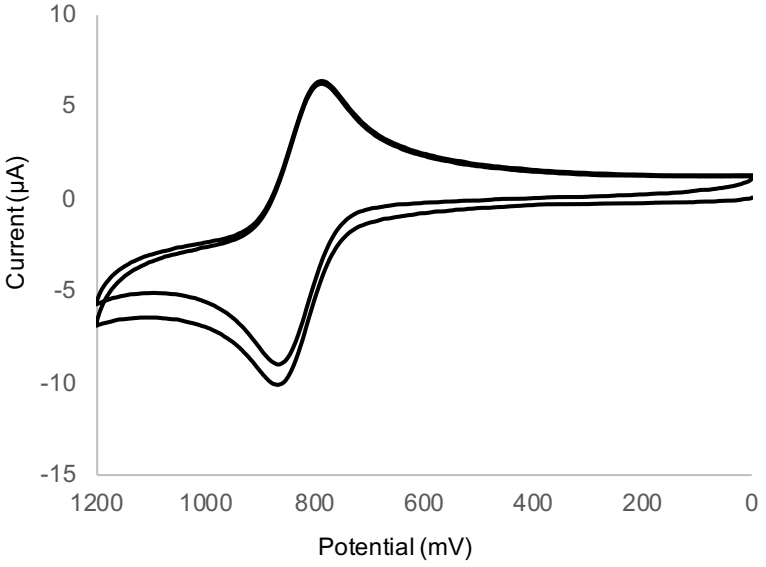

Figure S11 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 3.45 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.83 V vs. Ag/AgCl.

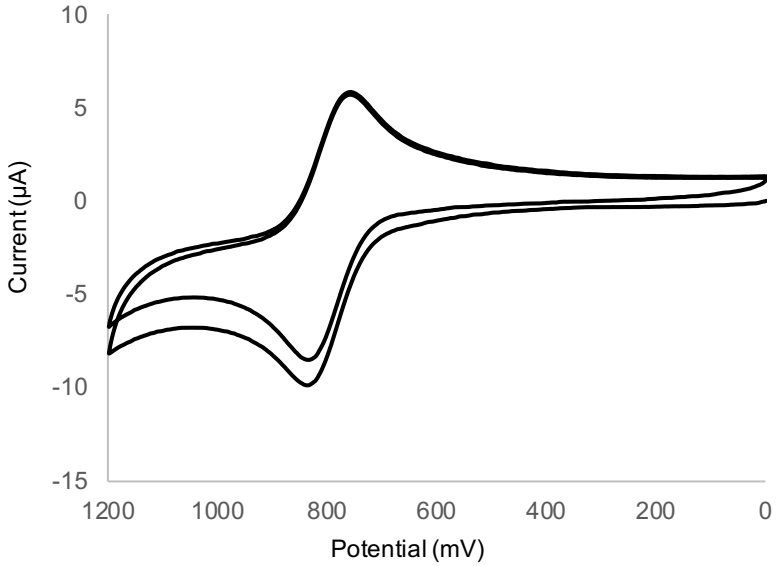

Figure S12 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 3.89 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.80 V vs. Ag/AgCl.

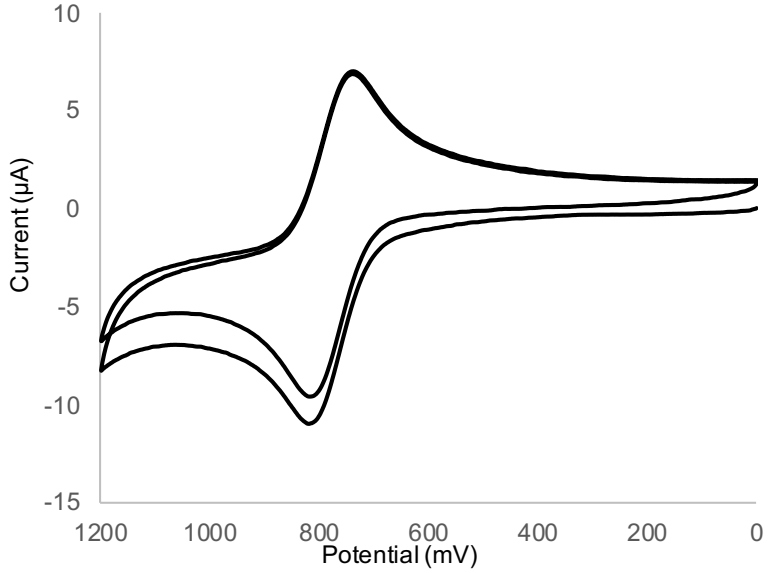

Figure S13 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 4.23 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.78 V vs. Ag/AgCl.

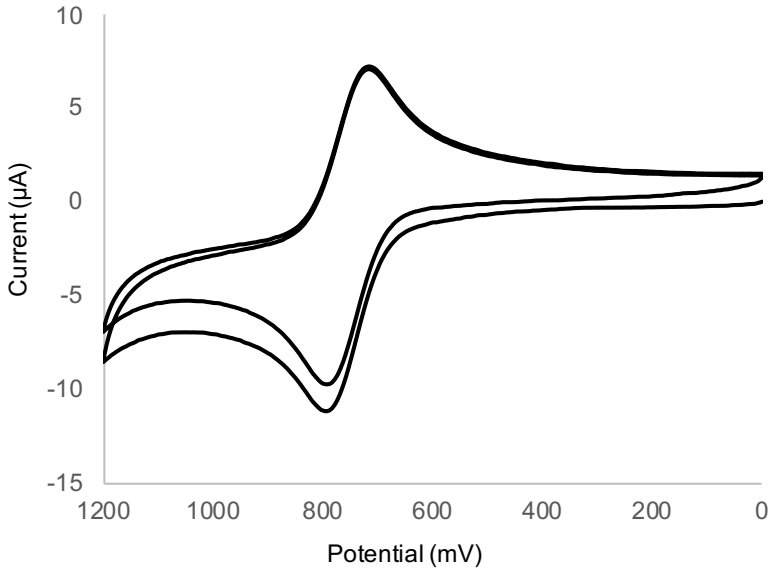

Figure S14 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 4.50 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.76 V vs. Ag/AgCl.

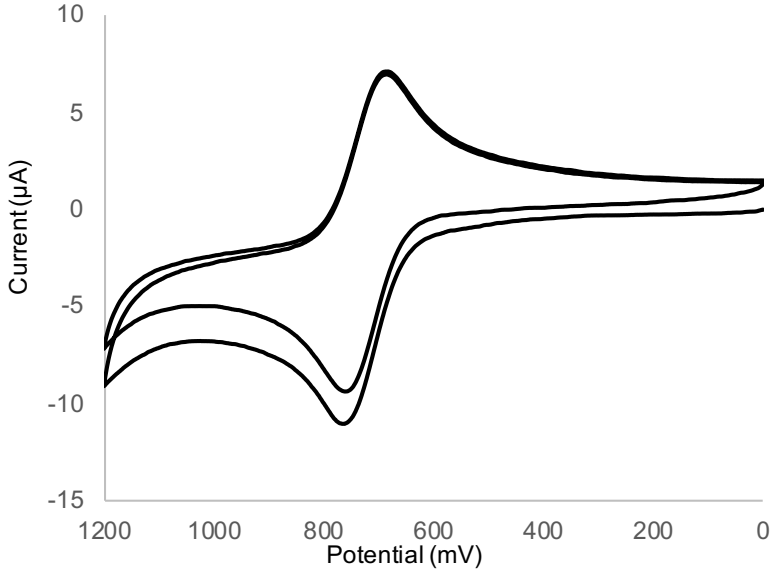

Figure S15 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 4.91 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.72 V vs. Ag/AgCl.

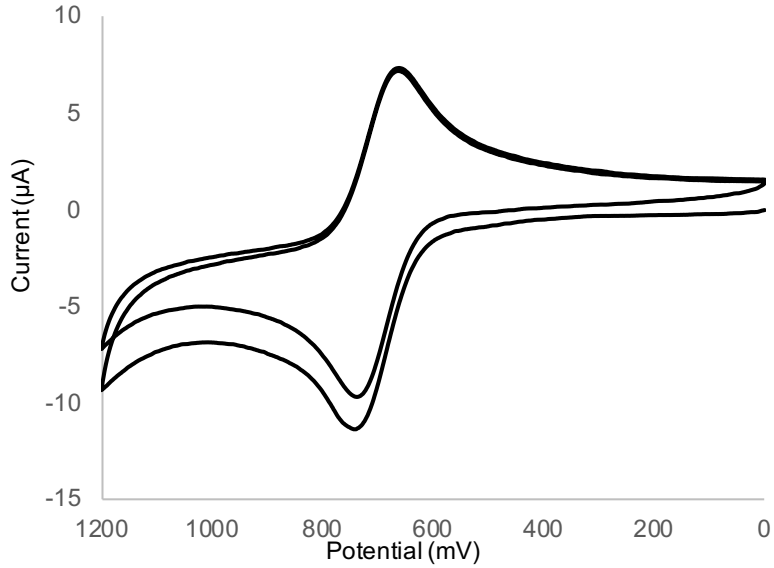

Figure S16 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 5.24 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.70 V vs. Ag/AgCl.

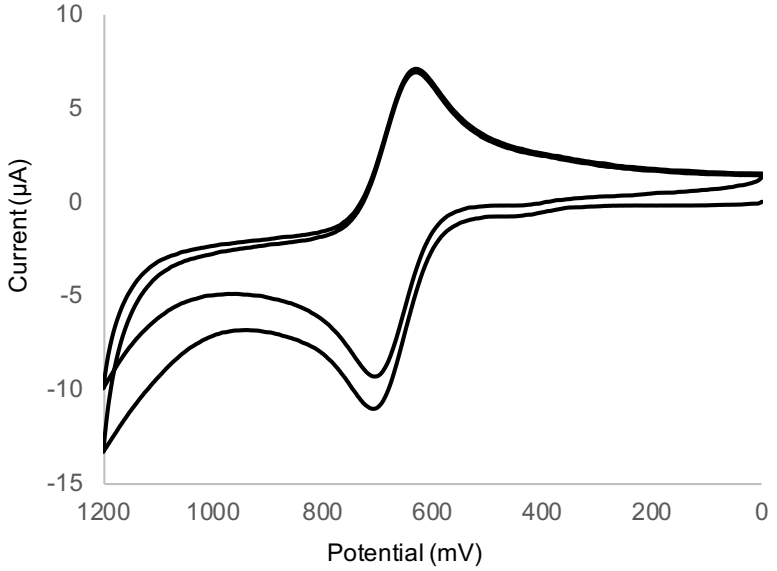

Figure S17 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 5.65 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.69 V vs. Ag/AgCl.

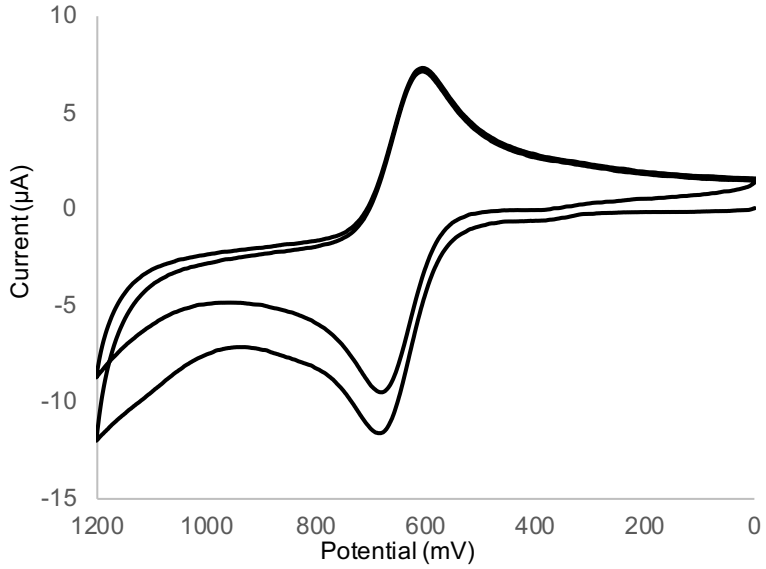

Figure S18 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 6.16 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.64 V vs. Ag/AgCl.

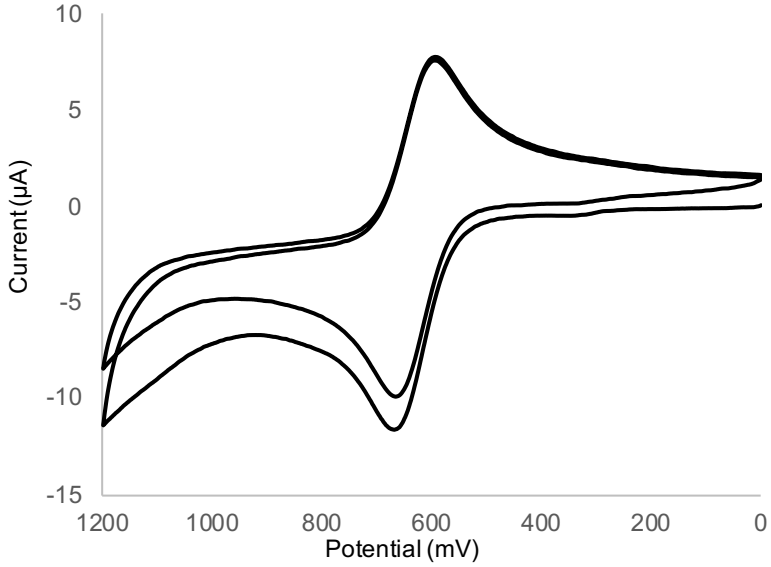

Figure S19 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 6.48 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.63 V vs. Ag/AgCl.

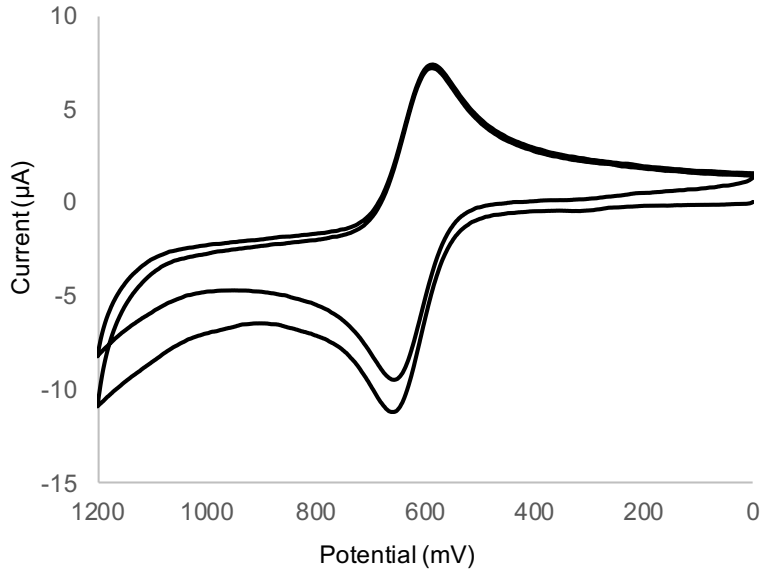

Figure S20 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 6.87 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.62 V vs. Ag/AgCl.

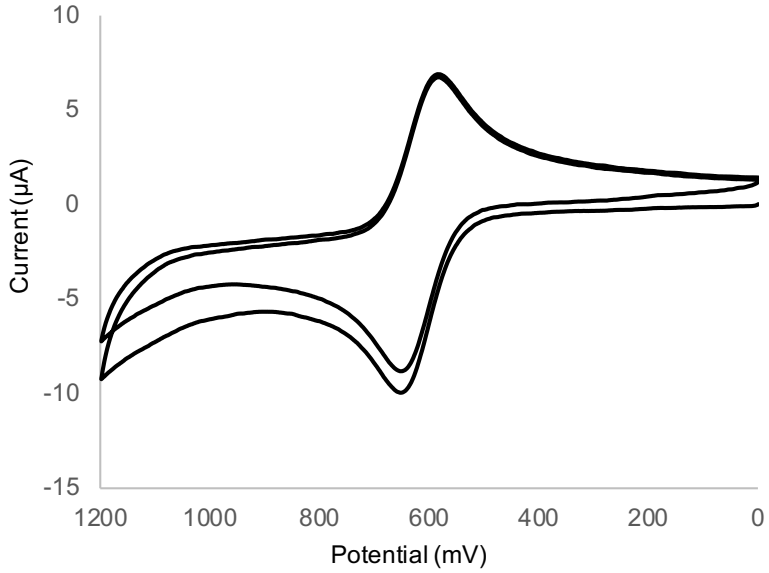

Figure S21 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 7.29 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.62 V vs. Ag/AgCl.

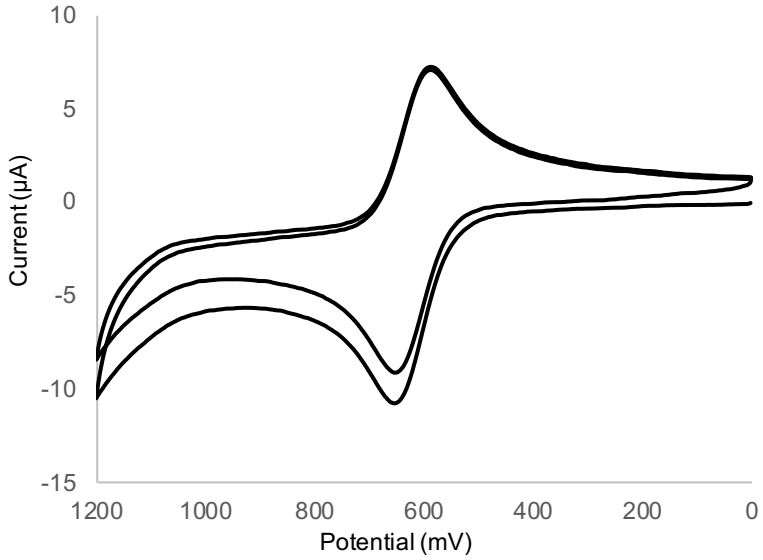

Figure S22 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 7.76 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.62 V vs. Ag/AgCl.

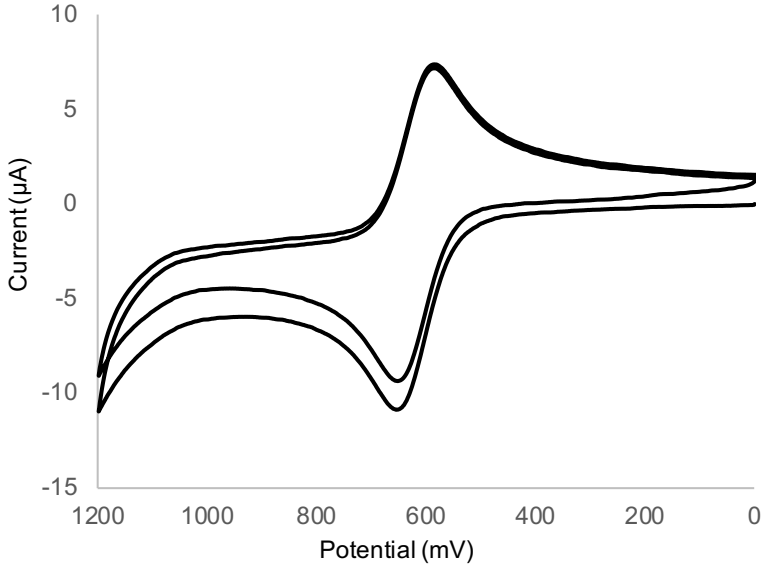

Figure S23 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 8.32 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.62 V vs. Ag/AgCl.

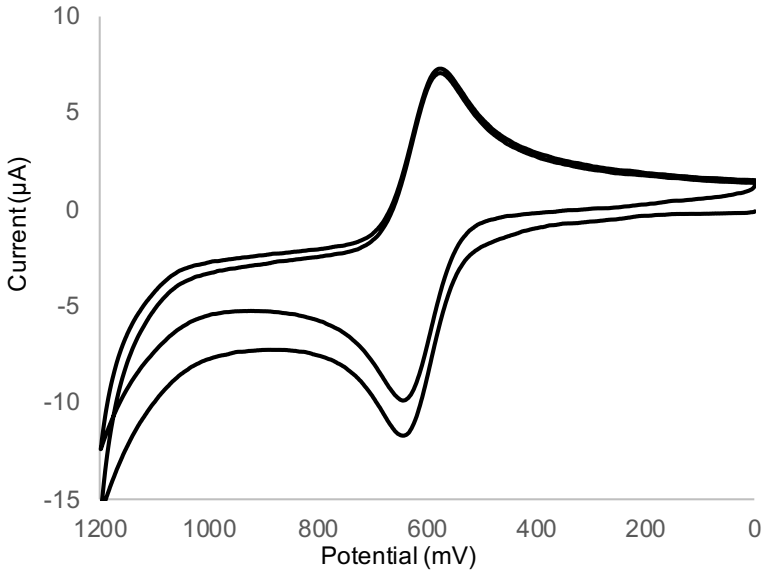

Figure S24 – Cyclic voltammogram of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ in pH 9.44 Britton-Robinson buffer. Scan rate is 100 mV/s. Reduction potential is 0.61 V vs. Ag/AgCl.

Spectroelectrochemistry

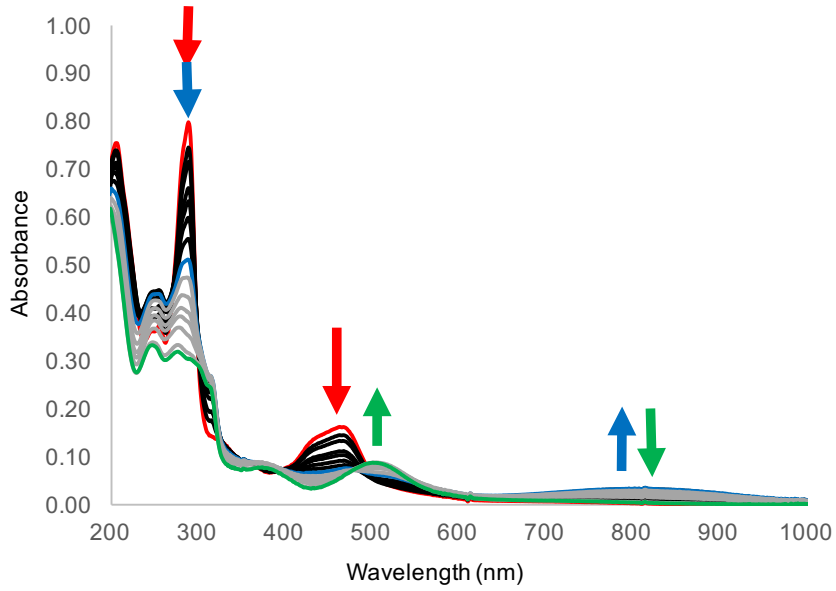

Figure S25 – Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ at pH = 1.55 at 1200 mV vs. AgCl reference. As the potential is held, initially there is a decrease in the 459 nm band (red) band and the appearance of a new broad absorbance band in the 800 nm region (blue). Over time, the 800 nm region band decreases and a higher energy band at 500 nm (green) appears. There is also a peak at 290 nm that decreases over time as the potential is held.

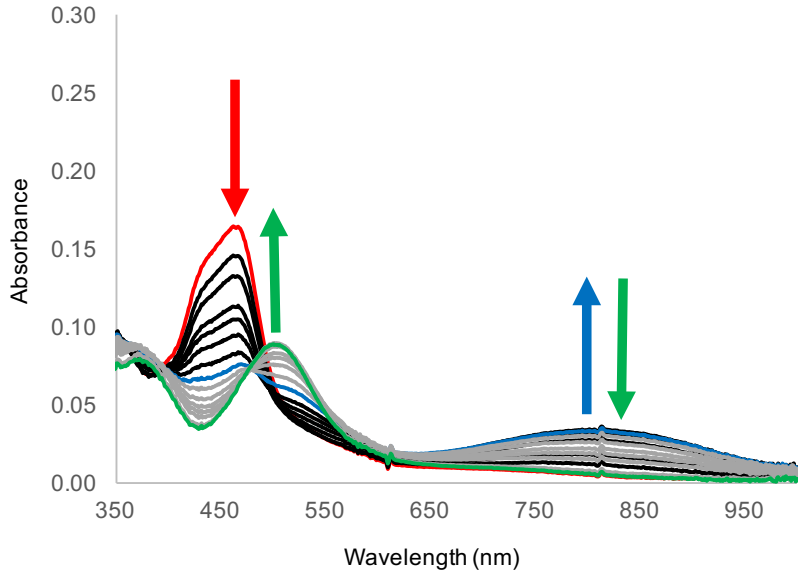

Figure S26 – Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ at pH = 1.55 at 1200 mV vs. AgCl reference. As the potential is held, initially there is a decrease in the 459 nm band (red) band and the appearance of a new broad absorbance band in the 800 nm region (blue). Over time, the 800 nm region band decreases and a higher energy band at 500 nm (green) appears.

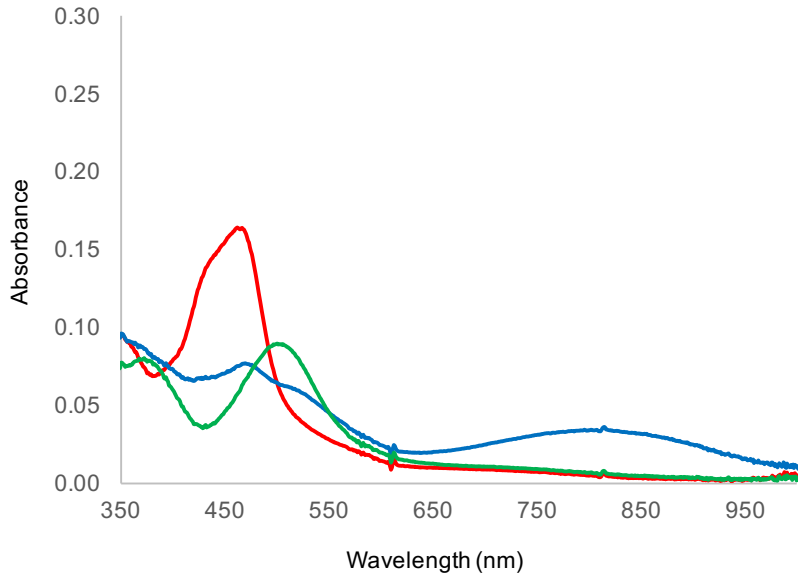

Figure S27 – Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ at pH = 1.55 at 1200 mV vs. AgCl reference depicting the three species that form at the potential is held: red = initial complex, blue = intermediate complex, green = final complex.

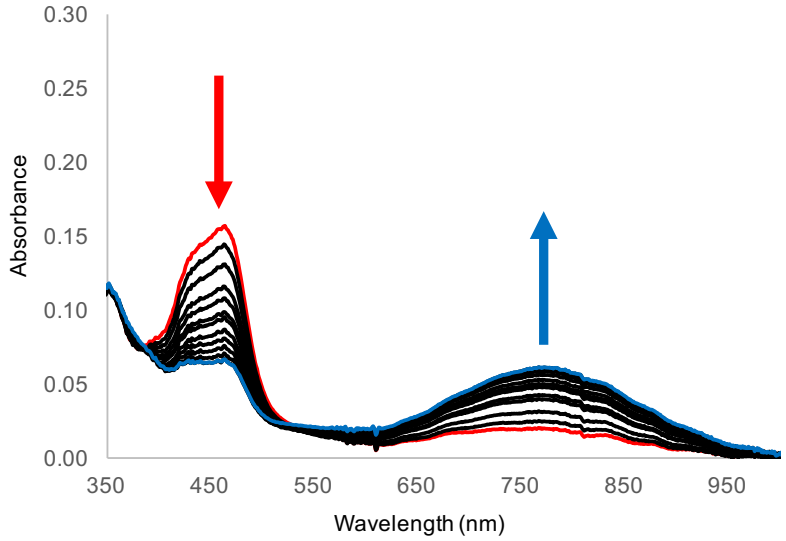

Figure S28 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ at pH = 2.86 at 1100 mV vs. AgCl reference. As the potential is held, the band at 450 nm region (red) decreases and a new broad band at 700-800 nm region (blue) appears.

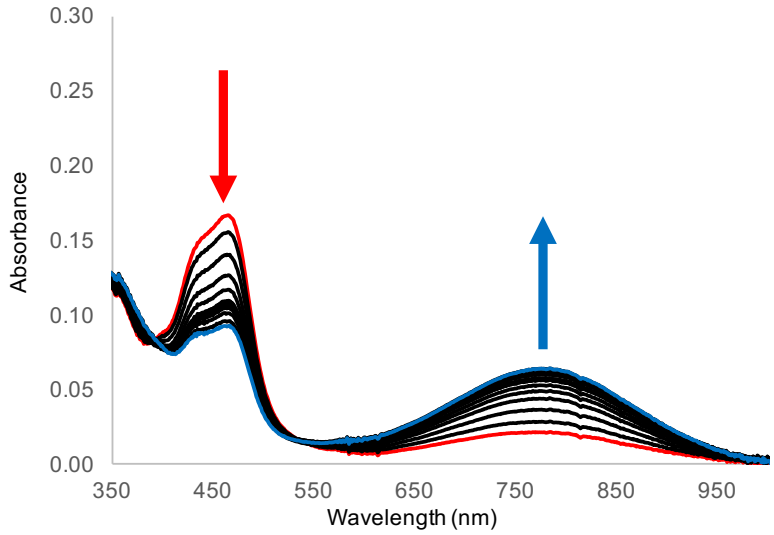

Figure S29 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ at pH = 3.98 at 1100 mV vs. AgCl reference. As the potential is held, the band at 450 nm region (red) decreases and a new broad band at 700-800 nm region (blue) appears.

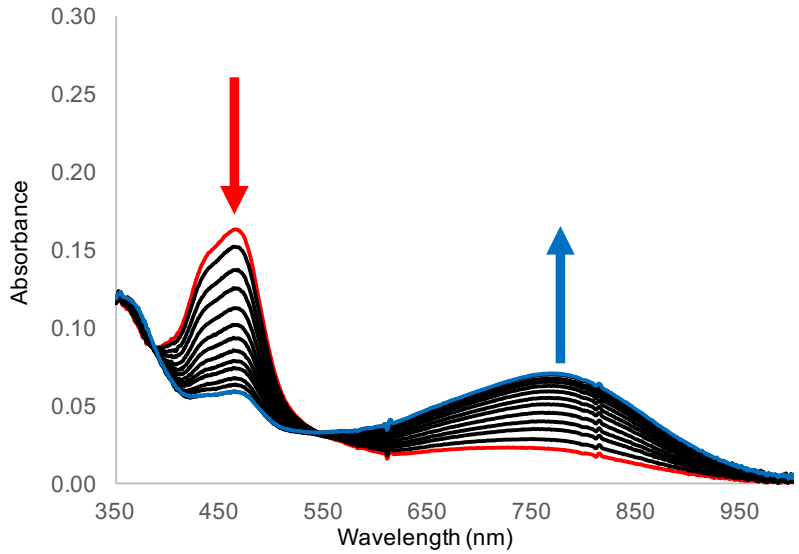

Figure S30 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ at pH = 4.92 at 1100 mV vs. AgCl reference. As the potential is held, the band at 450 nm region (red) decreases and a new broad band at 700-800 nm region (blue) appears.

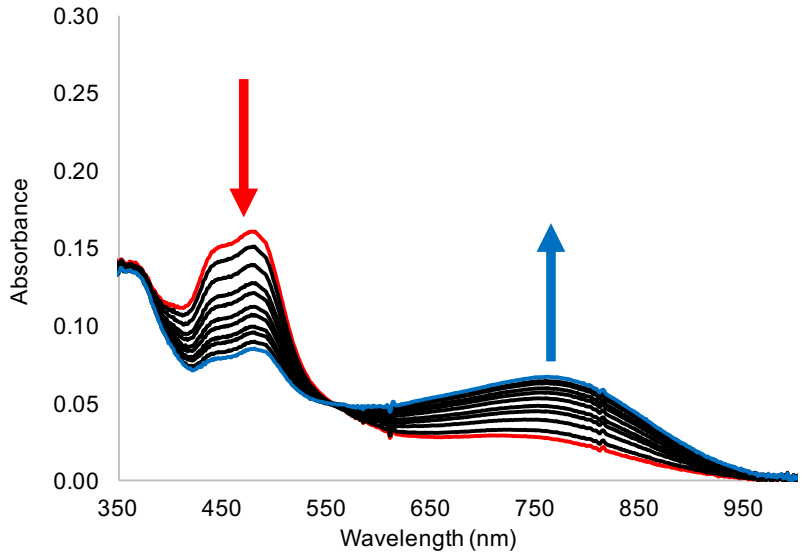

Figure S31 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ at pH = 6.04 at 1100 mV vs. AgCl reference. As the potential is held, the band at 450-500 nm region (red) decreases and a new broad band at 700-800 nm region (blue) appears.

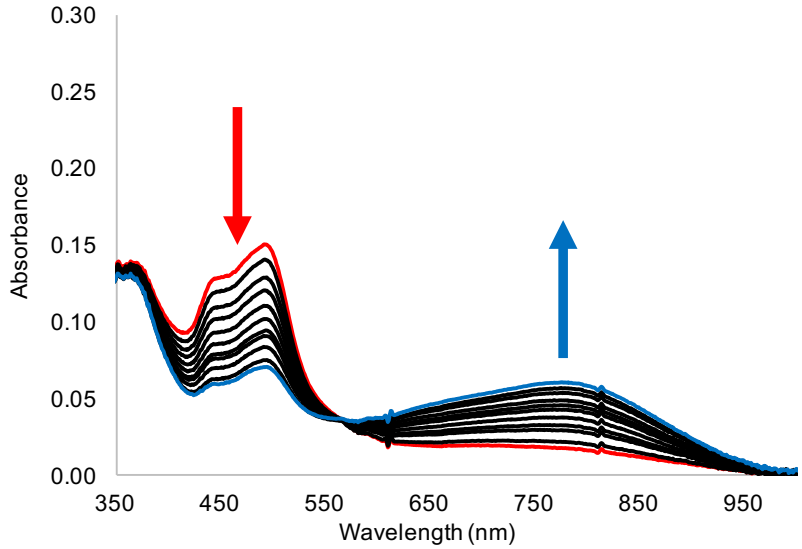

Figure S32 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ at pH = 6.87 at 1000 mV vs. AgCl reference. As the potential is held, the band at 450-500 nm region (red) decreases and a new broad band at 700-800 nm region (blue) appears.

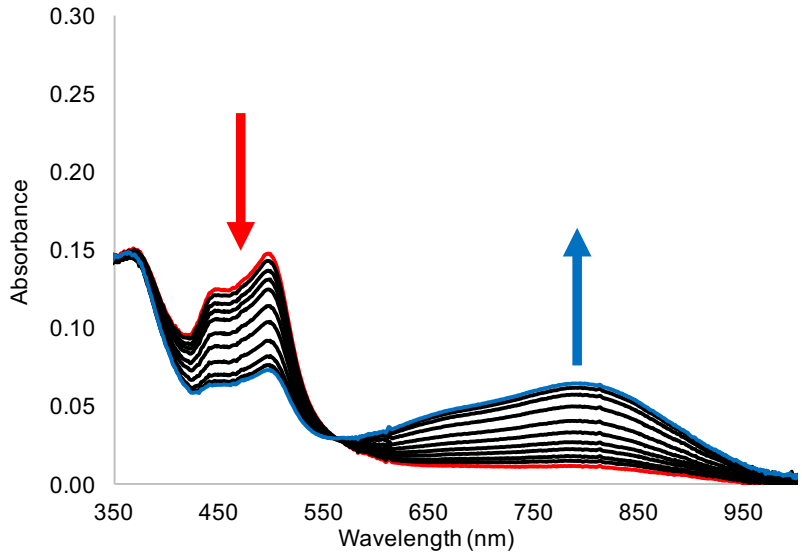

Figure S33 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ at pH = 8.10 at 900 mV vs. AgCl reference. As the potential is held, the band at 450-500 nm region (red) decreases and a new broad band at 700-800 nm region (blue) appears.

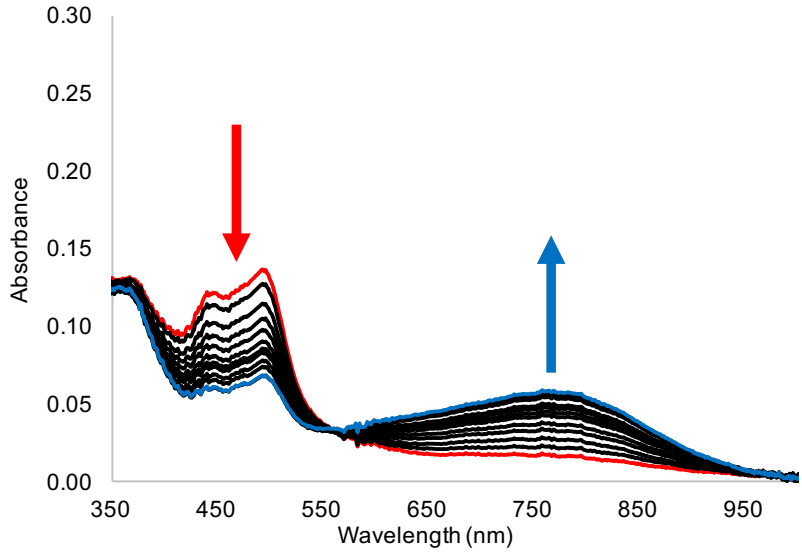

Figure S34 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ at pH = 8.84 at 1000 mV vs. AgCl reference. As the potential is held, the band at 450-500 nm region (red) decreases and a new broad band at 700-800 nm region (blue) appears.

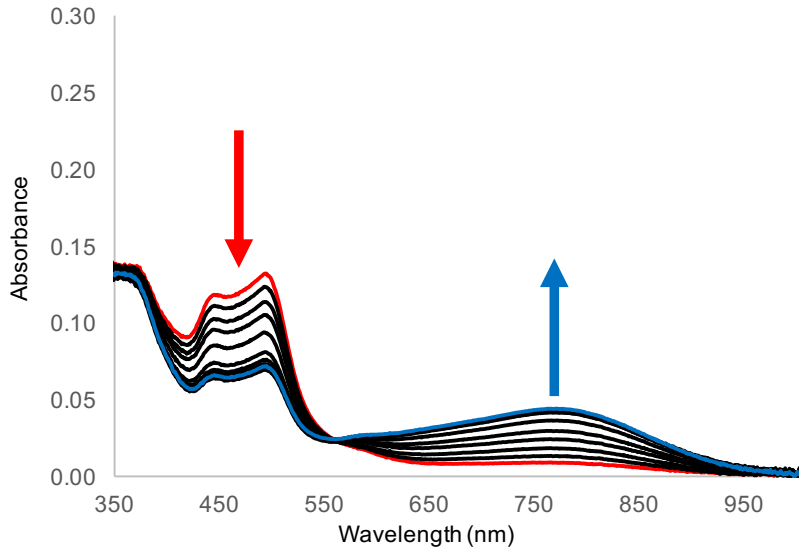

Figure S35 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ at pH = 9.85 at 1000 mV vs. AgCl reference. As the potential is held, the band at 450-500 nm region (red) decreases and a new broad band at 700-800 nm region (blue) appears.

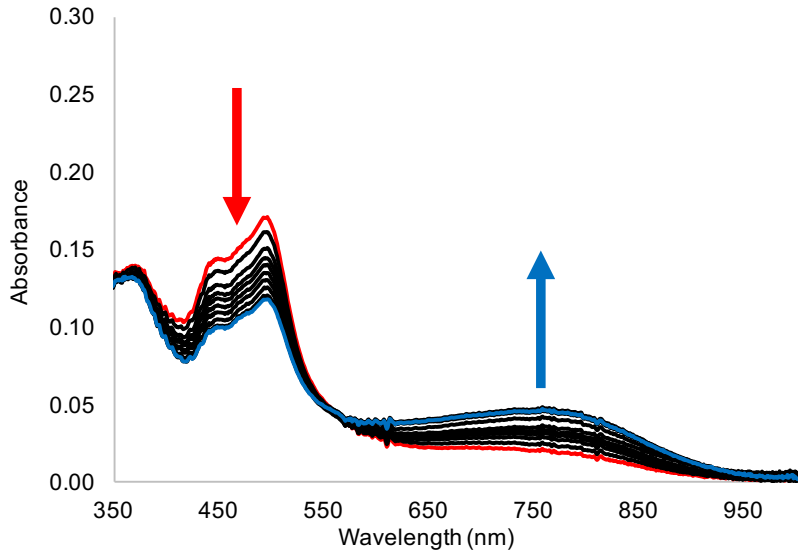

Figure S36 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OH)_2)][Cl]_2$ at pH = 11.21 at 900 mV vs. AgCl reference. As the potential is held, the band at 450-500 nm region (red) decreases and a new broad band at 700-800 nm region (blue) appears.

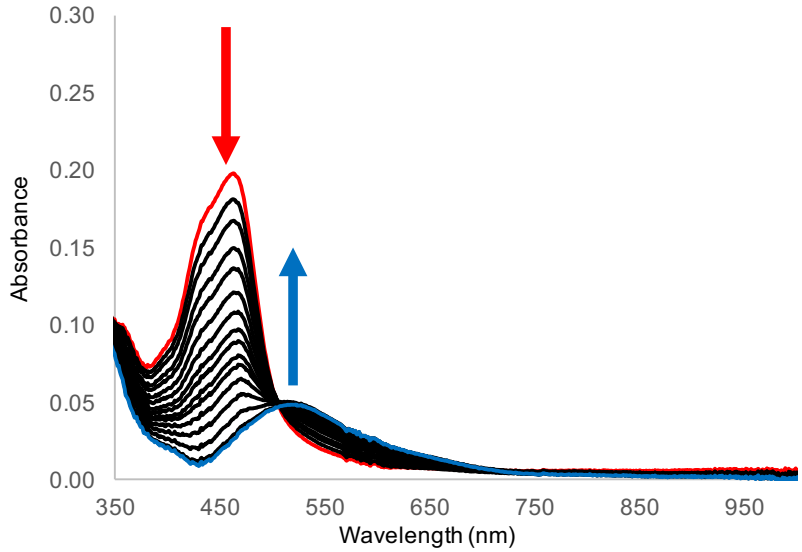

Figure S37 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OMe)_2)][Cl]_2$ at pH = 1.85 at 1200 mV vs. AgCl reference. As the potential is held, the band at 459 nm (red) decreases and a new broad band in the 500-550 nm region (blue) appears.

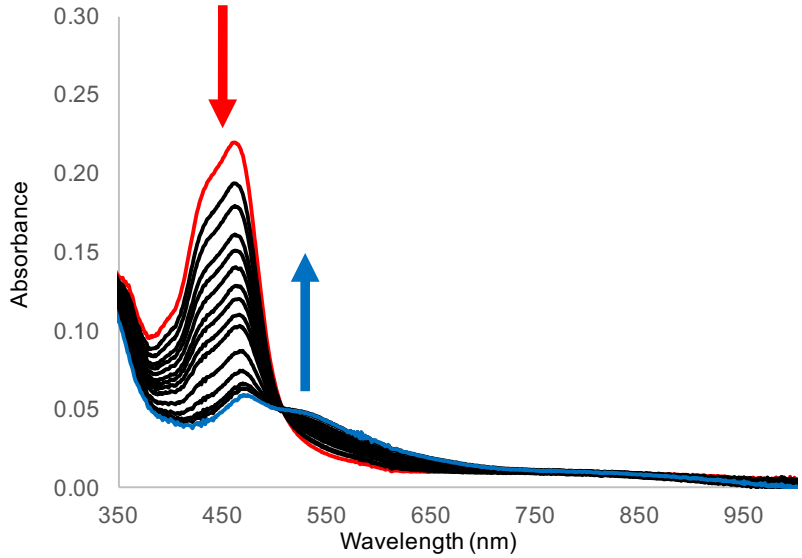

Figure S38 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OMe)_2)][Cl]_2$ at pH = 3.15 at 1200 mV vs. AgCl reference. As the potential is held, the band at 459 nm (red) decreases and a new broad band in the 500-550 nm region (blue) appears.

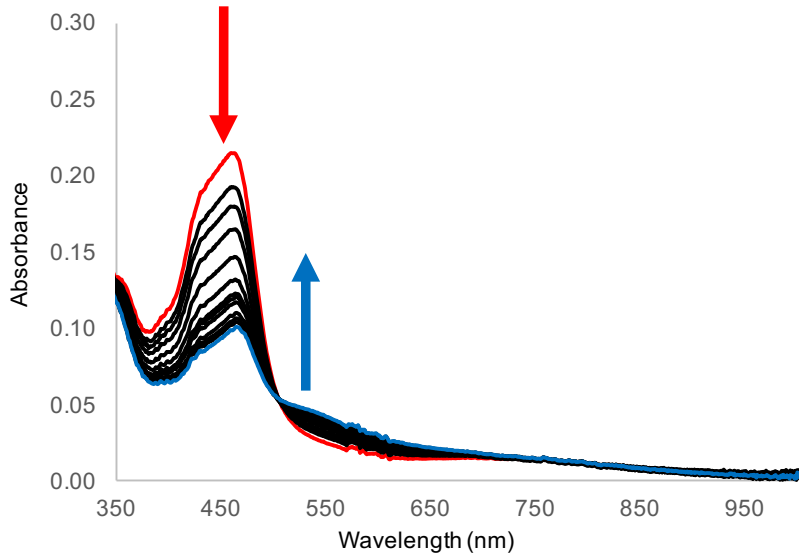

Figure S39 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OMe)_2)][Cl]_2$ at pH = 4.84 at 1200 mV vs. AgCl reference. As the potential is held, the band at 459 nm (red) decreases and a new broad band in the 500-550 nm region (blue) appears.

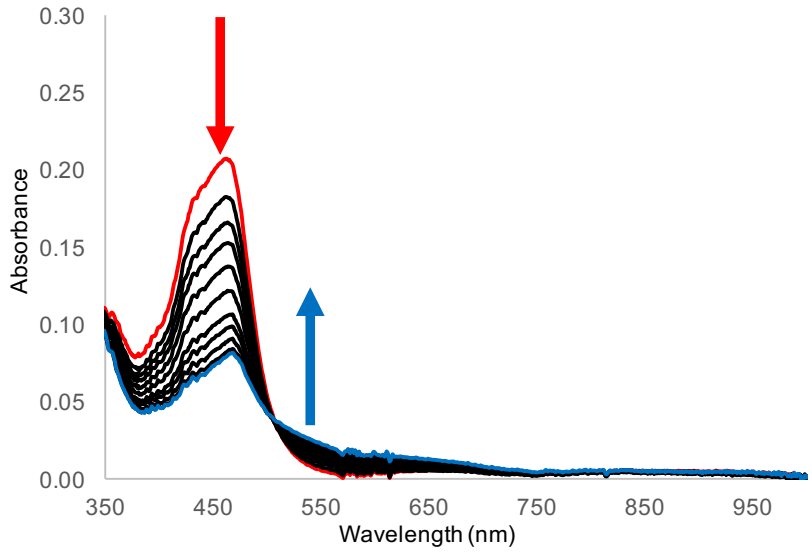

Figure S40 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OMe)_2)][Cl]_2$ at pH = 7.35 at 1200 mV vs. AgCl reference. As the potential is held, the band at 459 nm (red) decreases and a new broad band in the 500-550 nm region (blue) appears.

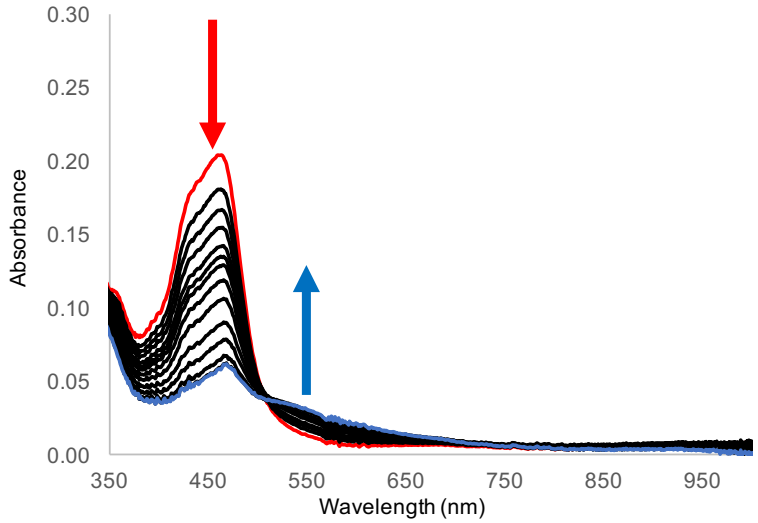

Figure S41 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OMe)_2)][Cl]_2$ at pH = 8.24 at 1200 mV vs. AgCl reference. As the potential is held, the band at 459 nm (red) decreases and a new broad band in the 500-550 nm region (blue) appears.

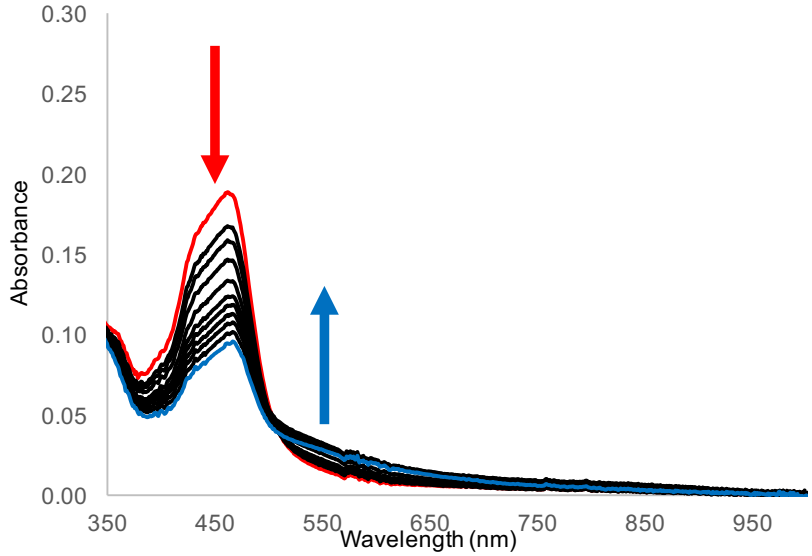

Figure S42 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OMe)_2)][Cl]_2$ at pH = 9.04 at 1200 mV vs. AgCl reference. As the potential is held, the band at 459 nm (red) decreases and a new broad band in the 500-550 nm region (blue) appears.

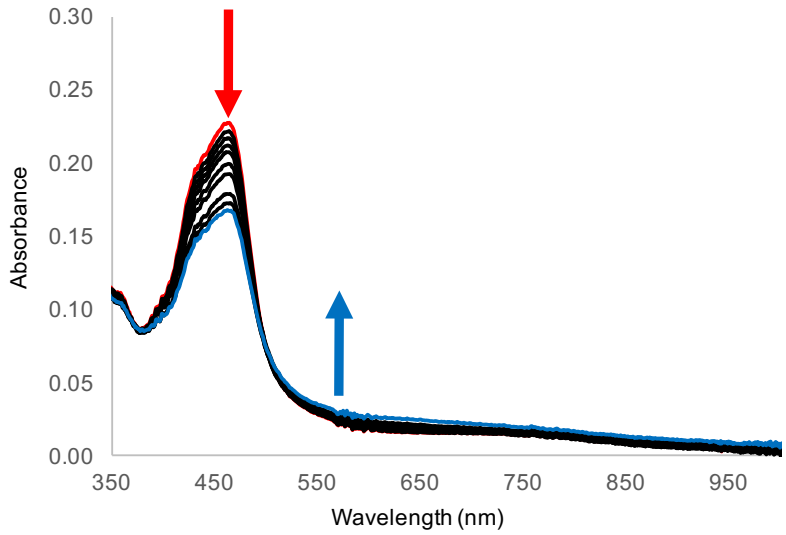

Figure S43 - Spectroelectrochemistry of $[Ru(bpy)_2(44'\text{-}bpy(OMe)_2)][Cl]_2$ at pH = 12.06 at 1200 mV vs. AgCl reference. As the potential is held, the band at 459 nm (red) decreases and a new broad band in the 500-550 nm region (blue) appears. At the high pH the decrease and relative increase in the absorbance bands are not as pronounced as they are at lower pH values.

X-Ray Crystallography

paul058 = $[Ru(bpy)_2(44'bpy(OCH_3)_2][Ce(NO_3)_6]$

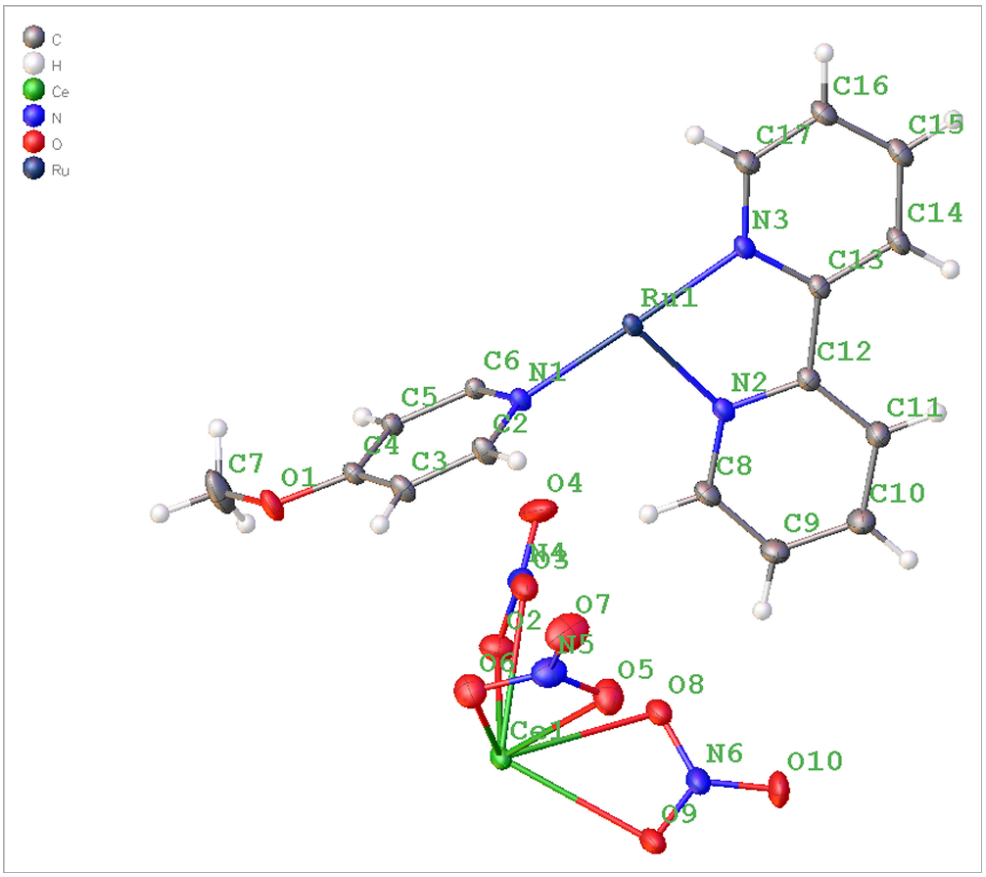

Table S1 Crystal data and structure refinement for paul058.

Identification code	paul058
Empirical formula	$C_{32}H_{28}CeN_{12}O_{20}Ru$
Formula weight	1141.85
Temperature/K	100.01
Crystal system	orthorhombic
Space group	Pnna
a/Å	19.0979(9)
b/Å	19.8019(9)
c/Å	12.9663(6)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4903.5(4)
Z	4
ρ_{calc}g/cm^3	1.547
μ/mm^{-1}	1.306
F(000)	2264.0

Crystal size/mm^3	0.2 × 0.15 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.754 to 74.078
Index ranges	-32 ≤ h ≤ 32, -33 ≤ k ≤ 33, -21 ≤ l ≤ 21
Reflections collected	382827
Independent reflections	12513 [R_{int} = 0.0418, R_{sigma} = 0.0123]
Data/restraints/parameters	12513/0/300
Goodness-of-fit on F^2	1.073
Final R indexes [I>=2σ (I)]	R_1 = 0.0346, wR_2 = 0.0805
Final R indexes [all data]	R_1 = 0.0453, wR_2 = 0.0877
Largest diff. peak/hole / e Å^{-3}	1.33/-1.22

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for paul058. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ce1	9197.1(2)	2500	2500	19.81(3)
Ru1	7500	5000	5553.5(2)	14.43(3)
O1	6574.4(8)	3325.7(7)	1810.4(10)	28.3(3)
N3	7738.5(7)	5697.1(6)	6687.9(9)	16.36(19)
O8	10072.5(7)	3309.7(7)	3492.9(11)	27.5(3)
O3	8634.8(7)	3648.5(8)	3026.5(12)	30.4(3)
O9	10323.6(7)	2253.3(7)	3605.7(12)	30.5(3)
N2	8561.2(7)	4846.0(7)	5717.4(10)	17.8(2)
N1	7301.7(7)	4370.2(6)	4328.5(9)	15.55(19)
O6	8079.8(8)	2266.2(9)	3583.3(13)	34.6(3)
O2	9306.3(9)	3703.1(8)	1686.8(13)	35.1(3)
O7	7938.6(10)	2474.2(11)	5219.1(14)	47.1(5)
O5	8955.1(9)	2615.6(10)	4488.2(12)	37.3(3)
O10	10938.8(9)	2984.7(10)	4457.3(13)	40.1(4)
O4	8915.8(9)	4627.5(8)	2382.1(17)	44.3(4)
N4	8949.0(8)	4009.8(9)	2367.0(14)	29.8(3)
C5	7149.1(8)	4320.9(7)	2492.5(11)	17.1(2)
N6	10453.4(8)	2850.7(9)	3866.9(13)	27.7(3)
N5	8314.2(10)	2451.3(10)	4449.9(14)	32.8(3)
C6	7359.2(7)	4653.0(7)	3378.7(10)	14.5(2)
C13	8414.0(8)	5697.7(7)	7010.0(11)	17.7(2)
C8	8936.7(9)	4376.2(9)	5208.9(13)	23.0(3)
C4	6857.9(8)	3678.5(8)	2584.4(12)	18.7(2)
C3	6831.5(9)	3375.2(8)	3558.5(12)	21.7(3)
C2	7051.8(9)	3733.5(8)	4400.4(12)	20.8(3)
C17	7286.7(9)	6146.5(8)	7088.2(13)	22.0(3)
C15	8182.4(10)	6628.0(9)	8140.2(12)	23.5(3)
C12	8864.1(8)	5194.5(8)	6508.8(12)	18.7(2)
C16	7492.9(10)	6619.2(9)	7815.0(13)	23.7(3)

C14	8647.9(9)	6157.7(9)	7742.7(13)	22.7(3)
C11	9546.8(9)	5058.5(9)	6810.4(13)	24.0(3)
C9	9617.8(10)	4222.4(10)	5485.2(15)	28.0(3)
C10	9925(1)	4566(1)	6298.9(16)	29.6(3)
C7	6594.8(17)	3615.7(13)	793.0(16)	45.6(6)

Table S3 Anisotropic Displacement Parameters ($Å^2×10^3$) for paul058. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ce1	15.97(5)	23.29(6)	20.16(5)	-7.41(4)	0	0
Ru1	19.10(6)	13.10(6)	11.08(6)	0	0	-2.07(5)
O1	41.0(7)	23.3(5)	20.7(5)	-8.0(4)	-5.8(5)	-6.0(5)
N3	19.9(5)	16.8(5)	12.3(4)	-2.3(4)	1.1(4)	-1.3(4)
O8	22.9(5)	29.3(6)	30.4(6)	-11.7(5)	-0.8(5)	1.8(5)
O3	23.3(6)	37.0(7)	31.0(7)	-12.3(6)	-1.5(5)	5.6(5)
O9	25.3(6)	29.3(6)	36.8(7)	-16.7(6)	-3.6(5)	2.6(5)
N2	22.3(5)	16.8(5)	14.3(5)	-2.1(4)	1.4(4)	-1.4(4)
N1	20.1(5)	13.5(4)	13.0(4)	0.2(4)	0.7(4)	-2.0(4)
O6	27.6(6)	42.0(8)	34.2(7)	-4.6(6)	4.7(6)	-2.6(6)
O2	36.4(7)	32.5(7)	36.4(7)	-5.6(6)	5.5(6)	6.3(6)
O7	44.5(9)	66.6(12)	30.2(8)	10.6(8)	17.2(7)	11.3(8)
O5	31.7(7)	52.8(10)	27.5(7)	-8.6(6)	2.2(6)	-0.2(7)
O10	31.7(7)	49.0(9)	39.8(8)	-16.0(7)	-16.8(6)	-1.2(7)
O4	31.1(7)	26.9(7)	75.0(13)	-9.1(7)	-7.5(8)	10.8(6)
N4	21.5(6)	27.6(7)	40.4(9)	-9.7(6)	-8.9(6)	6.4(5)
C5	21.7(6)	15.6(5)	14.0(5)	-0.9(4)	-1.5(4)	0.9(4)
N6	21.8(6)	34.9(8)	26.3(7)	-13.9(6)	-1.6(5)	3.5(5)
N5	32.1(8)	37.8(9)	28.6(8)	2.2(6)	9.7(6)	6.3(7)
C6	16.9(5)	13.1(5)	13.5(5)	0.3(4)	-0.1(4)	-0.5(4)
C13	21.3(6)	18.0(6)	13.8(5)	-2.3(4)	0.6(4)	-1.4(5)
C8	27.2(7)	23.0(7)	18.7(6)	-6.9(5)	3.2(5)	0.8(5)
C4	22.0(6)	16.0(5)	18.2(6)	-4.8(4)	-1.2(5)	0.2(4)
C3	29.7(7)	16.2(6)	19.3(6)	-3.4(5)	1.7(5)	-6.1(5)
C2	29.0(7)	15.4(5)	18.1(6)	0.0(5)	1.2(5)	-6.1(5)
C17	24.6(7)	22.1(6)	19.3(6)	-4.8(5)	1.6(5)	1.3(5)
C15	30.6(7)	22.8(7)	17.0(6)	-6.8(5)	2.4(5)	-3.5(6)
C12	21.5(6)	18.5(5)	16.2(5)	-2.0(4)	0.6(5)	-0.6(5)
C16	28.9(7)	22.3(6)	19.9(6)	-7.8(5)	2.9(6)	0.5(6)
C14	26.9(7)	22.8(7)	18.5(6)	-7.4(5)	-0.3(5)	-3.5(5)
C11	21.7(6)	26.8(7)	23.5(7)	-6.5(6)	-1.6(5)	1.4(5)
C9	26.5(7)	28.7(8)	28.8(8)	-8.3(6)	2.4(6)	5.5(6)
C10	24.1(7)	32.7(9)	32.0(9)	-8.9(7)	-0.4(6)	5.9(6)
C7	79.6(19)	36.7(11)	20.6(8)	-4.8(7)	-12.7(10)	-13.8(11)

Table S4 Bond Lengths for paul058.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ce1	O8	2.6501(13)	N2	C8	1.347(2)
Ce1	O8[1]	2.6501(13)	N2	C12	1.365(2)
Ce1	O3	2.6061(14)	N1	C6	1.3573(18)
Ce1	O3[1]	2.6062(14)	N1	C2	1.3513(19)
Ce1	O9	2.6309(14)	O6	N5	1.264(3)
Ce1	O9[1]	2.6309(14)	O2	N4	1.270(2)
Ce1	O6	2.5962(15)	O7	N5	1.229(2)
Ce1	O6[1]	2.5961(15)	O5	N5	1.267(3)
Ce1	O2[1]	2.6136(17)	O10	N6	1.231(2)
Ce1	O2	2.6136(17)	O4	N4	1.225(2)
Ce1	O5	2.6290(16)	C5	C6	1.383(2)
Ce1	O5[1]	2.6290(16)	C5	C4	1.393(2)
Ru1	N3[2]	2.0680(12)	C6	C6[2]	1.476(3)
Ru1	N3	2.0680(12)	C13	C12	1.468(2)
Ru1	N2[2]	2.0605(14)	C13	C14	1.390(2)
Ru1	N2	2.0605(14)	C8	C9	1.383(3)
Ru1	N1[2]	2.0547(12)	C4	C3	1.400(2)
Ru1	N1	2.0546(12)	C3	C2	1.368(2)
O1	C4	1.3373(19)	C17	C16	1.385(2)
O1	C7	1.439(3)	C15	C16	1.383(3)
N3	C13	1.356(2)	C15	C14	1.387(2)
N3	C17	1.344(2)	C12	C11	1.388(2)
O8	N6	1.261(2)	C11	C10	1.383(2)
O3	N4	1.266(3)	C9	C10	1.386(3)
O9	N6	1.255(2)			

[1]+X,1/2-Y,1/2-Z; [2]3/2-X,1-Y,+Z

Table S5 Bond Angles for paul058.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O8[1]	Ce1	O8	101.77(6)	O5	Ce1	O5[1]	159.75(7)
O3	Ce1	O8	66.72(4)	N3	Ru1	N3[2]	89.32(7)
O3[1]	Ce1	O8	156.23(5)	N2[2]	Ru1	N3[2]	78.98(5)
O3	Ce1	O8[1]	156.23(5)	N2	Ru1	N3	78.98(5)
O3[1]	Ce1	O8[1]	66.72(4)	N2[2]	Ru1	N3	92.55(5)
O3	Ce1	O3[1]	131.33(6)	N2	Ru1	N3[2]	92.55(5)
O3[1]	Ce1	O9[1]	110.87(4)	N2[2]	Ru1	N2	168.16(7)
O3[1]	Ce1	O9	108.52(5)	N1[2]	Ru1	N3[2]	174.63(5)
O3	Ce1	O9	110.87(4)	N1	Ru1	N3	174.63(5)
O3	Ce1	O9[1]	108.52(5)	N1	Ru1	N3[2]	95.98(5)
O3[1]	Ce1	O2	136.27(5)	N1[2]	Ru1	N3	95.98(5)
O3	Ce1	O2[1]	136.27(5)	N1[2]	Ru1	N2	89.33(5)
O3	Ce1	O2	48.93(5)	N1[2]	Ru1	N2[2]	99.86(5)
O3[1]	Ce1	O2[1]	48.94(5)	N1	Ru1	N2	99.86(5)

O3[1]	Ce1	O5	105.10(5)	N1	Ru1	N2[2]	89.33(5)
O3[1]	Ce1	O5[1]	66.09(5)	N1	Ru1	N1[2]	78.74(7)
O3	Ce1	O5	66.09(5)	C4	O1	C7	117.93(15)
O3	Ce1	O5[1]	105.09(5)	C13	N3	Ru1	115.42(10)
O9[1]	Ce1	O8	68.69(4)	C17	N3	Ru1	125.12(11)
O9[1]	Ce1	O8[1]	48.07(4)	C17	N3	C13	119.42(13)
O9	Ce1	O8[1]	68.69(4)	N6	O8	Ce1	96.59(10)
O9	Ce1	O8	48.07(4)	N4	O3	Ce1	96.94(10)
O9	Ce1	O9[1]	70.29(7)	N6	O9	Ce1	97.68(11)
O6	Ce1	O8[1]	132.33(5)	C8	N2	Ru1	125.13(11)
O6[1]	Ce1	O8[1]	111.32(5)	C8	N2	C12	119.44(14)
O6	Ce1	O8	111.32(5)	C12	N2	Ru1	114.79(10)
O6[1]	Ce1	O8	132.33(5)	C6	N1	Ru1	115.85(9)
O6	Ce1	O3[1]	69.36(5)	C2	N1	Ru1	125.32(10)
O6[1]	Ce1	O3[1]	71.05(5)	C2	N1	C6	118.43(12)
O6	Ce1	O3	71.05(5)	N5	O6	Ce1	97.94(11)
O6[1]	Ce1	O3	69.36(5)	N4	O2	Ce1	96.48(12)
O6[1]	Ce1	O9	179.47(5)	N5	O5	Ce1	96.26(12)
O6	Ce1	O9	110.13(5)	O3	N4	O2	116.98(17)
O6	Ce1	O9[1]	179.47(5)	O4	N4	O3	121.92(19)
O6[1]	Ce1	O9[1]	110.13(5)	O4	N4	O2	121.1(2)
O6[1]	Ce1	O6	69.45(8)	C6	C5	C4	118.60(13)
O6[1]	Ce1	O2	71.62(5)	O9	N6	O8	117.47(15)
O6	Ce1	O2[1]	71.62(5)	O10	N6	O8	121.21(17)
O6[1]	Ce1	O2[1]	116.51(5)	O10	N6	O9	121.31(18)
O6	Ce1	O2	116.51(5)	O6	N5	O5	116.83(17)
O6[1]	Ce1	O5	111.75(5)	O7	N5	O6	121.7(2)
O6	Ce1	O5[1]	111.74(5)	O7	N5	O5	121.5(2)
O6[1]	Ce1	O5[1]	48.74(5)	N1	C6	C5	122.27(13)
O6	Ce1	O5	48.74(5)	N1	C6	C6[2]	114.44(8)
O2[1]	Ce1	O8	107.77(5)	C5	C6	C6[2]	123.26(8)
O2[1]	Ce1	O8[1]	66.06(5)	N3	C13	C12	114.85(13)
O2	Ce1	O8	66.06(5)	N3	C13	C14	121.13(14)
O2	Ce1	O8[1]	107.77(5)	C14	C13	C12	124.01(15)
O2	Ce1	O9[1]	62.98(5)	N2	C8	C9	121.73(15)
O2	Ce1	O9	108.90(5)	O1	C4	C5	125.05(14)
O2[1]	Ce1	O9	62.98(5)	O1	C4	C3	116.01(14)
O2[1]	Ce1	O9[1]	108.90(5)	C5	C4	C3	118.90(13)
O2[1]	Ce1	O2	170.85(7)	C2	C3	C4	119.10(14)
O2	Ce1	O5	109.28(5)	N1	C2	C3	122.51(14)
O2[1]	Ce1	O5	72.41(6)	N3	C17	C16	121.85(16)
O2[1]	Ce1	O5[1]	109.29(5)	C16	C15	C14	119.25(15)
O2	Ce1	O5[1]	72.41(6)	N2	C12	C13	115.33(14)
O5	Ce1	O8	65.29(5)	N2	C12	C11	120.79(14)
O5	Ce1	O8[1]	129.79(5)	C11	C12	C13	123.87(14)
O5[1]	Ce1	O8	129.79(5)	C15	C16	C17	119.12(15)

O5[1]	Ce1	O8[1]	65.29(5)	C15	C14	C13	119.22(16)
O5[1]	Ce1	O9	131.45(5)	C10	C11	C12	119.50(16)
O5	Ce1	O9	68.01(5)	C8	C9	C10	119.16(16)
O5	Ce1	O9[1]	131.45(5)	C11	C10	C9	119.36(17)
O5[1]	Ce1	O9[1]	68.01(5)				

[1]+X,1/2-Y,1/2-Z; [2]3/2-X,1-Y,+Z

Table S6 Torsion Angles for paul058.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ce1	O8	N6	O9	4.31(17)	N2	C12	C11	C10	0.3(3)
Ce1	O8	N6	O10	-176.43(16)	C5	C4	C3	C2	4.0(2)
Ce1	O3	N4	O2	8.22(17)	C6	N1	C2	C3	-2.5(2)
Ce1	O3	N4	O4	-171.40(16)	C6	C5	C4	O1	173.53(15)
Ce1	O9	N6	O8	-4.35(17)	C6	C5	C4	C3	-4.2(2)
Ce1	O9	N6	O10	176.39(16)	C13	N3	C17	C16	0.8(2)
Ce1	O6	N5	O7	174.83(18)	C13	C12	C11	C10	178.93(17)
Ce1	O6	N5	O5	-4.8(2)	C8	N2	C12	C13	179.66(14)
Ce1	O2	N4	O3	-8.19(17)	C8	N2	C12	C11	-1.6(2)
Ce1	O2	N4	O4	171.43(16)	C8	C9	C10	C11	-0.6(3)
Ce1	O5	N5	O6	4.8(2)	C4	C5	C6	N1	1.1(2)
Ce1	O5	N5	O7	-174.91(18)	C4	C5	C6	C6[1]	-176.82(16)
Ru1	N3	C13	C12	-0.86(16)	C4	C3	C2	N1	-0.6(3)
Ru1	N3	C13	C14	177.70(12)	C2	N1	C6	C5	2.3(2)
Ru1	N3	C17	C16	-177.04(13)	C2	N1	C6	C6[1]	-179.65(16)
Ru1	N2	C8	C9	-168.51(14)	C17	N3	C13	C12	-178.93(14)
Ru1	N2	C12	C13	-9.02(17)	C17	N3	C13	C14	-0.4(2)
Ru1	N2	C12	C11	169.72(13)	C12	N2	C8	C9	1.8(3)
Ru1	N1	C6	C5	-170.88(11)	C12	C13	C14	C15	177.69(15)
Ru1	N1	C6	C6[1]	7.22(19)	C12	C11	C10	C9	0.8(3)
Ru1	N1	C2	C3	169.93(13)	C16	C15	C14	C13	1.4(3)
O1	C4	C3	C2	-173.92(16)	C14	C13	C12	N2	-171.98(15)
N3	C13	C12	N2	6.5(2)	C14	C13	C12	C11	9.3(3)
N3	C13	C12	C11	-172.16(15)	C14	C15	C16	C17	-0.9(3)
N3	C13	C14	C15	-0.7(2)	C7	O1	C4	C5	2.7(3)
N3	C17	C16	C15	-0.2(3)	C7	O1	C4	C3	-179.5(2)
N2	C8	C9	C10	-0.8(3)					

[1]3/2-X,1-Y,+Z

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for paul058.

Atom	*x*	*y*	*z*	U(eq)
H2AA	7202	4526	1835	21
H8	8728	4144	4646	28
H1AA	6663	2927	3634	26
H0AA	7028	3527	5061	25
H17	6813	6140	6867	26

H15	8336	6953	8630	28
H16	7165	6933	8086	28
H14	9121	6150	7968	27
H11	9753	5302	7364	29
H9	9872	3885	5122	34
H10	10391	4464	6503	36
H7A	6335	3326	314	68
H7B	7082	3653	564	68
H7C	6381	4065	808	68

Table S8 Solvent masks information for paul058.

Number	X	Y	Z	Volume	Electron count	Content
1	-0.807	-0.113	-0.888	1308.0	322.4	?

Crystal structure determination of [paul058]

Crystal Data for $C_{32}H_{28}CeN_{12}O_{20}Ru$ (M =1141.85 g/mol): orthorhombic, space group Pnna (no. 52), a = 19.0979(9) Å, b = 19.8019(9) Å, c = 12.9663(6) Å, V = 4903.5(4) Å^3, Z = 4, T = 100.01 K, μ(MoKα) = 1.306 mm^{-1}, *Dcalc* = 1.547 g/cm^3, 382827 reflections measured (3.754° ≤ 2Θ ≤ 74.078°), 12513 unique (R_{int} = 0.0418, R_{sigma} = 0.0123) which were used in all calculations. The final R_1 was 0.0346 (I > 2σ(I)) and wR_2 was 0.0877 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.
Details:
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2.a Aromatic/amide H refined with riding coordinates:
 C2AA(H2AA), C8(H8), C1AA(H1AA), C0AA(H0AA), C17(H17), C15(H15), C16(H16), C14(H14), C11(H11), C9(H9), C10(H10)
2.b Idealised Me refined as rotating group:
 C7(H7A,H7B,H7C)

Cartesian Coordinates of Computational Structures

$[Ru(bpy)_2(44'bpy(OCH_3)_2)]^{2+/3+}$

Ru^{2+}/B3LYP

Nuclear Repulsion Energy (a.u.) = 5141.1696845934

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)
Ru -0.59150 0.00000 0.00000
N 1.06418 -1.12721 -0.69076
N 1.06418 1.12721 0.69076
N -0.71604 1.30349 -1.65506
N -2.09931 1.34466 0.60522
N -2.09931 -1.34466 -0.60522
N -0.71604 -1.30349 1.65506
O 4.43116 -3.21071 -1.90224
O 4.43116 3.21071 1.90224
C 0.99311 -2.28312 -1.38492
C 2.10571 -2.98949 -1.79732
C 3.38069 -2.49053 -1.48196
C 3.46470 -1.29234 -0.76112
C 2.29311 -0.63586 -0.38027
C 2.29311 0.63586 0.38027
C 3.46470 1.29234 0.76112
C 3.38069 2.49053 1.48196
C 2.10571 2.98949 1.79732
C 0.99311 2.28312 1.38492
C 5.75721 -2.74767 -1.60845
C 5.75721 2.74767 1.60845
C 0.03199 1.22056 -2.77117
C -0.07887 2.12782 -3.81924
C -1.00052 3.16785 -3.70931
C -1.77815 3.25966 -2.55867
C -1.62297 2.31449 -1.54004
C -2.40652 2.32631 -0.28894
C -3.40174 3.26790 -0.00855
C -4.08814 3.20682 1.20067
C -3.76499 2.20020 2.10949
C -2.76814 1.29138 1.77250
C -2.76814 -1.29138 -1.77250
C -3.76499 -2.20020 -2.10949
C -4.08814 -3.20682 -1.20067
C -3.40174 -3.26790 0.00855
C -2.40652 -2.32631 0.28894
C -1.62297 -2.31449 1.54004
C -1.77815 -3.25966 2.55867
C -1.00052 -3.16785 3.70931
C -0.07887 -2.12782 3.81924
C 0.03199 -1.22056 2.77117
H 0.73254 -0.39607 2.81318

H -0.00323 -2.63974 -1.61438
H 2.00275 -3.91313 -2.35463
H 4.42730 -0.87828 -0.49950
H 4.42730 0.87828 0.49950
H 2.00275 3.91313 2.35463
H -0.00323 2.63974 1.61438
H 6.42635 -3.48743 -2.04660
H 5.92139 -2.69533 -0.52726
H 5.93854 -1.76914 -2.06475
H 6.42635 3.48743 2.04660
H 5.92139 2.69533 0.52726
H 5.93854 1.76914 2.06475
H 0.73254 0.39607 -2.81318
H 0.54820 2.01352 -4.69621
H -1.11488 3.89731 -4.50415
H -2.49709 4.06286 -2.45753
H -3.64223 4.04228 -0.72598
H -4.86146 3.93352 1.42613
H -4.27098 2.11162 3.06421
H -2.48407 0.49428 2.44806
H -2.48407 -0.49428 -2.44806
H -4.27098 -2.11162 -3.06421
H -4.86146 -3.93352 -1.42613
H -3.64223 -4.04228 0.72598
H -2.49709 -4.06286 2.45753
H -1.11488 -3.89731 4.50415
H 0.54820 -2.01352 4.69621

Ru^{2+}/M06-L

Nuclear Repulsion Energy (a.u.) = 5157.3188044538

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)
Ru -0.56956 0.00000 0.00000
N 1.08447 -1.11219 -0.69836
N 1.08447 1.11219 0.69836
N -0.71454 1.33047 -1.61791
N -2.07342 1.31578 0.63780
N -2.07342 -1.31578 -0.63780
N -0.71455 -1.33047 1.61791
O 4.43964 -3.23031 -1.84645
O 4.43964 3.23031 1.84645
C 1.01158 -2.26802 -1.38903
C 2.11956 -2.98423 -1.78302
C 3.39261 -2.49815 -1.45067
C 3.48030 -1.30032 -0.73708
C 2.31443 -0.63117 -0.37496
C 2.31443 0.63117 0.37496
C 3.48030 1.30031 0.73708
C 3.39261 2.49815 1.45067
C 2.11956 2.98423 1.78302

C 1.01158 2.26802 1.38903
C 5.74544 -2.75091 -1.52358
C 5.74544 2.75091 1.52358
C 0.03300 1.28414 -2.73561
C -0.12355 2.18532 -3.77753
C -1.09050 3.18010 -3.66463
C -1.86335 3.23644 -2.51405
C -1.66281 2.30298 -1.49762
C -2.42499 2.28970 -0.24844
C -3.43506 3.20271 0.05625
C -4.08591 3.12766 1.27941
C -3.71080 2.13621 2.18177
C -2.70621 1.25199 1.82287
C -2.70621 -1.25198 -1.82287
C -3.71080 -2.13620 -2.18177
C -4.08591 -3.12765 -1.27941
C -3.43506 -3.20270 -0.05625
C -2.42500 -2.28970 0.24844
C -1.66281 -2.30298 1.49762
C -1.86335 -3.23644 2.51405
C -1.09050 -3.18010 3.66463
C -0.12356 -2.18533 3.77753
C 0.03300 -1.28414 2.73561
H 0.76920 -0.48538 2.77897
H 0.00942 -2.61410 -1.62902
H 2.01535 -3.91150 -2.33756
H 4.44555 -0.89453 -0.45693
H 4.44555 0.89453 0.45693
H 2.01535 3.91150 2.33757
H 0.00942 2.61409 1.62902
H 6.43661 -3.48406 -1.93747
H 5.87996 -2.68623 -0.43801
H 5.92523 -1.77166 -1.98139
H 6.43661 3.48406 1.93747
H 5.87996 2.68622 0.43801
H 5.92523 1.77166 1.98139
H 0.76920 0.48537 -2.77897
H 0.50624 2.10210 -4.65800
H -1.24084 3.90407 -4.46068
H -2.62041 4.00672 -2.40534
H -3.71041 3.97053 -0.66030
H -4.87357 3.83497 1.52405
H -4.18730 2.04030 3.15257
H -2.37973 0.46131 2.49374
H -2.37973 -0.46131 -2.49374
H -4.18731 -2.04029 -3.15257
H -4.87358 -3.83496 -1.52405
H -3.71042 -3.97052 0.66030
H -2.62042 -4.00672 2.40534
H -1.24084 -3.90407 4.46068
H 0.50623 -2.10210 4.65800

Ru^{3+}/B3LYP

Nuclear Repulsion Energy (a.u.) = 5153.6597596383

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)

Ru -0.57113 0.00000 -0.00000
N 1.06654 -1.11157 -0.70411
N 1.06654 1.11157 0.70410
N -0.66608 1.44124 -1.54047
N -2.13212 1.27095 0.65779
N -2.13212 -1.27096 -0.65779
N -0.66607 -1.44125 1.54046
O 4.39365 -3.20873 -1.93280
O 4.39365 3.20873 1.93280
C 0.97190 -2.26755 -1.40023
C 2.07650 -2.97502 -1.82031
C 3.35950 -2.48648 -1.50765
C 3.46007 -1.29035 -0.77738
C 2.30115 -0.62787 -0.38948
C 2.30115 0.62787 0.38948
C 3.46007 1.29035 0.77738
C 3.35950 2.48648 1.50765
C 2.07650 2.97502 1.82031
C 0.97189 2.26755 1.40023
C 5.73456 -2.77067 -1.64477
C 5.73455 2.77067 1.64478
C 0.13724 1.45064 -2.62089
C 0.03468 2.42415 -3.60726
C -0.92573 3.42373 -3.46345
C -1.75190 3.41933 -2.34234
C -1.60746 2.41500 -1.38413
C -2.42379 2.31998 -0.16170
C -3.43931 3.21851 0.17003
C -4.15894 3.03617 1.34847
C -3.85254 1.95609 2.17412
C -2.83294 1.09212 1.79277
C -2.83294 -1.09213 -1.79277
C -3.85254 -1.95609 -2.17411
C -4.15893 -3.03617 -1.34846
C -3.43931 -3.21851 -0.17003
C -2.42379 -2.31998 0.16170
C -1.60746 -2.41500 1.38413
C -1.75189 -3.41934 2.34235
C -0.92572 -3.42373 3.46345
C 0.03469 -2.42415 3.60726
C 0.13725 -1.45064 2.62089
H 0.86396 -0.65199 2.69195
H -0.02761 -2.61427 -1.62795
H 1.96451 -3.89418 -2.38241
H 4.42718 -0.88821 -0.51450

H 4.42718 0.88822 0.51450
H 1.96451 3.89418 2.38241
H -0.02762 2.61428 1.62794
H 6.38301 -3.52111 -2.09412
H 5.90304 -2.73188 -0.56453
H 5.92594 -1.79357 -2.09791
H 6.38300 3.52112 2.09413
H 5.90304 2.73189 0.56454
H 5.92593 1.79357 2.09792
H 0.86395 0.65199 -2.69196
H 0.69752 2.38964 -4.46372
H -1.03339 4.20041 -4.21275
H -2.49955 4.19209 -2.21936
H -3.66935 4.05208 -0.48079
H -4.94925 3.72981 1.61411
H -4.38707 1.77604 3.09930
H -2.55986 0.24248 2.40536
H -2.55986 -0.24248 -2.40536
H -4.38708 -1.77605 -3.09929
H -4.94924 -3.72981 -1.61411
H -3.66935 -4.05209 0.48079
H -2.49954 -4.19209 2.21937
H -1.03338 -4.20041 4.21275
H 0.69753 -2.38964 4.46372

Ru^{3+}/M06-L

Nuclear Repulsion Energy (a.u.) = 5163.6320293714

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)
Ru -0.55521 0.00000 0.00000
N 1.09753 -1.09023 -0.71451
N 1.09753 1.09023 0.71451
N -0.65651 1.52197 -1.46249
N -2.13733 1.22992 0.68039
N -2.13733 -1.22992 -0.68039
N -0.65651 -1.52197 1.46249
O 4.40729 -3.16873 -1.98462
O 4.40729 3.16873 1.98462
C 0.99668 -2.23175 -1.42760
C 2.09527 -2.93203 -1.86411
C 3.37770 -2.45191 -1.54838
C 3.48558 -1.27125 -0.80206
C 2.33254 -0.61566 -0.39704
C 2.33254 0.61566 0.39704
C 3.48558 1.27125 0.80206
C 3.37770 2.45191 1.54838
C 2.09527 2.93203 1.86411
C 0.99668 2.23175 1.42760
C 5.73008 -2.71135 -1.67824

C 5.73008 2.71135 1.67824
C 0.16693 1.58903 -2.52205
C 0.05433 2.58906 -3.47521
C -0.93569 3.55365 -3.31951
C -1.77953 3.49160 -2.21912
C -1.62491 2.46395 -1.29202
C -2.45098 2.30195 -0.09683
C -3.49684 3.15040 0.25986
C -4.22330 2.89254 1.41459
C -3.89328 1.79016 2.19588
C -2.84482 0.97824 1.79403
C -2.84482 -0.97824 -1.79403
C -3.89328 -1.79016 -2.19588
C -4.22330 -2.89254 -1.41459
C -3.49683 -3.15041 -0.25986
C -2.45098 -2.30195 0.09683
C -1.62491 -2.46395 1.29202
C -1.77953 -3.49160 2.21912
C -0.93569 -3.55365 3.31951
C 0.05433 -2.58906 3.47521
C 0.16693 -1.58903 2.52205
H 0.91917 -0.80911 2.60038
H -0.01040 -2.56967 -1.65525
H 1.97935 -3.84317 -2.44151
H 4.45648 -0.87095 -0.53439
H 4.45648 0.87095 0.53439
H 1.97935 3.84317 2.44151
H -0.01040 2.56967 1.65525
H 6.39934 -3.44316 -2.12737
H 5.88509 -2.67950 -0.59488
H 5.90705 -1.72424 -2.11740
H 6.39934 3.44316 2.12737
H 5.88509 2.67950 0.59488
H 5.90705 1.72424 2.11740
H 0.91917 0.80911 -2.60038
H 0.73391 2.60154 -4.32101
H -1.05141 4.35011 -4.04896
H -2.55480 4.23837 -2.08275
H -3.74421 4.00574 -0.36047
H -5.04267 3.54669 1.69870
H -4.43642 1.55252 3.10470
H -2.54869 0.10855 2.37362
H -2.54869 -0.10855 -2.37362
H -4.43643 -1.55252 -3.10470
H -5.04267 -3.54669 -1.69870
H -3.74421 -4.00574 0.36047
H -2.55480 -4.23837 2.08275
H -1.05141 -4.35011 4.04896
H 0.73391 -2.60154 4.32101

$[Ru(bpy)_2(44'bpy(OH)_2)]^{2+/3+}$

Ru^{2+}/B3LYP

Nuclear Repulsion Energy (a.u.) = 4751.4814919507

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)

Ru	0.27871	0.00000	0.00000
N	-1.37431	1.01469	0.84991
N	-1.37431	-1.01469	-0.84991
N	0.40732	-1.52201	1.45632
N	1.78561	-1.24785	-0.78994
N	0.40732	1.52201	-1.45632
N	1.78561	1.24785	0.78994
O	-4.76075	2.85971	2.35780
O	-4.76075	-2.85971	-2.35780
C	-1.30381	2.05380	1.70704
C	-2.41710	2.68911	2.22691
C	-3.68615	2.23557	1.84322
C	-3.77216	1.16241	0.94923
C	-2.60448	0.57134	0.47056
C	-2.60448	-0.57134	-0.47056
C	-3.77216	-1.16241	-0.94923
C	-3.68615	-2.23557	-1.84322
C	-2.41710	-2.68911	-2.22691
C	-1.30381	-2.05380	-1.70704
C	-0.33891	-1.59446	2.57456
C	-0.21995	-2.63351	3.49098
C	0.70838	-3.64303	3.24133
C	1.48289	-3.57529	2.08699
C	1.31805	-2.50397	1.20356
C	2.09526	-2.34422	-0.04142
C	3.08567	-3.24042	-0.45576
C	3.76759	-3.01250	-1.64738
C	3.44380	-1.88834	-2.40546
C	2.44961	-1.03407	-1.94159
C	-0.33891	1.59446	-2.57456
C	-0.21995	2.63351	-3.49098
C	0.70838	3.64303	-3.24133
C	1.48289	3.57529	-2.08699
C	1.31805	2.50397	-1.20356
C	2.09526	2.34422	0.04142
C	3.08567	3.24042	0.45576
C	3.76759	3.01250	1.64738
C	3.44380	1.88834	2.40546
C	2.44961	1.03407	1.94158
H	-5.58275	2.45412	2.03158
H	-5.58275	-2.45412	-2.03158
H	-0.30799	2.37661	1.98423
H	-2.31222	3.51877	2.91596

H -4.74516 0.80320 0.63579
H -4.74516 -0.80320 -0.63579
H -2.31222 -3.51877 -2.91596
H -0.30799 -2.37661 -1.98423
H -1.04478 -0.78798 2.72906
H -0.84546 -2.64200 4.37637
H 0.82981 -4.47092 3.93181
H 2.20750 -4.35201 1.87817
H 3.32598 -4.10922 0.14404
H 4.53760 -3.70259 -1.97570
H 3.94637 -1.66892 -3.34065
H 2.16283 -0.15210 -2.50057
H -1.04478 0.78798 -2.72906
H -0.84546 2.64200 -4.37637
H 0.82981 4.47092 -3.93181
H 2.20750 4.35201 -1.87817
H 3.32598 4.10922 -0.14404
H 4.53760 3.70259 1.97570
H 3.94637 1.66892 3.34065
H 2.16283 0.15210 2.50057

Ru^{2+}/M06-L

Nuclear Repulsion Energy (a.u.) = 4766.4055374351

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)
Ru 0.27536 0.00000 0.00000
N -1.37553 1.00932 0.84044
N -1.37553 -1.00932 -0.84044
N 0.40596 -1.51216 1.44860
N 1.77527 -1.24539 -0.77392
N 0.40596 1.51216 -1.44860
N 1.77527 1.24539 0.77392
O -4.74400 2.83579 2.38193
O -4.74400 -2.83579 -2.38193
C -1.30148 2.04333 1.70093
C -2.40921 2.66950 2.23081
C -3.67915 2.21628 1.85526
C -3.76931 1.14982 0.95886
C -2.60741 0.56519 0.46824
C -2.60741 -0.56520 -0.46824
C -3.76931 -1.14982 -0.95886
C -3.67915 -2.21628 -1.85526
C -2.40921 -2.66950 -2.23081
C -1.30148 -2.04333 -1.70093

C -0.34171 -1.57229 2.56515
C -0.21161 -2.58964 3.49697
C 0.72826 -3.59068 3.26964
C 1.50068 -3.53855 2.11798
C 1.32639 -2.49094 1.21359
C 2.09285 -2.33955 -0.02476
C 3.07971 -3.23117 -0.44602
C 3.75078 -3.00348 -1.63885
C 3.42043 -1.88240 -2.39479
C 2.43140 -1.03126 -1.92876
C -0.34171 1.57229 -2.56515
C -0.21162 2.58963 -3.49697
C 0.72826 3.59068 -3.26964
C 1.50068 3.53855 -2.11799
C 1.32639 2.49094 -1.21359
C 2.09285 2.33955 0.02476
C 3.07971 3.23117 0.44601
C 3.75077 3.00348 1.63885
C 3.42043 1.88240 2.39479
C 2.43140 1.03126 1.92876
H -5.56414 2.42952 2.05543
H -5.56414 -2.42953 -2.05543
H -0.29920 2.36523 1.97233
H -2.30173 3.49617 2.92564
H -4.74443 0.78557 0.64812
H -4.74443 -0.78557 -0.64812
H -2.30173 -3.49618 -2.92564
H -0.29920 -2.36523 -1.97233
H -1.05723 -0.76548 2.70234
H -0.83881 -2.58918 4.38303
H 0.85951 -4.40226 3.98003
H 2.23877 -4.31056 1.92376
H 3.32367 -4.10075 0.15666
H 4.52074 -3.69316 -1.97365
H 3.91830 -1.66366 -3.33462
H 2.13516 -0.14687 -2.48696
H -1.05724 0.76548 -2.70234
H -0.83881 2.58918 -4.38303
H 0.85950 4.40226 -3.98003
H 2.23877 4.31056 -1.92376
H 3.32366 4.10075 -0.15666
H 4.52074 3.69317 1.97365
H 3.91830 1.66367 3.33462
H 2.13516 0.14687 2.48696

$\underline{Ru^{2+}/M06\text{-}L + 2\ H_2O}$

Nuclear Repulsion Energy (a.u.) = 5220.1461921041

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)
Ru 0.70345 -0.00000 0.00000
N -0.95113 -1.07343 -0.76236
N -0.95113 1.07342 0.76237
N 0.84309 1.41105 -1.54470
N 2.20113 1.28849 0.69959
N 0.84310 -1.41105 1.54470
N 2.20113 -1.28849 -0.69959
C -0.88458 -2.18492 -1.52107
C -1.99545 -2.87375 -1.95877
C -3.26918 -2.40778 -1.59739
C -3.34609 -1.24977 -0.81234
C -2.18229 -0.60841 -0.41121
C -2.18229 0.60841 0.41121
C -3.34609 1.24977 0.81234
C -3.26918 2.40777 1.59740
C -1.99545 2.87375 1.95878
C -0.88458 2.18491 1.52107
C 0.09855 1.40754 -2.66559
C 0.24767 2.35672 -3.66476
C 1.20425 3.35506 -3.50439
C 1.97343 3.36823 -2.34982
C 1.77975 2.38840 -1.37625
C 2.53879 2.31931 -0.12669
C 3.53239 3.22922 0.23658
C 4.18346 3.08930 1.45410
C 3.82718 2.03596 2.29171
C 2.83664 1.16033 1.87814
C 0.09855 -1.40754 2.66559
C 0.24767 -2.35673 3.66475
C 1.20425 -3.35507 3.50438
C 1.97343 -3.36823 2.34981
C 1.77975 -2.38840 1.37625
C 2.53880 -2.31931 0.12668
C 3.53240 -3.22921 -0.23658
C 4.18347 -3.08929 -1.45409
C 3.82719 -2.03595 -2.29171
C 2.83664 -1.16032 -1.87814
H 0.11649 -2.52027 -1.78221
H -1.88991 -3.76603 -2.56816
H -4.32072 -0.87100 -0.51865
H -4.32072 0.87100 0.51865
H -1.88991 3.76603 2.56816
H 0.11649 2.52027 1.78221
H -0.62852 0.60344 -2.74743
H -0.37852 2.30698 -4.55029
H 1.35015 4.11408 -4.26787
H 2.72385 4.13953 -2.20674

H 3.79464 4.04655 -0.42833
H 4.95760 3.79439 1.74438
H 4.30637 1.88813 3.25469
H 2.52378 0.32390 2.49811
H -0.62852 -0.60344 2.74743
H -0.37852 -2.30699 4.55028
H 1.35015 -4.11409 4.26787
H 2.72385 -4.13953 2.20674
H 3.79466 -4.04654 0.42833
H 4.95761 -3.79437 -1.74438
H 4.30638 -1.88812 -3.25468
H 2.52378 -0.32390 -2.49811
O -6.49423 1.81129 1.01689
H -7.11577 1.56631 1.71866
O -6.49423 -1.81129 -1.01689
H -7.00653 -2.39767 -0.44038
H -7.00654 2.39769 0.44040
H -7.11579 -1.56633 -1.71866
O -4.33803 -3.08174 -2.01082
H -5.16962 -2.64338 -1.67009
O -4.33803 3.08174 2.01082
H -5.16962 2.64338 1.67009

Ru^{3+}/B3LYP

Nuclear Repulsion Energy (a.u.) = 4765.0026851005

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)
Ru 0.26642 0.00000 0.00000
N -1.36683 0.99457 0.86587
N -1.36683 -0.99457 -0.86587
N 0.34151 -1.63956 1.33065
N 1.83450 -1.17402 -0.80615
N 0.34151 1.63956 -1.33065
N 1.83450 1.17402 0.80615
O -4.71454 2.82616 2.42095
O -4.71454 -2.82616 -2.42095
C -1.27408 2.02582 1.73459
C -2.38018 2.65186 2.27102
C -3.65642 2.20731 1.89034
C -3.75817 1.14624 0.97779
C -2.60199 0.55838 0.48303
C -2.60199 -0.55838 -0.48303
C -3.75817 -1.14624 -0.97779
C -3.65642 -2.20731 -1.89034
C -2.38018 -2.65186 -2.27102
C -1.27408 -2.02582 -1.73459
C -0.48423 -1.80094 2.38177
C -0.41022 -2.91155 3.21326
C 0.54413 -3.88991 2.94008
C 1.39568 -3.72647 1.85018

C 1.28169 -2.58697 1.05248
C 2.12504 -2.31789 -0.12477
C 3.16508 -3.14858 -0.54464
C 3.90580 -2.80426 -1.67250
C 3.59581 -1.63265 -2.36047
C 2.55454 -0.83942 -1.89284
C -0.48423 1.80094 -2.38177
C -0.41022 2.91155 -3.21326
C 0.54413 3.88991 -2.94008
C 1.39568 3.72646 -1.85018
C 1.28169 2.58697 -1.05248
C 2.12504 2.31789 0.12477
C 3.16508 3.14858 0.54464
C 3.90580 2.80426 1.67250
C 3.59581 1.63265 2.36047
C 2.55454 0.83942 1.89284
H -5.54856 2.43964 2.09947
H -5.54856 -2.43963 -2.09947
H -0.27543 2.33962 2.00986
H -2.26762 3.46988 2.97198
H -4.73493 0.79870 0.66448
H -4.73493 -0.79870 -0.66448
H -2.26762 -3.46988 -2.97198
H -0.27543 -2.33962 -2.00986
H -1.20765 -1.01537 2.55660
H -1.09171 -2.99790 4.05114
H 0.62623 -4.77269 3.56471
H 2.13650 -4.48219 1.62438
H 3.40050 -4.05347 0.00055
H 4.71525 -3.44463 -2.00562
H 4.14588 -1.32794 -3.24285
H 2.27751 0.07804 -2.39595
H -1.20765 1.01537 -2.55660
H -1.09171 2.99790 -4.05114
H 0.62623 4.77269 -3.56471
H 2.13650 4.48219 -1.62438
H 3.40050 4.05346 -0.00055
H 4.71525 3.44463 2.00562
H 4.14588 1.32794 3.24285
H 2.27751 -0.07804 2.39595

Ru^{3+}/M06-L

Nuclear Repulsion Energy (a.u.) = 4772.9422405808

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)

Ru	0.27539	0.00000	0.00000
N	-1.37286	0.98838	0.85452
N	-1.37286	-0.98838	-0.85452
N	0.32681	-1.68938	1.27008
N	1.86327	-1.16663	-0.78847
N	0.32681	1.68938	-1.27008
N	1.86327	1.16663	0.78847
O	-4.69545	2.79237	2.46297
O	-4.69545	-2.79238	-2.46297
C	-1.27198	2.01340	1.72478
C	-2.37086	2.62812	2.27877
C	-3.64845	2.18207	1.91212
C	-3.75794	1.13135	0.99383
C	-2.60844	0.55188	0.48186
C	-2.60844	-0.55188	-0.48186
C	-3.75794	-1.13135	-0.99383
C	-3.64845	-2.18207	-1.91212
C	-2.37086	-2.62812	-2.27877
C	-1.27198	-2.01340	-1.72478
C	-0.54913	-1.88200	2.26962
C	-0.51498	-3.01543	3.06555
C	0.45395	-3.98104	2.81256
C	1.35515	-3.78637	1.77435
C	1.27586	-2.62745	1.00490
C	2.14661	-2.32321	-0.12861
C	3.20236	-3.13201	-0.54106
C	3.96649	-2.75413	-1.63634
C	3.66342	-1.57151	-2.30300
C	2.60692	-0.79931	-1.84529
C	-0.54913	1.88200	-2.26962
C	-0.51498	3.01543	-3.06555
C	0.45395	3.98104	-2.81256
C	1.35515	3.78637	-1.77435
C	1.27585	2.62745	-1.00490
C	2.14660	2.32321	0.12861
C	3.20236	3.13202	0.54106
C	3.96649	2.75413	1.63634
C	3.66342	1.57151	2.30300
C	2.60692	0.79931	1.84528
H	-5.52859	2.40414	2.14455
H	-5.52859	-2.40415	-2.14455
H	-0.26525	2.32739	1.98605
H	-2.25281	3.44110	2.98703
H	-4.73817	0.77924	0.68745
H	-4.73817	-0.77924	-0.68745
H	-2.25281	-3.44110	-2.98703
H	-0.26525	-2.32739	-1.98605

H -1.28468 -1.09867 2.42765
H -1.24101 -3.13139 3.86340
H 0.50506 -4.88375 3.41434
H 2.10954 -4.53589 1.55937
H 3.42944 -4.04967 -0.00796
H 4.79340 -3.37787 -1.96358
H 4.23468 -1.24121 -3.16426
H 2.32902 0.13259 -2.33043
H -1.28468 1.09867 -2.42765
H -1.24102 3.13139 -3.86340
H 0.50505 4.88375 -3.41434
H 2.10954 4.53589 -1.55937
H 3.42944 4.04967 0.00796
H 4.79340 3.37788 1.96358
H 4.23468 1.24121 3.16426
H 2.32902 -0.13259 2.33042

Ru^{3+}/M06-L + 2 H_2O

Nuclear Repulsion Energy (a.u.) = 5230.2624273539

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)
Ru 0.68294 0.00000 -0.00000
N -0.95538 -1.04511 -0.78490
N -0.95538 1.04511 0.78490
N 0.76425 1.58446 -1.39195
N 2.26657 1.20780 0.72387
N 0.76425 -1.58446 1.39195
N 2.26657 -1.20780 -0.72387
C -0.85897 -2.13492 -1.57521
C -1.95925 -2.79134 -2.07298
C -3.24365 -2.32521 -1.73735
C -3.34326 -1.20018 -0.90077
C -2.19310 -0.58524 -0.44089
C -2.19310 0.58524 0.44089
C -3.34326 1.20018 0.90077
C -3.24364 2.32521 1.73735
C -1.95924 2.79134 2.07298
C -0.85897 2.13492 1.57521
C -0.08281 1.70248 -2.42808
C -0.00043 2.75454 -3.32588
C 0.98438 3.71886 -3.13797
C 1.85319 3.60402 -2.06140
C 1.72845 2.52421 -1.19038
C 2.57543 2.30587 -0.01843
C 3.63643 3.13115 0.34709
C 4.37995 2.82823 1.47952

C 4.05113 1.70398 2.22967
C 2.98995 0.91364 1.81662
C -0.08281 -1.70248 2.42808
C -0.00043 -2.75454 3.32588
C 0.98437 -3.71886 3.13797
C 1.85319 -3.60402 2.06140
C 1.72845 -2.52421 1.19038
C 2.57543 -2.30587 0.01843
C 3.63642 -3.13115 -0.34709
C 4.37994 -2.82823 -1.47951
C 4.05113 -1.70398 -2.22967
C 2.98995 -0.91364 -1.81662
H 0.14783 -2.46527 -1.81680
H -1.84173 -3.65788 -2.71533
H -4.32460 -0.82814 -0.62153
H -4.32460 0.82814 0.62153
H -1.84173 3.65788 2.71533
H 0.14783 2.46527 1.81680
H -0.83148 0.92230 -2.53275
H -0.70032 2.80868 -4.15331
H 1.07450 4.55774 -3.82217
H 2.62144 4.35250 -1.89785
H 3.88335 4.00242 -0.25096
H 5.21106 3.46418 1.77070
H 4.60630 1.43226 3.12148
H 2.69431 0.02638 2.36989
H -0.83148 -0.92230 2.53275
H -0.70033 -2.80868 4.15331
H 1.07450 -4.55774 3.82217
H 2.62143 -4.35250 1.89785
H 3.88335 -4.00242 0.25096
H 5.21105 -3.46418 -1.77069
H 4.60630 -1.43226 -3.12148
H 2.69431 -0.02638 -2.36989
O -6.45788 1.73209 1.27685
H -7.02319 1.40078 1.99109
O -6.45788 -1.73209 -1.27685
H -7.02853 -2.33855 -0.78105
H -7.02853 2.33855 0.78105
H -7.02319 -1.40078 -1.99109
O -4.29244 -2.96599 -2.21856
H -5.14358 -2.53720 -1.89836
O -4.29244 2.96599 2.21856
H -5.14358 2.53720 1.89836

$[Ru(bpy)_2(44'bpy(O^-)(OH))]^{+/2+}$

Ru^{2+}/B3LYP

Nuclear Repulsion Energy (a.u.) = 4722.8644581525

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)

Ru	-0.27375	0.00007	-0.00430
N	1.43537	0.92679	-0.84371
N	1.31450	-1.07245	0.88470
N	-0.44553	-1.52306	-1.44619
N	-1.84228	-1.17184	0.77219
N	-0.33338	1.53057	1.44304
N	-1.71059	1.33176	-0.81164
O	4.91310	2.60494	-2.33543
O	4.65407	-2.98847	2.43071
C	1.41768	1.95074	-1.72266
C	2.56051	2.53183	-2.23960
C	3.80350	2.03235	-1.82614
C	3.83400	0.97384	-0.91489
C	2.63876	0.43459	-0.43622
C	2.58225	-0.69279	0.52473
C	3.71022	-1.31395	1.02457
C	3.63661	-2.41292	1.96651
C	2.27703	-2.76857	2.30801
C	1.20571	-2.10074	1.76332
C	0.31331	-1.63723	-2.55301
C	0.17078	-2.68271	-3.45837
C	-0.79571	-3.65702	-3.21077
C	-1.58234	-3.54768	-2.06814
C	-1.39213	-2.47137	-1.19527
C	-2.17867	-2.26928	0.03660
C	-3.20391	-3.12630	0.45030
C	-3.89451	-2.85841	1.62812
C	-3.54499	-1.73234	2.37261
C	-2.51691	-0.91872	1.91004
C	0.40882	1.56109	2.56625
C	0.34607	2.60879	3.47850
C	-0.51804	3.67209	3.21963
C	-1.28823	3.64696	2.06075
C	-1.18259	2.56422	1.18156
C	-1.96155	2.44587	-0.06742
C	-2.89931	3.39528	-0.48738
C	-3.58864	3.20310	-1.68104
C	-3.32529	2.06021	-2.43527
C	-2.38212	1.15322	-1.96501
H	5.70957	2.17225	-1.98244
H	0.43788	2.30475	-2.01921
H	2.49954	3.35150	-2.94578
H	4.78560	0.57570	-0.58239
H	4.70197	-0.99486	0.72237
H	2.10557	-3.58200	3.00747

H 0.19091 -2.37986 2.02916
H 1.05078 -0.85892 -2.70533
H 0.80846 -2.72423 -4.33427
H -0.93631 -4.48869 -3.89313
H -2.33644 -4.29588 -1.85900
H -3.46401 -3.99622 -0.13985
H -4.69079 -3.51817 1.95632
H -4.05358 -1.48163 3.29675
H -2.20962 -0.03723 2.45899
H 1.06228 0.71154 2.72132
H 0.96506 2.58369 4.36835
H -0.59345 4.50843 3.90663
H -1.96325 4.46560 1.84512
H -3.09364 4.27702 0.11034
H -4.31797 3.93420 -2.01374
H -3.83644 1.86663 -3.37166
H -2.14291 0.25407 -2.51985

Ru^{2+}/M06-L

Nuclear Repulsion Energy (a.u.) = 4737.5953299518

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)
Ru -0.26917 -0.00213 -0.00197
N 1.42774 0.94965 -0.82146
N 1.32928 -1.04445 0.88580
N -0.41000 -1.50443 -1.44710
N -1.81247 -1.20415 0.74276
N -0.37147 1.50765 1.44836
N -1.71276 1.30568 -0.79846
O 4.87028 2.62535 -2.36606
O 4.67534 -2.88100 2.49133
C 1.39595 1.96847 -1.70315
C 2.52756 2.54711 -2.23551
C 3.77597 2.05412 -1.83681
C 3.82124 1.00430 -0.92070
C 2.63757 0.46574 -0.42387
C 2.59301 -0.64666 0.53625
C 3.72188 -1.24307 1.05760
C 3.65762 -2.32924 2.00747
C 2.30215 -2.70308 2.33452
C 1.22677 -2.06323 1.77284
C 0.35213 -1.58077 -2.55437
C 0.21669 -2.59536 -3.48760
C -0.74335 -3.58130 -3.27415
C -1.52926 -3.51482 -2.13274

C -1.34956 -2.46976 -1.22590
C -2.13164 -2.30193 -0.00116
C -3.13727 -3.17724 0.41121
C -3.82754 -2.92947 1.58858
C -3.49800 -1.80293 2.33796
C -2.48963 -0.96979 1.88212
C 0.36108 1.53580 2.57703
C 0.25127 2.55266 3.51224
C -0.65069 3.58690 3.27727
C -1.40658 3.56746 2.11393
C -1.25376 2.51991 1.20522
C -2.00366 2.40608 -0.04739
C -2.94766 3.33828 -0.48095
C -3.60153 3.14627 -1.68968
C -3.29798 2.01900 -2.44856
C -2.35284 1.12705 -1.96842
H 5.66882 2.19379 -2.01969
H 0.40617 2.31622 -1.98982
H 2.45568 3.36365 -2.94683
H 4.77895 0.60706 -0.59507
H 4.71122 -0.90209 0.75974
H 2.13459 -3.51227 3.04311
H 0.20764 -2.35382 2.02857
H 1.08497 -0.78784 -2.68094
H 0.85605 -2.60565 -4.36511
H -0.87902 -4.39035 -3.98664
H -2.28363 -4.27344 -1.94753
H -3.38027 -4.05008 -0.18745
H -4.61200 -3.60621 1.91638
H -4.01171 -1.56725 3.26527
H -2.19299 -0.08246 2.43586
H 1.04489 0.70128 2.71353
H 0.86535 2.52772 4.40735
H -0.76496 4.39855 3.99067
H -2.11449 4.36594 1.91312
H -3.17140 4.21193 0.12386
H -4.33679 3.86805 -2.03474
H -3.78312 1.82795 -3.40111
H -2.07753 0.23571 -2.52714

Ru^{2+}/M06-L + 2 H_2O

Nuclear Repulsion Energy (a.u.) = 5194.5378069326

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)

Ru	0.69891	-0.00082	-0.01281
N	-0.92347	1.10702	0.76090
N	-0.98189	-1.04129	-0.76876
N	0.79995	-1.38479	1.55656
N	2.15830	-1.35085	-0.69611
N	0.85656	1.38915	-1.56649
N	2.21690	1.26669	0.67182
C	-0.84838	2.21461	1.53418
C	-1.94306	2.90680	1.99221
C	-3.27689	2.48771	1.66131
C	-3.31956	1.31200	0.83858
C	-2.17392	0.66894	0.41988
C	-2.19862	-0.54076	-0.41463
C	-3.37695	-1.14886	-0.82684
C	-3.33284	-2.30026	-1.61951
C	-2.07349	-2.80517	-1.98033
C	-0.94528	-2.15081	-1.53363
C	0.06809	-1.33145	2.68516
C	0.20256	-2.25833	3.70721
C	1.13000	-3.28689	3.56406
C	1.88391	-3.35215	2.40146
C	1.70538	-2.39346	1.40391
C	2.45485	-2.38016	0.14742
C	3.40288	-3.34284	-0.20301
C	4.05318	-3.25694	-1.42563
C	3.74317	-2.20162	-2.27991
C	2.79624	-1.27349	-1.87800
C	0.11347	1.38483	-2.68935
C	0.26341	2.33198	-3.68986
C	1.21925	3.33199	-3.53119
C	1.98682	3.34683	-2.37582
C	1.79268	2.36861	-1.40039
C	2.55138	2.30110	-0.15170
C	3.54316	3.21291	0.21320
C	4.19774	3.07066	1.42829
C	3.84832	2.01066	2.26121
C	2.85892	1.13462	1.84692
H	0.16179	2.53615	1.78713
H	-1.80130	3.78969	2.61235
H	-4.30053	0.94526	0.54357
H	-4.33948	-0.74228	-0.53208
H	-1.99240	-3.69628	-2.59527
H	0.04713	-2.51293	-1.79367
H	-0.63333	-0.50302	2.74848
H	-0.41171	-2.16771	4.59812
H	1.26517	-4.02852	4.34651
H	2.61296	-4.14614	2.27126

H 3.62810 -4.15923 0.47654
H 4.79037 -4.00396 -1.70718
H 4.22458 -2.09284 -3.24709
H 2.51877 -0.43383 -2.51090
H -0.61497 0.58171 -2.76936
H -0.36262 2.28056 -4.57558
H 1.36505 4.08995 -4.29580
H 2.73687 4.11868 -2.23259
H 3.80058 4.03398 -0.44915
H 4.96942 3.77780 1.72032
H 4.33153 1.85940 3.22178
H 2.55104 0.29408 2.46396
O -6.52537 -1.55382 -1.02400
H -7.09706 -1.20069 -1.72193
O -6.52731 1.70803 1.11849
H -5.77393 2.25126 1.46406
H -7.11041 -2.12617 -0.50576
H -6.56116 0.97226 1.74330
O -4.31655 3.09495 2.05607
O -4.42601 -2.93470 -2.04227
H -5.23743 -2.46455 -1.70034

Ru^{3+}/B3LYP

Nuclear Repulsion Energy (a.u.) = 4735.1749244391

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)
Ru -0.22214 -0.01380 0.00204
N 1.54967 0.68002 -0.92018
N 1.14050 -1.27428 0.79790
N -0.76714 -1.45299 -1.43320
N -1.93654 -0.88788 0.88519
N 0.02836 1.56049 1.40509
N -1.51761 1.52220 -0.75501
O 5.20653 1.94970 -2.35795
O 4.12014 -3.66819 2.30950
C 1.65335 1.69487 -1.80213
C 2.86375 2.13577 -2.30260
C 4.03821 1.50228 -1.87036
C 3.93709 0.44267 -0.96076
C 2.68167 0.05264 -0.50411
C 2.46687 -1.06211 0.44478
C 3.47534 -1.84924 0.93714
C 3.20896 -2.94939 1.85177
C 1.80629 -3.13746 2.17594
C 0.85560 -2.31411 1.64536
C -0.10290 -1.68467 -2.58108
C -0.49780 -2.66687 -3.48166
C -1.62030 -3.43656 -3.18046
C -2.31090 -3.19788 -1.99492
C -1.86911 -2.19600 -1.12810

C -2.53469 -1.86335 0.14701
C -3.70065 -2.48780 0.59675
C -4.25634 -2.10898 1.81618
C -3.63435 -1.11082 2.56322
C -2.47699 -0.52452 2.06132
C 0.83944 1.50042 2.47757
C 0.99761 2.56886 3.35319
C 0.29095 3.74437 3.10859
C -0.55026 3.80909 2.00140
C -0.66996 2.70260 1.15690
C -1.54093 2.67616 -0.03446
C -2.34891 3.74722 -0.42464
C -3.13963 3.63287 -1.56478
C -3.10774 2.44633 -2.29441
C -2.28438 1.41523 -1.85508
H 5.95242 1.44806 -1.98488
H 0.72530 2.15951 -2.11066
H 2.90719 2.95531 -3.00981
H 4.83117 -0.06543 -0.61967
H 4.50864 -1.68474 0.65638
H 1.52397 -3.94114 2.84707
H -0.19167 -2.44194 1.88594
H 0.76054 -1.05945 -2.76888
H 0.06846 -2.81800 -4.39325
H -1.95757 -4.21416 -3.85742
H -3.18306 -3.79083 -1.75083
H -4.17446 -3.25936 0.00372
H -5.16158 -2.58797 2.17359
H -4.03015 -0.78328 3.51762
H -1.95843 0.25303 2.60806
H 1.36421 0.56655 2.63197
H 1.66196 2.46911 4.20370
H 0.38884 4.59989 3.76820
H -1.10667 4.71523 1.79944
H -2.36434 4.66257 0.15276
H -3.76960 4.45964 -1.87495
H -3.70485 2.31076 -3.18871
H -2.22604 0.47922 -2.39562

Ru^{3+}/M06-L

Nuclear Repulsion Energy (a.u.) = 4746.7465474431

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)

Ru	-0.23872	-0.01089	-0.01571
N	1.54857	0.60584	-0.95353
N	1.09426	-1.33548	0.75092
N	-0.87152	-1.43643	-1.42336
N	-1.96955	-0.80485	0.88556
N	0.13219	1.53345	1.38297
N	-1.46291	1.58860	-0.71720
O	5.22325	1.75909	-2.41175
O	4.01413	-3.75008	2.32492
C	1.67682	1.60456	-1.84710
C	2.89410	2.00401	-2.35423
C	4.05117	1.34705	-1.91643
C	3.92418	0.30439	-0.99555
C	2.66351	-0.04707	-0.53269
C	2.42299	-1.14200	0.41609
C	3.41237	-1.93880	0.93117
C	3.12034	-3.02448	1.84366
C	1.71449	-3.19639	2.13841
C	0.78106	-2.36726	1.58709
C	-0.23103	-1.70195	-2.57484
C	-0.67568	-2.67120	-3.45974
C	-1.82162	-3.39289	-3.13976
C	-2.48644	-3.12029	-1.95213
C	-1.99653	-2.13323	-1.09874
C	-2.62125	-1.76569	0.17354
C	-3.79873	-2.33438	0.65755
C	-4.31249	-1.91384	1.87659
C	-3.63837	-0.93039	2.59282
C	-2.47126	-0.40101	2.06364
C	0.96735	1.41945	2.42939
C	1.20194	2.46537	3.30851
C	0.55021	3.67583	3.09803
C	-0.31439	3.79686	2.01958
C	-0.51243	2.71204	1.16636
C	-1.40414	2.73983	0.00538
C	-2.15580	3.85360	-0.36577
C	-2.97203	3.78907	-1.48608
C	-3.02373	2.60691	-2.21726
C	-2.25775	1.52947	-1.79873
H	5.95279	1.24232	-2.02996
H	0.75456	2.08866	-2.15814
H	2.95925	2.81300	-3.07431
H	4.80558	-0.22736	-0.64901
H	4.45308	-1.78299	0.66090
H	1.40780	-3.99583	2.80722
H	-0.27724	-2.48096	1.80712
H	0.65701	-1.10859	-2.77478

H -0.12643 -2.85327 -4.37803
H -2.19675 -4.16212 -3.80905
H -3.38037 -3.67676 -1.68875
H -4.31332 -3.09883 0.08414
H -5.23072 -2.34917 2.26082
H -4.00465 -0.57090 3.54921
H -1.90529 0.36479 2.58749
H 1.44575 0.45254 2.55880
H 1.88529 2.32217 4.13956
H 0.71012 4.51703 3.76663
H -0.83348 4.73302 1.84036
H -2.10469 4.76672 0.21848
H -3.56114 4.65228 -1.78232
H -3.64740 2.51053 -3.10029
H -2.26380 0.58714 -2.34044

Ru^{3+}/M06-L + 2 H_2O

Nuclear Repulsion Energy (a.u.) = 5203.9071511950

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)
Ru 0.64199 0.01455 0.01660
N -0.89045 1.10620 0.78242
N -1.02551 -1.01168 -0.76683
N 0.72535 -1.47434 1.51611
N 2.13278 -1.32688 -0.70541
N 0.87977 1.41779 -1.52632
N 2.21843 1.21973 0.73493
C -0.75366 2.22979 1.54414
C -1.81288 2.94459 2.02561
C -3.16439 2.53808 1.72583
C -3.27634 1.35599 0.90717
C -2.16784 0.68429 0.46345
C -2.23091 -0.50545 -0.39334
C -3.42210 -1.07326 -0.81599
C -3.39487 -2.20164 -1.64782
C -2.14253 -2.71906 -2.01938
C -1.00062 -2.10096 -1.55906
C -0.04661 -1.48241 2.61711
C 0.06021 -2.46474 3.58966
C 0.99817 -3.47709 3.41940
C 1.79092 -3.47669 2.28070
C 1.63982 -2.46633 1.33244
C 2.42038 -2.38718 0.09653
C 3.38490 -3.32189 -0.27883

C 4.05207 -3.17269 -1.48688
C 3.74332 -2.08800 -2.30094
C 2.78195 -1.18622 -1.87294
C 0.13814 1.44156 -2.64717
C 0.34336 2.37822 -3.64725
C 1.34981 3.32422 -3.47902
C 2.11684 3.30310 -2.32194
C 1.86957 2.33783 -1.34753
C 2.62091 2.22165 -0.09537
C 3.67628 3.05981 0.26103
C 4.32218 2.87106 1.47523
C 3.89915 1.84710 2.31581
C 2.84482 1.04324 1.90946
H 0.27014 2.52207 1.76117
H -1.64458 3.82783 2.63517
H -4.28106 1.03195 0.64251
H -4.37699 -0.65453 -0.51127
H -2.07894 -3.59262 -2.66025
H -0.01520 -2.47087 -1.83189
H -0.75687 -0.66562 2.71160
H -0.58356 -2.42539 4.46253
H 1.11284 -4.25961 4.16406
H 2.52598 -4.26071 2.13086
H 3.61157 -4.16481 0.36598
H 4.80283 -3.89790 -1.78808
H 4.23590 -1.93332 -3.25564
H 2.50799 -0.32581 -2.47721
H -0.63082 0.67795 -2.72800
H -0.27847 2.36037 -4.53630
H 1.53766 4.07391 -4.24241
H 2.90483 4.03535 -2.17942
H 3.99372 3.85619 -0.40489
H 5.14704 3.51813 1.76013
H 4.37304 1.66620 3.27542
H 2.47344 0.23355 2.53254
O -6.57178 -1.39503 -1.14310
H -7.10106 -1.01607 -1.86102
O -6.42210 1.74922 1.08971
H -5.74704 2.33160 1.49855
H -7.19526 -1.95449 -0.65615
H -6.63623 1.13238 1.80231
O -4.17069 3.16700 2.13691
O -4.49014 -2.79926 -2.09833
H -5.30376 -2.31852 -1.76698

$[Ru(bpy)_2(44'bpy(O^-)_2)]^{0/+}$

Ru^{2+}/B3LYP

Nuclear Repulsion Energy (a.u.) = 4694.2137771640

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)

Ru	0.26337	0.00000	0.00000
N	-1.38374	-0.99011	-0.87487
N	-1.38374	0.99011	0.87487
N	0.37244	1.52541	-1.44040
N	1.76685	1.26087	0.79026
N	0.37244	-1.52541	1.44040
N	1.76685	-1.26087	-0.79026
O	-4.81283	-2.72427	-2.43677
O	-4.81283	2.72427	2.43677
C	-1.32543	-2.00534	-1.77379
C	-2.42769	-2.61551	-2.32384
C	-3.76655	-2.20259	-1.96495
C	-3.78346	-1.12151	-1.00381
C	-2.62919	-0.55700	-0.49364
C	-2.62919	0.55700	0.49364
C	-3.78346	1.12151	1.00381
C	-3.76655	2.20259	1.96495
C	-2.42769	2.61551	2.32384
C	-1.32543	2.00534	1.77379
C	-0.38162	1.59134	-2.55504
C	-0.28768	2.63851	-3.46474
C	0.62149	3.66633	-3.21413
C	1.40233	3.60649	-2.06403
C	1.26354	2.52578	-1.18631
C	2.04940	2.37243	0.05325
C	3.02392	3.28576	0.47110
C	3.71983	3.05954	1.65450
C	3.42637	1.91795	2.40051
C	2.44683	1.04903	1.93356
C	-0.38162	-1.59134	2.55504
C	-0.28768	-2.63851	3.46474
C	0.62149	-3.66633	3.21413
C	1.40233	-3.60649	2.06403
C	1.26354	-2.52578	1.18631
C	2.04940	-2.37243	-0.05325
C	3.02392	-3.28576	-0.47110
C	3.71983	-3.05954	-1.65450
C	3.42637	-1.91795	-2.40051
C	2.44683	-1.04903	-1.93356
H	-0.32486	-2.32287	-2.05164
H	-2.29771	-3.42265	-3.03991
H	-4.75608	-0.75867	-0.68834
H	-4.75608	0.75867	0.68834
H	-2.29771	3.42265	3.03991
H	-0.32486	2.32287	2.05164

H -1.07202 0.77020 -2.70317
H -0.91830 2.64127 -4.34691
H 0.72225 4.50096 -3.90004
H 2.11190 4.39674 -1.85280
H 3.24048 4.16642 -0.12082
H 4.47700 3.76244 1.98595
H 3.94164 1.69793 3.32891
H 2.18299 0.15360 2.48354
H -1.07202 -0.77020 2.70317
H -0.91830 -2.64127 4.34691
H 0.72225 -4.50096 3.90004
H 2.11190 -4.39674 1.85280
H 3.24048 -4.16642 0.12082
H 4.47700 -3.76244 -1.98595
H 3.94164 -1.69793 -3.32891
H 2.18299 -0.15360 -2.48354

Ru^{2+}/M06-L

Nuclear Repulsion Energy (a.u.) = 4709.0116968328

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)
Ru 0.25428 0.00000 0.00000
N -1.39060 -0.98756 -0.86285
N -1.39060 0.98756 0.86285
N 0.37587 1.48786 -1.45821
N 1.74429 1.26972 0.76321
N 0.37587 -1.48786 1.45821
N 1.74429 -1.26972 -0.76321
O -4.80174 -2.66115 -2.50430
O -4.80174 2.66115 2.50430
C -1.32575 -1.98814 -1.77418
C -2.42371 -2.57621 -2.34807
C -3.76268 -2.15717 -2.00704
C -3.78367 -1.09279 -1.03386
C -2.63617 -0.54704 -0.49543
C -2.63617 0.54704 0.49543
C -3.78367 1.09279 1.03386
C -3.76268 2.15717 2.00704
C -2.42371 2.57621 2.34807
C -1.32575 1.98814 1.77418
C -0.36625 1.52263 -2.58228
C -0.23768 2.52278 -3.53210
C 0.69357 3.53716 -3.32070
C 1.45750 3.51335 -2.16305
C 1.28557 2.48290 -1.23788

C 2.04525 2.36400 0.00650
C 3.00991 3.28156 0.42728
C 3.67565 3.08113 1.62770
C 3.36374 1.95849 2.39146
C 2.39786 1.08248 1.92499
C -0.36625 -1.52263 2.58228
C -0.23768 -2.52278 3.53210
C 0.69357 -3.53716 3.32070
C 1.45750 -3.51335 2.16305
C 1.28558 -2.48290 1.23788
C 2.04525 -2.36400 -0.00650
C 3.00991 -3.28156 -0.42728
C 3.67565 -3.08113 -1.62770
C 3.36374 -1.95849 -2.39147
C 2.39786 -1.08248 -1.92499
H -0.31715 -2.30731 -2.03960
H -2.28766 -3.37474 -3.07575
H -4.75739 -0.71679 -0.72558
H -4.75739 0.71679 0.72558
H -2.28766 3.37474 3.07575
H -0.31716 2.30731 2.03960
H -1.07396 0.70544 -2.70070
H -0.86040 2.50135 -4.42155
H 0.82341 4.33478 -4.04712
H 2.18917 4.29456 -1.97937
H 3.23898 4.15121 -0.18158
H 4.42626 3.79177 1.96304
H 3.85810 1.76054 3.33802
H 2.11453 0.19652 2.48869
H -1.07395 -0.70544 2.70070
H -0.86040 -2.50135 4.42155
H 0.82342 -4.33478 4.04712
H 2.18917 -4.29456 1.97937
H 3.23898 -4.15121 0.18158
H 4.42626 -3.79177 -1.96304
H 3.85810 -1.76054 -3.33802
H 2.11453 -0.19652 -2.48869

Ru^{2+}/M06-L + 2 H_2O

Nuclear Repulsion Energy (a.u.) = 5170.9025788983

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)

Ru	0.00000	0.00000	0.72178
N	0.45159	1.24200	-0.92525
N	-0.45159	-1.24200	-0.92525
N	-2.02054	0.52614	0.81887
N	-0.73320	-1.30741	2.18931
N	2.02054	-0.52614	0.81887
N	0.73320	1.30741	2.18931
C	0.88261	2.52454	-0.87938
C	1.09995	3.30257	-1.99082
C	0.86789	2.78493	-3.31118
C	0.40955	1.42736	-3.31893
C	0.22815	0.69995	-2.16170
C	-0.22815	-0.69995	-2.16170
C	-0.40955	-1.42736	-3.31893
C	-0.86789	-2.78493	-3.31118
C	-1.09995	-3.30257	-1.99082
C	-0.88261	-2.52454	-0.87938
C	-2.60518	1.49864	0.09416
C	-3.95900	1.78194	0.17664
C	-4.75383	1.02916	1.03849
C	-4.16045	0.02422	1.78789
C	-2.79076	-0.21482	1.66827
C	-2.07403	-1.23566	2.43024
C	-2.68403	-2.09296	3.34731
C	-1.92199	-3.02954	4.02979
C	-0.55163	-3.08789	3.78534
C	0.00000	-2.21254	2.86403
C	2.60518	-1.49864	0.09416
C	3.95900	-1.78194	0.17664
C	4.75383	-1.02916	1.03849
C	4.16045	-0.02422	1.78789
C	2.79076	0.21482	1.66827
C	2.07403	1.23566	2.43024
C	2.68403	2.09296	3.34731
C	1.92199	3.02954	4.02979
C	0.55163	3.08789	3.78534
C	-0.00000	2.21254	2.86403
H	1.04795	2.92321	0.12177
H	1.44892	4.32674	-1.87240
H	0.18760	0.97983	-4.28433
H	-0.18760	-0.97983	-4.28433
H	-1.44892	-4.32674	-1.87240
H	-1.04795	-2.92321	0.12177
H	-1.94200	2.05449	-0.56449
H	-4.37786	2.57901	-0.43073
H	-5.81967	1.22208	1.12588
H	-4.76078	-0.57514	2.46593

H -3.75330 -2.02784 3.52588
H -2.38985 -3.70264 4.74299
H 0.08699 -3.80169 4.29728
H 1.06272 -2.22354 2.63349
H 1.94200 -2.05449 -0.56449
H 4.37786 -2.57901 -0.43073
H 5.81967 -1.22208 1.12588
H 4.76078 0.57514 2.46593
H 3.75330 2.02784 3.52588
H 2.38985 3.70264 4.74299
H -0.08699 3.80169 4.29728
H -1.06272 2.22354 2.63349
O -0.37582 -1.85464 -6.54031
H -0.63413 -2.45997 -5.79850
O 0.37582 1.85464 -6.54031
H 1.04863 1.16267 -6.50171
H -1.04863 -1.16267 -6.50171
H 0.63413 2.45997 -5.79850
O 1.04838 3.46080 -4.36990
O -1.04838 -3.46080 -4.36990

Ru^{3+}/B3LYP

Nuclear Repulsion Energy (a.u.) = 4706.3525715330

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)
Ru 0.20608 -0.01311 -0.00772
N -1.20664 -1.22184 -0.78958
N -1.50904 0.71533 0.95726
N -0.02253 1.57169 -1.39773
N 1.55499 1.48643 0.73517
N 0.71675 -1.47142 1.41760
N 1.89651 -0.95145 -0.90821
O -4.27757 -3.49634 -2.30279
O -5.13474 2.02178 2.46197
C -0.96441 -2.26122 -1.65226
C -1.94649 -3.04477 -2.18361
C -3.33926 -2.81167 -1.84157
C -3.55639 -1.71900 -0.91029
C -2.52119 -0.96767 -0.41344
C -2.68721 0.13952 0.55801
C -3.90901 0.55554 1.04200
C -4.03075 1.62907 2.00979
C -2.75307 2.19124 2.39650
C -1.57724 1.72431 1.86348
C -0.85412 1.53738 -2.45526
C -0.99906 2.61217 -3.32548
C -0.25685 3.76786 -3.09108
C 0.60387 3.80692 -1.99794
C 0.70800 2.69491 -1.15809

C 1.59461 2.64319 0.02085
C 2.43122 3.69443 0.40592
C 3.23312 3.55712 1.53551
C 3.18351 2.36776 2.25992
C 2.33216 1.35765 1.82515
C 0.04452 -1.67956 2.56514
C 0.40834 -2.67307 3.46671
C 1.50574 -3.47856 3.16566
C 2.20248 -3.26481 1.97883
C 1.79252 -2.25030 1.11055
C 2.46462 -1.94336 -0.16888
C 3.60784 -2.60888 -0.61935
C 4.17163 -2.25437 -1.84238
C 3.58081 -1.23867 -2.59150
C 2.44549 -0.61223 -2.08710
H 0.07629 -2.42088 -1.90358
H -1.69884 -3.84931 -2.86769
H -4.57864 -1.52120 -0.61047
H -4.82620 0.08142 0.70947
H -2.73233 2.99965 3.12154
H -0.62503 2.15327 2.15802
H -1.40768 0.61873 -2.60011
H -1.68109 2.53302 -4.16420
H -0.34294 4.62741 -3.74718
H 1.18725 4.69757 -1.80283
H 2.45954 4.61235 -0.16707
H 3.88505 4.36820 1.84191
H 3.78813 2.21468 3.14642
H 2.25895 0.42014 2.36162
H -0.79767 -1.02332 2.74497
H -0.16158 -2.80574 4.37901
H 1.81852 -4.26571 3.84348
H 3.05395 -3.88734 1.73504
H 4.05796 -3.39339 -0.02471
H 5.05890 -2.76530 -2.20081
H 3.98426 -0.92882 -3.54871
H 1.95128 0.18138 -2.63415

Ru^{3+}/M06-L

Nuclear Repulsion Energy (a.u.) = 4719.3094911386

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)
Ru 0.23126 0.00000 0.00000
N -1.36498 -0.94868 -0.90010
N -1.36498 0.94868 0.90010

N 0.31727 1.62343 -1.33788
N 1.78056 1.20404 0.81129
N 0.31726 -1.62343 1.33788
N 1.78056 -1.20404 -0.81129
O -4.73952 -2.62465 -2.55081
O -4.73952 2.62465 2.55081
C -1.27794 -1.94334 -1.82295
C -2.36884 -2.52862 -2.40382
C -3.70924 -2.12170 -2.04668
C -3.75553 -1.08018 -1.04676
C -2.61518 -0.53048 -0.50955
C -2.61518 0.53048 0.50955
C -3.75553 1.08018 1.04676
C -3.70924 2.12170 2.04668
C -2.36884 2.52862 2.40382
C -1.27794 1.94334 1.82295
C -0.48714 1.76121 -2.40531
C -0.42806 2.86631 -3.23928
C 0.49339 3.86969 -2.95605
C 1.32654 3.73144 -1.85464
C 1.22739 2.59548 -1.05130
C 2.05858 2.34916 0.12967
C 3.07921 3.20047 0.55179
C 3.82036 2.87691 1.67950
C 3.52834 1.70326 2.36734
C 2.50433 0.89387 1.89971
C -0.48714 -1.76121 2.40531
C -0.42806 -2.86631 3.23928
C 0.49339 -3.86969 2.95605
C 1.32654 -3.73144 1.85464
C 1.22739 -2.59548 1.05130
C 2.05858 -2.34916 -0.12967
C 3.07921 -3.20047 -0.55179
C 3.82036 -2.87691 -1.67950
C 3.52834 -1.70326 -2.36734
C 2.50433 -0.89387 -1.89971
H -0.26620 -2.24207 -2.09124
H -2.23362 -3.31080 -3.14662
H -4.73583 -0.73896 -0.72437
H -4.73583 0.73896 0.72437
H -2.23362 3.31080 3.14662
H -0.26620 2.24207 2.09124
H -1.18995 0.95056 -2.57927
H -1.09865 2.93284 -4.09023
H 0.56230 4.75335 -3.58426
H 2.04795 4.50700 -1.61770
H 3.29882 4.10908 -0.00042
H 4.61813 3.53366 2.01539
H 4.08315 1.41090 3.25336
H 2.23514 -0.03117 2.40421
H -1.18995 -0.95056 2.57927
H -1.09865 -2.93284 4.09023
H 0.56230 -4.75335 3.58426
H 2.04795 -4.50700 1.61770
H 3.29882 -4.10908 0.00042
H 4.61813 -3.53366 -2.01539

H 4.08315 -1.41090 -3.25336
H 2.23514 0.03117 -2.40421

Ru^{3+}/M06-L + 2 H_2O

Nuclear Repulsion Energy (a.u.) = 5178.5601615642

Imaginary Frequencies = 0

Cartesian Coordinates (Angstroms)
Ru 0.00000 0.00000 0.66389
N 0.50871 1.21086 -0.93365
N -0.50871 -1.21086 -0.93365
N -2.03828 0.53108 0.75796
N -0.74034 -1.25839 2.20339
N 2.03828 -0.53108 0.75796
N 0.74034 1.25839 2.20339
C 1.06208 2.44966 -0.86083
C 1.36719 3.20439 -1.96194
C 1.11614 2.70422 -3.28940
C 0.55132 1.38254 -3.32725
C 0.27680 0.67963 -2.17887
C -0.27680 -0.67963 -2.17887
C -0.55132 -1.38254 -3.32725
C -1.11614 -2.70422 -3.28940
C -1.36719 -3.20439 -1.96194
C -1.06208 -2.44966 -0.86083
C -2.61988 1.45995 -0.01911
C -3.97116 1.75672 0.06747
C -4.75169 1.06145 0.98599
C -4.15570 0.09769 1.78667
C -2.79084 -0.15777 1.66104
C -2.07067 -1.14554 2.46592
C -2.67202 -1.93083 3.44868
C -1.90446 -2.83326 4.17150
C -0.54310 -2.93181 3.90148
C -0.00000 -2.12644 2.91218
C 2.61988 -1.45995 -0.01911
C 3.97116 -1.75672 0.06747
C 4.75169 -1.06145 0.98599
C 4.15570 -0.09769 1.78667
C 2.79084 0.15777 1.66104
C 2.07067 1.14554 2.46592
C 2.67202 1.93083 3.44868
C 1.90446 2.83326 4.17150
C 0.54310 2.93181 3.90148
C 0.00000 2.12644 2.91218
H 1.23728 2.82545 0.14528
H 1.79819 4.19448 -1.83866
H 0.34144 0.95450 -4.30469

H -0.34144 -0.95450 -4.30469
H -1.79819 -4.19448 -1.83866
H -1.23728 -2.82545 0.14528
H -1.96478 1.97057 -0.72011
H -4.39536 2.51743 -0.58025
H -5.81474 1.26594 1.07871
H -4.75083 -0.45417 2.50724
H -3.73455 -1.83822 3.65004
H -2.36537 -3.45007 4.93793
H 0.09650 -3.62071 4.44428
H 1.05654 -2.17043 2.65989
H 1.96478 -1.97057 -0.72011
H 4.39536 -2.51743 -0.58025
H 5.81474 -1.26594 1.07871
H 4.75083 0.45417 2.50724
H 3.73455 1.83822 3.65004
H 2.36537 3.45007 4.93793
H -0.09650 3.62071 4.44428
H -1.05654 2.17043 2.65989
O -0.58243 -1.79384 -6.53442
H -0.88845 -2.40229 -5.82244
O 0.58243 1.79384 -6.53442
H 1.30690 1.15869 -6.60560
H -1.30690 -1.15869 -6.60560
H 0.88845 2.40229 -5.82244
O 1.37470 3.36571 -4.33212
O -1.37470 -3.36571 -4.33212