Electronic Supplementary Information for Dalton Transactions

Supplementary Information:

S1. $[Ru(bpy)(Obpy)]^{2+}$

a. Cartesian Coordinates from calculations
b. TDDFT Singlet Results
c. TDDFT Spectra Comparison
d. TDDFT Triplet Results

S2. $[(Ru(bpy)_2)_2Obpy]^{4+}$

a. Cartesian Coordinates from calculations
b. TDDFT Triplet Results

S3. $[Ru(bpy)_3]^{2+}$

a. Cartesian Coordinates from calculations
b. TDDFT Triplet Results
c.

S4. Graphical Representation of Orbital Distribution

S5. Inter atom bond distances of O-bpy dimer

S6. TDDFT Triplet State Results

S1.a. Cartesian Coordinates from calculations

Atom	Coordinates		
	X	Y	Z
Re	-0.013778	0.063187	-0.001508
N	-0.072699	0.020134	2.105339
C	1.153888	-0.206737	2.690007
C	-1.180205	0.127362	2.895992
C	1.254941	-0.591278	4.038474
C	-1.135899	-0.264224	4.246138
C	0.084109	-0.684874	4.808600
H	2.219806	-0.797839	4.486506
H	-2.035004	-0.206519	4.850614
H	0.131132	-1.010526	5.842936
N	0.404744	-2.006188	0.068220
C	1.622494	-2.589106	0.270643
C	-0.703243	-2.825019	-0.038399
C	1.789470	-3.971723	0.415380
H	2.477420	-1.928944	0.306244
C	-0.595715	-4.219781	0.120359
C	0.656797	-4.804544	0.359133
H	2.782854	-4.378584	0.570744
H	-1.475955	-4.847578	0.053384
H	0.747948	-5.878741	0.483536
N	-1.877266	-0.771837	-0.507964
C	-1.958615	-2.144197	-0.405108
C	-2.959219	-0.090204	-0.987681
C	-3.149843	-2.828100	-0.719537
C	-4.159989	-0.719244	-1.332395
H	-2.849703	0.981809	-1.082423
C	-4.266365	-2.115194	-1.178620

H	-3.204119	-3.906052	-0.627333
H	-4.988031	-0.127801	-1.707946
H	-5.187148	-2.633834	-1.425234
N	-0.697037	2.045735	-0.247771
C	-0.410966	2.555360	-1.511025
C	-1.402051	2.831092	0.636491
C	-0.713873	3.879057	-1.863775
C	-1.738507	4.161278	0.293282
C	-1.370016	4.705411	-0.941852
H	-0.459660	4.262483	-2.843718
H	-2.285701	4.763881	1.010494
H	-1.610467	5.733846	-1.190545
N	1.954769	0.529485	0.544477
C	2.297495	0.148410	1.828740
C	2.931178	1.013086	-0.275791
C	3.629325	0.216204	2.278182
C	4.269121	1.116146	0.124211
H	2.626386	1.315133	-1.268863
C	4.629888	0.699428	1.420440
H	3.881013	-0.084880	3.288446
H	5.006392	1.512817	-0.565322
H	5.659910	0.761005	1.756667
N	0.349610	0.317068	-2.023740
C	0.165743	1.602929	-2.484703
C	0.811602	-0.639013	-2.879254
C	0.479351	1.937214	-3.817760
C	1.129214	-0.361946	-4.213479
H	0.927506	-1.634662	-2.471145
C	0.967706	0.953211	-4.690626
H	0.341138	2.948073	-4.180863
H	1.493498	-1.155522	-4.856778
H	1.210724	1.204493	-5.718056

C	-2.325414	0.921488	2.314445
C	-1.835503	2.384731	2.034850
H	-1.015782	2.615004	2.731767
H	-2.649874	3.058719	2.319518
H	-2.739799	0.465301	1.416840
H	-3.132227	0.970425	3.052568

S1.b. TDDFT Singlet Excited States

Excited State 1: Singlet-A 2.4193 eV 512.47 nm f=0.0098
135 ->138 -0.11687
136 ->138 0.29885
136 ->139 -0.15070
137 ->138 0.44733
137 ->139 -0.36172

This state for optimization and/or second-order correction.
Total Energy, E(RPA) = -1657.86807045
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.4833 eV 499.28 nm f=0.0046
136 ->138 0.24347
137 ->138 0.28964
137 ->139 0.56168
137 ->140 0.11921

Excited State 3: Singlet-A 2.5426 eV 487.62 nm f=0.0161
135 ->138 -0.12194
135 ->139 0.19803
136 ->138 0.34125

136 ->139	-0.31571	
136 ->140	-0.34206	
137 ->138	-0.22502	
137 ->140	-0.17968	

Excited State 4: Singlet-A 2.5591 eV 484.49 nm f=0.0185

135 ->138	0.29884
135 ->140	-0.20427
136 ->138	0.13478
136 ->139	-0.27550
136 ->140	0.23566
137 ->138	-0.20187
137 ->140	0.39319

Excited State 5: Singlet-A 2.5738 eV 481.71 nm f=0.0102

135 ->138	0.27867
135 ->139	-0.15366
136 ->138	0.40588
136 ->139	0.41543
136 ->140	-0.10703
137 ->138	-0.12024
137 ->139	-0.13869

Excited State 6: Singlet-A 2.6425 eV 469.19 nm f=0.0398

135 ->138	0.53553
135 ->139	0.11509
135 ->140	0.16373
136 ->138	-0.11621
136 ->139	-0.16787
136 ->140	-0.14714
137 ->138	0.23377

137 ->140 -0.17563

Excited State 7: Singlet-A 2.7352 eV 453.29 nm f=0.0314
135 ->139 0.11229
135 ->140 0.49080
136 ->138 0.10643
136 ->140 0.39992
137 ->138 -0.15739
137 ->139 0.10002
137 ->140 -0.12057

Excited State 8: Singlet-A 2.8009 eV 442.66 nm f=0.1046
135 ->139 0.49281
135 ->140 -0.30545
136 ->139 0.21610
136 ->140 0.19309
137 ->140 -0.20170

Excited State 9: Singlet-A 2.9946 eV 414.03 nm f=0.0007
135 ->139 0.33259
135 ->140 0.24014
136 ->139 0.14511
136 ->140 -0.22296
136 ->144 -0.11937
137 ->140 0.36408
137 ->144 -0.10417
137 ->145 -0.12400

Excited State 10: Singlet-A 3.3515 eV 369.93 nm f=0.0111
136 ->141 0.13499
137 ->141 0.67920

Excited State 11: Singlet-A 3.4529 eV 359.07 nm f=0.0065
136 ->141 0.67171
137 ->141 -0.13623

Excited State 12: Singlet-A 3.5078 eV 353.45 nm f=0.0046
135 ->142 -0.10908
136 ->144 -0.10346
137 ->142 0.46020
137 ->143 0.19560
137 ->144 0.21097
137 ->145 -0.21218
137 ->146 -0.16689
137 ->151 0.17857

Excited State 13: Singlet-A 3.5513 eV 349.12 nm f=0.0034
135 ->141 0.68625

Excited State 14: Singlet-A 3.5788 eV 346.44 nm f=0.0102
135 ->142 -0.17450
135 ->151 -0.10366
136 ->142 0.31516
136 ->145 -0.10963
136 ->150 -0.14006
136 ->151 0.13291
137 ->142 0.29736
137 ->143 -0.25123
137 ->144 -0.30977
137 ->150 -0.11768

Excited State 15: Singlet-A 3.6060 eV 343.83 nm f=0.0061

135 ->142 -0.12817
135 ->151 -0.10470
136 ->142 0.37651
136 ->145 -0.10868
136 ->151 0.16380
137 ->142 -0.22152
137 ->143 0.38310
137 ->144 0.10345

Excited State 16: Singlet-A 3.6363 eV 340.96 nm f=0.0089
135 ->142 0.17873
135 ->144 0.12502
135 ->151 0.11269
136 ->143 0.17652
136 ->145 0.14785
137 ->142 0.24228
137 ->143 0.36138
137 ->144 -0.32098
137 ->145 0.15395
137 ->146 0.15192

Excited State 17: Singlet-A 3.6750 eV 337.37 nm f=0.0091
134 ->138 0.10180
135 ->142 0.14273
135 ->143 0.16774
135 ->144 0.13104
136 ->142 0.27594
136 ->145 0.12717
137 ->142 0.16479
137 ->143 -0.18511
137 ->144 0.39341

137 ->145 0.19076
137 ->146 0.14963

Excited State 18: Singlet-A 3.6875 eV 336.23 nm f=0.0286
132 ->138 0.10390
136 ->143 0.41030
136 ->144 0.28468
136 ->145 0.12012
136 ->146 -0.12595
136 ->150 0.11382
137 ->143 -0.19755
137 ->145 -0.29060
137 ->146 -0.12296
137 ->150 0.10831

Excited State 19: Singlet-A 3.7183 eV 333.45 nm f=0.0166
136 ->143 -0.38030
136 ->144 0.39254
136 ->145 -0.12445
137 ->145 -0.24440
137 ->146 0.25860

Excited State 20: Singlet-A 3.7236 eV 332.97 nm f=0.0061
135 ->142 0.36403
135 ->143 -0.12617
135 ->145 -0.21985
135 ->151 0.11376
136 ->142 0.26634
136 ->143 -0.16200
136 ->144 -0.15549
136 ->146 -0.10740

137 ->145 -0.15045
137 ->146 -0.29641

Excited State 21: Singlet-A 3.7459 eV 330.98 nm f=0.0304
135 ->143 -0.25468
135 ->145 -0.11223
135 ->150 -0.14759
136 ->143 0.22711
136 ->144 -0.15209
136 ->145 -0.13653
136 ->150 -0.12158
137 ->144 0.15055
137 ->145 -0.21852
137 ->146 0.33311
137 ->150 -0.22205

Excited State 22: Singlet-A 3.7724 eV 328.66 nm f=0.0015
135 ->142 -0.12527
135 ->143 -0.14234
135 ->144 -0.22216
135 ->146 0.15196
135 ->150 -0.12091
136 ->143 -0.11306
136 ->144 0.13318
136 ->145 0.51233
136 ->150 -0.12985

Excited State 23: Singlet-A 3.7878 eV 327.32 nm f=0.0033
136 ->144 0.30270
136 ->146 0.45877
136 ->150 -0.19023

137 ->146 -0.20293
137 ->150 -0.18071

Excited State 24: Singlet-A 3.8264 eV 324.03 nm f=0.0023
135 ->142 0.22295
135 ->143 0.33466
135 ->144 -0.30372
135 ->146 0.17794
136 ->142 -0.13575
136 ->146 -0.30993
136 ->150 -0.16175

Excited State 25: Singlet-A 3.8468 eV 322.30 nm f=0.0192
133 ->139 0.12891
135 ->142 0.12673
135 ->144 0.34081
135 ->145 0.39923
135 ->146 -0.12802
136 ->145 0.18048
136 ->146 -0.15601
136 ->150 -0.16263
137 ->150 -0.13869

Excited State 26: Singlet-A 3.8709 eV 320.30 nm f=0.0239
135 ->142 -0.23618
135 ->143 0.17888
135 ->144 0.35657
135 ->145 -0.34080
135 ->146 0.15141
136 ->146 -0.16637
136 ->150 -0.12252

137 ->146 -0.11357
137 ->150 -0.13650

Excited State 27: Singlet-A 3.8792 eV 319.61 nm f=0.0015
133 ->139 -0.15759
135 ->142 0.21321
135 ->143 -0.28400
135 ->144 0.16524
135 ->146 0.48916
137 ->145 0.12200
137 ->150 0.13451

Excited State 28: Singlet-A 4.0099 eV 309.19 nm f=0.0344
134 ->138 0.44879
134 ->140 0.10378
135 ->143 -0.14977
135 ->144 -0.12910
135 ->150 0.23309
136 ->142 -0.15498
136 ->151 0.24151
137 ->151 -0.14732

Excited State 29: Singlet-A 4.0662 eV 304.91 nm f=0.0146
133 ->138 -0.15206
134 ->138 0.37093
134 ->140 0.24080
135 ->143 0.10232
135 ->150 -0.20458
136 ->151 -0.17368
137 ->146 0.12442
137 ->150 0.11288

137 ->151 0.20598

Excited State 30: Singlet-A 4.0814 eV 303.78 nm f=0.0064
133 ->138 0.45647
135 ->142 0.10248
135 ->145 -0.17775
135 ->146 -0.17721
135 ->151 -0.22886
136 ->150 -0.19080
137 ->150 0.15389
137 ->151 0.15633

Excited State 31: Singlet-A 4.0856 eV 303.46 nm f=0.0082
133 ->138 0.50588
134 ->138 0.12700
134 ->140 0.11737
135 ->145 0.16319
135 ->146 0.17381
135 ->151 0.18646
136 ->150 0.16203
136 ->151 -0.13749
137 ->150 -0.10814

Excited State 32: Singlet-A 4.1054 eV 302.00 nm f=0.0014
134 ->138 0.11043
134 ->139 0.68506

Excited State 33: Singlet-A 4.2261 eV 293.38 nm f=0.0094
132 ->138 -0.11257
132 ->139 0.12351
133 ->139 0.14643

133 ->140 0.17852
134 ->140 -0.12893
135 ->143 -0.21568
135 ->146 -0.15982
135 ->150 -0.19463
136 ->144 0.15161
136 ->145 -0.16725
136 ->146 -0.16240
137 ->145 0.25506

Excited State 34: Singlet-A 4.2583 eV 291.16 nm f=0.0732
132 ->138 0.41158
132 ->140 -0.17529
134 ->138 -0.12052
134 ->140 0.41151
136 ->146 -0.10417

Excited State 35: Singlet-A 4.2873 eV 289.19 nm f=0.0473
132 ->138 -0.25739
132 ->139 -0.26656
132 ->140 0.13795
133 ->139 -0.30051
133 ->140 0.40564
134 ->140 0.17093

Excited State 36: Singlet-A 4.3050 eV 288.00 nm f=0.0311
132 ->138 -0.12468
132 ->139 0.60683
132 ->140 0.12106
133 ->140 0.10758
134 ->140 0.20752

Excited State 37: Singlet-A 4.3239 eV 286.74 nm f=0.0357
132 ->138 0.24247
132 ->140 -0.20111
133 ->139 0.14067
133 ->140 0.53250
134 ->140 -0.13601

Excited State 38: Singlet-A 4.4165 eV 280.73 nm f=0.3605
132 ->139 -0.17395
132 ->140 0.32259
133 ->139 0.40460
134 ->140 0.16168
135 ->145 -0.12228

Excited State 39: Singlet-A 4.4432 eV 279.04 nm f=0.0117
135 ->150 0.12037
135 ->151 -0.15526
136 ->150 0.25167
136 ->151 0.11937
137 ->147 -0.14744
137 ->150 -0.30899
137 ->151 0.37710

Excited State 40: Singlet-A 4.5285 eV 273.79 nm f=0.4936
132 ->138 0.25555
132 ->140 0.46185
132 ->141 -0.11322
133 ->139 -0.15422
134 ->140 -0.16411

Excited State 41: Singlet-A 4.5423 eV 272.95 nm f=0.0144
135 ->147 -0.15208
135 ->150 -0.33686
136 ->146 0.10643
136 ->148 0.14482
136 ->149 0.12465
136 ->150 0.12524
136 ->151 0.38152
136 ->152 -0.10698
137 ->151 -0.12116

Excited State 42: Singlet-A 4.6633 eV 265.87 nm f=0.0282
135 ->148 0.10361
135 ->151 0.43313
135 ->152 -0.10630
136 ->150 -0.14807
136 ->151 0.21452
137 ->148 0.12940
137 ->151 0.28385

Excited State 43: Singlet-A 4.8462 eV 255.84 nm f=0.0067
134 ->141 0.65238
134 ->144 0.10519

Excited State 44: Singlet-A 4.9033 eV 252.86 nm f=0.0150
133 ->141 0.59473
137 ->147 -0.21936

Excited State 45: Singlet-A 4.9420 eV 250.88 nm f=0.0085
131 ->138 0.15684
132 ->141 -0.18915

133 ->141 0.22150
134 ->142 -0.14850
137 ->147 0.49389
137 ->150 -0.15638

Excited State 46: Singlet-A 4.9874 eV 248.59 nm f=0.0264
131 ->138 -0.22644
134 ->142 0.42040
134 ->145 -0.12218
134 ->146 -0.15243
136 ->147 0.19941
136 ->149 0.11020
136 ->150 -0.10202
137 ->147 0.21212
137 ->148 -0.12159

Excited State 47: Singlet-A 5.0028 eV 247.83 nm f=0.0023
132 ->141 -0.31913
133 ->145 0.11069
134 ->142 0.14271
136 ->147 -0.20883
137 ->148 0.41462
137 ->149 -0.19707

Excited State 48: Singlet-A 5.0315 eV 246.41 nm f=0.0126
132 ->141 0.22835
134 ->141 -0.10342
134 ->143 -0.28649
136 ->147 0.31863
137 ->148 0.33379
137 ->149 0.17405

137 ->150 -0.14380
137 ->151 -0.10589

Excited State 49: Singlet-A 5.0445 eV 245.78 nm f=0.0077
130 ->138 -0.11208
134 ->143 0.17618
134 ->144 -0.16842
136 ->147 0.41988
136 ->148 -0.11989
136 ->149 -0.11566
137 ->149 -0.33715

Excited State 50: Singlet-A 5.0711 eV 244.49 nm f=0.0159
129 ->138 -0.13560
131 ->138 -0.26816
132 ->141 0.34837
133 ->142 -0.11241
134 ->142 -0.10941
134 ->143 0.15626
136 ->147 -0.17977
136 ->148 0.16616
136 ->149 -0.10751
137 ->147 0.19300
137 ->148 0.12887
137 ->149 -0.19281

S1.c. TDDFT

Shown in Figure S1c are the simulated and experimental absorption spectra for the $[Ru(bpy)(O\text{-}bpy)]^{2+}$ complex. The simulated spectrum for $[(Ru(bpy)_2)_2(O\text{-}bpy)]^{4+}$ was not calculated due to computational expense. The simulated spectrum was calculated in the gas phase and closely agrees with the experimental spectra. The low energy band maximum is the same for both the experimental and calculated spectra, 454 nm. The π to π^* transition for the experimental spectrum is found at 290 nm, where it is blue shifted for the calculated spectrum by 12 nm. The shoulder located at 360 nm in the calculated spectrum is not resolved in the experimental one.

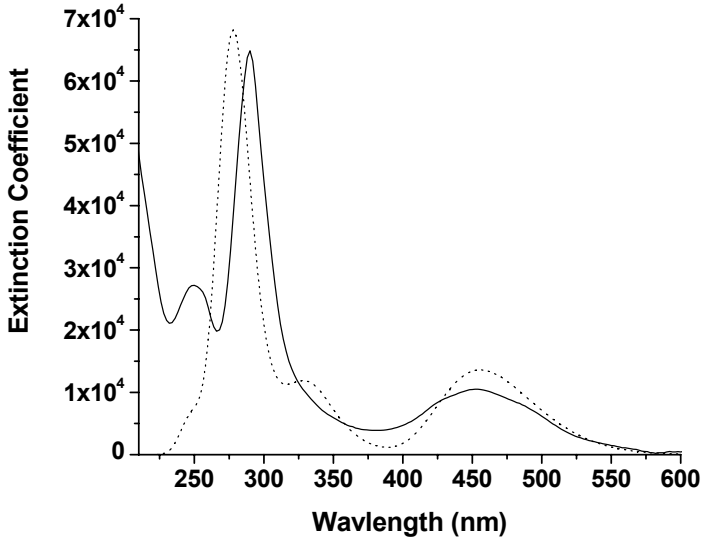


Figure S1c. Simulated (----, gas phase) and experimental (—, acetonitrile) $[Ru(bpy)(O\text{-}bpy)]^{2+}$

S1.d. TDDFT Triplet Results

Excited State 1: ?Spin -A 0.1327 eV 9343.73 nm f=0.0005
138A ->139A 0.26048
124B ->137B -0.12604
126B ->137B 0.10917
131B ->137B -0.11442
132B ->137B -0.14136
133B ->137B 0.17262
134B ->137B 0.20078
135B ->137B -0.44609
136B ->137B 1.05012
136B ->140B -0.12428

This state for optimization and/or second-order correction.
Total Energy, E(RPA) = -1657.87361623
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: ?Spin -A 0.1675 eV 7400.79 nm f=0.0051
138A ->139A 0.54919
136B ->137B -0.42165

Excited State 3: ?Spin -A 0.2294 eV 5405.33 nm f=0.0073
138A ->140A 0.57428
132B ->137B 0.10888
135B ->137B 0.50650
136B ->137B 0.13122

Excited State 4: ?Spin -A 0.2678 eV 4629.10 nm f=0.0036
138A ->140A -0.28583
123B ->137B 0.12000

132B ->137B 0.19626
134B ->137B 0.20372
135B ->137B 0.80255
135B ->140B -0.10006
136B ->137B 0.30066

Excited State 5: ?Spin -A 0.9335 eV 1328.11 nm f=0.0027
138A ->141A 1.00104

S2.a. Cartesian Coordinates from Calculation

Atom	Coordinates		
	X	Y	Z
Ru	0.000000	0.000000	0.000000
N	0.000000	0.000000	2.089145
C	1.245325	0.000000	2.687705
C	-1.109592	0.030470	2.882421
C	1.377519	0.038061	4.088698
C	-1.035683	0.072387	4.280656
H	-2.065956	0.035053	2.375814
C	0.230255	0.079228	4.897695
H	2.358947	0.042539	4.548968
H	-1.948054	0.108438	4.866300
H	0.320240	0.121995	5.978463
N	2.048980	-0.212937	0.422894
C	2.385375	-0.027925	1.750203
C	3.044944	-0.224919	-0.509994
C	3.725665	0.166220	2.139605
C	4.393001	-0.035778	-0.179258
H	2.736704	-0.366235	-1.538580
C	4.741027	0.173588	1.170388

H	3.972665	0.346580	3.179443
H	5.142178	-0.025246	-0.963917
H	5.771344	0.362199	1.455877
N	-0.837537	-2.029462	-0.050679
C	-0.230562	-3.269568	0.078052
C	-2.203376	-2.000103	-0.308162
C	-0.972020	-4.454751	-0.086528
C	-2.962931	-3.172798	-0.475626
C	-2.342228	-4.416811	-0.371946
H	-0.481690	-5.411019	0.010279
H	-4.022383	-3.117854	-0.685286
H	-2.911833	-5.330755	-0.504808
N	0.200311	0.164260	-2.084433
C	-0.007506	-0.835065	-2.988434
C	0.522054	1.423536	-2.550581
C	0.094130	-0.636348	-4.371185
H	-0.265801	-1.804190	-2.581219
C	0.637845	1.679823	-3.929767
C	0.421876	0.645205	-4.853445
H	-0.087877	-1.462150	-5.050463
H	0.884185	2.672581	-4.287038
H	0.501914	0.835496	-5.918912
N	-2.028086	0.408537	-0.228206
C	-2.855436	-0.675943	-0.391827
C	-2.570059	1.661181	-0.255012
C	-4.240363	-0.503050	-0.595208
C	-3.937250	1.889936	-0.447691
H	-1.890881	2.489147	-0.114659
C	-4.791379	0.786567	-0.627359
H	-4.895899	-1.354244	-0.725093
H	-4.316503	2.906064	-0.458150
H	-5.856162	0.925812	-0.784026

N	0.515522	2.017185	-0.211628
C	0.662547	2.909254	0.810294
C	0.719249	2.448732	-1.506761
C	1.011290	4.249052	0.597528
H	0.480264	2.537031	1.809885
C	1.074170	3.783925	-1.777179
C	1.223734	4.696447	-0.720588
H	1.108966	4.921077	1.443349
H	1.230396	4.115963	-2.796562
H	1.493640	5.728565	-0.920199
C	1.260798	-3.349614	0.399357
H	1.804884	-2.843331	-0.407920
H	1.444348	-2.761785	1.306611
C	1.820813	-4.792067	0.590461
H	1.236841	-5.320547	1.354052
H	1.694250	-5.361730	-0.338771
C	3.292181	-4.865109	0.996930
C	4.073598	-3.693530	1.003505
N	3.840017	-6.084265	1.362965
C	5.418991	-3.725269	1.389507
H	3.635895	-2.755786	0.696748
Ru	3.030105	-8.128655	1.252404
C	5.161504	-6.098750	1.791848
C	5.961919	-4.941686	1.801818
H	6.026111	-2.826216	1.374599
N	3.654528	-8.213526	-0.747641
N	1.199668	-7.963225	0.227287
N	4.904245	-8.484500	2.084086
N	2.230738	-8.197992	3.185085
N	2.474082	-10.136749	1.396448
C	5.719048	-7.390248	2.247391
H	6.996307	-4.990545	2.113926

C	2.646006	-8.191834	-1.691163
C	4.948061	-8.289991	-1.174369
C	1.277491	-8.146484	-1.139704
C	-0.029232	-7.977573	0.820244
C	5.359746	-9.709512	2.479185
C	1.754596	-9.430335	3.587632
C	2.198018	-7.160745	4.069212
C	1.865497	-10.504352	2.580348
C	2.650028	-11.077724	0.425036
C	7.000400	-7.522695	2.821356
C	2.936451	-8.239821	-3.067599
C	5.293791	-8.346403	-2.530845
H	5.710711	-8.320795	-0.407288
C	0.116234	-8.338851	-1.914505
C	-1.213997	-8.180615	0.101200
H	-0.044913	-7.842612	1.894665
C	6.625460	-9.899371	3.045491
H	4.695768	-10.548050	2.329604
C	1.229925	-9.618688	4.880310
C	1.689726	-7.292615	5.367500
H	2.601373	-6.219824	3.716116
C	1.421877	-11.824194	2.785582
C	2.233112	-12.406342	0.579530
H	3.146236	-10.752347	-0.479914
C	7.463699	-8.783819	3.224799
H	7.637816	-6.660136	2.966713
C	4.270799	-8.319275	-3.497889
H	2.137397	-8.220748	-3.799690
H	6.337672	-8.417544	-2.817075
C	-1.142362	-8.365709	-1.293959
H	0.192126	-8.506116	-2.982558
H	-2.161711	-8.219834	0.628232

H	6.939385	-10.895212	3.339174
C	1.193518	-8.543831	5.782354
H	1.693440	-6.440360	6.038469
C	1.602910	-12.787527	1.779603
H	0.944462	-12.106071	3.716585
H	2.401857	-13.119999	-0.219679
H	8.448608	-8.892342	3.667357
H	4.506142	-8.366227	-4.556331
H	-2.038100	-8.550320	-1.878742
H	0.798488	-8.681663	6.783780
H	1.267061	-13.808525	1.930302
H	0.864562	-10.590496	5.190403

S2.b. TDDFT Triplet Results

Excited state symmetry could not be determined.
Excited State 1: ?Spin -?Sym 0.1014 eV 12225.55 nm f=0.0033
268A ->269A -0.72652
268A ->270A -0.12753

This state for optimization and/or second-order correction.
Total Energy, E(RPA) = -3238.24009815
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited state symmetry could not be determined.
Excited State 2: ?Spin -?Sym 0.1225 eV 10124.90 nm f=0.0034
268A ->269A 0.20897
268A ->270A -0.47798

Excited state symmetry could not be determined.
Excited State 3: ?Spin -?Sym 0.2835 eV 4373.23 nm f=0.0000

238B ->267B 0.19968
256B ->267B 0.10802
259B ->267B -0.18012
260B ->267B 0.39735
262B ->267B 0.74383
263B ->267B 0.63812

Excited state symmetry could not be determined.
Excited State 4: ?Spin -?Sym 0.3336 eV 3716.06 nm f=0.0003
234B ->267B 0.12559
237B ->267B -0.14027
258B ->267B -0.59718
259B ->267B -0.54307
261B ->267B -0.32758
262B ->267B 0.37613
263B ->267B -0.46467

Excited state symmetry could not be determined.
Excited State 5: ?Spin -?Sym 0.5149 eV 2407.76 nm f=0.0018
268A ->271A 0.99143

S3.a. Cartesian Coordinates from calculations

Atom	Coordinates		
	X	Y	Z
Ru	-0.005579	0.060399	-0.059220
N	-0.048855	-0.003083	2.030848
C	1.173270	-0.179353	2.648027
C	-1.169278	0.087796	2.802966
C	1.271028	-0.263199	4.049799
C	-1.129138	0.013140	4.200695

H	-2.105609	0.226208	2.277884
C	0.113704	-0.166731	4.837871
H	2.234047	-0.405038	4.525810
H	-2.048869	0.092242	4.770143
H	0.179040	-0.230734	5.919254
N	2.020744	-0.193225	0.390672
C	2.329307	-0.266898	1.734324
C	3.032141	-0.265445	-0.521520
C	3.661333	-0.416420	2.164598
C	4.373457	-0.415844	-0.148898
H	2.746518	-0.203822	-1.563841
C	4.696279	-0.492013	1.219664
H	3.894169	-0.470779	3.221424
H	5.141066	-0.469289	-0.913323
H	5.726361	-0.606245	1.541566
N	-0.494445	-1.972821	-0.091888
C	0.387287	-3.002304	0.058973
C	-1.834300	-2.262128	-0.256757
C	-0.012508	-4.344213	0.048975
H	1.427530	-2.731232	0.186006
C	-2.291209	-3.593586	-0.273521
C	-1.377307	-4.647571	-0.119613
H	0.728188	-5.126904	0.172298
H	-3.344941	-3.810925	-0.401730
H	-1.719996	-5.677246	-0.129842
N	0.240019	0.275721	-2.124357
C	0.161028	-0.731063	-3.041056
C	0.478850	1.561653	-2.566415
C	0.317326	-0.512876	-4.415281
H	-0.026848	-1.723531	-2.651988
C	0.643173	1.837549	-3.937121
C	0.562648	0.795698	-4.874043

H	0.246142	-1.347962	-5.103740
H	0.828861	2.850112	-4.275192
H	0.686550	0.998768	-5.932887
N	-2.076920	0.135301	-0.336368
C	-2.714184	-1.087021	-0.410573
C	-2.817391	1.272861	-0.467753
C	-4.104487	-1.167089	-0.616151
C	-4.202585	1.251069	-0.671485
H	-2.276682	2.208095	-0.402373
C	-4.860129	0.008233	-0.748421
H	-4.596515	-2.130643	-0.676145
H	-4.746645	2.184321	-0.768675
H	-5.932333	-0.043619	-0.907912
N	0.328758	2.118753	-0.224999
C	0.373194	3.001626	0.813671
C	0.545448	2.586282	-1.505931
C	0.625703	4.366910	0.632006
H	0.198008	2.594217	1.801076
C	0.805425	3.948937	-1.745360
C	0.846911	4.851530	-0.671468
H	0.649366	5.028272	1.491348
H	0.976953	4.306491	-2.753725
H	1.047401	5.903695	-0.846130

S3.b. TDDFT Triplet Results

Excited state symmetry could not be determined.
Excited State 1: ?Spin -?Sym 0.0889 eV 13946.41 nm f=0.0018
131A ->132A 0.42552

This state for optimization and/or second-order correction.

Total Energy, E(RPA) = -1580.48243672
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited state symmetry could not be determined.
Excited State 2: ?Spin -?Sym 0.0935 eV 13260.08 nm f=0.0020
131A ->133A 0.43745

Excited state symmetry could not be determined.
Excited State 3: ?Spin -?Sym 0.2604 eV 4760.62 nm f=0.0001
116B ->130B -0.18723
117B ->130B 0.12604
126B ->130B 0.11543
127B ->130B 0.35893
128B ->130B 0.76862
129B ->130B -0.67532

Excited state symmetry could not be determined.
Excited State 4: ?Spin -?Sym 0.2606 eV 4757.14 nm f=0.0001
116B ->130B 0.12589
117B ->130B 0.18739
126B ->130B 0.35677
127B ->130B -0.11642
128B ->130B 0.67614
129B ->130B 0.76831

Excited state symmetry could not be determined.
Excited State 5: ?Spin -?Sym 0.8508 eV 1457.26 nm f=0.0000
131A ->134A 1.01491

S4. Graphical Representation of Orbital Distribution

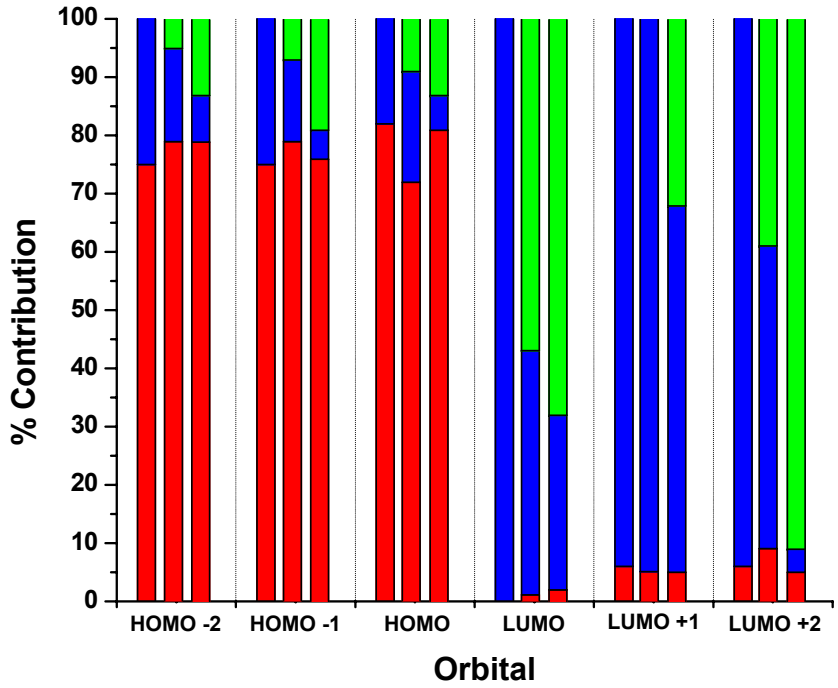
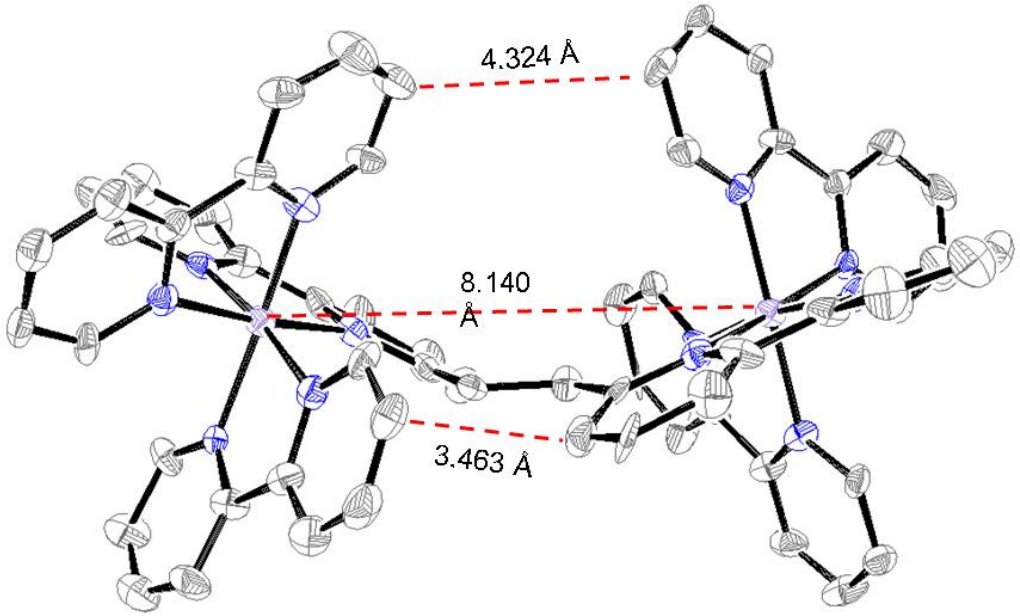


Figure S4. Graphical representation of the orbital contributions: Red – Ruthenium orbitals, Blue – bpy, Green – O-bpy. The order of the columns in each set of three is $[Ru(bpy)_3]^{2+}$, $[Ru(bpy)(O\text{-}bpy)]^{2+}$, $[(Ru(bpy)_2)_2(O\text{-}bpy)]^{4+}$

S5. Inter atom bond distances of O-bpy dimer



S6. TDDFT Triplet State Results

Compound	State	f	Transition	Type			Energy	
				Singlet Triplet Energy Gap			**17.2**	**^{3}MLLCT**
	1	0.001	H-2 → H-1 (0.7)	Ru(0.6)	→	Ru(0.7)	18.2	^{3}d-d
				Bpy(0.4),O-				
O-Bpy	2	0.005	H → L (0.6)	Bpy(0.6)	→	O-Bpy(0.9)	18.5	^{3}ILCT
			H-2 → H-1 (0.4)	Ru(0.6)	→	Ru(0.7)		^{3}d-d
				Bpy(0.4),O-		Bpy(0.6),O-		
	3	0.007	H → L+1 (0.5)	Bpy(0.6)	→	Bpy(0.4)	19.0	^{3}ILCT
			H-3 → H-1 (0.4)	Ru(0.6)	→	Ru(0.7)		^{3}d-d
	4	0.004	H-3 → H-1 (0.7)	Ru(0.6)	→	Ru(0.7)	19.3	^{3}d-d
				Singlet Triplet Energy Gap			**17.6**	**^{3}MLLCT**
				Bpy(0.6),O-		Bpy(0.9),O-		
	1	0.003	H → L (1.0)	Bpy(0.4)	→	Bpy(0.1)	18.4	^{3}ILCT
			H→L+1	Bpy(0.6),O-		Bpy(0.5),O-		
O-Bpy	2	0.003	(0.8)	Bpy(0.4)	→	Bpy(0.5)	18.6	^{3}ILCT
Dimer	3	0.000	H-6→H-1 (0.5)	Ru(0.4), L(0.6)	→	Ru(0.8)	19.9	^{3}MLMCT
			H-5→H-1 (0.3)	Ru(0.3), L(0.7)	→	Ru(0.8)		^{3}MLMCT
	4	0.000	H-9→H-1 (0.4)	Ru(0.3), L(0.7)	→	Ru(0.8)	20.3	^{3}MLMCT
			H-8→H-1 (0.3)	Ru(0.2), L(0.8)	→	Ru(0.8)		^{3}MLMCT
				Singlet Triplet Energy Gap			**17.7**	**^{3}MLLCT**
	1	0.002	H → L (1.0)	Bpy(1.0)	→	Bpy(1.0)	18.4	^{3}ILCT
			H→L+1					
Bpy	2	0.002	(1.0)	Bpy(1.0)	→	Bpy(1.0)	18.4	^{3}ILCT
	3	0.000	H-3→H-1 (0.5)	Ru(0.6), Bpy(0.4)	→	Ru(0.8)	19.8	^{3}MLMCT
			H-2→H-1 (0.4)	Ru(0.6), Bpy(0.4)	→	Ru(0.8)		^{3}MLMCT
	4	0.000	H-3→H-1 (0.4)	Ru(0.6), Bpy(0.4)	→	Ru(0.8)	19.8	^{3}MLMCT
			H-2→H-1 (0.5)	Ru(0.6), Bpy(0.4)	→	Ru(0.8)		^{3}MLMCT