Electronic Structure of the Water Oxidation Catalyst, *cis,cis*-$[(bpy)_2(H_2O)Ru^{III}ORu^{III}(OH_2)(bpy)_2]^{4+}$, The Blue Dimer

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- Supporting Information -

Table of Contents

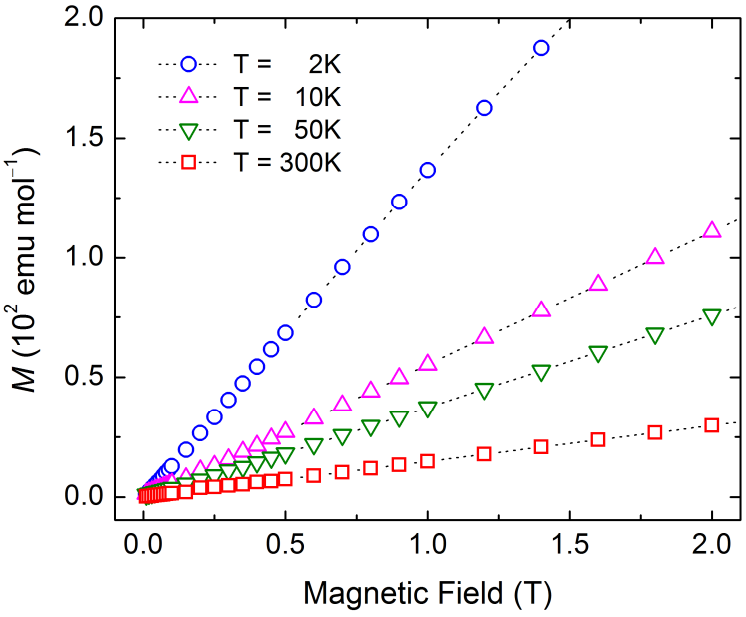

Figure S1. Field dependence of the magnetization for the blue dimer at various temperatures.

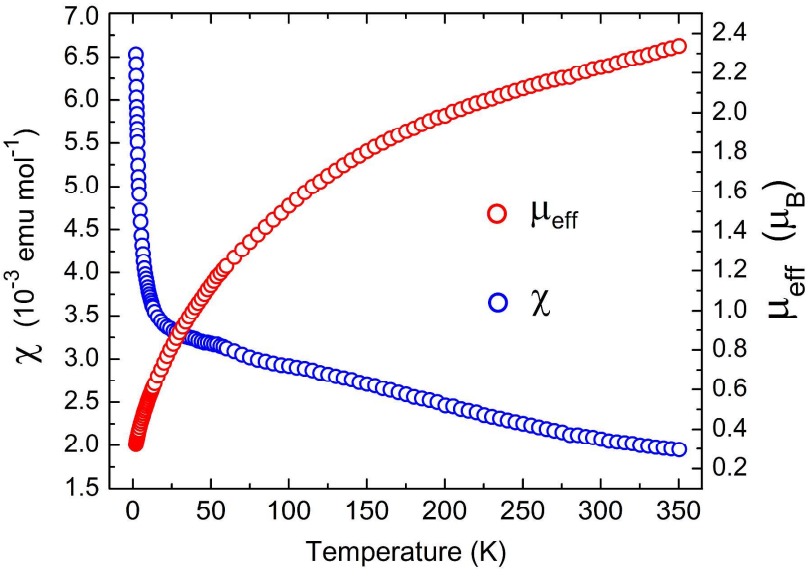

Figure S2. Temperature dependence of χ (magnetic susceptibility per formula unit) and of μ_{eff} (magnetic moment per formula unit) for the hexafluorophosphate salt of the blue dimer, $[(bpy)_2(H_2O)Ru(\mu\text{-}O)Ru(OH_2)(bpy)_2](PF_6)_4$, in a magnetic field of 1000 G (0.10 T).

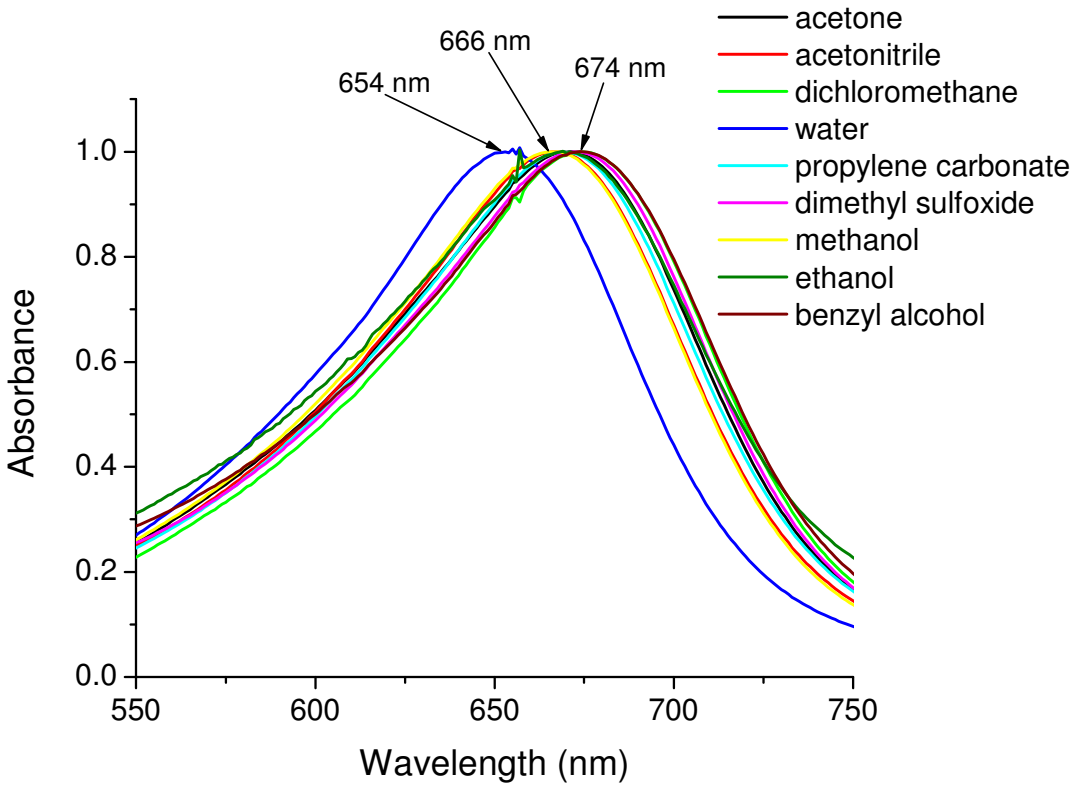

Figure S3. Solvent dependence on visible absorption band for *cis,cis*-$[(bpy)_2ClRuORuCl(bpy)_2](PF_6)_2$.

Computational Methods

Theoretical calculations were carried out by using Density Functional Theory (DFT) as implemented in Gaussian03, revision D.02.[1] Becke's three-parameter hybrid functional[2-5] with the LYP correlation functional[6] (B3LYP) was used with Los Alamos effective core potential LanL2DZ basis set. Frequency calculations were performed in the optimized geometries to ensure that the geometries correspond to a minimum in the potential energy surface. Franck-Condon vertical excitation energies and oscillator strengths were obtained with non-equilibrium Time-Dependent Density Functional Theory (TD-DFT)[7-9] as implemented in Gaussian03. Solvent-specific interactions and counterion effects were modeled by explicitly adding hydrogen-bonded water molecules and chloride anions, respectively. The bulk of the solvent was modeled by means of the Integral Equation Formalism Polarizable Continum Model (IEF-PCM)[12-15], as implemented in Gaussian03. Pauling's radii were used in all cases. The electronic spectra were modeled as the convolution of gaussian bands associated with each transition.[16] Estimation of redox potentials with DFT calculations is well documented in the literature.[17-19]

Geometries

Closed-shell singlets.

***cis,cis*-$[(bpy)_2(H_2O)Ru^{III}ORu^{III}(OH_2)bpy)_2]^{4+}$ (BD)**: The coordinates of the x-ray structure[20] of $[(bpy)_2(H_2O)Ru^{III}ORu^{III}(OH_2)bpy)_2]^{4+}$ were used as input geometry in Gaussian03. Although three isomers are possible for the blue dimer (enantiomeric pair and meso), all the known x-ray structures for the family $[(bpy)_2(L)RuORu(L)bpy)_2]^{n+}$ (L: H_2O, Cl, NO_2, NH_3)[20-23] contain only the enantiomeric pair and all studies reported here focus on a single enantiomer with the enantiomer chosen (Δ,Δ or Λ,Λ) irrelevant to the results. The ground state was assumed to be a closed-shell singlet and the structure was optimized at DFT level (B3LYP, LANL2DZ) with no symmetry restrictions. Tight convergence criteria were used for both the SCF and the optimization itself. The calculation converged to a final C_2 symmetry, which was used to calculate the gas phase absorption spectrum and to build the structures with hydrogen-bonded water molecules and counterions.

***cis,cis*-$[(bpy)_2(H_2O)Ru^{III}ORu^{III}(OH_2)(bpy)_2]^{4+}\times4H_2O$ ($BD\times4H_2O$)**: Two water molecules were hydrogen-bonded to each of the two aquo ligands of the optimized gas phase structure with a hydrogen-bond distance of 1.500 Å and the resulting "hydrate" was fully optimized under C_2 symmetry.

***cis,cis*-$[(bpy)_2(H_2O)Ru^{III}ORu^{III}(OH_2)(bpy)_2](Cl)_4\times4H_2O$ ($BDCl_4\times4H_2O$)**: Four chloride anions were added to $BD\times4H_2O$, each hydrogen-bonded to one of the hydrogen-bonded water molecules with a hydrogen-bond distance of 1.700 Å. The resulting structure was fully optimized under C_2 symmetry.

Broken symmetry singlet.

BS-BD: For the broken symmetry state, we used the geometry of the closed-shell singlet as the starting point. The methodology described in the Gaussian official website was employed (http://www.gaussian.com/g_news/sum05/newsletter_g03_tips.htm). Martin *et al.*[24] were unable to optimize the structure of the broken symmetry state using the LANL2 relativistic effective core potential with the corresponding uncontracted basis set for Ru. We were able to optimize the structure of the broken symmetry state using the LANL2DZ basis set. The resulting structure was used for the comparison shown in Table1.

$Ru^{IV}ORu^{III}$ structures containing coordinated aqua or chloride ligands were optimized as a ground state doublet with strong coupling. The Ru-μ-O bond distances were shorter in this oxidation state relative to their $Ru^{III}ORu^{III}$ analogues as expected.

Energies. As previously reported by Baik *et al.*[19] and Martin *et al.*[24], the results from DFT calculations place the triplet state as the lowest in energy for the blue dimer, followed by the broken symmetry state, and the closed-shell singlet is the highest in energy. In our work, we disregard the energy ordering obtained from the calculations and we focused our attention in the comparison of calculated *vs* experimental properties for the different electronic configurations.

Spectra. Figure S6 shows a comparison between the experimental absorption spectrum for the blue dimer in H_2O at pH 7 and the calculated spectrum for $BDCl_4{\times}4H_2O$. Figures S5 to S10 show calculated and experimental absorption spectra for complexes discussed in the manuscript. Tables S1 to S5 show selected excitation energies and oscillators strengths of transitions from time-dependent DFT calculations.

Geometries. Tables S6 through S15 contain the Cartesian coordinates for the different structures. Figures S1 and S2 show the optimized structures for $BD{\times}4H_2O$ and $BDCl_4{\times}4H_2O$, respectively. Some significant features are also shown in the figures.

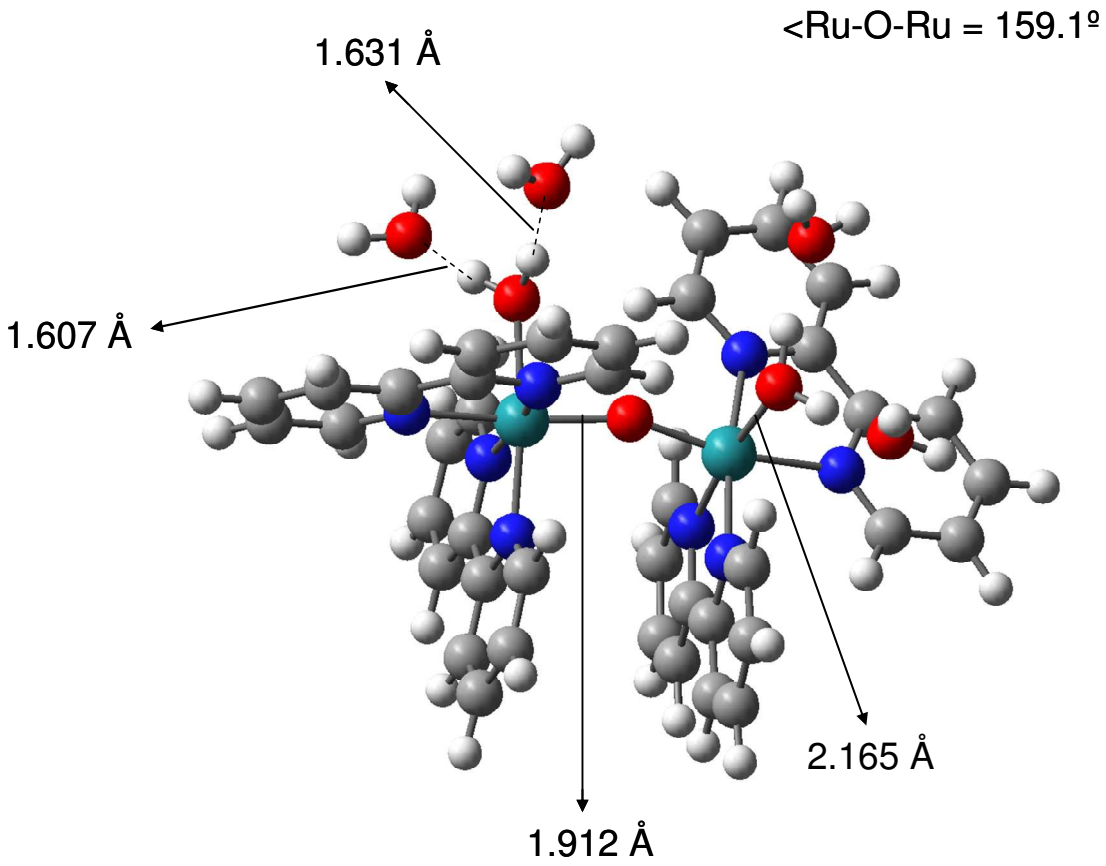

Figure S3. Optimized structure for BD×4H_2O.

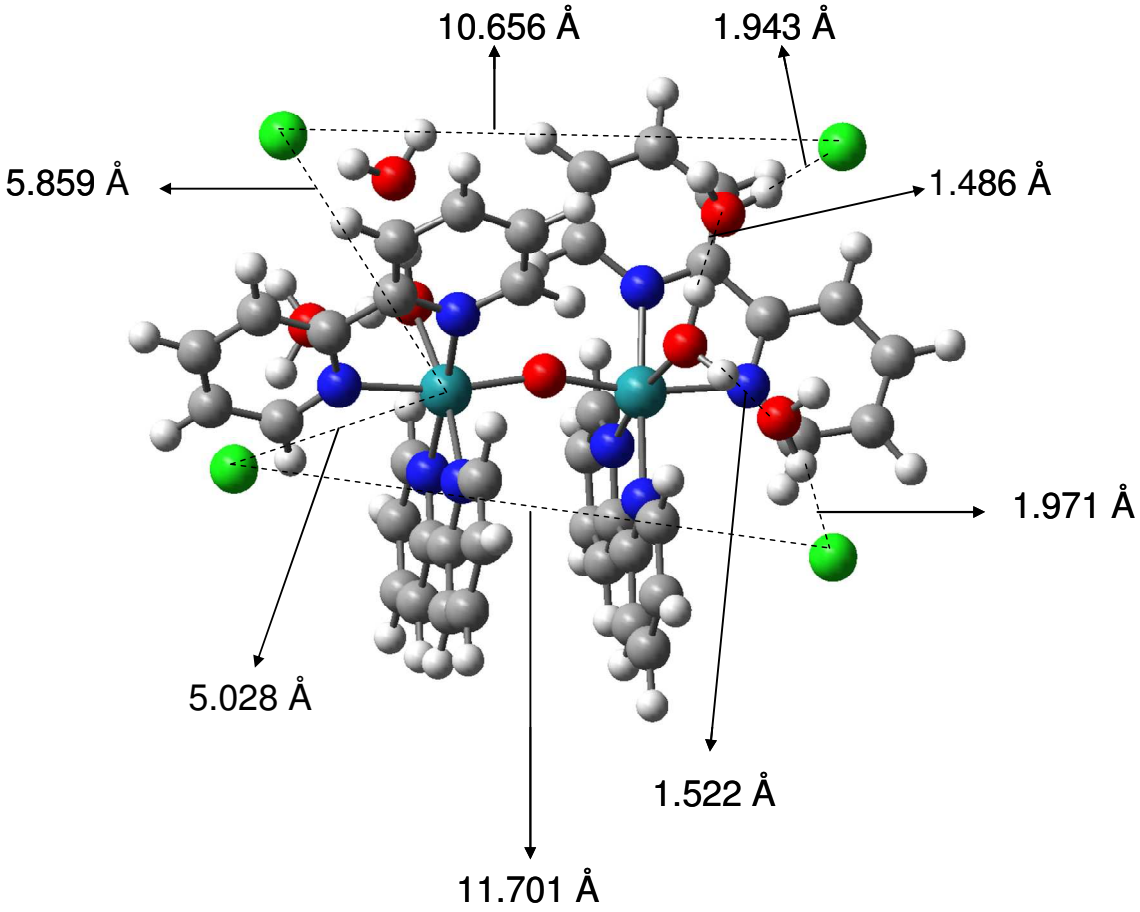

Figure S4. Optimized structure for $BDCl_4 \times 4H_2O$.

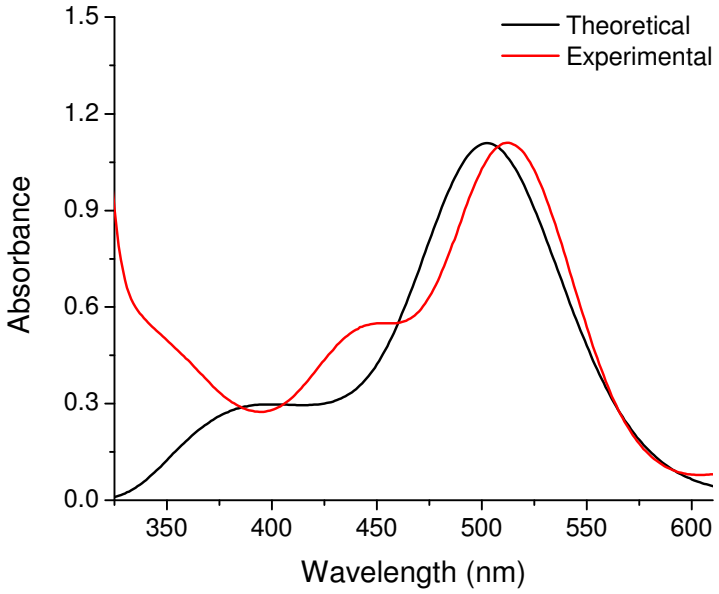

Figure S5. Comparison between calculated and experimental absorption spectra for $[(HO)Ru^{IV}ORu^{III}(OH_2)]^{4+}$ in acetonitrile and with IEF-PCM (acetonitrile).

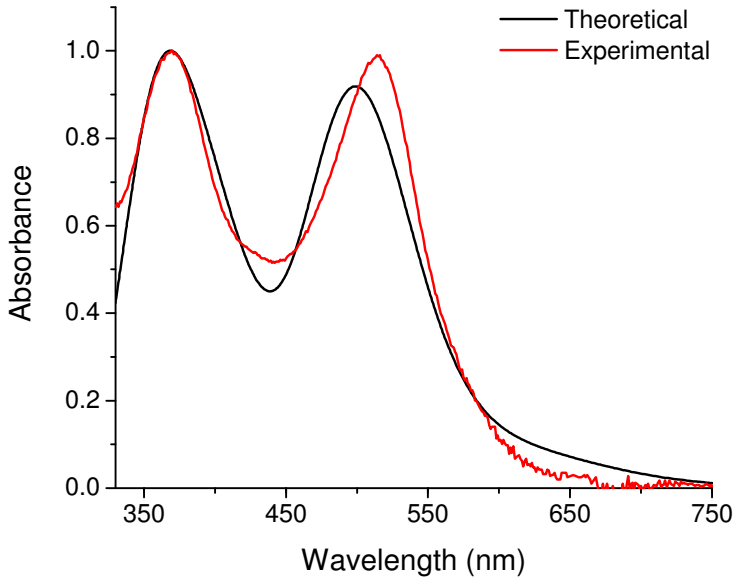

Figure S6. Comparison between calculated and experimental absorption spectra for $Ru(bpy)_2Cl_2$ in water (experimental) and with IEF-PCM (water).

Table S1. Excitation energies and oscillator strengths for $BDCl_4 \times 4H_2O$. The results on each state include: the spin and spatial symmetry, the excitation energy, the oscillator strength, and (on the second line for each state) the largest coefficients in the CI expansion.

Excited State 1:	Singlet-B	0.1282 eV	9669.87 nm	f=0.0001
228 ->229	0.37467			
Excited State 2:	Singlet-A	1.3372 eV	927.21 nm	f=0.0000
226 ->229	0.65143			
Excited State 3:	Singlet-A	1.5587 eV	795.42 nm	f=0.0004
225 ->229	0.65465			
Excited State 4:	Singlet-B	1.5762 eV	786.59 nm	f=0.0027
224 ->229	0.65517			
Excited State 5:	Singlet-B	2.0706 eV	598.78 nm	f=0.3430
226 ->230	0.13271			
227 ->229	0.44420			
228 ->231	-0.40105			
228 ->233	-0.14636			
Excited State 6:	Singlet-A	2.1990 eV	563.82 nm	f=0.0588
228 ->230	0.66736			
228 ->232	0.15805			
Excited State 7:	Singlet-B	2.2872 eV	542.09 nm	f=0.0737
227 ->229	0.18344			
228 ->231	0.50105			
228 ->233	-0.40359			
Excited State 8:	Singlet-A	2.2991 eV	539.28 nm	f=0.0017
228 ->230	-0.13769			
228 ->232	0.67004			
Excited State 9:	Singlet-B	2.3649 eV	524.28 nm	f=0.0344
222 ->229	-0.11381			
227 ->229	0.24695			
228 ->231	0.25581			
228 ->233	0.53515			
Excited State 10:	Singlet-A	2.4592 eV	504.16 nm	f=0.0090
223 ->229	0.69224			
Excited State 11:	Singlet-B	2.5115 eV	493.66 nm	f=0.0097

222 ->229 0.68352

Excited State 12: Singlet-A 2.5960 eV 477.59 nm f=0.0052
221 ->229 0.68644

Excited State 13: Singlet-B 2.6117 eV 474.73 nm f=0.0040
220 ->229 0.68736

Excited State 14: Singlet-B 2.7749 eV 446.81 nm f=0.0013
216 ->229 0.11346
219 ->229 0.68561

Excited State 15: Singlet-A 2.7786 eV 446.22 nm f=0.0000
217 ->229 0.11782
218 ->229 0.68469

Table S2. Excitation energies and oscillator strengths for BS-BD. The results on each state include: the spin and spatial symmetry, the excitation energy, the oscillator strength, and (on the second line for each state) the largest coefficients in the CI expansion.

Excited state symmetry could not be determined.
Excited State 1: ?Spin -?Sym 0.2110 eV 5876.37 nm f=0.0001
191A ->193A -0.12037
192A ->193A -1.10207
192A ->197A 0.15515
191B ->193B 0.12212
192B ->193B 1.10209
192B ->197B 0.15439

Excited state symmetry could not be determined.
Excited State 2: ?Spin -?Sym 0.6436 eV 1926.35 nm f=0.0000
188A ->193A 0.12656
191A ->193A -0.23390
192A ->193A 0.61860
188B ->193B -0.12578
191B ->193B -0.23307
192B ->193B 0.61843

Excited state symmetry could not be determined.
Excited State 3: ?Spin -?Sym 1.0200 eV 1215.51 nm f=0.0001
191A ->193A 0.86253
191A ->197A -0.10292
191B ->193B 0.86136
191B ->197B 0.10248

Excited state symmetry could not be determined.
Excited State 4: ?Spin -?Sym 1.3674 eV 906.70 nm f=0.0005
187A ->193A 0.17683
190A ->193A 0.54412
187B ->193B 0.24649
188B ->193B -0.13447
190B ->193B 0.74183

Excited state symmetry could not be determined.
Excited State 5: ?Spin -?Sym 1.3720 eV 903.67 nm f=0.0001
187A ->193A 0.25751
188A ->193A -0.10654
190A ->193A 0.74010
187B ->193B -0.19114
190B ->193B -0.53912

Excited state symmetry could not be determined.
Excited State 6: ?Spin -?Sym 1.9374 eV 639.96 nm f=0.0000
184A ->193A 0.29797
186A ->193A 0.29228
187A ->193A 0.27130
188A ->193A 0.44215
189A ->193A -0.15173
192A ->193A -0.13791
184B ->193B 0.29080
186B ->193B 0.27619
187B ->193B -0.29951
188B ->193B -0.43740
189B ->193B 0.14524
192B ->193B -0.13876

Excited state symmetry could not be determined.
Excited State 7: ?Spin -?Sym 2.0374 eV 608.54 nm f=0.1641
184A ->193A -0.20001
186A ->193A -0.21542
187A ->193A -0.17952
188A ->193A -0.32625
189A ->193A 0.11306
191A ->193A -0.40746
184B ->193B 0.19631
186B ->193B 0.20627
187B ->193B -0.20186
188B ->193B -0.32688
189B ->193B 0.10943
191B ->193B 0.40936

Excited state symmetry could not be determined.
Excited State 8: ?Spin -?Sym 2.1667 eV 572.22 nm f=0.0174
184A ->193A -0.12877
186A ->193A -0.42549
187A ->193A 0.17872
188A ->193A 0.26215
189A ->193A 0.63637
191A ->193A 0.13056
186B ->193B 0.24773
189B ->193B 0.34716
191B ->193B -0.12408

Excited state symmetry could not be determined.
Excited State 9: ?Spin -?Sym 2.1722 eV 570.78 nm f=0.0018
186A ->193A 0.19408
187A ->193A -0.15383
188A ->193A -0.22738
189A ->193A -0.33498
186B ->193B 0.40602
187B ->193B 0.21929
188B ->193B 0.30843
189B ->193B 0.63929

Excited state symmetry could not be determined.
Excited State 10: ?Spin -?Sym 2.2122 eV 560.47 nm f=0.2072
168A ->193A -0.12521
181A ->193A -0.12187
184A ->193A 0.15419
187A ->193A 0.25883
188A ->193A 0.35965
191A ->193A -0.36466
192A ->195A -0.10857
168B ->193B -0.12485
181B ->193B -0.12462
184B ->193B -0.15005
187B ->193B 0.27769
188B ->193B 0.35093
191B ->193B 0.36576
192B ->195B -0.10905

Excited state symmetry could not be determined.
Excited State 11: ?Spin -?Sym 2.4266 eV 510.93 nm f=0.0002
191A ->198A -0.12873
191A ->199A -0.11958
191A ->205A -0.12298

192A ->194A 0.27518
192A ->197A -0.10538
192A ->198A 0.38883
192A ->199A 0.35920
191B ->198B -0.11354
191B ->199B -0.11217
191B ->205B -0.12103
192B ->194B -0.27974
192B ->197B -0.10878
192B ->198B 0.38792
192B ->199B 0.37550

Excited state symmetry could not be determined.
Excited State 12: ?Spin -?Sym 2.5076 eV 494.44 nm f=0.0024
191A ->198A 0.19833
191A ->199A 0.19217
192A ->194A 0.24838
192A ->197A -0.14920
192A ->198A 0.32830
192A ->199A 0.30927
192A ->200A 0.15552
192A ->204A -0.13729
192A ->205A -0.15787
191B ->198B -0.19366
191B ->199B -0.19849
192B ->194B 0.23855
192B ->197B 0.14659
192B ->198B -0.31167
192B ->199B -0.30585
192B ->200B -0.14866
192B ->204B 0.13627
192B ->205B 0.15794

Excited state symmetry could not be determined.
Excited State 13: ?Spin -?Sym 2.5956 eV 477.68 nm f=0.0005
187A ->193A -0.41351
188A ->193A 0.30284
189A ->196A -0.14345
190A ->193A 0.19815
192A ->196A -0.11682
187B ->193B 0.52485
188B ->193B -0.41674
189B ->196B -0.11247
190B ->193B -0.26138
192B ->196B 0.11140

Excited state symmetry could not be determined.
Excited State 14: ?Spin -?Sym 2.6008 eV 476.72 nm f=0.0053

187A ->193A	0.56461
188A ->193A	-0.40964
189A ->196A	-0.10894
190A ->193A	-0.26947
187B ->193B	0.43806
188B ->193B	-0.34451
189B ->196B	0.14056
190B ->193B	-0.21737

Excited state symmetry could not be determined.
Excited State 15: ?Spin -?Sym 2.6300 eV 471.42 nm f=0.0084

187A ->193A	-0.18232
188A ->193A	0.13625
188A ->199A	0.10120
191A ->198A	0.17039
191A ->199A	0.17483
192A ->194A	-0.18090
192A ->196A	0.20750
192A ->198A	-0.20402
192A ->199A	-0.17942
192A ->200A	0.15136
192A ->204A	-0.17084
192A ->205A	-0.22965
192A ->208A	-0.11090
187B ->193B	0.15508
188B ->193B	-0.12941
188B ->199B	0.10222
191B ->198B	-0.16815
191B ->199B	-0.18138
192B ->194B	-0.18289
192B ->196B	-0.20766
192B ->198B	0.20076
192B ->199B	0.18995
192B ->200B	-0.15495
192B ->204B	0.17056
192B ->205B	0.23028
192B ->208B	0.10816

Table S3. Excitation energies and oscillator strengths for BD - triplet electronic state. The results on each state include: the spin and spatial symmetry, the excitation energy, the oscillator strength, and (on the second line for each state) the largest coefficients in the CI expansion.

Excited State 1: ?Spin -A 0.8214 eV 1509.41 nm f=0.0000
190B ->193B 0.27705
191B ->192B 1.02744
191B ->197B -0.14867
This state for optimization and/or second-order correction.
Total Energy, E(RPA) = -2396.04963507
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: ?Spin -A 0.8951 eV 1385.18 nm f=0.0002
190B ->192B 0.93453
190B ->194B -0.10686
190B ->197B -0.15950
191B ->193B -0.90688
191B ->196B -0.10793

Excited State 3: ?Spin -A 1.1141 eV 1112.84 nm f=0.0000
190B ->193B 1.01971
191B ->192B 0.22557

Excited State 4: ?Spin -A 1.6077 eV 771.18 nm f=0.0016
187B ->192B 0.18409
188B ->193B -0.39120
189B ->192B 0.82682
189B ->193B -0.26425
189B ->197B -0.11137

Excited State 5: ?Spin -A 1.6184 eV 766.09 nm f=0.0002
186B ->192B 0.17712
188B ->192B 0.81751
188B ->193B 0.26079
188B ->197B -0.11159
189B ->193B -0.41512

Excited State 6: ?Spin -A 1.8964 eV 653.77 nm f=0.0000
187B ->193B 0.18985
188B ->192B 0.37715
188B ->193B 0.16197
189B ->192B 0.31078
189B ->193B 0.81254

Excited State 7: ?Spin -A 1.9034 eV 651.38 nm f=0.0002

186B ->193B 0.18861
188B ->192B -0.31438
188B ->193B 0.82655
189B ->192B 0.34787
189B ->193B -0.15012

Excited State 8: ?Spin -A 2.1843 eV 567.61 nm f=0.4716
192A ->195A -0.14349
190B ->192B 0.55078
190B ->199B 0.12595
191B ->193B 0.59763

Excited State 9: ?Spin -A 2.5678 eV 482.84 nm f=0.0054
184A ->200A 0.11047
184A ->203A 0.14423
185A ->198A -0.10354
188A ->203A 0.11713
192A ->200A -0.12097
192A ->203A -0.13597
193A ->194A -0.32758
193A ->197A -0.23344
193A ->198A 0.76193
193A ->209A 0.12531
191B ->196B -0.10047
191B ->205B -0.16000
191B ->207B -0.14896

Excited State 10: ?Spin -A 2.6085 eV 475.31 nm f=0.0032
184A ->198A -0.16371
185A ->203A 0.11553
186A ->200A 0.10258
186A ->203A 0.12168
192A ->194A -0.26215
192A ->197A -0.20088
192A ->198A 0.68788
192A ->209A 0.11780
193A ->196A -0.15290
193A ->200A -0.20536
193A ->203A -0.24708
193A ->205A -0.11026
190B ->205B -0.10640
191B ->194B -0.12647
191B ->199B 0.19854

Excited State 11: ?Spin -A 2.6711 eV 464.18 nm f=0.0000
184A ->198A -0.18027

188A ->194A	0.12691
188A ->198A	-0.16692
192A ->194A	0.14453
192A ->198A	-0.36037
193A ->195A	-0.10556
193A ->196A	-0.15100
193A ->200A	-0.19398
193A ->203A	-0.23878
193A ->205A	-0.10100
185B ->192B	-0.16700
191B ->194B	-0.46401
191B ->199B	0.53189
191B ->203B	-0.10673
191B ->209B	0.12314

Excited State 12: ?Spin -A 2.6952 eV 460.02 nm f=0.0049

190A ->196A	0.12654
191A ->197A	-0.16737
186B ->192B	-0.17555
186B ->193B	-0.12843
187B ->192B	0.85390
187B ->193B	-0.19961
189B ->192B	-0.20099
189B ->197B	-0.10667

Excited State 13: ?Spin -A 2.6995 eV 459.29 nm f=0.0028

190A ->196A	-0.11283
190A ->197A	-0.15463
191A ->196A	0.13885
186B ->192B	0.84599
186B ->193B	0.20177
187B ->192B	0.17134
187B ->193B	-0.13882
188B ->192B	-0.19097
188B ->197B	-0.10242
189B ->196B	-0.10287

Excited State 14: ?Spin -A 2.7301 eV 454.15 nm f=0.0007

185A ->198A	-0.12888
186A ->198A	-0.15151
187A ->200A	-0.16426
187A ->203A	-0.20169
188A ->200A	-0.10559
188A ->203A	-0.12878
189A ->198A	-0.25008
189A ->208A	-0.12223

190A ->200A -0.16059
190A ->203A -0.20017
191A ->198A -0.27995
191A ->208A -0.12568
186B ->192B -0.11302
187B ->192B 0.12534
188B ->196B 0.14652
188B ->199B -0.16546
188B ->201B -0.10568
188B ->205B 0.26614
188B ->207B 0.26353
188B ->210B -0.10061
189B ->194B -0.11432
189B ->199B 0.40430
189B ->208B -0.16468
189B ->209B 0.15443
190B ->199B 0.12287

Excited State 15: ?Spin -A 2.7338 eV 453.53 nm f=0.0001
187A ->198A -0.27425
187A ->208A -0.12709
188A ->198A -0.16496
189A ->200A -0.18096
189A ->203A -0.21947
190A ->198A -0.27987
190A ->208A -0.12480
191A ->200A -0.17517
191A ->203A -0.21298
186B ->192B 0.14928
187B ->192B 0.10972
188B ->194B -0.11522
188B ->199B 0.41777
188B ->208B -0.16834
188B ->209B 0.15803
189B ->196B 0.14460
189B ->199B 0.13163
189B ->200B 0.10137
189B ->201B -0.12596
189B ->205B 0.27318
189B ->207B 0.26804
189B ->210B -0.10468

Excited State 16: ?Spin -A 2.7552 eV 450.00 nm f=0.0000
185A ->195A 0.14366
186A ->195A -0.15610
187A ->194A 0.10826

188A ->194A -0.20865
188A ->198A -0.12205
193A ->195A 0.29149
193A ->196A -0.14579
193A ->200A -0.15029
193A ->203A -0.15406
184B ->195B 0.20030
185B ->192B 0.59408
185B ->194B 0.17920
191B ->194B 0.33038
191B ->197B 0.24169
191B ->199B 0.27162

Excited State 17: ?Spin -A 2.7605 eV 449.14 nm f=0.0006
185A ->194A 0.11658
186A ->194A -0.19190
187A ->195A 0.11519
188A ->195A -0.22208
189A ->198A -0.12206
192A ->200A 0.15014
192A ->203A 0.12055
193A ->194A 0.27048
193A ->197A -0.10960
193A ->198A 0.12944
182B ->192B -0.12349
184B ->192B 0.55030
184B ->194B 0.18293
185B ->195B 0.19388
190B ->194B 0.21877
190B ->199B -0.28565
191B ->195B 0.36406

Excited State 18: ?Spin -A 2.7707 eV 447.49 nm f=0.0138
185A ->194A -0.11286
185A ->198A 0.14180
186A ->198A 0.20021
188A ->195A 0.13110
189A ->198A -0.20998
192A ->196A 0.21645
192A ->200A 0.23342
192A ->203A 0.30646
192A ->205A 0.12383
193A ->194A -0.25584
184B ->192B -0.20591
184B ->194B -0.10079
190B ->194B 0.32139

190B ->199B	-0.45135		
190B ->209B	-0.11374		
191B ->195B	-0.32490		
Excited State 19:	?Spin -A	2.8366 eV	437.09 nm f=0.0033
193A ->194A	-0.22218		
193A ->198A	-0.10337		
168B ->192B	-0.19750		
169B ->192B	-0.12022		
181B ->192B	0.17083		
182B ->192B	-0.33314		
183B ->193B	-0.11322		
184B ->192B	0.60223		
190B ->199B	0.10911		
191B ->195B	-0.50937		
191B ->196B	0.18149		
Excited State 20:	?Spin -A	2.8855 eV	429.68 nm f=0.0000
193A ->195A	-0.25049		
193A ->196A	0.10864		
193A ->200A	0.11419		
185B ->192B	0.73053		
191B ->194B	-0.51935		
191B ->197B	-0.16264		

Table S4. Excitation energies and oscillator strengths for optimized $[(bpy)_2(H_2O)RuORu(OH_2)(bpy)_2]^{5+}$ with IEF-PCM (acetonitrile). The results on each state include: the spin and spatial symmetry, the excitation energy, the oscillator strength, and (on the second line for each state) the largest coefficients in the CI expansion.

Excited State 1:	?Spin -B	-0.8652 eV	-1432.99 nm f=-0.0005
171A ->193A	-0.16209		
175A ->193A	-0.23022		
187A ->193A	-0.77554		
189A ->193A	0.26327		
190A ->193A	0.29371		
192A ->193A	0.11119		
170B ->192B	0.15138		
174B ->192B	-0.12521		
176B ->192B	-0.19086		
186B ->192B	0.78256		
188B ->193B	0.12855		
189B ->192B	-0.28835		

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

Total Energy, E(RPA) = -2396.59773146
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2:	?Spin -B	0.2143 eV 5785.83 nm f=0.0002
174A ->193A	-0.10839	
175A ->193A	0.11239	
187A ->193A	0.41254	
189A ->193A	-0.21845	
190A ->193A	0.60819	
192A ->193A	0.72050	
176B ->192B	0.10024	
186B ->192B	-0.38752	
188B ->193B	0.35647	
189B ->192B	0.14979	

Excited State 3:	?Spin -A	0.5859 eV 2116.19 nm f=0.0001
172B ->192B	0.11721	
188B ->192B	0.90927	
191B ->192B	-0.14043	

Excited State 4:	?Spin -A	0.9383 eV 1321.31 nm f=0.0000
176A ->193A	-0.13735	
177A ->193A	-0.10809	
184A ->193A	0.13661	
186A ->193A	-0.38731	
191A ->193A	-0.13375	
174B ->193B	0.14957	
177B ->192B	0.23875	
184B ->193B	0.41592	
185B ->192B	0.76625	
191B ->192B	0.21775	

Excited State 5:	?Spin -B	0.9436 eV 1313.93 nm f=0.0005
185A ->193A	-0.30775	
187A ->193A	-0.25273	
189A ->193A	0.14288	
172B ->193B	0.12039	
174B ->192B	0.18952	
179B ->192B	-0.10485	
184B ->192B	0.59705	
185B ->193B	0.29998	
186B ->192B	-0.21312	
188B ->193B	0.63058	
189B ->192B	0.11817	
190B ->192B	0.18259	

Excited State 6: ?Spin -B 0.9610 eV 1290.19 nm f=0.0001

175A ->193A	-0.11414
185A ->193A	0.25628
187A ->193A	-0.28481
189A ->193A	0.15789
190A ->193A	0.14789
192A ->193A	-0.11952
174B ->192B	-0.12637
177B ->193B	-0.13017
184B ->192B	-0.48740
185B ->193B	-0.31828
186B ->192B	-0.25121
188B ->193B	0.70761
189B ->192B	0.14692
191B ->193B	-0.17083

Excited State 7: ?Spin -A 1.2324 eV 1006.01 nm f=0.0004

184A ->193A	-0.32989
186A ->193A	0.10136
188A ->193A	0.12410
191A ->193A	0.80548
184B ->193B	0.14134
185B ->192B	0.14731
186B ->193B	0.36097
188B ->192B	0.15278
189B ->193B	-0.17267

Excited State 8: ?Spin -B 1.2607 eV 983.42 nm f=0.0003

185A ->193A	0.33530
187A ->193A	0.12620
189A ->193A	-0.14643
190A ->193A	0.62203
192A ->193A	-0.61027
184B ->192B	0.16956
185B ->193B	0.14149

Excited State 9: ?Spin -A 1.2688 eV 977.15 nm f=0.0000

153A ->193A	0.12846
155A ->193A	0.13100
170A ->193A	-0.12858
179A ->193A	-0.11931
184A ->193A	-0.31412
186A ->193A	-0.47411
188A ->193A	0.19452
191A ->193A	-0.36544
185B ->192B	-0.11364

186B ->193B 0.63722
188B ->192B 0.25727
189B ->193B -0.30541

Excited State 10: ?Spin -A 1.3847 eV 895.38 nm f=0.0000
176A ->193A 0.16747
177A ->193A 0.13011
184A ->193A -0.19144
186A ->193A 0.64890
188A ->193A 0.15961
191A ->193A -0.39702
184B ->193B 0.10935
186B ->193B 0.16926
188B ->192B 0.14552
190B ->193B 0.10943
191B ->192B 0.46315

Excited State 11: ?Spin -B 1.3928 eV 890.20 nm f=0.0001
173A ->193A 0.12191
175A ->193A -0.12095
178A ->193A 0.13903
185A ->193A 0.70388
189A ->193A 0.13342
190A ->193A -0.22599
192A ->193A 0.28496
185B ->193B 0.10248
190B ->192B 0.49780
191B ->193B 0.14183

Excited State 12: ?Spin -A 1.4512 eV 854.35 nm f=0.0032
186A ->193A -0.31373
188A ->193A -0.16887
191A ->193A 0.17031
184B ->193B -0.18706
185B ->192B -0.25125
190B ->193B 0.14136
191B ->192B 0.81879

Excited State 13: ?Spin -B 1.4518 eV 854.02 nm f=0.0027
185A ->193A -0.34474
189A ->193A -0.28080
192A ->193A -0.13018
184B ->192B -0.22173
185B ->193B -0.17230
190B ->192B 0.79653
191B ->193B 0.12548

Excited State 14:	?Spin -B	1.4640 eV	846.90 nm	f=0.0056
185A ->193A	-0.16305			
187A ->193A	0.36806			
189A ->193A	0.86021			
190A ->193A	0.15456			
188B ->193B	-0.10943			
190B ->192B	0.18621			
Excited State 15:	?Spin -A	1.5273 eV	811.79 nm	f=0.0008
186A ->193A	-0.10498			
188A ->193A	0.93363			
186B ->193B	-0.24473			
187B ->192B	0.11199			
188B ->192B	-0.12591			
189B ->193B	0.11318			
Excited State 16:	?Spin -B	1.6112 eV	769.53 nm	f=0.0066
186B ->192B	0.34479			
187B ->193B	-0.16550			
189B ->192B	0.91606			
Excited State 17:	?Spin -A	1.6205 eV	765.09 nm	f=0.0002
170A ->193A	0.13807			
172A ->193A	0.11454			
176A ->193A	-0.10035			
179A ->193A	-0.13072			
184A ->193A	0.72489			
186A ->193A	0.12288			
186B ->193B	0.29340			
187B ->192B	0.37664			
188B ->192B	0.15712			
189B ->193B	-0.28228			
Excited State 18:	?Spin -A	1.6763 eV	739.63 nm	f=0.0012
184A ->193A	-0.31653			
188A ->193A	-0.12512			
186B ->193B	-0.19027			
187B ->192B	0.89523			
188B ->192B	-0.10024			
Excited State 19:	?Spin -B	1.8801 eV	659.46 nm	f=0.0022
184B ->192B	-0.18767			
185B ->193B	0.15554			
188B ->193B	0.15059			
190B ->192B	-0.19130			

191B ->193B 0.93419

Excited State 20: ?Spin -A 1.8891 eV 656.31 nm f=0.0014
184B ->193B 0.16020
185B ->192B -0.16201
190B ->193B 0.94613
191B ->192B -0.18466

Excited State 21: ?Spin -A 2.0723 eV 598.30 nm f=0.0000
184B ->193B 0.28067
185B ->192B -0.16522
186B ->193B 0.38651
187B ->192B 0.18250
189B ->193B 0.83051

Excited State 22: ?Spin -B 2.0836 eV 595.05 nm f=0.0029
177B ->193B 0.15114
184B ->192B -0.46639
185B ->193B 0.72294
187B ->193B -0.39390
191B ->193B -0.22103

Excited State 23: ?Spin -A 2.0989 eV 590.72 nm f=0.0001
174B ->193B 0.15179
184B ->193B 0.75140
185B ->192B -0.47217
186B ->193B -0.20399
189B ->193B -0.26147
190B ->193B -0.22114

Excited State 24: ?Spin -B 2.1219 eV 584.30 nm f=0.0022
184B ->192B -0.17995
185B ->193B 0.32761
186B ->192B 0.10864
187B ->193B 0.89892
189B ->192B 0.12715

Excited State 25: ?Spin -B 2.4556 eV 504.90 nm f=0.5279
171A ->193A -0.11752
175A ->193A -0.23166
178A ->193A -0.14491
187A ->193A 0.43812
172B ->193B -0.10135
176B ->192B 0.17524
186B ->192B 0.42999
188B ->193B 0.38317

188B ->196B 0.12227

Excited State 26: ?Spin -A 2.5057 eV 494.81 nm f=0.0004
153A ->193A -0.21650
155A ->193A -0.23879
161A ->193A 0.10821
163A ->193A -0.12721
164A ->193A -0.15739
176A ->193A 0.12080
179A ->193A 0.74322
152B ->192B 0.26465
154B ->192B 0.12724
178B ->192B -0.39960
179B ->193B 0.15158
186B ->193B 0.19819
188B ->192B 0.12028

Excited State 27: ?Spin -A 2.6215 eV 472.96 nm f=0.0004
180A ->193A 0.11082
182A ->193A 0.93795
184A ->193A -0.12732
182B ->192B -0.24301

Excited State 28: ?Spin -B 2.6260 eV 472.14 nm f=0.0117
181A ->193A 0.13496
183A ->193A 0.94245
183B ->192B -0.24117

Excited State 29: ?Spin -A 2.6359 eV 470.36 nm f=0.0024
182A ->193A 0.11417
184A ->199A 0.16303
184A ->209A 0.13089
190A ->194A 0.35450
190A ->196A 0.46594
190A ->198A 0.26419
192A ->194A 0.36190
192A ->196A 0.47604
192A ->198A 0.25524
186B ->196B 0.13607
188B ->199B -0.15981

Excited State 30: ?Spin -B 2.7101 eV 457.48 nm f=0.0033
173A ->193A -0.10448
175A ->193A -0.16107
178A ->193A 0.59018
183A ->193A -0.12739

185A ->193A -0.11423
155B ->192B 0.11718
163B ->192B 0.11532
165B ->192B 0.10363
174B ->192B 0.10584
179B ->192B 0.66453
183B ->192B -0.16931

Excited State 31: ?Spin -B 2.7401 eV 452.48 nm f=0.0458
178A ->193A 0.14780
181A ->193A 0.11677
183A ->193A 0.21173
179B ->192B 0.11485
181B ->192B 0.11364
182B ->193B -0.22724
183B ->192B 0.90174

Excited State 32: ?Spin -A 2.7406 eV 452.40 nm f=0.0185
180A ->193A 0.13212
182A ->193A 0.23654
180B ->192B 0.10497
182B ->192B 0.91394
183B ->193B -0.22042

Excited State 33: ?Spin -A 2.7729 eV 447.12 nm f=0.0001
176A ->193A 0.35940
177A ->193A 0.30407
179A ->193A -0.19177
180A ->193A 0.81135
186A ->193A -0.16181
180B ->192B -0.11501

Excited State 34: ?Spin -B 2.7840 eV 445.34 nm f=0.0044
173A ->193A -0.21526
174A ->193A 0.15347
175A ->193A 0.14191
178A ->193A -0.40740
181A ->193A 0.74202
185A ->193A 0.17082
179B ->192B 0.31606
181B ->192B -0.11261

Excited State 35: ?Spin -B 2.8012 eV 442.61 nm f=0.0020
178A ->193A 0.55749
181A ->193A 0.56632
183A ->193A -0.12991

179B ->192B -0.52450

Excited State 36: ?Spin -A 2.8497 eV 435.08 nm f=0.0000
176A ->193A 0.42935
177A ->193A 0.65026
179A ->193A -0.12030
180A ->193A -0.51577
182A ->193A 0.12673
184A ->193A 0.13721
186A ->193A -0.19780
177B ->192B -0.12236

Excited State 37: ?Spin -B 2.8701 eV 431.98 nm f=0.0049
173A ->193A -0.13188
175A ->193A 0.25210
178A ->193A 0.13740
181A ->193A -0.13792
184A ->194A -0.15389
184A ->196A -0.21973
184A ->198A -0.10207
184A ->200A -0.10222
190A ->197A -0.13512
190A ->199A -0.35306
192A ->197A -0.19902
192A ->199A -0.33300
186B ->199B -0.14880
188B ->194B -0.28187
188B ->196B 0.45400
188B ->198B 0.29142

Excited State 38: ?Spin -A 2.9037 eV 426.99 nm f=0.0001
176A ->193A 0.11289
191A ->197A 0.10789
172B ->192B 0.14849
175B ->192B -0.13804
177B ->192B 0.36962
180B ->192B 0.77880
181B ->193B -0.17507
185B ->192B -0.13862
191B ->197B -0.12332

Excited State 39: ?Spin -B 2.9134 eV 425.56 nm f=0.0030
181A ->193A 0.13837
185A ->199A -0.13096
186A ->194A -0.10005
186A ->196A -0.14902

190A ->197A -0.11111
174B ->192B -0.32166
176B ->192B 0.10723
180B ->193B -0.17235
181B ->192B 0.72462
184B ->192B 0.11578
184B ->199B 0.15238
185B ->196B 0.15938
190B ->197B 0.14876

Excited State 40: ?Spin -A 2.9210 eV 424.46 nm f=0.0022
172A ->193A 0.13046
176A ->193A 0.11750
179A ->193A 0.39667
172B ->192B 0.12570
177B ->192B -0.11647
178B ->192B 0.78517
179B ->193B 0.24667

Excited State 41: ?Spin -B 2.9312 eV 422.98 nm f=0.0135
173A ->193A -0.18942
175A ->193A 0.51721
185A ->197A 0.10373
185A ->199A 0.20009
186A ->194A 0.14750
186A ->196A 0.20296
186A ->200A 0.12017
174B ->192B 0.11467
176B ->192B 0.31165
181B ->192B 0.40008
184B ->199B -0.23054
185B ->194B 0.13020
185B ->196B -0.20937
185B ->198B -0.12173
185B ->200B -0.12720
186B ->192B 0.10049

Excited State 42: ?Spin -A 2.9352 eV 422.40 nm f=0.0008
176A ->199A -0.13843
177A ->199A -0.10731
185A ->194A -0.20534
185A ->196A -0.28863
185A ->198A -0.11888
185A ->200A -0.20230
186A ->197A -0.14237
186A ->199A -0.30620

191A ->197A -0.13726
174B ->196B 0.10954
177B ->199B 0.14815
178B ->192B -0.17281
180B ->192B 0.28332
184B ->194B -0.20211
184B ->196B 0.34083
184B ->198B 0.18201
184B ->200B 0.20299
185B ->197B 0.15477
185B ->199B 0.36695
190B ->196B 0.11303
191B ->197B 0.13628

Excited State 43: ?Spin -B 2.9370 eV 422.14 nm f=0.0229
173A ->193A 0.40602
174A ->193A -0.20729
175A ->193A -0.36997
181A ->193A 0.16834
184A ->196A -0.13155
185A ->193A -0.14480
185A ->199A 0.22662
186A ->194A 0.11026
186A ->196A 0.15231
186A ->200A 0.12947
192A ->197A -0.13363
174B ->192B -0.20759
176B ->192B -0.10786
181B ->192B 0.12403
184B ->197B -0.10314
184B ->199B -0.25936
185B ->194B 0.13976
185B ->196B -0.24244
185B ->198B -0.13614
185B ->200B -0.14418
191B ->196B -0.10031

Excited State 44: ?Spin -B 2.9509 eV 420.16 nm f=0.0089
173A ->193A 0.52261
174A ->193A -0.46344
175A ->193A 0.38943
181A ->193A 0.14124
187A ->193A -0.10364
176B ->192B 0.35604
178B ->193B 0.11965
179B ->192B 0.15638

181B ->192B	-0.26628	

Excited State 45:	?Spin -A	2.9875 eV 415.01 nm f=0.0027
172A ->193A	0.24938	
176A ->193A	0.40590	
177A ->193A	-0.21682	
180A ->193A	-0.10541	
188A ->195A	0.10815	
189A ->194A	0.10979	
191A ->197A	0.14036	
192A ->198A	0.11193	
172B ->192B	-0.14559	
177B ->192B	0.55932	
179B ->193B	-0.11117	
180B ->192B	-0.30534	
184B ->193B	-0.10058	
185B ->192B	-0.11624	
185B ->199B	0.12192	
187B ->195B	0.10091	
190B ->198B	0.13457	
191B ->197B	-0.14469	

Excited State 46:	?Spin -A	2.9924 eV 414.33 nm f=0.0003
172A ->193A	-0.13512	
176A ->193A	-0.44517	
177A ->193A	0.45974	
188A ->195A	-0.17707	
189A ->194A	-0.19564	
175B ->192B	-0.14531	
177B ->192B	0.49436	
180B ->192B	-0.28881	
185B ->192B	-0.13338	
187B ->195B	-0.17078	
189B ->194B	-0.18939	

Excited State 47:	?Spin -B	3.0002 eV 413.25 nm f=0.0004
180A ->212A	-0.10253	
181A ->213A	-0.10283	
185A ->199A	0.13044	
190A ->197A	-0.27923	
191A ->196A	-0.22017	
191A ->198A	0.39884	
191A ->205A	-0.10754	
192A ->197A	0.34814	
192A ->199A	-0.14956	
180B ->212B	0.10237	

181B ->192B -0.17317
181B ->213B 0.10289
184B ->199B -0.14316
185B ->198B -0.11435
190B ->197B 0.43707
190B ->199B -0.11759
190B ->206B -0.10923
191B ->194B -0.13682
191B ->196B 0.19420
191B ->198B -0.38081
191B ->205B 0.10001

Excited State 48: ?Spin -A 3.0012 eV 413.12 nm f=0.0000
176A ->193A -0.18185
177A ->193A 0.13712
190A ->196A 0.14407
190A ->198A -0.21551
191A ->197A 0.42471
191A ->199A -0.12831
191A ->206A -0.12063
192A ->196A -0.16583
192A ->198A 0.31811
177B ->192B -0.29404
185B ->199B 0.10560
190B ->194B 0.14415
190B ->196B -0.19633
190B ->198B 0.35347
191B ->197B -0.41847
191B ->199B 0.11459
191B ->206B 0.10162

Excited State 49: ?Spin -A 3.0129 eV 411.51 nm f=0.0002
172A ->193A -0.25531
176A ->193A -0.20402
177A ->193A 0.22733
188A ->195A 0.37967
189A ->194A 0.42383
189A ->196A -0.17508
189A ->201A 0.12309
172B ->192B 0.16801
177B ->192B 0.10054
178B ->192B 0.12271
179B ->193B 0.10688
187B ->195B 0.38226
187B ->202B 0.11047
189B ->194B 0.41345

189B ->196B 0.16797
189B ->201B -0.11605

Excited State 50: ?Spin -B 3.0142 eV 411.33 nm f=0.0011
173A ->193A 0.12873
188A ->194A 0.41673
188A ->196A -0.20935
188A ->201A 0.14218
189A ->195A 0.50334
173B ->210B -0.10250
176B ->192B -0.10751
187B ->194B -0.41207
187B ->196B -0.19145
187B ->201B 0.13355
189B ->195B -0.50352
189B ->202B -0.11027

Excited State 51: ?Spin -B 3.0376 eV 408.17 nm f=0.0175
173A ->193A 0.24044
174A ->193A -0.11847
173B ->192B 0.13785
174B ->192B 0.70992
176B ->192B -0.33046
177B ->193B 0.17189
181B ->192B 0.34511
184B ->192B -0.19912
185B ->193B -0.14549

Excited State 52: ?Spin -A 3.0658 eV 404.41 nm f=0.0018
169A ->193A -0.16848
172A ->193A 0.63533
176A ->193A -0.34360
177A ->193A 0.28515
184A ->193A -0.12420
169B ->192B 0.11233
172B ->192B -0.42515
175B ->192B 0.12993
179B ->193B -0.11378
180B ->192B 0.16616

Excited State 53: ?Spin -B 3.1043 eV 399.39 nm f=0.0051
171A ->193A -0.19107
173A ->193A 0.54587
174A ->193A 0.69888
175A ->193A 0.26618
174B ->192B -0.11448

176B ->192B -0.16361

Excited State 54: ?Spin -B 3.1319 eV 395.87 nm f=0.0375
171A ->193A 0.42950
173A ->193A 0.10679
174A ->193A 0.39475
175A ->193A -0.25715
170B ->192B 0.11285
174B ->192B 0.26484
176B ->192B 0.59841
178B ->193B 0.17745
182B ->193B -0.10037

Excited State 55: ?Spin -A 3.1348 eV 395.51 nm f=0.0002
172A ->193A -0.44716
169B ->192B 0.10517
172B ->192B -0.53213
175B ->192B 0.55632
177B ->192B 0.16583
178B ->192B 0.19873
180B ->192B 0.15038

Excited State 56: ?Spin -A 3.1697 eV 391.16 nm f=0.0002
172A ->193A -0.12406
184A ->199A 0.14385
187A ->194A 0.32452
187A ->196A 0.41807
187A ->198A 0.24047
189A ->196A -0.22927
189A ->198A -0.11198
190A ->200A 0.22599
192A ->200A 0.21448
172B ->192B -0.11681
175B ->192B -0.32634
186B ->194B 0.19428
186B ->196B -0.31537
186B ->198B -0.20759
188B ->209B 0.12083
189B ->196B 0.17781

Excited State 57: ?Spin -A 3.1834 eV 389.48 nm f=0.0005
155A ->193A 0.10424
172A ->193A 0.15405
179A ->193A 0.14066
187A ->194A 0.13794
187A ->196A 0.21419

169B ->192B -0.12346
172B ->192B 0.46380
173B ->193B -0.10991
175B ->192B 0.65357
179B ->193B -0.11863
183B ->193B -0.10570
186B ->196B -0.13636

Excited State 58: ?Spin -B 3.1992 eV 387.55 nm f=0.0001
184A ->200A 0.16287
190A ->197A 0.14912
190A ->199A 0.32439
192A ->197A 0.16940
192A ->199A 0.34299
174B ->192B -0.13570
182B ->193B -0.28230
186B ->209B -0.12693
188B ->194B -0.29049
188B ->196B 0.42912
188B ->198B 0.29764
188B ->200B -0.31020

Excited State 59: ?Spin -A 3.2019 eV 387.22 nm f=0.0000
184A ->199A 0.17522
184A ->209A -0.11359
190A ->198A -0.10371
190A ->200A 0.49319
192A ->198A -0.11151
192A ->200A 0.46945
183B ->193B -0.11740
186B ->194B -0.15128
186B ->196B 0.23444
186B ->198B 0.13822
186B ->200B 0.15593
188B ->197B -0.16159
188B ->199B -0.42270
189B ->196B -0.11774

Excited State 60: ?Spin -A 3.2149 eV 385.66 nm f=0.0078
153A ->193A -0.16056
155A ->193A -0.17391
161A ->193A 0.10852
163A ->193A -0.13796
164A ->193A -0.13754
169A ->193A -0.35092
172A ->193A 0.16696

179A ->193A -0.32401
155B ->193B 0.10139
172B ->192B 0.14945
174B ->193B 0.13968
175B ->192B 0.13532
177B ->192B 0.10233
179B ->193B 0.66082
183B ->193B -0.18960

Excited State 61: ?Spin -B 3.2183 eV 385.25 nm f=0.0174
192A ->199A 0.11508
173B ->192B -0.34379
178B ->193B 0.12641
182B ->193B 0.80962
183B ->192B 0.22068
188B ->196B 0.15241
188B ->198B 0.10465
188B ->200B -0.11096

Excited State 62: ?Spin -A 3.2249 eV 384.46 nm f=0.0092
175B ->192B 0.11753
179B ->193B 0.17139
181B ->193B 0.10351
182B ->192B 0.24097
183B ->193B 0.90845

Excited State 63: ?Spin -B 3.2438 eV 382.22 nm f=0.0020
173B ->192B 0.86753
174B ->192B -0.13291
175B ->193B -0.19078
177B ->193B -0.10273
182B ->193B 0.35835

Excited State 64: ?Spin -B 3.2750 eV 378.58 nm f=0.0095
171A ->193A 0.75628
175A ->193A 0.12431
170B ->192B -0.42424
172B ->193B -0.22221
176B ->192B -0.17921
178B ->193B -0.26075

Excited State 65: ?Spin -A 3.3038 eV 375.28 nm f=0.0004
170A ->193A 0.92766
172A ->193A -0.12038
184A ->193A -0.17084
171B ->192B -0.21673

Excited State 66:	?Spin -B	3.3385 eV	371.37 nm	f=0.0353
171A ->193A	0.14286			
152B ->193B	-0.13359			
170B ->192B	-0.18298			
174B ->192B	-0.13822			
176B ->192B	-0.26270			
177B ->193B	0.10652			
178B ->193B	0.85696			
182B ->193B	-0.11799			
Excited State 67:	?Spin -A	3.3788 eV	366.95 nm	f=0.0001
169A ->193A	0.70975			
172A ->193A	0.18798			
152B ->192B	-0.13483			
169B ->192B	-0.28779			
172B ->192B	-0.20296			
174B ->193B	-0.14398			
178B ->192B	-0.15293			
179B ->193B	0.40136			
181B ->193B	0.10718			
Excited State 68:	?Spin -A	3.3955 eV	365.14 nm	f=0.0003
170A ->193A	0.14464			
170B ->193B	-0.14039			
171B ->192B	0.67183			
176B ->193B	-0.34046			
180B ->192B	-0.13299			
181B ->193B	-0.50304			
Excited State 69:	?Spin -B	3.3973 eV	364.95 nm	f=0.0035
172B ->193B	0.11314			
174B ->192B	-0.12249			
175B ->193B	-0.12597			
177B ->193B	0.23512			
178B ->193B	-0.17830			
180B ->193B	0.88530			
181B ->192B	0.19471			
Excited State 70:	?Spin -A	3.4096 eV	363.63 nm	f=0.0002
169A ->193A	-0.23701			
170A ->193A	0.10994			
172A ->193A	-0.11913			
171B ->192B	0.42146			
174B ->193B	-0.14079			
176B ->193B	-0.13523			

180B ->192B 0.16145
181B ->193B 0.77025

Excited State 71: ?Spin -B 3.4345 eV 360.99 nm f=0.0008
171A ->193A 0.15259
185A ->199A 0.10938
170B ->192B 0.57473
171B ->193B -0.18497
172B ->193B -0.17198
174B ->192B -0.17883
175B ->193B -0.10494
177B ->193B 0.52186
180B ->193B -0.21773
185B ->193B -0.13770
185B ->198B 0.10065
188B ->194B 0.14372
188B ->196B 0.10845

Excited State 72: ?Spin -A 3.4668 eV 357.63 nm f=0.0000
153A ->193A -0.14770
155A ->193A -0.17245
164A ->193A -0.13959
169A ->193A 0.31905
179A ->193A -0.13905
152B ->192B 0.19100
170B ->193B -0.10427
171B ->192B 0.29114
172B ->192B 0.13490
174B ->193B 0.52444
176B ->193B 0.29900
177B ->192B -0.10106
179B ->193B -0.18259
181B ->193B 0.18336
184B ->193B -0.10489
184B ->200B 0.11406
186B ->193B 0.15717

Excited State 73: ?Spin -B 3.4779 eV 356.49 nm f=0.0008
184A ->196A 0.27430
184A ->198A 0.11752
186A ->196A 0.22532
186A ->198A 0.10765
186A ->200A -0.16277
187A ->197A 0.14048
187A ->199A 0.26273
189A ->199A -0.11674

190A ->195A -0.23092
190A ->209A 0.19990
192A ->195A -0.24550
192A ->209A 0.18704
172B ->193B 0.25800
180B ->193B -0.15113
185B ->200B 0.11792
186B ->199B -0.24357
188B ->194B -0.19628
188B ->200B 0.30684
188B ->201B -0.10009
189B ->199B 0.11511

Excited State 74: ?Spin -B 3.4920 eV 355.05 nm f=0.0360
171A ->193A -0.21226
185A ->199A -0.11015
190A ->195A 0.10934
192A ->195A 0.12601
170B ->192B -0.44733
171B ->193B 0.15145
174B ->192B -0.11509
176B ->192B 0.14953
177B ->193B 0.67101
180B ->193B -0.15739
185B ->193B -0.13174
185B ->196B -0.15706

Excited State 75: ?Spin -A 3.5036 eV 353.88 nm f=0.0000
176A ->199A -0.10731
185A ->200A -0.35657
186A ->197A -0.12043
186A ->199A -0.26673
186A ->209A 0.14582
171B ->192B 0.12618
174B ->193B -0.34883
176B ->193B 0.40396
177B ->192B 0.10989
179B ->193B 0.14993
181B ->193B -0.14887
184B ->193B 0.13339
184B ->194B 0.17931
184B ->196B -0.24842
184B ->198B -0.20807
184B ->200B 0.13905
185B ->209B -0.16343

Table S5. Excitation energies and oscillator strengths for $Ru(bpy)_2Cl_2$ with IEF-PCM (water). The results on each state include: the spin and spatial symmetry, the excitation energy, the oscillator strength, and (on the second line for each state) the largest coefficients in the CI expansion.

Excited State 1: Singlet-B 1.9758 eV 627.51 nm f=0.0142 <S**2>=0.000
97 -> 98 0.68959
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1114.55663734
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.0020 eV 619.31 nm f=0.0020 <S**2>=0.000
95 -> 99 -0.18434
97 -> 99 0.66984

Excited State 3: Singlet-B 2.2315 eV 555.61 nm f=0.0047 <S**2>=0.000
95 -> 98 -0.38997
96 -> 99 0.57863

Excited State 4: Singlet-A 2.2875 eV 542.02 nm f=0.0000 <S**2>=0.000
95 -> 99 -0.39775
96 -> 98 0.57383

Excited State 5: Singlet-B 2.4438 eV 507.35 nm f=0.1560 <S**2>=0.000
95 -> 98 0.57210
96 -> 99 0.37558
97 -> 98 0.11633

Excited State 6: Singlet-A 2.6006 eV 476.76 nm f=0.0097 <S**2>=0.000
95 -> 99 0.51180
96 -> 98 0.35466
97 -> 99 0.19236
97 ->103 0.23482

Excited State 7: Singlet-B 2.8871 eV 429.45 nm f=0.0179 <S**2>=0.000
97 ->100 0.64558
97 ->102 -0.14293
97 ->104 0.21918

Excited State 8: Singlet-B 2.9661 eV 418.00 nm f=0.0162 <S**2>=0.000
95 ->104 0.10862
97 ->100 -0.25243
97 ->102 -0.19246
97 ->104 0.59785

Excited State 9: Singlet-A 3.0997 eV 399.99 nm f=0.0000 <S**2>=0.000
96 ->100 -0.17941
97 ->101 0.65877

Excited State 10: Singlet-A 3.1379 eV 395.11 nm f=0.0046 <S**2>=0.000
96 ->100 0.61393
97 ->101 0.21320
97 ->103 0.24884

Excited State 11: Singlet-B 3.1925 eV 388.36 nm f=0.0270 <S**2>=0.000
95 ->100 -0.35626
95 ->104 0.10770
97 ->102 0.55109
97 ->104 0.19978

Excited State 12: Singlet-B 3.2358 eV 383.17 nm f=0.0585 <S**2>=0.000
95 ->100 0.59668
96 ->101 0.10467
97 ->102 0.31900

Excited State 13: Singlet-A 3.2435 eV 382.25 nm f=0.0188 <S**2>=0.000
95 -> 99 -0.13348
95 ->101 -0.15354
95 ->103 -0.21273
96 ->100 -0.25534
96 ->102 -0.30369
96 ->104 0.24244
97 ->103 0.40648

Excited State 14: Singlet-B 3.3468 eV 370.46 nm f=0.0329 <S**2>=0.000
96 ->103 0.66892
96 ->107 -0.14849

Excited State 15: Singlet-B 3.3742 eV 367.45 nm f=0.0308 <S**2>=0.000
95 ->102 -0.18027
95 ->104 0.24363
96 ->101 0.59749
96 ->103 0.11457
96 ->107 0.10248
97 ->102 -0.11455

Excited State 16: Singlet-A 3.4017 eV 364.47 nm f=0.0116 <S**2>=0.000
95 ->101 0.46461
95 ->103 -0.23967
95 ->107 0.14507
96 ->102 -0.22169

96 ->104 0.22317
97 ->103 -0.26480
97 ->107 -0.14279

Excited State 17: Singlet-A 3.4571 eV 358.64 nm f=0.0149 <S**2>=0.000
95 ->101 -0.22894
95 ->103 -0.37694
95 ->107 0.10758
96 ->102 0.44169
96 ->104 0.25693
97 ->103 -0.12563

Excited State 18: Singlet-B 3.4741 eV 356.89 nm f=0.0232 <S**2>=0.000
95 ->102 -0.10296
95 ->104 0.53151
96 ->101 -0.31829
96 ->107 0.26863

Excited State 19: Singlet-A 3.5073 eV 353.51 nm f=0.0007 <S**2>=0.000
95 ->101 -0.15882
95 ->103 0.46555
95 ->107 0.20385
96 ->104 0.40944
97 ->103 -0.12750
97 ->107 -0.12686

Excited State 20: Singlet-B 3.5193 eV 352.30 nm f=0.0526 <S**2>=0.000
95 ->102 0.65520
95 ->104 0.17366
96 ->101 0.12546

Table S6. Cartesian Coordinates for BD (optimized geometry, strong coupling)

Element	x	y	z
H	-2.29462	-2.45960	-0.71279
H	-6.54091	2.55688	-0.62755
H	4.05373	4.17512	3.82234
H	-5.54382	-2.49042	2.76632
H	-4.06360	2.34967	-0.67864
H	-7.88417	0.82383	0.62555
H	-6.68443	-1.02644	1.77455
H	-0.67761	-2.11229	2.05471
H	-1.56358	-3.99934	3.47100
H	-1.22218	3.39603	0.84830
H	-1.06996	5.37488	-0.69046
H	-1.34172	5.00097	-3.17073
H	-1.73118	2.69040	-4.01323
H	-2.72119	-3.35267	-3.00737
H	-2.66083	-1.75951	-4.96497
H	-2.15667	0.64336	-4.54697
H	2.15671	-0.64333	-4.54697
H	4.06361	-2.34966	-0.67865
H	1.56355	3.99933	3.47099
H	0.67759	2.11229	2.05470
H	1.22217	-3.39604	0.84828
H	-4.05375	-4.17511	3.82233
H	2.29461	2.45961	-0.71278
H	2.72121	3.35268	-3.00735
H	7.88416	-0.82384	0.62559
H	1.34172	-5.00095	-3.17076
H	2.66087	1.75954	-4.96495
H	6.54092	-2.55688	-0.62754
H	6.68442	1.02643	1.77459
H	5.54380	2.49042	2.76633
H	1.06995	-5.37488	-0.69050
H	1.73119	-2.69038	-4.01324
H	2.67709	-1.94942	2.72987
H	1.43107	-1.06294	3.23012
H	-1.43103	1.06291	3.23010
H	-2.67708	1.94937	2.72989
C	-2.25517	-1.80917	-1.57691

C	-6.05495	1.73343	-0.11501
C	-2.24087	-3.28081	3.02125
C	-1.23190	4.37963	-1.09112
C	-2.49153	-2.30164	-2.86713
C	-3.63300	-3.37835	3.21665
C	-1.38301	4.16656	-2.47701
C	-2.45640	-1.41073	-3.95730
C	-6.11848	-0.27649	1.23469
C	-4.47257	-2.42537	2.61747
C	-1.31463	3.28097	-0.22536
C	-2.17282	-0.05561	-3.71836
C	-4.71455	-0.33831	1.17815
C	-3.91613	-1.39398	1.83621
C	-1.68163	1.79352	-2.03665
C	-1.94386	0.39009	-2.40382
C	1.60370	-2.86123	-2.95029
C	-6.80074	0.76726	0.58534
C	-4.65833	1.61945	-0.14675
C	-1.73854	-2.23589	2.23527
C	2.45643	1.41075	-3.95728
C	6.11847	0.27649	1.23472
C	2.24085	3.28081	3.02124
C	4.47255	2.42537	2.61748
C	1.23190	-4.37962	-1.09115
C	1.94387	-0.39007	-2.40382
C	2.49154	2.30165	-2.86711
C	2.17285	0.05563	-3.71836
C	4.65833	-1.61945	-0.14674
C	4.71454	0.33831	1.17817
C	3.91611	1.39398	1.83622
C	1.31463	-3.28097	-0.22538
C	1.68164	-1.79351	-2.03666
C	2.25517	1.80917	-1.57690
C	1.38302	-4.16655	-2.47704
C	1.73853	2.23589	2.23526
C	-1.60369	2.86124	-2.95027
C	6.80074	-0.76726	0.58537
C	6.05495	-1.73343	-0.11499
C	3.63297	3.37835	3.21665
N	-2.55392	-1.31074	1.65211

N	-1.54112	2.01742	-0.68339
N	-1.99421	-0.49284	-1.34248
N	1.54113	-2.01742	-0.68340
N	1.99421	0.49284	-1.34247
N	-3.99029	0.61164	0.48628
N	2.55391	1.31074	1.65211
N	3.99029	-0.61164	0.48628
O	-1.86800	1.47047	2.45621
O	0.00000	0.00001	0.88512
O	1.86802	-1.47048	2.45620
Ru	-1.86067	0.34863	0.52173
Ru	1.86067	-0.34864	0.52173

Table S7. Cartesian Coordinates for BD×4H_2O (optimized geometry, strong coupling)

Element	x	y	z
H	-5.17180	-1.58605	-1.41008
H	-4.56435	-1.81287	-3.84729
H	-2.16197	-1.95828	-4.48691
H	3.84056	-2.26848	-2.99006
H	1.84344	-6.43895	1.44160
H	-0.05778	-2.18096	-4.84475
H	0.05778	2.18096	-4.84475
H	1.78745	4.29870	-1.11187
H	-3.75724	0.96647	3.52485
H	-1.80896	0.35537	2.04749
H	2.41243	-2.40788	-5.06703
H	3.33111	1.55416	0.29040
H	4.37584	-3.39710	3.76895
H	2.72540	-1.93595	-0.78071
H	-1.58235	-6.78199	-1.16227
H	-4.37584	3.39710	3.76895
H	-2.72540	1.93595	-0.78071
H	3.04759	-5.10541	2.55308
H	-1.78745	-4.29870	-1.11187
H	-3.84056	2.26848	-2.99006
H	-0.28484	7.87561	0.13879
H	0.28484	-7.87561	0.13879
H	4.56435	1.81287	-3.84729
H	-2.41243	2.40788	-5.06703

H	1.58235	6.78199	-1.16227
H	-1.84344	6.43895	1.44160
H	1.80896	-0.35537	2.04749
H	3.75724	-0.96647	3.52485
H	-3.04759	5.10541	2.55308
H	-3.33111	-1.55416	0.29040
H	5.17180	1.58605	-1.41008
H	2.16197	1.95828	-4.48691
H	2.27929	2.59986	2.01830
H	-2.27929	-2.59986	2.01830
H	4.38175	3.19590	2.70973
H	-4.38175	-3.19590	2.70973
H	-3.69556	-4.41343	1.93361
H	3.69556	4.41343	1.93361
H	1.00485	2.08188	2.91825
H	-1.00485	-2.08188	2.91825
H	0.13869	3.11381	4.81035
H	0.95334	1.79524	5.21089
H	-0.95334	-1.79524	5.21089
H	-0.13869	-3.11381	4.81035
C	2.14396	-1.98392	-1.69215
C	-0.88285	-6.18971	-0.58186
C	3.20174	-1.73745	3.00147
C	-4.13518	-1.64901	-1.72388
C	2.76227	-2.16690	-2.93541
C	2.12731	-1.38330	2.17339
C	3.54518	-3.09530	3.13896
C	-3.79241	-1.77311	-3.08506
C	1.96330	-2.24135	-4.09278
C	1.03708	-5.98340	0.87921
C	2.79359	-4.05942	2.44850
C	-3.11299	-1.62472	-0.76633
C	0.57096	-2.11465	-3.96439
C	0.86455	-4.58682	0.87506
C	1.72661	-3.65244	1.62731
C	-1.44864	-1.82866	-2.44095
C	0.00000	-1.93326	-2.69106
C	2.43656	1.85721	-3.44314
C	-1.72661	3.65244	1.62731
C	-0.86455	4.58682	0.87506

C	1.00104	4.79344	-0.55728
C	-0.57096	2.11465	-3.96439
C	-2.76227	2.16690	-2.93541
C	-3.20174	1.73745	3.00147
C	0.00000	1.93326	-2.69106
C	-1.00104	-4.79344	-0.55728
C	4.13518	1.64901	-1.72388
C	-2.79359	4.05942	2.44850
C	-1.03708	5.98340	0.87921
C	-1.96330	2.24135	-4.09278
C	0.15860	-6.79738	0.14520
C	3.11299	1.62472	-0.76633
C	1.44864	1.82866	-2.44095
C	-2.14396	1.98392	-1.69215
C	3.79241	1.77311	-3.08506
C	-2.12731	1.38330	2.17339
C	-2.43656	-1.85721	-3.44314
C	-0.15860	6.79738	0.14520
C	0.88285	6.18971	-0.58186
C	-3.54518	3.09530	3.13896
N	0.79285	-1.87989	-1.56270
N	-1.79939	-1.72269	-1.11131
N	1.41506	-2.32097	1.49146
N	-1.41506	2.32097	1.49146
N	-0.79285	1.87989	-1.56270
N	-0.14964	-4.00105	0.15257
N	1.79939	1.72269	-1.11131
N	0.14964	4.00105	0.15257
O	0.00000	0.00000	0.58094
O	-1.44340	-2.03515	2.01210
O	-3.63026	-3.46150	2.14383
O	1.44340	2.03515	2.01210
O	3.63026	3.46150	2.14383
O	0.56266	2.30112	4.47233
O	-0.56266	-2.30112	4.47233
Ru	0.21891	1.86800	0.23423
Ru	-0.21891	-1.86800	0.23423

Table S8. Cartesian Coordinates for $BDCl_4 \times 4H_2O$ (optimized geometry, strong coupling)

Element	x	y	z
H	3.93391	1.95873	-3.22966
H	2.54202	1.96396	-5.33533
H	0.05492	1.90886	-5.13024
H	-5.10076	1.76450	-1.72773
H	-1.71205	6.04030	2.49046
H	-2.04204	2.01883	-4.77204
H	2.04204	-2.01883	-4.77204
H	-0.57710	-4.52403	-1.60878
H	2.94471	-0.22819	4.09336
H	1.54957	0.03211	2.00972
H	-4.45934	1.97985	-4.16534
H	-2.78354	-1.87718	-1.02216
H	-3.48573	2.56016	4.90192
H	-3.28373	1.63602	-0.01773
H	0.41367	6.93377	-1.17905
H	3.48573	-2.56016	4.90192
H	3.28373	-1.63602	-0.01773
H	-2.65885	4.51389	3.59995
H	0.57710	4.52403	-1.60878
H	5.10076	-1.76450	-1.72773
H	0.77995	-7.73839	0.91748
H	-0.77995	7.73839	0.91748
H	-2.54202	-1.96396	-5.33533
H	4.45934	-1.97985	-4.16534
H	-0.41367	-6.93377	-1.17905
H	1.71205	-6.04030	2.49046
H	-1.54957	-0.03211	2.00972
H	-2.94471	0.22819	4.09336
H	2.65885	-4.51389	3.59995
H	2.78354	1.87718	-1.02216
H	-3.93391	-1.95873	-3.22966
H	-0.05492	-1.90886	-5.13024
H	-2.20229	-2.88049	0.87287
H	2.20229	2.88049	0.87287
H	3.23969	4.25156	-0.55827
H	-3.23969	-4.25156	-0.55827
H	-1.25632	-2.51235	2.23599

H	1.25632	2.51235	2.23599
H	-0.63399	-3.75988	3.99394
H	0.63399	3.75988	3.99394
H	1.40510	2.37503	4.41985
H	-1.40510	-2.37503	4.41985
H	-3.88845	-4.24581	0.95823
H	3.88845	4.24581	0.95823
C	-3.05263	1.71964	-1.07148
C	-0.07824	6.24987	-0.49664
C	-2.60517	1.10474	3.55113
C	2.85329	1.90198	-3.19075
C	-4.06123	1.79218	-2.03649
C	-1.83299	0.94247	2.39209
C	-2.91789	2.40339	3.99004
C	2.07347	1.90755	-4.35777
C	-3.69899	1.90779	-3.39360
C	-1.29470	5.73360	1.54020
C	-2.46980	3.50939	3.25025
C	2.21549	1.86314	-1.94231
C	-2.34056	1.92818	-3.73405
C	-1.19902	4.37011	1.22065
C	-1.72220	3.29073	2.07852
C	0.08626	1.86607	-2.96639
C	-1.36196	1.84541	-2.72404
C	-0.67542	-1.89022	-4.24119
C	1.72220	-3.29073	2.07852
C	1.19902	-4.37011	1.22065
C	0.00000	-4.87322	-0.76009
C	2.34056	-1.92818	-3.73405
C	4.06123	-1.79218	-2.03649
C	2.60517	-1.10474	3.55113
C	1.36196	-1.84541	-2.72404
C	0.00000	4.87322	-0.76009
C	-2.85329	-1.90198	-3.19075
C	2.46980	-3.50939	3.25025
C	1.29470	-5.73360	1.54020
C	3.69899	-1.90779	-3.39360
C	-0.73481	6.68296	0.66565
C	-2.21549	-1.86314	-1.94231
C	-0.08626	-1.86607	-2.96639

C	3.05263	-1.71964	-1.07148
C	-2.07347	-1.90755	-4.35777
C	1.83299	-0.94247	2.39209
C	0.67542	1.89022	-4.24119
C	0.73481	-6.68296	0.66565
C	0.07824	-6.24987	-0.49664
C	2.91789	-2.40339	3.99004
N	-1.73111	1.75589	-1.39951
N	0.86475	1.85353	-1.82662
N	-1.40426	2.01687	1.67893
N	1.40426	-2.01687	1.67893
N	1.73111	-1.75589	-1.39951
N	-0.54449	3.95689	0.08009
N	-0.86475	-1.85353	-1.82662
N	0.54449	-3.95689	0.08009
O	0.00000	0.00000	0.26261
O	1.44258	2.29014	1.23896
O	3.32511	3.75534	0.33300
O	-1.44258	-2.29014	1.23896
O	-3.32511	-3.75534	0.33300
O	-1.07747	-2.88948	3.66234
O	1.07747	2.88948	3.66234
Cl	-2.94452	-5.05533	-2.33408
Cl	2.94452	5.05533	-2.33408
Cl	0.27939	-5.32084	4.70475
Cl	-0.27939	5.32084	4.70475
Ru	0.19273	-1.87245	-0.03060
Ru	-0.19273	1.87245	-0.03060

Table S9. Cartesian Coordinates for BS-BD (optimized geometry, broken symmetry state)

Element	x	y	z
H	1.02740	-0.30874	-0.14170
H	-0.78234	0.10034	6.06145
H	4.09156	9.36460	1.26178
H	4.13286	-1.91220	2.92354
H	-0.62323	1.73638	4.18876
H	0.89823	-1.78030	6.17962
H	2.66039	-1.93338	4.43239
H	3.62576	1.73016	-0.36739

H	5.52876	0.09491	-0.63101
H	0.58459	4.84765	3.22107
H	-1.51710	6.03620	3.89697
H	-3.73449	5.09559	3.14460
H	-3.76320	3.03428	1.74878
H	-0.85944	-1.66635	-1.06465
H	-3.22691	-0.89292	-0.65285
H	-3.60429	1.20283	0.63634
H	-2.71083	4.06616	-3.44523
H	1.80301	4.55788	-4.61305
H	3.41044	7.39398	2.67666
H	2.49251	5.34310	1.52644
H	2.95345	1.80775	-2.85785
H	5.76733	-1.75899	1.05845
H	0.09069	6.64957	-0.31179
H	-2.25324	7.40830	-0.74677
H	3.22912	8.48719	-5.69802
H	-0.40385	0.47166	-5.23693
H	-3.67677	6.08717	-2.36006
H	2.33770	6.22710	-6.38555
H	3.55722	8.96933	-3.28158
H	3.84695	9.22268	-1.20688
H	1.99283	0.17997	-4.50313
H	-1.73714	2.35093	-4.29424
H	4.54503	3.88362	-2.43699
H	4.70275	4.15707	-0.86241
H	3.66992	3.22845	2.78546
H	2.56655	3.28636	3.95018
C	0.00000	0.00000	0.00000
C	0.00000	0.00000	5.31664
C	4.82813	0.00000	0.19200
C	-1.56650	5.14254	3.28362
C	-1.06282	-0.75308	-0.51558
C	4.96114	-1.03608	1.13709
C	-2.80303	4.61534	2.86063
C	-2.38226	-0.31843	-0.28478
C	1.93474	-1.12974	4.39059
C	4.03480	-1.12065	2.19003
C	-0.38741	4.48006	2.91323
C	-2.59250	0.86474	0.44409

C	1.98010	-0.17349	3.36034
C	2.99445	-0.17649	2.28343
C	-1.60168	2.82345	1.73780
C	-1.49175	1.58616	0.93996
C	-0.70798	2.21271	-3.98285
C	0.93898	-1.04676	5.38021
C	0.08628	0.92276	4.26543
C	3.77331	0.91327	0.32898
C	-2.66144	5.77738	-2.13186
C	3.17448	8.00234	-3.58607
C	3.31158	7.36298	1.59662
C	3.55197	8.38145	-0.59084
C	1.38098	0.98442	-4.10844
C	-0.78754	4.26089	-2.46286
C	-1.86982	6.51719	-1.23234
C	-2.11308	4.63713	-2.74404
C	2.19034	5.53303	-4.34757
C	2.86292	7.01892	-2.63046
C	3.03513	7.20828	-1.17302
C	1.92590	1.89491	-3.19165
C	-0.10755	3.09894	-3.06892
C	-0.55499	6.10138	-0.98526
C	0.04184	1.14924	-4.51501
C	2.80032	6.21906	0.96771
C	-2.81636	3.44954	2.07481
C	2.98967	7.73348	-4.95412
C	2.49177	6.47486	-5.34069
C	3.69242	8.46428	0.80481
N	2.87308	0.83006	1.34917
N	-0.40031	3.34137	2.16856
N	-0.20488	1.13933	0.71676
N	1.20665	2.93544	-2.68976
N	-0.02015	5.00483	-1.58960
N	1.05314	0.84860	3.30549
N	2.66196	6.13960	-0.38595
N	2.37097	5.78855	-3.01959
O	2.71374	3.29643	2.98203
O	1.71557	3.33648	0.15749
O	4.09806	3.84673	-1.56638
Ru	1.27961	2.18923	1.67312

Ru	1.94894	4.44242	-1.43259

Table S10. Cartesian Coordinates for optimized BD (triplet electronic state).

Element	x	y	z
C	2.505916	1.489464	1.89724
C	6.127657	-0.11612	-1.69829
C	2.047071	-3.10214	3.200659
C	1.277496	1.433552	-4.28564
C	2.838527	2.733736	2.449435
H	2.483445	0.594116	2.504507
C	3.422793	-3.38202	3.317536
C	1.550517	2.785812	-3.9987
C	2.872117	3.864565	1.61149
C	6.075513	-1.51026	0.283681
C	4.313504	-2.81748	2.389373
C	1.333463	0.497762	-3.24283
C	2.55856	3.713068	0.249671
C	4.678286	-1.35816	0.334418
C	3.822443	-1.9859	1.364766
C	1.903404	2.173119	-1.67138
C	2.229649	2.442615	-0.25569
H	6.657867	0.37937	-2.50467
N	2.47384	-1.71585	1.264045
N	1.649752	0.852158	-1.96788
N	2.214145	1.341503	0.576146
O	1.8149	-2.34628	-1.5583
O	-0.00296	-0.52471	-0.00532
H	-3.81259	-3.93222	-4.18659
Ru	1.912947	-0.46956	-0.35573
H	5.372696	-3.03167	2.470094
N	-1.64822	0.816175	1.98384
N	-2.21504	1.358399	-0.54907
O	-1.81503	-2.37818	1.501678
Ru	-1.9202	-0.47173	0.346285
H	4.182462	0.595638	-2.31948
N	4.016867	-0.59786	-0.60905
H	7.890578	-0.99949	-0.78554
H	6.594693	-2.10559	1.025347
H	0.562613	-2.02016	2.030115
H	1.332281	-3.52512	3.89879
C	-1.82338	3.110049	2.734797

N	-2.48611	-1.68272	-1.29681
H	1.13643	-0.55305	-3.42144
H	1.042374	1.109503	-5.29408
H	1.533059	3.532277	-4.78701
H	2.073759	4.193692	-2.44915
C	6.811832	-0.88608	-0.73897
H	3.083646	2.807131	3.50368
H	3.146714	4.838265	2.005681
H	2.590164	4.575811	-0.40577
C	4.735084	0.007233	-1.59862
C	1.609484	-2.26565	2.164295
N	-4.02318	-0.59861	0.599715
H	-2.53923	4.580048	0.490903
C	-2.8423	3.908322	-1.53691
H	-4.18258	0.561665	2.332981
H	-1.35079	-3.44003	-3.96898
C	-6.08536	-1.48948	-0.30661
H	-0.57672	-1.97405	-2.06959
C	-2.06389	-3.03008	-3.26142
C	-4.32902	-2.75839	-2.44146
H	-1.15646	-0.62215	3.412701
C	-1.26874	1.350705	4.311728
H	3.792928	-4.02588	4.109455
C	-2.21079	2.444851	0.301843
C	-2.82927	2.791884	-2.39444
C	-2.52357	3.728584	-0.17967
C	-4.73836	-0.0106	1.601677
C	-4.68808	-1.33915	-0.35726
C	-3.83517	-1.94832	-1.40105
C	-1.33797	0.434458	3.252541
C	-1.88359	2.145666	1.71135
C	-2.51136	1.533632	-1.86575
H	-2.50468	0.64895	-2.48878
C	-1.52078	2.711842	4.048834
C	-1.6238	-2.21543	-2.20886
H	-3.07869	2.887021	-3.44594
H	-7.89733	-0.99536	0.775543
C	1.858657	3.156142	-2.6777
H	-1.4919	3.443877	4.850248
H	-3.10509	4.892566	-1.91253
H	-6.65876	0.348653	2.517798
H	-6.60785	-2.06945	-1.0582
C	-6.81844	-0.88326	0.729072

C	-6.1311	-0.13273	1.701277
H	-5.38874	-2.9687	-2.52457
C	-3.4403	-3.30534	-3.38215
H	-1.03929	1.005249	5.314355
H	-2.0234	4.154548	2.524883
H	-2.49211	-2.54021	2.190555
H	-1.63398	-3.20382	1.008389
H	1.650853	-3.19022	-1.09074
H	2.482866	-2.47634	-2.26244

Table S11. Cartesian Coordinates for BD×12H_2O (optimized geometry, strong coupling).

Element	x	y	z
C	-2.60395	1.034324	2.465118
C	-5.2813	-3.37186	1.062336
C	-2.96853	2.494085	-2.02333
C	0.198	-4.57909	2.009925
C	-2.9642	1.445104	3.754742
C	-2.17758	1.543402	-1.36238
C	-4.36339	2.320275	-2.06477
C	0	-4.40391	3.394262
C	-2.67679	0.602557	4.846245
C	-5.92568	-1.36502	-0.12677
C	-4.92637	1.185026	-1.45848
C	-0.22833	-3.5748	1.131207
C	-2.02418	-0.6168	4.606708
C	-4.57481	-0.97412	-0.15601
C	-4.09138	0.260355	-0.80597
C	-1.02214	-2.24825	2.929783
C	-1.68387	-0.98119	3.290316
C	0.611852	3.226362	3.854808
C	4.091379	-0.26036	-0.80597
C	4.574813	0.974117	-0.15601
C	3.952909	2.929704	1.008897
C	2.024178	0.616797	4.606708
C	2.964195	-1.4451	3.754742
C	2.968526	-2.49409	-2.02333
C	1.683865	0.981185	3.290316
C	-3.95291	-2.9297	1.008897
C	-0.198	4.579094	2.009925
C	4.926371	-1.18503	-1.45848

C	5.92568	1.365015	-0.12677
C	2.676786	-0.60256	4.846245
C	-6.28821	-2.57189	0.492589
C	0.228334	3.574798	1.131207
C	1.022144	2.248246	2.929783
C	2.603949	-1.03432	2.465118
C	0	4.403907	3.394262
C	2.177577	-1.5434	-1.36238
C	-0.61185	-3.22636	3.854808
C	6.288213	2.571893	0.492589
C	5.281296	3.371864	1.062336
C	4.363393	-2.32028	-2.06477
H	0.660758	-5.47693	1.615266
H	0.308162	-5.17078	4.098468
H	-0.7737	-3.08442	4.917215
H	-3.4736	2.392617	3.894865
H	-6.69039	-0.74248	-0.57614
H	-1.80453	-1.28042	5.435217
H	1.804534	1.280419	5.435217
H	3.155294	3.527858	1.426786
H	2.492677	-3.34479	-2.49747
H	1.095991	-1.62134	-1.32188
H	-2.96467	0.882848	5.854708
H	0.116001	3.666031	0.058578
H	-5.00094	3.04551	-2.56119
H	-2.81875	1.64931	1.600616
H	-5.51616	-4.31568	1.542437
H	5.000938	-3.04551	-2.56119
H	2.818745	-1.64931	1.600616
H	-5.99858	1.032387	-1.49295
H	-3.15529	-3.52786	1.426786
H	3.473597	-2.39262	3.894865
H	7.328647	2.879396	0.528885
H	-7.32865	-2.8794	0.528885
H	-0.30816	5.170775	4.098468
H	2.964669	-0.88285	5.854708
H	5.51616	4.315677	1.542437
H	6.69039	0.742479	-0.57614
H	-1.09599	1.621341	-1.32188
H	-2.49268	3.344786	-2.49747
H	5.998583	-1.03239	-1.49295
H	-0.116	-3.66603	0.058578
H	-0.66076	5.476928	1.615266

H	0.773696	3.084422	4.917215
H	1.660548	3.050213	-1.50399
H	-1.66055	-3.05021	-1.50399
N	-1.98757	-0.15612	2.226755
N	-0.83185	-2.4388	1.578257
N	-2.73109	0.460962	-0.75052
N	2.731089	-0.46096	-0.75052
N	1.987568	0.156115	2.226755
N	-3.60105	-1.75332	0.424141
N	0.831851	2.438796	1.578257
N	3.601046	1.753319	0.424141
O	0	0	0.031781
Ru	1.622834	0.958416	0.348771
Ru	-1.62283	-0.95842	0.348771
O	-1.26839	-2.0511	-1.44177
O	-2.21529	-4.31132	-1.65628
O	1.268385	2.051101	-1.44177
O	2.215288	4.311318	-1.65628
O	1.196581	6.717437	-1.14316
O	-4.08579	-4.23602	-3.42413
O	-1.19658	-6.71744	-1.14316
O	4.08579	4.236023	-3.42413
H	1.33321	1.606595	-2.33839
H	-1.33321	-1.6066	-2.33839
O	1.456239	1.212012	-4.03074
O	-1.45624	-1.21201	-4.03074
O	-3.35292	-2.72464	-5.60718
O	1.108888	-1.25118	-4.5726
O	-1.10889	1.251176	-4.5726
O	3.352924	2.724641	-5.60718
H	1.524051	-1.84944	-5.21723
H	0.127339	-1.4306	-4.40824
H	2.92248	3.268724	-6.29928
H	4.065903	2.186435	-6.00934
H	-2.92248	-3.26872	-6.29928
H	-4.0659	-2.18644	-6.00934
H	-0.12734	1.430602	-4.40824
H	-1.52405	1.849436	-5.21723
H	1.695277	7.34798	-0.58786
H	0.631696	7.202814	-1.77544
H	4.885618	4.786978	-3.49282
H	3.89875	3.717224	-4.24722
H	-0.6317	-7.20281	-1.77544

H	-1.69528	-7.34798	-0.58786
H	-4.88562	-4.78698	-3.49282
H	-3.89875	-3.71722	-4.24722
H	-2.99562	-4.34665	-2.30111
H	-1.8109	-5.20424	-1.46708
H	2.995621	4.346651	-2.30111
H	1.810899	5.204238	-1.46708
H	-2.12953	-1.73917	-4.52742
H	-1.48172	-0.21046	-4.26009
H	1.481723	0.210461	-4.26009
H	2.129532	1.739174	-4.52742

Table S12. Cartesian Coordinates for $[(bpy)_2(H_2O)RuORu(OH_2)(bpy)_2]^{5+}$ (optimized geometry). [3,4]-bis-aqua.

Element	x	y	z
C	2.675367	-1.81754	-1.45803
C	0.321702	-6.31355	0.157042
C	3.67822	-0.88882	3.142578
C	-3.57356	-2.68864	-1.51061
C	3.337871	-2.02515	-2.6743
C	2.575838	-0.79855	2.281613
C	4.210446	-2.15902	3.443244
C	-3.18237	-2.92363	-2.84542
C	2.585524	-2.38679	-3.81036
C	2.16476	-5.63518	1.581185
C	3.613777	-3.29862	2.875462
C	-2.59377	-2.33584	-0.57131
C	1.188469	-2.51504	-3.69372
C	1.798154	-4.29189	1.394299
C	2.505554	-3.15632	2.018976
C	-0.88314	-2.4372	-2.21254
C	0.565869	-2.29767	-2.45296
C	1.8261	2.786442	-3.19693
C	-2.50555	3.156324	2.018976
C	-1.79815	4.291892	1.394299
C	0	4.960571	-0.00606
C	-1.18847	2.515039	-3.69372
C	-3.33787	2.025148	-2.6743
C	-3.67822	0.88882	3.142578
C	-0.56587	2.297672	-2.45296
C	0	-4.96057	-0.00606

C	3.573562	2.688635	-1.51061
C	-3.61378	3.298616	2.875462
C	-2.16476	5.635181	1.581185
C	-2.58552	2.38679	-3.81036
C	1.425828	-6.66092	0.960714
C	2.593767	2.335839	-0.57131
C	0.883135	2.437203	-2.21254
C	-2.67537	1.817535	-1.45803
C	3.182369	2.923625	-2.84542
C	-2.57584	0.798547	2.281613
C	-1.8261	-2.78644	-3.19693
C	-1.42583	6.66092	0.960714
C	-0.3217	6.313551	0.157042
C	-4.21045	2.159018	3.443244
H	-4.60947	-2.79156	-1.20321
H	-3.915	-3.2168	-3.59207
H	-1.51903	-2.97123	-4.2204
H	4.417527	-1.92655	-2.72377
H	3.01346	-5.89694	2.202515
H	0.604871	-2.80105	-4.5616
H	-0.60487	2.801048	-4.5616
H	0.843655	4.673672	-0.61789
H	-4.11291	-0.00881	3.570458
H	-2.12813	-0.1552	2.0298
H	3.07552	-2.57619	-4.76135
H	2.855872	2.15095	0.464424
H	5.065353	-2.26069	4.105596
H	3.221476	-1.5566	-0.56093
H	-0.27776	-7.0738	-0.33346
H	-5.06535	2.260687	4.105596
H	-3.22148	1.556601	-0.56093
H	4.013886	-4.27867	3.107995
H	-0.84366	-4.67367	-0.61789
H	-4.41753	1.926549	-2.72377
H	-1.7037	7.701486	1.103182
H	1.703702	-7.70149	1.103182
H	3.915001	3.216799	-3.59207
H	-3.07552	2.576185	-4.76135
H	0.277759	7.073802	-0.33346
H	-3.01346	5.89694	2.202515
H	2.128131	0.155202	2.0298
H	4.112908	0.008806	3.570458
H	-4.01389	4.278673	3.107995

H	-2.85587	-2.15095	0.464424
H	4.609471	2.791564	-1.20321
H	1.519027	2.971227	-4.2204
H	1.429823	2.967511	2.412722
H	0.403742	1.982062	3.157301
H	-0.40374	-1.98206	3.157301
H	-1.42982	-2.96751	2.412722
N	1.322011	-1.95521	-1.3448
N	-1.27788	-2.22334	-0.90719
N	1.999779	-1.90546	1.725563
N	-1.99978	1.905461	1.725563
N	-1.32201	1.95521	-1.3448
N	0.714312	-3.95947	0.596758
N	1.277876	2.223336	-0.90719
N	-0.71431	3.959472	0.596758
O	0.843963	2.188421	2.306157
O	0	0	0.461038
O	-0.84396	-2.18842	2.306157
Ru	-0.30751	1.889156	0.434039
Ru	0.307507	-1.88916	0.434039

Table S13. Cartesian Coordinates for optimized geometry of $[(bpy)_2ClRuORuCl(bpy)_2]^{2+}$.

Element	x	y	z
C	2.947524	-1.90895	-0.58106
C	-0.34089	-6.26278	-0.3326
C	2.028051	-1.36428	4.109978
C	-2.79333	-1.93904	-3.13721
C	4.025349	-1.99202	-1.47043
C	1.447854	-1.13004	2.854154
C	2.13095	-2.68522	4.580794
C	-1.9267	-2.01841	-4.2457
C	3.764442	-2.06812	-2.85277
C	0.631487	-5.85518	1.848131
C	1.668106	-3.73475	3.770349
C	-2.25028	-1.85835	-1.84812
C	2.434235	-2.04163	-3.29736
C	0.617052	-4.47521	1.574816
C	1.10486	-3.44577	2.514751
C	-0.04383	-1.93001	-2.71211
C	1.386725	-1.95182	-2.36103
C	0.540329	2.01143	-4.0273

C	-1.10486	3.445772	2.514751
C	-0.61705	4.475212	1.574816
C	0.329513	4.879644	-0.54974
C	-2.43424	2.041628	-3.29736
C	-4.02535	1.992021	-1.47043
C	-2.02805	1.364275	4.109978
C	-1.38673	1.951815	-2.36103
C	-0.32951	-4.87964	-0.54974
C	2.79333	1.939038	-3.13721
C	-1.66811	3.734752	3.770349
C	-0.63149	5.855183	1.848131
C	-3.76444	2.06812	-2.85277
C	0.147226	-6.759	0.890325
C	2.250276	1.858348	-1.84812
C	0.043826	1.930014	-2.71211
C	-2.94752	1.908949	-0.58106
C	1.926702	2.018405	-4.2457
C	-1.44785	1.130041	2.854154
C	-0.54033	-2.01143	-4.0273
C	-0.14723	6.759	0.890325
C	0.340891	6.262777	-0.3326
C	-2.13095	2.685217	4.580794
N	1.656763	-1.89952	-1.01136
N	-0.90337	-1.85772	-1.63565
N	0.991846	-2.14814	2.077562
N	-0.99185	2.148139	2.077562
N	-1.65676	1.899517	-1.01136
N	0.134151	-4.00322	0.378711
N	0.903368	1.857722	-1.63565
N	-0.13415	4.003222	0.378711
O	0	0	0.510403
Ru	0	1.885067	0.238105
Ru	0	-1.88507	0.238105
Cl	2.128003	2.159445	1.481136
Cl	-2.128	-2.15945	1.481136
H	3.101555	-1.84801	0.488622
H	-0.72827	-6.92681	-1.09756
H	2.389564	-0.52391	4.692525
H	-3.87084	-1.9556	-3.26203
H	5.039289	-2.00244	-1.08536
H	1.355035	-0.13066	2.446456
H	2.567378	-2.89639	5.552103
H	-2.32231	-2.09857	-5.25359

H	4.579547	-2.1488	-3.56523
H	1.005669	-6.22444	2.795415
H	1.749292	-4.75835	4.116344
H	-2.86519	-1.82464	-0.95553
H	2.218008	-2.09925	-4.35803
H	-0.14025	2.08574	-4.86798
H	0.713341	4.459327	-1.47032
H	-2.21801	2.099254	-4.35803
H	-5.03929	2.00244	-1.08536
H	-2.38956	0.523907	4.692525
H	-0.71334	-4.45933	-1.47032
H	3.870839	1.955598	-3.26203
H	-1.74929	4.758347	4.116344
H	-1.00567	6.224439	2.795415
H	-4.57955	2.148798	-3.56523
H	0.14704	-7.82512	1.094568
H	2.865189	1.824637	-0.95553
H	-3.10156	1.848008	0.488622
H	2.32231	2.098568	-5.25359
H	-1.35504	0.13066	2.446456
H	0.140248	-2.08574	-4.86798
H	-0.14704	7.825116	1.094568
H	0.728269	6.926807	-1.09756
H	-2.56738	2.896386	5.552103

Table S14. Cartesian Coordinates for optimized geometry of $[(bpy)_2ClRuORuCl(bpy)_2]^{3+}$.

Element	x	y	z
C	-2.53983	0.370549	-2.70707
C	-6.09067	0.16568	1.447959
C	-1.5004	-4.1169	-1.70589
C	-1.72864	3.455935	2.737899
C	-2.9112	1.153424	-3.80848
C	-1.22947	-2.82708	-1.22641
C	-2.78092	-4.66445	-1.51055
C	-2.08679	4.457744	1.816394
C	-3.07396	2.540075	-3.63165
C	-5.73857	-2.0445	0.520716
C	-3.75868	-3.89197	-0.86165
C	-1.62597	2.128145	2.294292
C	-2.84629	3.100877	-2.36263
C	-4.4083	-1.69299	0.234498

C	-3.44004	-2.59875	-0.41152
C	-2.21304	2.759276	0.082232
C	-2.47004	2.27207	-1.29113
C	2.32799	4.104402	-0.47582
C	3.440075	-2.59864	0.411449
C	4.408163	-1.693	-0.23498
C	4.75668	0.461955	-1.14517
C	2.847348	3.100515	2.362838
C	2.912314	1.152941	3.808512
C	1.500677	-4.11662	1.706422
C	2.470636	2.271866	1.291369
C	-4.75712	0.462256	1.143913
C	1.727912	3.45639	-2.73722
C	3.758819	-3.89178	0.86176
C	5.738328	-2.04461	-0.52156
C	3.075282	2.539574	3.631746
C	-6.59049	-1.11156	1.133537
C	1.625267	2.128547	-2.29377
C	2.213224	2.759277	-0.08183
C	2.540502	0.370222	2.707136
C	2.086532	4.458019	-1.8157
C	1.229641	-2.82689	1.226795
C	-2.32779	4.104358	0.476373
C	6.590048	-1.11186	-1.13496
C	6.090114	0.16527	-1.44963
C	2.781188	-4.66417	1.510963
N	-2.32912	0.914499	-1.47915
N	-1.86463	1.790956	0.998735
N	-2.17414	-2.08715	-0.58481
N	2.174194	-2.08706	0.584888
N	2.32956	0.914296	1.479312
N	-3.93076	-0.44156	0.550873
N	1.86438	1.79113	-0.99835
N	3.93053	-0.44164	-0.55151
O	-1.6E-05	-0.13913	0.000252
Ru	1.853928	-0.17503	-0.24461
Ru	-1.85403	-0.17509	0.244735
Cl	1.672923	-1.21879	-2.45376
Cl	-1.67367	-1.21931	2.453692
H	-2.40741	-0.69953	-2.79908
H	-6.71365	0.913329	1.926413
H	-0.72225	-4.66677	-2.224
H	-1.55214	3.687711	3.782765

H	-3.07357	0.683567	-4.77243
H	-0.26118	-2.36677	-1.37918
H	-3.01851	-5.66291	-1.86401
H	-2.19073	5.490449	2.135194
H	-3.37565	3.170853	-4.46221
H	-6.11187	-3.03253	0.279862
H	-4.75378	-4.29567	-0.71885
H	-1.38417	1.308933	2.961948
H	-2.97284	4.167365	-2.21736
H	2.617327	4.867996	0.236886
H	4.336619	1.425541	-1.39682
H	2.974019	4.166997	2.217634
H	3.074838	0.682972	4.772375
H	0.722632	-4.66643	2.224749
H	-4.33716	1.425928	1.395391
H	1.551039	3.688336	-3.78198
H	4.753906	-4.29549	0.718869
H	6.11169	-3.03258	-0.28057
H	3.377301	3.170236	4.462272
H	-7.61743	-1.37666	1.364545
H	1.383146	1.309461	-2.96146
H	2.407924	-0.69984	2.799109
H	2.1905	5.490758	-2.13438
H	0.261362	-2.36656	1.379653
H	-2.61675	4.868087	-0.23634
H	7.616899	-1.37705	-1.36626
H	6.712908	0.912756	-1.92858
H	3.018868	-5.66256	1.864554

Table S15. Cartesian Coordinates for $Ru(bpy)_2Cl_2$ (optimized geometry).

Element	x	y	z
Ru	0	0	0.532821
N	0.572083	1.982683	0.511597
C	1.020042	4.755154	0.542165
C	-0.21201	2.819617	-0.25203
C	1.557327	2.511449	1.290303
C	1.808888	3.888638	1.325788
C	0	4.211801	-0.25158
H	2.103777	1.790987	1.89089
H	2.597169	4.268933	1.967445
H	-0.62977	4.862095	-0.84897

H	1.189403	5.827973	0.559633
N	-0.57208	-1.98268	0.511597
C	-1.02004	-4.75515	0.542165
C	0.212013	-2.81962	-0.25203
C	-1.55733	-2.51145	1.290303
C	-1.80889	-3.88864	1.325788
C	0	-4.2118	-0.25158
H	-2.10378	-1.79099	1.89089
H	-2.59717	-4.26893	1.967445
H	0.629773	-4.8621	-0.84897
H	-1.1894	-5.82797	0.559633
N	-1.29982	0.764532	-0.85557
C	-3.094	2.030902	-2.61837
C	-2.22857	0.042308	-1.54352
C	-1.25126	2.133051	-1.03371
C	-2.14238	2.77876	-1.91257
C	-3.13449	0.633853	-2.42831
H	-2.23741	-1.0237	-1.35217
H	-2.09588	3.855013	-2.03788
H	-3.85913	0.014024	-2.94662
H	-3.78932	2.52046	-3.29373
N	1.299819	-0.76453	-0.85557
C	3.094002	-2.0309	-2.61837
C	1.251261	-2.13305	-1.03371
C	2.228567	-0.04231	-1.54352
C	3.134489	-0.63385	-2.42831
C	2.142376	-2.77876	-1.91257
H	2.237414	1.023701	-1.35217
H	3.859134	-0.01402	-2.94662
H	2.095879	-3.85501	-2.03788
H	3.78932	-2.52046	-3.29373
Cl	1.697236	-0.67459	2.237535
Cl	-1.69724	0.674589	2.237535

References

1. Frisch, M. J. ; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; J.A. Montgomery, J.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, revision D.01; Gaussian Inc., Wallingford, CT, 2004.

2. Becke, A. D. *Phys. Rev., Ser. A* **1988**, *38*, 3098-3100.

3. Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 1372-1377.

4. Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648-5652.

5. Stevens, P. J.; Devlin, F. J.; Chablowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623-11627.

6. Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev.* **1988**, *B37*, 785-789.

7. Stratmann, R. E.; Scuseria, G. E.; Frisch, M. J. *J. Chem. Phys.* **1998**, *109*, 8218-8224.

8. Bauernschmitt, R.; Ahlrichs, R. *Chem. Phys. Lett.* **1996**, *256*, 454-464.

9. Casida, M. E. ; Jamorski, C.; Casida, K. C.; Salahub, D. R. *J. Chem. Phys.* **1998**, *108*, 4439-4449.

10. Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995-2001.

11. Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. *J. Comp. Chem.* **2003**, *24*, 669-681.

12. Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev.* **2005**, *105* (8), 2999-3093.

13. Cance`s, E.; Mennucci, B.; Tomasi, J. *J. Chem. Phys.* **1997**, *107*, 3032.

14. Mennucci, B.; Cance`s, E.; Tomasi, J. *J. Phys. Chem. B* **1997**, *101*, 10506.

15. Cance`s, E.; Mennucci, B. *J. Math. Chem.* **1998**, *23*, 309.

16. Nazeeruddin, M. K.; Wang, Q.; Cevey, L.; Aranyos, V.; Liska, P.; Figgemeier, E.; Klein, C.; Hirata, N.; Koops, S.; Haque, S. A.; Durrant, J. R.; Hagfeldt, A.; Lever, A. B. P.; Graetzel, M. *Inorg. Chem.* **2006**, *45*(2), 787-797.

17. Baik, M.-H.; Friesner, R. A. *J. Phys. Chem. A* **2002**, *106*(32), 7407-7412.

18. Yang, X.; Baik, M.-H. *J. Am. Chem. Soc.* **2004**, *126*(41), 13222-13223.

19. Yang, X.; Baik, M.-H. *J. Am. Chem. Soc.* **2006**, *128*(23), 7476-7485.

20. Gilbert, J. A.; Eggleston, D. S.; Murphy, W. R. Jr.; Geselowitz, D. A.; Gersten, S. W.; Hodgson, D. J.; Meyer, T. J. *J. Am. Chem. Soc.* **1985**, *107*(13), 3855-3864.

21. Ishitani, O.; White, P. S.; Meyer, T. J. *Inorg. Chem.* **1996**, *35*, 2167-2168.

22. Phelps, D. W.; Kahn, E. M.; Hodgson, D. J. *Inorg. Chem.* **1975**, *14*, 2486.

23. Concepcion, J. J.; Meyer, T. J. *Unpublished Results*.

24. Batista, E. R.; Martin, R. L. *J. Am. Chem. Soc.* **2007**, *129*(23), 7224-7225.