SUPPORTING INFORMATION

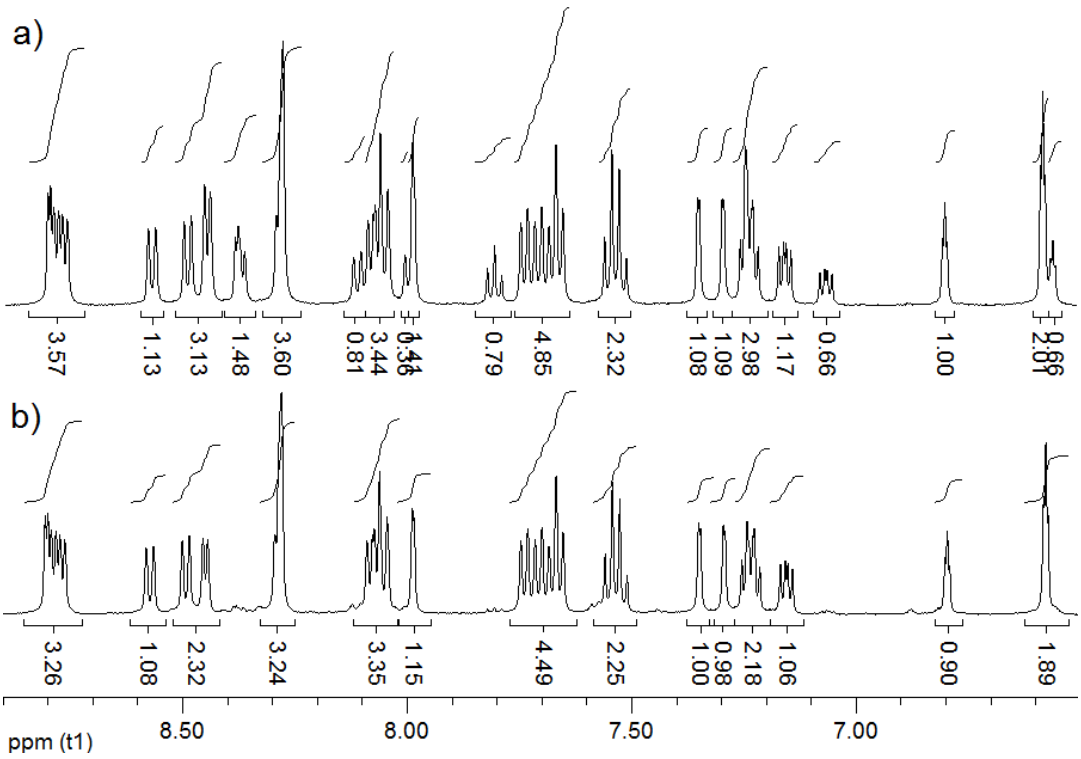

Figure S1. ^{1}H-NMR spectra of (a) *mer/fac mixture* of $[Ru(Q1Pz)_3]^{2+}$ and (b) *mer*-$[Ru(Q1Pz)_3]^{2+}$ isolated product after light illumination.

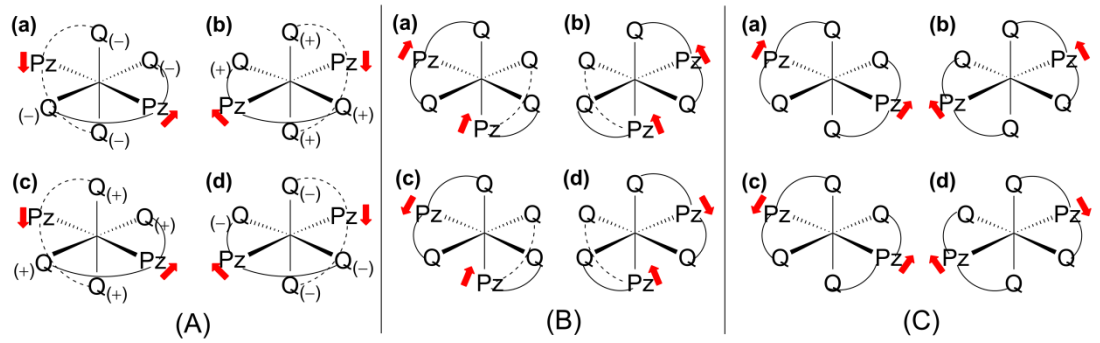

Figure S2. Illustrations of different stereoisomers for which optimized total energies have been calculated (A, left) *meridional*, (B, centre) *cis-facial* and (C, right) *trans-facial* isomers. The red arrow indicates the plane and direction of the polarity of the pyrazole group. In (A) the subscript (+) and (–) indicate the sign of the dihedral angle between the *trans*-quinolines as defined in Figure S2 and the stereochemical labels for each isomer is (a) C-S_a, (b) A-R_a, (c) C-R_a and (d) A-S_a respectively. No stereochemical labels have been assigned to the *fac* isomers.

Table S1. Calculated total energy (eV) of each calculated isomer of $[Ru(DQPz)_2]^{2+}$, referenced to the lowest energy isomer of each complex. Isomers shown in Figure S2.

	mer-	*trans-fac-*	*cis-fac-*
(a)	0	0	0
(b)	0	0.000001	0.01
(c)	0.002	0.01	0.003
(d)	0.002	0.006	0.003

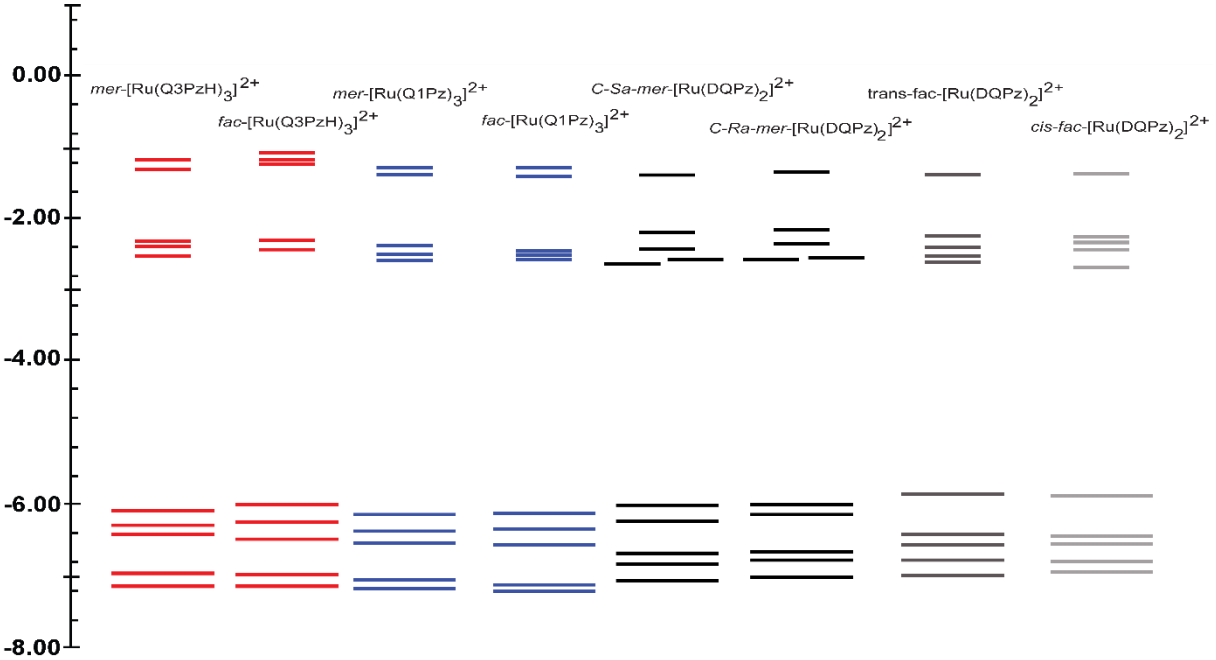

Figure S3: The first 5 HOMO and LUMOs of representative calculated complex isomers.

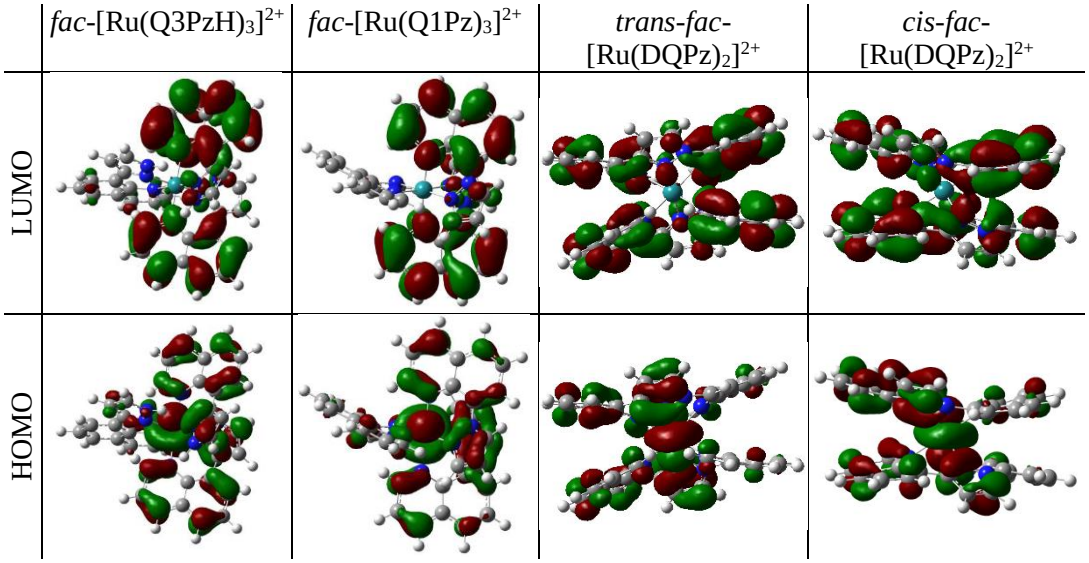

Figure S4. Frontier molecular orbitals of the *fac*-isomers of three complexes.

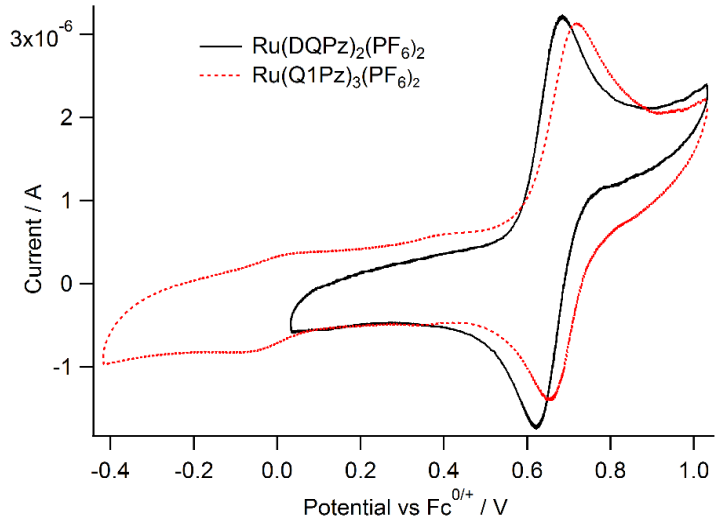

Figure S5. Cyclic voltammetry for the oxidations of *mer*-/*fac*-$[Ru(Q1Pz)_3]^{2+}$ and *mer*-$[Ru(DQPz)_2]^{2+}$.

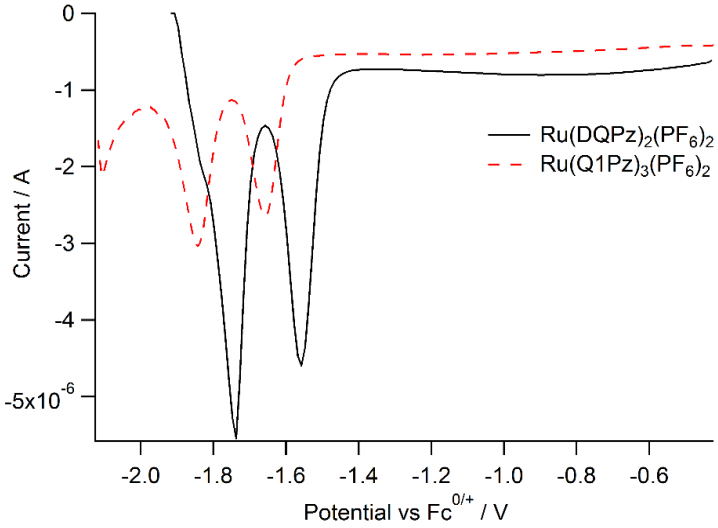

Figure S6. Differential pulse voltammetry for the reductions of *mer*-/*fac*-$[Ru(Q1Pz)_3]^{2+}$ and *mer*-$[Ru(DQPz)_2]^{2+}$.

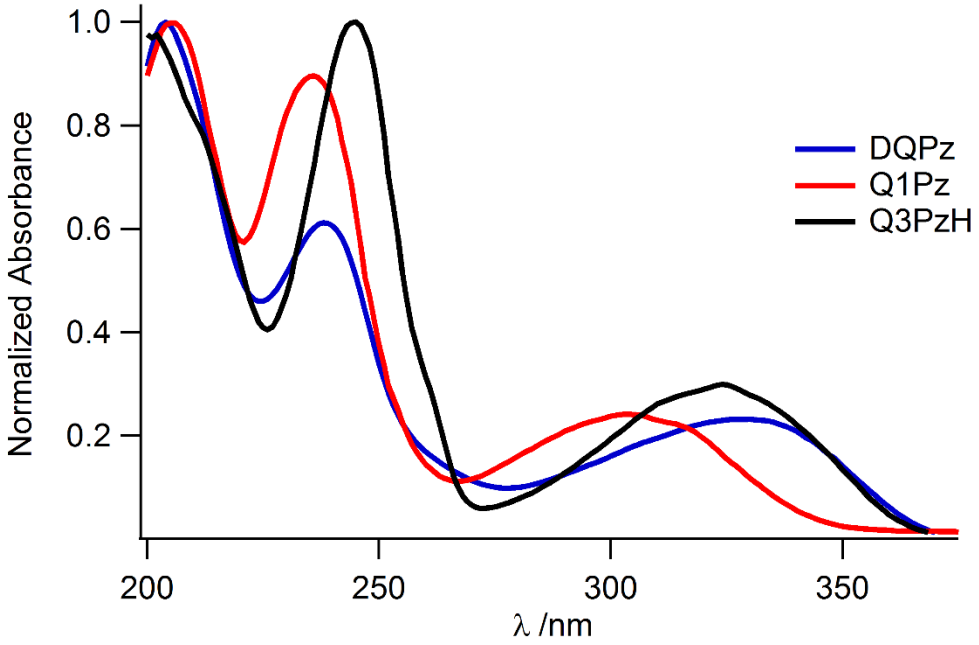

Figure S7. Electronic absorption spectra of ligands Q3PzH, Q1Pz and DQPz in neat acetonitrile.

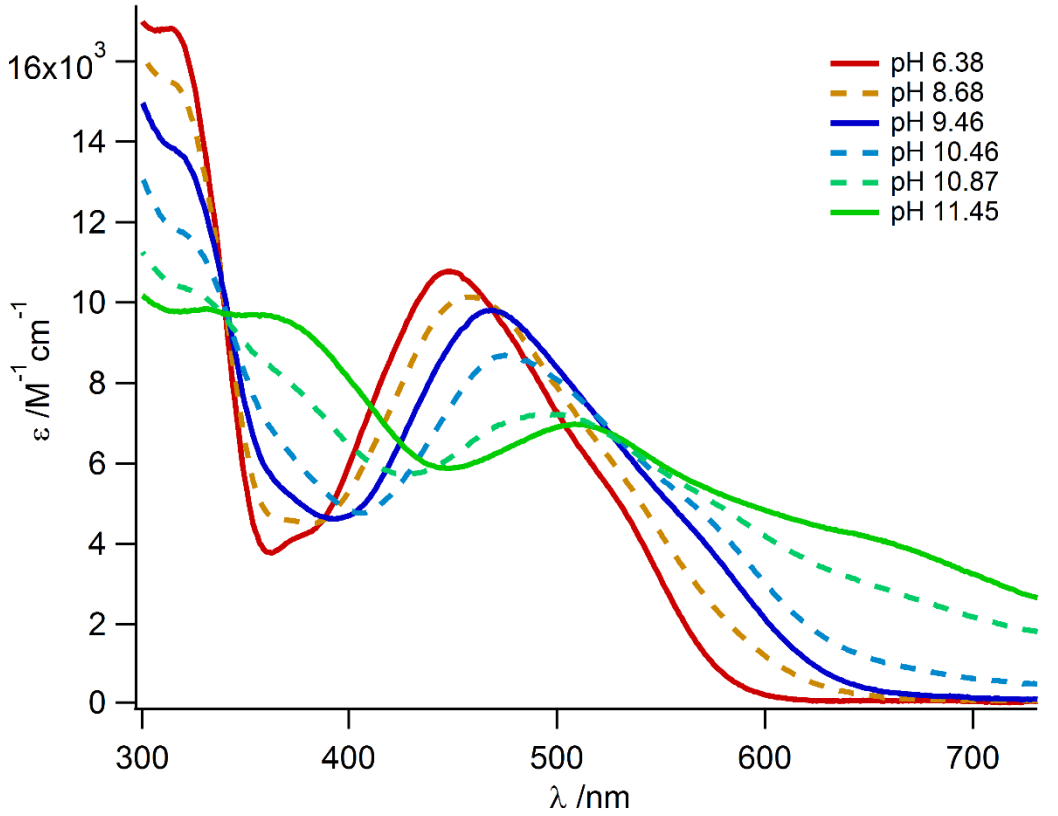

Figure S8. UV-Vis absorption spectra of *mer*-$[Ru(Q3PzH)_3]^{2+}$ in H_2O at different measured pH (set by HCl and NaOH).

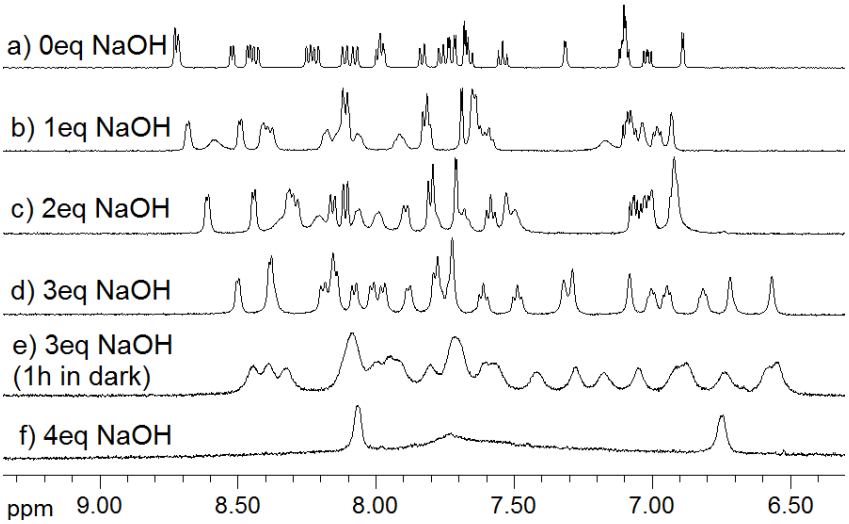

Figure S9. ^{1}H-NMR spectra of $[Ru(Q3PzH)_3]^{2+}$ in CD_3CN titrated with NaOH(aq). Number of equivalents: (a) 0, (b) 1.0, (c) 2.0, (d) 3.0, (e) 3.0 after 1 h at room temperature in the dark and (f) 4.0 (*i.e.* +1 equivalent to sample in e).

Table S2: Electro-spray ionization high resolution mass spectrometry on *mer*-$[Ru(Q3PzH)_3]^{2+}$, *mer*-$[Ru(Q1Pz)_3]^{2+}$ and *mer*-$[Ru(DQPz)_2]^{2+}$ after 5 h light with 10 equivalences of triflic acid[a]

Complex	***Species after 5h of irradiation[b]***	***m/z***	***Rel. int. (%)***	***Species without irradiation***	***m/z***	***Rel. int. (%)***
mer-$[Ru(Q3PzH)_3]^{2+}$	$[L+H^+]^+$ $[M]^{2+}$ $[M\text{-}L+CD_3CN]^{2+}$	196.08724 343.57125 266.54442	100 57 9	$[L+H^+]^+$ $[M]^{2+}$	196.08693 343.57159	20 100
mer-$[Ru(Q1Pz)_3]^{2+}$	$[L+H^+]^+$ $[M]^{2+}$ $[M\text{-}L]^{2+}$ $[M\text{-}L+CD_3CN]^{2+}$ $[M\text{-}L+2CD_3CN]^{2+}$	196.08657 343.57063 246.03088 266.54426 290.07610	100 20 9 9 5	$[L+H^+]^+$ $[M]^{2+}$ $[M^{2+}+PF_6^-]^+$ $[M^{2+}\text{-}L+DMSO+Cl^-]^+$	196.08657 343.57063 832.10831 605.04637	10 100 10 5[c]
mer-$[Ru(DQPz)_2]^{2+}$	$[M]^{2+}$	373.07371	100	$[M]^{2+}$	373.07377	100

[a] The sample with $[Ru(DQPz)_2]^{2+}$ had 20 equivalences triflic acid. [b] L represents the respective ligand. [c] A minor contamination from the synthesis.

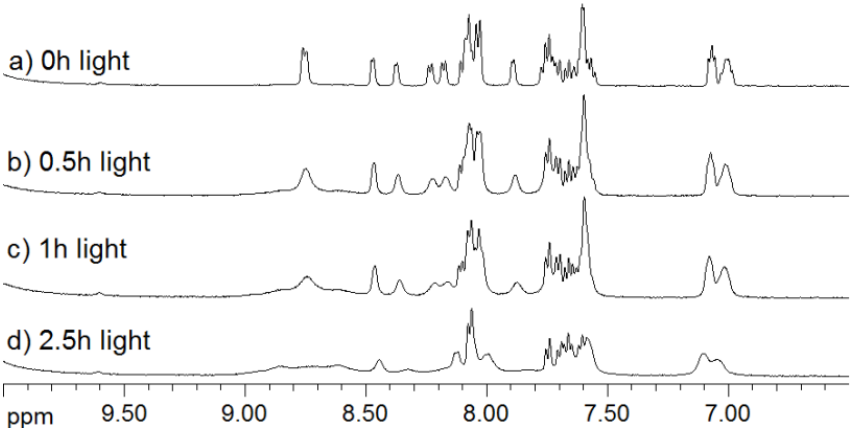

Figure S10. ^{1}H-NMR spectra of $[Ru(DQPz)_2]^{2+}$ with 20 equiv. triflic acid after exposure to visible light for (a) 0 h after keeping the sample in the dark for 2 h, (b) 0.5 h, (c) 1 h and (d) 2.5 h.

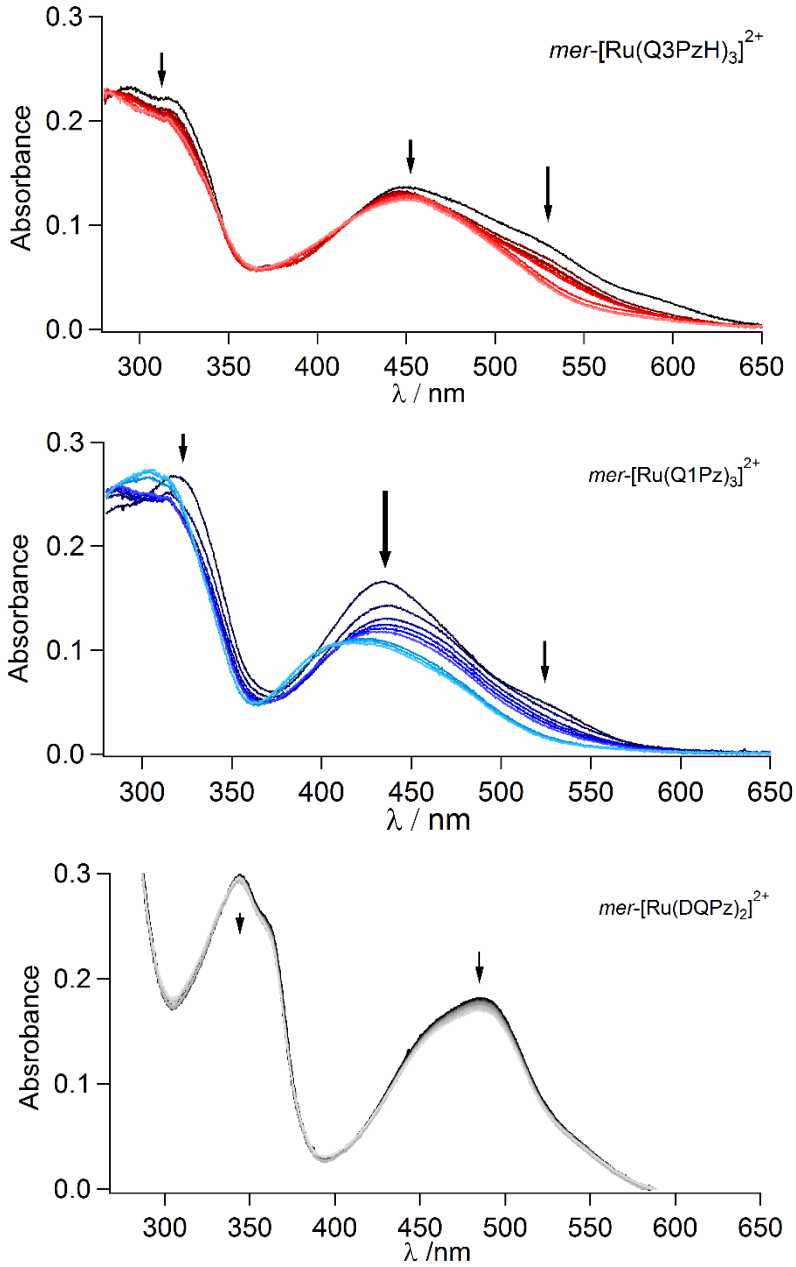

Figure S11. Absorption changes with continuous broad band visible light irradiation for (Top) *mer*-$[Ru(Q3PzH)_3]^{2+}$, (Middle) *mer*-$[Ru(Q1Pz)_3]^{2+}$ and (Bottom) *mer*-$[Ru(DQPz)_2]^{2+}$ in neat acetonitrile (without triflic acid).

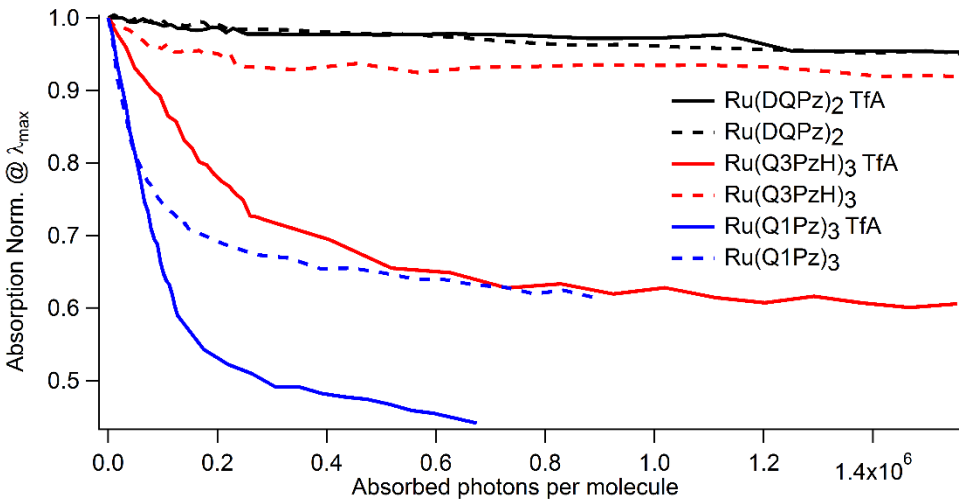

Figure S12: Kinetic traces following the changes in UV/vis absorption at specified wavelengths as a function of photons absorbed per molecule in the light experiment for *mer*-$[Ru(Q3PzH)_3]^{2+}$ (a) and *mer*-$[Ru(Q1Pz)_3]^{2+}$ (b). Solid lines are for experiments without acid and dashed lines are with 10 equiv. triflic acid.

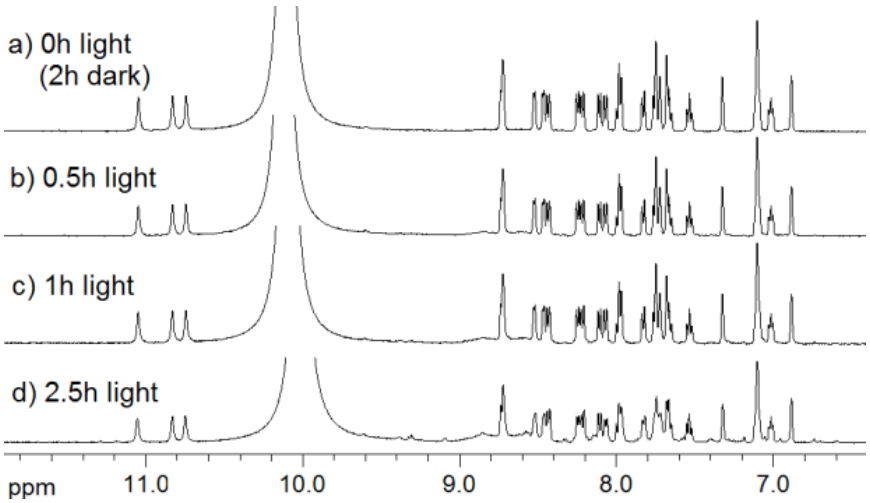

Figure S13. ^{1}H-NMR spectra of *mer*-$[Ru(Q3PzH)_3]^{2+}$ with 10 equiv. triflic acid after exposure to visible light for (a) 0 h after keeping the sample in the dark for 2 h, (b) 0.5 h, (c) 1 h and (d) 2.5 h.

TDDFT calculated transitions for *fac*-$[Ru(Q3PzH)_3]^{2+}$ **(Table S3)**, *fac*-$[Ru(Q3PzH)_2(Q3Pz)]^{+}$ **(Table S4)**, *fac*-$[Ru(Q3PzH)(Q3Pz)_2]$ **(Table S5),** *fac*-$[Ru(Q3Pz)_3]^{-}$ **(Table S6),** *mer*-$[Ru(Q3PzH)_3]^{2+}$ **(Table S7),** *mer*-$[Ru(Q3PzH)_2(Q3Pz_a)]^{+}$ **(Table S8),** *mer*-$[Ru(Q3PzH)_2(Q3Pz_b)]^{+}$ **(Table S9),** *mer*-$[Ru(Q3PzH)_2(Q3Pz_c)]^{+}$ **(Table S10),** *mer*-$[Ru(Q3PzH_a)(Q3Pz)_2]$ **(Table S11),** *mer*-$[Ru(Q3PzH_b)(Q3Pz)_2]$ **(Table S12),** *mer*-$[Ru(Q3PzH_c)(Q3Pz)_2]$ **(Table S13),** *mer*-$[Ru(Q3Pz)_3]^{-}$ **(Table S14),** *fac*-$[Ru(Q1Pz)_3]^{2+}$**(Table S15),** *mer*-$[Ru(Q1Pz)_3]^{2+}$**(Table S16),** *cis-fac*-$[Ru(DQPz)_2]^{2+}$ **(Table S17),** *trans-fac*-$[Ru(DQPz)_2]^{2+}$ **(Table S18),** *C-R$_a$-mer*-$[Ru(DQPz)_2]^{2+}$ **(Table S19),** *C-S$_a$-mer*-$[Ru(DQPz)_2]^{2+}$ **(Table S20).**

Table S3. TDDFT calculated transitions for *fac*-$[Ru(Q3PzH)_3]^{2+}$.

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	2.6983	459.48	0.0199	160	→	161	0.17523
				160	→	162	0.67352
2	2.7374	452.93	0.0831	160	→	161	0.64617
				160	→	162	-0.17321
				160	→	163	-0.18627
3	2.8519	434.74	0.0508	159	→	161	-0.40809
				159	→	163	0.15969
				160	→	161	0.17516
				160	→	163	0.49971
4	2.8972	427.94	0.0486	158	→	162	0.1094
				159	→	161	0.12853
				159	→	162	0.64844
				159	→	163	-0.14987
				160	→	163	0.11858
5	2.9109	425.93	0.0202	158	→	162	-0.11042
				159	→	161	0.52244
				159	→	163	0.34499
				160	→	161	0.10375
				160	→	163	0.25514
6	2.9773	416.43	0.0037	158	→	162	0.26407
				159	→	161	-0.14231
				159	→	162	0.15287
				159	→	163	0.53776
				160	→	163	-0.26483
7	3.1097	398.71	0.0091	158	→	161	0.66699
				158	→	162	0.14543
				158	→	163	0.1162
8	3.1911	388.53	0.0511	158	→	162	-0.1647
				158	→	163	0.65001
				160	→	163	-0.12731
9	3.204	386.96	0.0782	158	→	161	-0.141
				158	→	162	0.57048
				158	→	163	0.17836
				159	→	162	-0.19346
				159	→	163	-0.13544
				160	→	163	0.16151

10	3.6411	340.51	0.0031	160	→	164	0.25414
				160	→	165	0.42522
				160	→	169	-0.1187
				160	→	173	0.13151
				160	→	174	0.3236
				160	→	175	0.11661
11	3.7505	330.58	0.0009	158	→	174	0.11408
				158	→	175	-0.13734
				159	→	165	0.10576
				159	→	174	0.17126
				160	→	164	0.21208
				160	→	165	-0.15849
				160	→	166	-0.15704
				160	→	167	0.18701
				160	→	168	0.17487
				160	→	170	0.13123
				160	→	171	-0.17011
				160	→	175	0.28627
				160	→	177	-0.10436
12	3.8268	323.99	0.0056	158	→	165	-0.12856
				158	→	174	-0.23017
				159	→	165	-0.15858
				159	→	167	0.15902
				159	→	168	0.11082
				159	→	170	0.16253
				159	→	171	-0.20701
				159	→	172	-0.10561
				159	→	174	-0.10271
				159	→	175	0.33503
				159	→	177	-0.12639
				160	→	165	-0.20335
13	3.8579	321.38	0.0916	157	→	161	0.55978
				157	→	162	0.31005
				157	→	163	-0.18636
14	3.8809	319.48	0.0392	157	→	161	-0.23442
				157	→	163	-0.15171
				159	→	164	-0.19617
				159	→	165	-0.16474
				159	→	174	-0.15728
				160	→	164	0.34514
				160	→	165	-0.30778
				160	→	166	0.12518
15	3.9145	316.73	0.0396	155	→	161	-0.11339
				156	→	161	-0.1072
				156	→	162	-0.1276
				157	→	161	-0.21489

				157	→	162	0.3641
				157	→	163	-0.32516
				158	→	174	-0.10053
				160	→	165	0.23033
				160	→	166	-0.16443
				160	→	174	-0.12727
16	3.9314	315.37	0.0274	156	→	161	0.1104
				157	→	161	0.14147
				157	→	162	-0.12065
				157	→	163	0.18319
				158	→	165	-0.13173
				158	→	174	-0.19866
				160	→	164	0.40802
				160	→	165	0.12283
				160	→	166	-0.20789
				160	→	174	-0.19134
				160	→	175	-0.12927
17	3.976	311.83	0.0841	156	→	161	-0.2279
				156	→	162	0.48988
				157	→	162	-0.23466
				157	→	163	-0.29073
				160	→	166	-0.16052
18	4.0056	309.53	0.0061	155	→	161	-0.13729
				156	→	161	-0.19019
				156	→	162	-0.13447
				157	→	161	0.1255
				157	→	162	-0.20193
				157	→	163	-0.15954
				158	→	175	-0.10934
				160	→	165	0.14585
				160	→	166	0.41167
				160	→	167	0.1127
				160	→	174	-0.13138
19	4.0151	308.79	0.0312	155	→	161	0.13785
				155	→	162	-0.11103
				156	→	161	0.10149
				156	→	162	0.36399
				157	→	162	0.32086
				157	→	163	0.15814
				159	→	165	0.15823
				160	→	166	0.26397
20	4.0378	307.06	0.0135	155	→	161	0.13237
				155	→	162	0.1783
				156	→	161	0.34454
				157	→	162	-0.13267
				157	→	163	-0.31156

				159	→	164	0.2407
				159	→	165	0.1361
				160	→	164	0.12934
				160	→	166	0.11469
				160	→	168	-0.20421
21	4.0558	305.7	0.0199	155	→	162	-0.11113
				156	→	161	-0.33911
				157	→	163	0.18733
				159	→	164	0.3427
				159	→	166	0.18063
				159	→	167	0.1009
				160	→	164	0.19604
				160	→	167	-0.17145
				160	→	168	-0.21008
22	4.079	303.96	0.0627	155	→	161	-0.14086
				155	→	162	-0.19981
				155	→	163	0.12889
				156	→	162	-0.13618
				156	→	163	0.25809
				158	→	164	0.1142
				159	→	164	-0.13831
				159	→	165	0.3889
				159	→	166	-0.16342
				160	→	167	-0.1659
				160	→	168	-0.10449
23	4.1003	302.38	0.0026	155	→	161	-0.17088
				155	→	162	-0.21043
				155	→	163	0.12239
				156	→	161	0.29021
				156	→	163	0.38397
				159	→	164	0.18943
				159	→	165	-0.2438
24	4.1704	297.3	0.0036	155	→	161	0.10124
				158	→	174	-0.10702
				158	→	175	0.11395
				159	→	164	0.21173
				159	→	165	0.28163
				159	→	166	0.11742
				159	→	167	-0.12366
				159	→	168	-0.12819
				160	→	167	0.28815
				160	→	168	0.28257
25	4.1837	296.35	0.0026	155	→	161	0.52792
				155	→	162	-0.14209
				155	→	163	0.11758
				156	→	162	-0.14159

				156	→	163	0.13402
				157	→	163	-0.11285
				160	→	167	0.16531
				160	→	168	-0.18066
26	4.1986	295.3	0.003	155	→	161	-0.16664
				155	→	162	0.376
				156	→	163	0.21797
				158	→	164	-0.18992
				158	→	166	-0.10206
				159	→	166	-0.13027
				159	→	167	-0.14206
				160	→	166	-0.11345
				160	→	167	0.21163
				160	→	168	-0.23553
27	4.2084	294.61	0.0087	158	→	164	-0.14729
				159	→	164	-0.30996
				159	→	166	0.48837
				159	→	167	0.11396
				159	→	168	-0.12371
				160	→	167	0.11281
				160	→	168	-0.19032
				160	→	169	-0.11165
28	4.2162	294.06	0.0061	155	→	161	0.17653
				155	→	162	0.37936
				156	→	161	-0.10705
				156	→	163	0.32357
				158	→	164	0.11045
				159	→	164	-0.10482
				159	→	166	0.13472
				160	→	167	-0.22499
				160	→	168	0.22313
29	4.2349	292.77	0.005	155	→	162	0.13709
				155	→	163	0.12587
				156	→	163	-0.13925
				158	→	164	0.39103
				158	→	165	-0.19848
				158	→	166	0.17984
				158	→	167	0.22155
				160	→	167	0.20031
				160	→	168	-0.1968
30	4.2719	290.23	0.0061	154	→	163	-0.11454
				155	→	163	0.46345
				156	→	162	0.1054
				156	→	163	-0.19056
				158	→	164	-0.14418
				158	→	166	-0.14576

				159	→	164	-0.11956
				160	→	169	0.2925
31	4.2834	289.45	0.0038	154	→	163	-0.11864
				155	→	163	-0.26989
				158	→	164	0.11894
				158	→	165	0.29495
				159	→	166	0.14438
				159	→	174	-0.10191
				160	→	169	0.40259
32	4.3006	288.3	0.0256	154	→	163	0.1103
				155	→	163	0.23458
				158	→	164	0.15348
				158	→	165	0.45484
				158	→	174	-0.12514
				160	→	169	-0.24443
				160	→	174	-0.1764
33	4.351	284.96	0.0076	152	→	162	0.11852
				153	→	162	-0.20498
				158	→	164	-0.12408
				158	→	166	0.2153
				158	→	167	-0.12429
				158	→	168	-0.10787
				159	→	165	0.10365
				159	→	166	-0.13843
				159	→	167	0.47681
				160	→	167	0.13386
34	4.379	283.14	0.0015	158	→	164	-0.18907
				158	→	166	0.36363
				158	→	167	0.17972
				158	→	168	-0.10085
				159	→	166	0.10908
				159	→	168	0.30683
				159	→	169	0.10671
				159	→	174	-0.16087
35	4.4284	279.98	0.0055	155	→	163	0.13641
				158	→	166	0.32654
				158	→	168	-0.16455
				158	→	171	0.12527
				158	→	175	-0.20549
				159	→	167	-0.22003
				159	→	168	-0.2403
				159	→	171	-0.11175
				159	→	175	0.11995
				160	→	171	0.10398
				160	→	175	-0.12215
36	4.4569	278.19	0.0042	158	→	164	0.10324

				159	→	168	0.40369
				159	→	173	0.10401
				159	→	174	0.29574
				160	→	167	0.1211
				160	→	170	-0.13629
				160	→	171	0.16147
				160	→	174	0.14495
				160	→	175	-0.17873
37	4.4758	277.01	0.0208	154	→	161	-0.14022
				158	→	164	-0.23547
				158	→	165	0.12128
				158	→	166	0.10784
				158	→	167	0.33327
				158	→	168	0.23507
				159	→	165	-0.11486
				159	→	166	-0.15166
				159	→	168	-0.23216
				159	→	174	0.21592
				160	→	169	0.10818
38	4.5354	273.37	0.0477	152	→	163	0.10392
				153	→	162	-0.17245
				154	→	161	-0.21861
				158	→	167	-0.24636
				158	→	168	0.27239
				158	→	169	0.15737
				158	→	174	-0.14364
				159	→	167	-0.11553
				159	→	169	0.29712
				160	→	174	0.10908
39	4.5646	271.62	0.0031	153	→	162	0.15228
				158	→	166	-0.11339
				158	→	167	0.18992
				158	→	168	-0.21124
				158	→	175	-0.11297
				159	→	165	0.12537
				159	→	167	0.15842
				159	→	169	0.49597
40	4.6115	268.86	0.064	152	→	161	-0.1763
				153	→	161	-0.14889
				154	→	161	0.11008
				154	→	162	-0.14978
				154	→	163	0.28567
				157	→	164	0.24948
				157	→	166	-0.17256
				158	→	168	-0.10606
				158	→	169	0.1784

				159	→	169	-0.14636
				160	→	169	0.3043
41	4.6195	268.39	0.0683	154	→	161	0.35652
				156	→	164	0.11758
				157	→	165	0.17038
				157	→	169	0.11222
				158	→	164	-0.11672
				158	→	165	0.11221
				158	→	166	0.17
				158	→	168	0.14234
				158	→	174	-0.2139
				158	→	175	-0.12063
				159	→	175	-0.1027
				160	→	166	-0.11559
				160	→	168	-0.13222
				160	→	174	0.12952
42	4.6401	267.2	0.0149	154	→	161	0.17199
				158	→	164	-0.10943
				158	→	166	0.10237
				158	→	168	0.244
				158	→	173	0.11391
				158	→	174	0.24856
				158	→	175	0.15888
				159	→	169	0.28339
				159	→	174	0.14382
				159	→	175	0.17705
				160	→	174	-0.15433
				160	→	175	-0.1199
43	4.7575	260.61	0.0125	153	→	162	0.21373
				156	→	164	-0.14821
				156	→	166	-0.12984
				158	→	165	-0.12297
				158	→	168	0.36013
				158	→	170	-0.10391
				158	→	171	0.14358
				158	→	175	-0.18015
				159	→	167	0.1758
				159	→	174	-0.15694
44	4.8021	258.19	0.0448	152	→	162	-0.1357
				153	→	162	0.15807
				154	→	162	0.17806
				156	→	164	-0.1353
				156	→	166	-0.12071
				158	→	166	0.16686
				158	→	167	-0.20591
				158	→	169	0.44112

				158	→	175	0.1388
45	4.812	257.66	0.0122	153	→	162	-0.14696
				154	→	162	0.22492
				158	→	166	-0.11204
				158	→	167	0.2854
				158	→	169	0.35878
				158	→	170	-0.10182
				158	→	171	0.13685
				158	→	174	0.11114
				158	→	175	-0.15606
				159	→	168	0.12853
				159	→	174	-0.1511
46	4.8197	257.24	0.0034	152	→	161	-0.19928
				153	→	161	-0.26985
				154	→	161	-0.13131
				154	→	162	0.50624
				158	→	169	-0.24558
47	4.8604	255.09	0.0074	152	→	162	-0.2383
				152	→	163	0.27951
				153	→	162	-0.23724
				153	→	163	0.31269
				154	→	161	0.36117
				157	→	165	-0.19226
48	4.8714	254.51	0.0023	152	→	161	0.20579
				153	→	161	0.33356
				154	→	162	0.28895
				154	→	163	0.49969
49	4.9373	251.12	0.0038	152	→	161	0.48452
				152	→	162	0.11836
				153	→	161	-0.45667
				154	→	163	0.11961
50	4.988	248.56	0.0027	152	→	162	0.50188
				152	→	163	0.21814
				153	→	162	0.29585
				153	→	163	0.22934
				157	→	165	-0.16826

Table S4. TDDFT calculated transitions for *fac*-[Ru(Q3PzH)$_2$(Q3Pz)]$^+$.

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	2.3545	526.58	0.0783	160	→	161	0.63228
				160	→	162	-0.26438
				160	→	163	0.10197
2	2.3638	524.51	0.0205	160	→	161	0.24693
				160	→	162	0.64027
				160	→	163	0.1308
3	2.5132	493.34	0.0344	158	→	163	0.14216

				160	→	161	-0.11369
				160	→	163	0.6489
4	2.5762	481.28	0.0039	159	→	161	0.68966
				159	→	163	-0.10882
5	2.7164	456.43	0.0406	157	→	161	-0.20092
				158	→	161	0.52985
				158	→	162	-0.10788
				159	→	162	-0.37521
6	2.742	452.16	0.0218	157	→	161	-0.12984
				158	→	161	0.35111
				158	→	162	0.25273
				159	→	162	0.43168
				159	→	163	0.29316
7	2.7997	442.85	0.0005	157	→	162	0.13722
				158	→	162	-0.38361
				159	→	163	0.54783
8	2.9018	427.27	0.0989	157	→	162	-0.11536
				157	→	163	0.11601
				158	→	161	-0.11059
				158	→	162	0.4116
				158	→	163	-0.28505
				159	→	162	-0.34943
				159	→	163	0.24963
9	3.0133	411.45	0.0714	157	→	163	-0.20172
				158	→	162	0.20743
				158	→	163	0.57107
				159	→	162	-0.13441
				160	→	163	-0.16034
10	3.2224	384.76	0.0572	157	→	161	0.49846
				157	→	162	0.31295
				157	→	163	0.27575
				158	→	161	0.18685
				158	→	162	0.13029
				158	→	163	0.1316
11	3.2457	381.99	0.0012	157	→	161	-0.35819
				157	→	162	0.56178
				158	→	161	-0.12546
				158	→	162	0.16375
12	3.3368	371.57	0.0091	157	→	161	-0.22488
				157	→	162	-0.1726
				157	→	163	0.59163
				158	→	163	0.20643
13	3.3905	365.68	0.0085	160	→	164	0.5194
				160	→	165	-0.38558
				160	→	166	0.1424
				160	→	167	0.10682

14	3.5669	347.6	0.005	160	→	164	0.42812
				160	→	165	0.524
				160	→	166	-0.12329
15	3.661	338.66	0.0274	159	→	164	-0.19503
				159	→	166	-0.11207
				160	→	165	0.17103
				160	→	166	0.5236
				160	→	167	-0.1476
				160	→	168	0.10362
				160	→	169	-0.10916
				160	→	173	-0.15415
				160	→	176	0.10666
16	3.7932	326.86	0.0058	158	→	164	-0.18581
				158	→	165	0.13144
				159	→	164	0.39426
				159	→	165	-0.10007
				159	→	173	0.10096
				159	→	175	0.13944
				159	→	177	-0.1118
				160	→	166	0.24809
				160	→	168	0.16381
				160	→	173	0.15078
				160	→	175	0.15021
				160	→	177	-0.10857
17	3.805	325.85	0.0047	158	→	165	-0.10082
				159	→	164	-0.28612
				160	→	164	-0.11853
				160	→	166	-0.17986
				160	→	167	0.15206
				160	→	168	0.41382
				160	→	169	0.14578
				160	→	175	0.1827
				160	→	177	-0.15246
18	3.8442	322.52	0.0046	157	→	173	0.11291
				158	→	164	0.14104
				158	→	165	-0.14508
				158	→	166	0.14212
				158	→	173	-0.16508
				159	→	164	0.11351
				159	→	166	0.11212
				159	→	173	-0.19141
				160	→	165	0.11861
				160	→	166	0.1917
				160	→	167	0.41587
19	3.8605	321.16	0.0138	156	→	161	0.11427
				158	→	165	-0.12088

				159	→	164	0.25815
				159	→	165	0.4106
				159	→	166	0.12026
				159	→	167	-0.12389
				160	→	167	-0.29937
				160	→	168	0.13614
20	3.8708	320.3	0.0065	155	→	161	-0.1169
				157	→	173	-0.13814
				158	→	164	0.14241
				158	→	173	0.17077
				159	→	164	0.18178
				159	→	165	0.13922
				159	→	169	0.11354
				159	→	173	0.22669
				159	→	176	-0.12111
				160	→	167	0.30252
				160	→	173	-0.15085
				160	→	176	0.12424
21	3.8871	318.96	0.0325	155	→	161	0.19721
				156	→	161	0.37677
				158	→	164	-0.20319
				159	→	164	-0.17312
				159	→	165	0.26742
				159	→	166	0.113
				160	→	167	0.1707
22	3.9104	317.06	0.0875	156	→	161	0.47908
				156	→	162	-0.36655
				158	→	164	0.12107
				159	→	165	-0.2195
				160	→	167	-0.11531
23	3.9316	315.35	0.0582	155	→	161	0.531
				156	→	162	0.30312
				158	→	164	0.18048
				159	→	165	-0.15966
				160	→	168	-0.12174
24	3.9537	313.59	0.0617	155	→	161	-0.33187
				156	→	161	0.29609
				156	→	162	0.47413
				159	→	165	-0.11706
25	3.956	313.41	0.0031	155	→	161	0.10851
				158	→	164	-0.26325
				159	→	164	0.17866
				159	→	165	-0.17487
				159	→	168	-0.12504
				159	→	173	-0.10225
				159	→	175	-0.15864

				159	→	177	0.1281
				160	→	166	-0.10096
				160	→	167	0.10634
				160	→	168	0.27024
				160	→	169	-0.17808
				160	→	173	-0.23079
				160	→	175	-0.13711
26	3.9836	311.24	0.0163	156	→	161	0.10358
				157	→	164	-0.10093
				158	→	164	0.3595
				158	→	165	0.28435
				158	→	168	0.10547
				159	→	166	-0.14754
				159	→	173	-0.10299
				160	→	168	0.26462
				160	→	175	-0.10695
				160	→	176	-0.10497
				160	→	177	0.10757
27	4.0057	309.52	0.0069	157	→	165	-0.15643
				158	→	165	0.48049
				158	→	167	-0.12349
				158	→	173	-0.14062
				158	→	176	0.10925
				159	→	166	0.15434
				160	→	173	-0.11295
				160	→	175	0.1096
				160	→	176	0.13691
				160	→	177	-0.11972
28	4.0679	304.79	0.0278	158	→	173	0.12479
				159	→	164	-0.11758
				159	→	165	-0.20552
				159	→	166	0.49382
				159	→	168	0.15202
				160	→	168	0.17113
				160	→	169	-0.14863
29	4.1057	301.98	0.0038	155	→	162	-0.15196
				155	→	163	-0.25573
				156	→	163	0.15478
				157	→	168	-0.11661
				158	→	164	-0.10037
				158	→	166	0.47093
				158	→	167	-0.18394
				158	→	168	0.16345
30	4.1341	299.91	0.0139	155	→	162	0.32601
				155	→	163	0.3728
				156	→	163	-0.30147

				158	→	164	-0.12773
				158	→	166	0.25377
				158	→	168	0.10654
				159	→	166	-0.11284
31	4.1512	298.67	0.0204	154	→	163	-0.12748
				155	→	162	0.17728
				155	→	163	0.21356
				156	→	163	0.35216
				158	→	168	0.10534
				159	→	166	0.15412
				159	→	167	0.2125
				159	→	168	-0.25522
				160	→	169	0.2103
32	4.1755	296.93	0.0088	151	→	162	-0.11248
				155	→	162	-0.11144
				156	→	163	-0.3527
				159	→	165	0.12261
				159	→	166	0.15701
				159	→	167	0.4269
				159	→	168	-0.25005
33	4.2072	294.7	0.0016	154	→	162	0.20023
				155	→	162	0.46582
				155	→	163	-0.27648
				156	→	163	0.15576
				159	→	167	0.15283
				160	→	169	-0.20994
34	4.2244	293.5	0.0325	155	→	162	-0.18617
				155	→	163	0.35568
				156	→	163	0.24449
				158	→	166	0.102
				159	→	167	0.19456
				159	→	168	0.10996
				160	→	169	-0.32749
35	4.2679	290.51	0.0049	152	→	163	-0.13325
				157	→	164	0.15722
				157	→	165	0.15077
				157	→	166	-0.16338
				158	→	167	0.34554
				158	→	168	0.27916
				159	→	167	0.22742
				159	→	168	0.25575
36	4.2861	289.27	0.0065	154	→	161	0.11867
				157	→	164	-0.11237
				157	→	165	-0.11393
				158	→	167	-0.19846
				158	→	168	-0.11519

				159	→	167	0.29251
				159	→	168	0.38055
				160	→	169	0.27526
				160	→	173	-0.10078
37	4.2987	288.42	0.0047	157	→	167	0.12432
				157	→	168	-0.14136
				158	→	165	-0.14232
				158	→	166	-0.29452
				158	→	167	-0.32256
				158	→	168	0.40068
				159	→	166	-0.10092
				160	→	169	-0.11959
38	4.3343	286.05	0.0038	154	→	161	0.60524
				154	→	162	-0.24156
				155	→	162	0.16199
39	4.3672	283.9	0.0026	154	→	161	0.27003
				154	→	162	0.57206
				155	→	162	-0.15646
				156	→	163	0.10907
				157	→	164	0.12336
40	4.3886	282.52	0.0046	154	→	162	-0.12869
				157	→	164	0.52335
				157	→	165	0.13079
				157	→	167	0.17267
				158	→	164	0.20856
				158	→	167	-0.23626

Table S5. TDDFT calculated transitions for *fac*-[Ru(Q3PzH)(Q3Pz)$_2$].

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	1.9402	639.03	0.0046	160	→	161	0.64529
				160	→	162	-0.25531
2	2.0912	592.88	0.0716	160	→	161	0.27445
				160	→	162	0.60922
				160	→	163	0.20157
3	2.2749	545.02	0.0871	159	→	161	-0.16369
				159	→	162	0.1151
				159	→	163	0.19381
				160	→	162	-0.21516
				160	→	163	0.59334
4	2.4691	502.13	0.0046	158	→	161	0.53299
				158	→	162	-0.17201
				158	→	163	-0.11339
				159	→	161	-0.25017
				159	→	162	-0.29858
				159	→	163	0.10816
5	2.4856	498.81	0.0142	158	→	161	0.39239

				159	→	161	0.28986
				159	→	162	0.46926
				159	→	163	-0.13587
6	2.5626	483.82	0.061	158	→	161	0.13891
				158	→	162	0.52468
				159	→	161	-0.37705
				159	→	162	0.19029
				159	→	163	-0.1051
7	2.5816	480.27	0.0707	158	→	161	0.14075
				158	→	162	0.31347
				158	→	163	0.18759
				159	→	161	0.33533
				159	→	162	-0.12133
				159	→	163	0.45585
8	2.6364	470.28	0.0152	158	→	162	-0.19993
				158	→	163	0.65475
9	2.7411	452.32	0.0561	158	→	162	-0.18115
				159	→	161	-0.22496
				159	→	162	0.32409
				159	→	163	0.43109
				160	→	163	-0.27658
10	3.0971	400.32	0.0075	157	→	161	0.69552
11	3.1574	392.68	0.0649	157	→	162	0.58825
				157	→	163	0.34543
12	3.2099	386.25	0.0182	160	→	164	0.68664
13	3.2446	382.12	0.0032	160	→	165	0.66984
14	3.3196	373.49	0.0606	156	→	161	0.37494
				156	→	162	0.48525
				157	→	162	-0.12055
				157	→	163	0.2766
				160	→	166	-0.1176
15	3.3525	369.82	0.0078	156	→	161	-0.19035
				156	→	162	-0.21288
				157	→	162	-0.32899
				157	→	163	0.53186
16	3.444	360	0.0099	156	→	161	0.15432
				160	→	166	0.6587
17	3.4633	357.99	0.0052	156	→	161	0.53863
				156	→	162	-0.44192
18	3.4707	357.23	0.0211	156	→	163	0.69445
19	3.5671	347.57	0.0004	159	→	164	0.64204
				159	→	166	0.13188
				159	→	167	0.15867
20	3.6097	343.47	0.0235	158	→	164	0.14943
				159	→	164	-0.12424
				159	→	165	0.12389

				160	→	167	0.615
				160	→	168	-0.11486
21	3.6631	338.46	0.0086	159	→	165	0.17163
				160	→	165	0.13311
				160	→	168	0.44195
				160	→	169	0.3382
				160	→	174	0.11588
				160	→	176	-0.23121
22	3.7396	331.54	0.0011	158	→	164	-0.25136
				159	→	165	0.56384
				160	→	167	-0.13298
				160	→	168	-0.18351
23	3.7645	329.35	0.0401	158	→	164	0.58791
				158	→	167	0.13956
				159	→	165	0.11898
				160	→	167	-0.21959
				160	→	168	-0.16056
24	3.819	324.65	0.0024	158	→	165	0.59889
				158	→	169	-0.10934
				158	→	175	0.12515
				160	→	169	-0.22057
25	3.8345	323.34	0.0161	158	→	164	-0.14446
				158	→	165	0.2433
				159	→	165	-0.27432
				160	→	168	-0.25939
				160	→	169	0.41161
				160	→	175	-0.18197
26	3.8508	321.97	0.0969	155	→	161	0.63629
				155	→	162	-0.14711
				159	→	166	-0.15253
				159	→	167	-0.12305
27	3.8924	318.53	0.0182	155	→	161	0.20993
				159	→	164	-0.16302
				159	→	166	0.5703
				159	→	167	0.27222
28	3.9636	312.81	0.0038	154	→	161	-0.10886
				155	→	162	-0.20138
				158	→	165	-0.11463
				158	→	166	0.32769
				158	→	169	-0.12617
				158	→	175	0.17524
				159	→	167	-0.10776
				159	→	176	-0.11139
				160	→	168	-0.22176
				160	→	169	0.11669
				160	→	175	0.20172

				160	→	176	-0.16495
29	3.9744	311.96	0.0064	155	→	162	-0.14649
				158	→	165	-0.15671
				158	→	166	0.26789
				158	→	169	-0.12434
				158	→	175	0.12291
				159	→	166	-0.14561
				159	→	167	0.32052
				159	→	168	-0.15977
				159	→	175	-0.11994
				159	→	176	0.17239
				160	→	168	0.15296
				160	→	175	-0.1127
				160	→	176	0.11601
30	3.9931	310.5	0.0054	154	→	161	0.40598
				155	→	161	0.1211
				155	→	162	0.35382
				155	→	163	0.12967
				158	→	166	0.29926
				158	→	167	0.1548
31	4.0182	308.56	0.008	154	→	161	0.27553
				158	→	166	-0.13709
				158	→	167	-0.21105
				158	→	175	0.11194
				159	→	166	-0.19556
				159	→	167	0.29353
				159	→	168	0.10927
				159	→	169	0.163
				159	→	175	-0.14081
				159	→	176	-0.10566
				160	→	169	0.18277
				160	→	175	0.14263
32	4.0231	308.18	0.003	154	→	161	0.4472
				154	→	162	-0.18881
				154	→	163	-0.12423
				155	→	162	-0.40607
				159	→	167	-0.1674
33	4.0491	306.2	0.0041	155	→	162	-0.10503
				158	→	165	0.13133
				158	→	166	0.20259
				158	→	167	0.25324
				158	→	168	0.13579
				158	→	169	0.19238
				158	→	175	-0.22746
				158	→	176	-0.1561
				159	→	165	0.10039

				159	→	167	0.123
				159	→	168	0.17388
				159	→	169	0.16355
				159	→	176	-0.14992
				160	→	168	0.11694
				160	→	176	0.15659
34	4.0915	303.03	0.0042	154	→	162	0.33997
				154	→	163	0.11069
				155	→	162	-0.27191
				155	→	163	0.29723
				159	→	167	0.22577
				159	→	169	-0.12948
				159	→	175	0.15235
				160	→	168	-0.12571
				160	→	176	-0.16688
35	4.1082	301.8	0.0004	154	→	162	-0.24518
				155	→	163	-0.27925
				158	→	166	-0.14785
				158	→	167	0.30009
				158	→	175	-0.13111
				159	→	166	-0.11435
				159	→	167	0.19411
				159	→	169	-0.11099
				159	→	175	0.18062
				160	→	169	-0.12989
				160	→	176	-0.15905
36	4.1573	298.23	0.0072	154	→	162	0.18499
				158	→	166	-0.31781
				158	→	167	0.44716
				158	→	168	-0.10965
				158	→	175	0.17843
				159	→	169	0.11225
				159	→	175	-0.14176
37	4.1937	295.64	0.0027	153	→	161	0.11951
				153	→	162	0.17432
				154	→	162	0.40239
				154	→	163	-0.27925
				155	→	163	-0.38389
				157	→	164	0.12092
38	4.225	293.45	0.0007	153	→	163	0.13193
				154	→	163	0.12781
				157	→	164	0.41048
				157	→	165	-0.2989
				157	→	166	-0.24017
				158	→	168	-0.10928
				159	→	168	0.19424

39	4.2631	290.83	0.0044	154	→	162	0.11931
				154	→	163	0.12956
				155	→	163	-0.15574
				157	→	164	-0.19894
				158	→	168	-0.28527
				159	→	168	0.4046
				160	→	169	-0.10211
				160	→	171	-0.10306
				160	→	175	-0.21343
40	4.3051	287.99	0.0036	153	→	163	0.10213
				154	→	163	0.50613
				155	→	163	-0.29372
				156	→	165	-0.11622
				159	→	168	-0.25592
				159	→	169	0.10842

Table S6. TDDFT calculated transitions for *fac*-[Ru(Q3Pz)$_3$]$^-$.

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	1.9016	651.98	0.0087	160	→	162	0.69055
2	1.9295	642.58	0.0578	160	→	161	0.66462
				160	→	163	0.18093
3	2.1123	586.95	0.0546	158	→	162	0.12946
				158	→	163	-0.11111
				159	→	161	0.478
				159	→	162	-0.10123
				160	→	161	0.18884
				160	→	163	-0.41893
4	2.1537	575.67	0.0048	158	→	161	-0.12106
				159	→	161	0.21652
				159	→	162	0.47191
				159	→	163	-0.44071
5	2.1846	567.53	0.0435	158	→	162	-0.21594
				158	→	163	0.1778
				159	→	161	0.43178
				159	→	162	-0.26191
				160	→	161	-0.10282
				160	→	163	0.37818
6	2.2314	555.62	0.0006	158	→	161	-0.11708
				158	→	162	-0.20073
				159	→	162	0.37985
				159	→	163	0.52618
7	2.2699	546.21	0.0122	158	→	161	0.6073
				158	→	163	-0.2948
				159	→	162	0.12975
8	2.3861	519.61	0.1233	158	→	161	0.28431

				158	→	163	0.58686
				160	→	163	-0.20784
9	2.5923	478.27	0.0756	158	→	162	0.58413
				159	→	161	0.12138
				159	→	162	0.14428
				160	→	163	0.28266
10	3.0508	406.4	0.0478	155	→	161	-0.17166
				157	→	161	0.58304
				157	→	162	-0.20629
				160	→	164	-0.23432
11	3.0523	406.2	0.0046	157	→	161	0.2169
				160	→	164	0.64514
12	3.1479	393.87	0.0689	155	→	162	-0.11096
				156	→	161	0.34023
				157	→	161	-0.12183
				157	→	162	-0.32179
				157	→	163	0.4742
13	3.1594	392.43	0.0544	155	→	161	0.26088
				155	→	163	0.13152
				156	→	161	0.39259
				156	→	162	-0.22838
				156	→	163	0.23189
				157	→	161	0.17982
				157	→	162	0.14163
				157	→	163	-0.12543
				160	→	165	0.25207
				160	→	166	-0.10539
14	3.1834	389.47	0.0469	155	→	162	0.10888
				156	→	161	-0.19821
				156	→	163	-0.10235
				157	→	163	0.16755
				160	→	165	0.59925
				160	→	166	-0.1273
15	3.1907	388.58	0.0574	155	→	161	0.30092
				155	→	162	0.35663
				155	→	163	-0.10769
				156	→	161	-0.1112
				156	→	162	-0.13481
				157	→	161	0.10382
				157	→	162	0.22653
				157	→	163	0.35516
				160	→	165	-0.15244
				160	→	166	0.10936
16	3.2402	382.65	0.0064	155	→	161	-0.32717
				155	→	162	0.20369
				155	→	163	0.15271

				156	→	161	0.28728
				156	→	162	0.31252
				157	→	162	0.34633
17	3.2518	381.28	0.0188	155	→	161	0.35563
				155	→	163	-0.20204
				156	→	162	0.53447
18	3.2904	376.81	0.0018	157	→	162	-0.10593
				160	→	165	0.16899
				160	→	166	0.64254
19	3.3352	371.74	0.0076	155	→	162	0.50845
				156	→	161	0.10911
				157	→	161	-0.11743
				157	→	162	-0.36471
				157	→	163	-0.21392
20	3.3612	368.87	0.0029	158	→	164	-0.11735
				159	→	164	0.67607
21	3.3972	364.96	0.0056	155	→	163	0.55642
				156	→	161	-0.22132
				156	→	162	0.13871
				156	→	163	0.25219
				157	→	163	0.17275
22	3.3997	364.69	0.0037	155	→	161	-0.20833
				155	→	162	0.14627
				155	→	163	-0.25144
				156	→	163	0.57938
				157	→	161	-0.10573
23	3.4532	359.04	0.0003	158	→	164	0.64294
				158	→	165	-0.10729
				159	→	164	0.11212
				159	→	165	-0.1357
				159	→	166	-0.1028
24	3.4937	354.88	0.0016	158	→	164	0.12722
				159	→	165	0.67762
25	3.5681	347.48	0.0091	158	→	165	0.64823
				160	→	169	0.16206
26	3.6025	344.16	0.0042	158	→	165	-0.17139
				159	→	166	0.543
				160	→	167	-0.17074
				160	→	169	0.29871
				160	→	175	0.11205
27	3.6306	341.5	0.0038	158	→	164	-0.15633
				158	→	165	-0.11615
				158	→	166	0.16738
				159	→	166	-0.32504
				160	→	168	-0.12748
				160	→	169	0.44842

				160	→	174	-0.15438
				160	→	175	0.11929
28	3.6829	336.65	0.0084	160	→	167	0.31472
				160	→	168	0.54851
				160	→	169	0.15382
				160	→	175	0.13867
29	3.6927	335.76	0.0118	158	→	166	0.64486
				159	→	166	0.12706
				160	→	169	-0.12179
30	3.7273	332.64	0.0551	154	→	162	0.10159
				159	→	166	0.12185
				159	→	169	-0.14458
				160	→	167	0.50926
				160	→	168	-0.35641
				160	→	169	0.11034
31	3.8092	325.49	0.0017	158	→	174	-0.1562
				159	→	166	-0.1392
				159	→	167	0.22769
				159	→	168	0.17591
				159	→	169	-0.3138
				159	→	174	0.34214
				160	→	167	-0.19797
				160	→	175	0.14591
32	3.9102	317.08	0.0141	154	→	161	0.59652
				154	→	162	-0.12935
				154	→	163	0.16388
				159	→	167	0.1317
				159	→	169	-0.12715
33	3.9357	315.02	0.0144	154	→	161	0.24183
				158	→	167	-0.23938
				158	→	169	0.23605
				158	→	174	-0.17341
				159	→	168	0.29633
				159	→	169	0.18901
				159	→	175	0.18115
				160	→	169	0.15973
				160	→	174	0.19267
34	3.949	313.96	0.0158	154	→	162	-0.10566
				159	→	167	0.59343
				159	→	168	-0.14132
				159	→	169	0.20577
35	3.9741	311.98	0.0133	154	→	162	0.34982
				154	→	163	-0.13138
				158	→	167	0.24757
				158	→	174	0.16639
				158	→	175	0.20649

				159	→	168	0.18169
				160	→	169	-0.10251
				160	→	175	0.24757
36	3.9818	311.38	0.0029	154	→	162	-0.20918
				154	→	163	0.19829
				158	→	168	0.25906
				158	→	169	0.21486
				158	→	175	0.23669
				159	→	167	-0.13464
				159	→	168	-0.23019
				160	→	175	0.27647
37	4.0183	308.55	0.0067	154	→	162	0.47517
				158	→	167	-0.3102
				159	→	168	-0.2873
				160	→	167	-0.11208
38	4.0557	305.7	0.0067	154	→	162	0.11696
				158	→	167	0.44847
				158	→	168	-0.17522
				158	→	169	0.26688
				158	→	174	-0.15574
				159	→	168	-0.23425
39	4.0727	304.43	0.0064	152	→	161	0.14162
				153	→	161	-0.19791
				154	→	162	0.11823
				154	→	163	0.54883
				158	→	167	0.10213
				159	→	168	0.22743
				160	→	175	-0.10413
40	4.1041	302.1	0.0073	148	→	163	0.12528
				155	→	164	-0.1023
				155	→	165	-0.11287
				157	→	164	0.55468
				157	→	165	0.23259
				159	→	168	-0.11502

Table S7. TDDFT calculated transitions for *mer*-$[Ru(Q3PzH)_3]^{2+}$.

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	2.731	453.99	0.1438	159	→	161	0.14756
				160	→	161	0.66451
				160	→	162	0.14543
2	2.8101	441.21	0.0175	159	→	161	-0.1347
				160	→	161	-0.12092
				160	→	162	0.66208
				160	→	163	0.13349
3	2.8521	434.72	0.0561	159	→	161	0.64847
				160	→	161	-0.16601

				160	→	162	0.12942
				160	→	163	-0.15037
4	2.9389	421.87	0.0303	158	→	161	-0.29867
				159	→	161	0.1245
				159	→	162	-0.26671
				159	→	163	0.27546
				160	→	163	0.47159
5	2.9549	419.59	0.0096	158	→	161	0.53195
				158	→	162	0.14898
				159	→	162	-0.41028
6	2.9876	415	0.03	158	→	161	0.153
				159	→	162	0.17915
				159	→	163	0.62369
				160	→	163	-0.16043
7	3.0211	410.4	0.0034	158	→	161	0.27513
				158	→	162	-0.3027
				158	→	163	-0.22086
				159	→	162	0.35481
				159	→	163	-0.12157
				160	→	163	0.34007
8	3.0962	400.43	0.0155	158	→	162	-0.37113
				158	→	163	0.56929
9	3.2321	383.61	0.105	158	→	162	0.46789
				158	→	163	0.30806
				159	→	162	0.2873
				160	→	163	0.24396
10	3.5989	344.51	0.0016	158	→	172	0.15121
				158	→	174	0.12216
				159	→	175	-0.10007
				160	→	164	0.14697
				160	→	165	-0.26368
				160	→	166	0.18571
				160	→	168	0.19788
				160	→	170	-0.11003
				160	→	171	-0.15001
				160	→	172	0.27206
				160	→	173	-0.1548
				160	→	174	0.2213
11	3.7469	330.9	0.0046	157	→	161	0.29799
				158	→	172	-0.13332
				158	→	174	-0.10889
				159	→	165	0.18962
				159	→	168	-0.10191
				159	→	172	-0.20676
				159	→	173	0.15912
				159	→	174	-0.16129

				159	→	175	-0.12962
				160	→	164	-0.14224
				160	→	165	-0.14136
				160	→	175	0.18755
12	3.7635	329.44	0.0014	157	→	161	0.61624
				159	→	172	0.10317
13	3.7929	326.88	0.0016	158	→	172	-0.12215
				160	→	164	0.592
				160	→	165	0.16475
				160	→	166	0.1066
14	3.8964	318.2	0.0537	156	→	161	-0.2411
				157	→	162	-0.12267
				157	→	163	0.25336
				158	→	171	0.15746
				158	→	172	-0.11623
				158	→	175	0.19144
				159	→	171	-0.11498
				159	→	175	-0.1809
				160	→	164	-0.12317
				160	→	171	-0.16847
				160	→	172	0.11313
				160	→	175	-0.23647
15	3.8989	318	0.1532	155	→	161	0.11994
				156	→	161	-0.30244
				157	→	162	-0.23348
				157	→	163	0.40818
				158	→	175	-0.11877
				159	→	175	0.12752
				160	→	164	0.15475
				160	→	171	0.10834
				160	→	175	0.12169
16	3.9306	315.43	0.0298	156	→	161	0.13949
				156	→	162	0.10276
				157	→	162	-0.10613
				158	→	171	-0.11029
				158	→	172	0.1692
				158	→	174	0.13436
				159	→	164	-0.11201
				159	→	165	0.15542
				159	→	172	-0.12069
				160	→	165	0.4495
				160	→	169	0.10594
17	3.9451	314.27	0.0094	156	→	161	0.50031
				156	→	162	0.14841
				157	→	162	-0.35486
				157	→	163	0.14705

				160	→	165	-0.14582
18	3.9877	310.92	0.0215	155	→	161	0.1239
				156	→	161	0.2357
				156	→	162	-0.21529
				157	→	162	0.45182
				157	→	163	0.40739
19	4.0153	308.78	0.0403	155	→	162	0.19343
				156	→	162	0.52007
				157	→	162	0.25583
				159	→	164	0.205
				160	→	166	-0.1737
20	4.0243	308.09	0.0344	156	→	162	0.26391
				159	→	164	-0.38547
				160	→	166	0.38661
				160	→	168	0.13893
21	4.058	305.53	0.0211	159	→	164	0.45275
				159	→	165	0.14787
				159	→	166	0.11176
				159	→	175	0.12493
				160	→	166	0.40053
22	4.1149	301.31	0.0075	155	→	161	0.61142
				156	→	163	0.20125
				157	→	163	-0.23146
23	4.124	300.64	0.0135	156	→	163	0.40883
				158	→	164	0.21713
				158	→	165	-0.16258
				159	→	164	0.12314
				159	→	165	-0.20227
				159	→	166	-0.31141
				159	→	168	-0.10515
24	4.1395	299.52	0.0129	155	→	161	-0.16281
				156	→	163	0.45448
				158	→	164	-0.40282
				158	→	167	-0.11004
				159	→	166	0.1522
25	4.1513	298.66	0.0146	156	→	163	0.2141
				158	→	164	0.36564
				158	→	165	0.13279
				158	→	166	0.13753
				159	→	165	0.28811
				159	→	166	0.24262
				160	→	165	-0.10434
				160	→	167	-0.24856
26	4.1681	297.46	0.008	152	→	161	-0.12405
				153	→	161	0.12898
				153	→	163	-0.10089

				158	→	164	0.26219
				158	→	165	0.15455
				159	→	166	0.13428
				160	→	164	-0.11617
				160	→	165	0.1933
				160	→	167	0.44131
				160	→	168	0.1273
27	4.1907	295.86	0.0029	154	→	161	-0.1093
				158	→	166	-0.10404
				159	→	175	0.10391
				160	→	165	0.10145
				160	→	166	-0.16703
				160	→	167	-0.21909
				160	→	168	0.5262
				160	→	169	-0.16031
28	4.2436	292.17	0.0117	155	→	163	-0.10854
				158	→	165	0.304
				158	→	166	0.38821
				158	→	168	0.1341
				159	→	166	-0.25463
				159	→	168	-0.19829
				160	→	168	0.16358
				160	→	175	-0.13054
29	4.2556	291.35	0.0151	155	→	163	0.29751
				158	→	165	0.24698
				159	→	165	-0.23431
				159	→	175	-0.11872
				160	→	165	0.15546
				160	→	166	0.14225
				160	→	167	-0.22816
				160	→	168	-0.12905
				160	→	169	-0.21316
30	4.2849	289.35	0	155	→	162	0.50782
				155	→	163	-0.32133
				156	→	162	-0.14449
				159	→	165	-0.12917
				160	→	169	-0.17488
31	4.2938	288.75	0.0016	155	→	162	-0.24519
				155	→	163	-0.17862
				158	→	165	-0.17543
				158	→	166	0.27511
				158	→	169	-0.10227
				159	→	165	-0.27349
				159	→	166	0.26777
				159	→	172	-0.13616
32	4.3144	287.37	0.0015	155	→	162	0.14996

				155	→	163	0.233
				158	→	168	0.10191
				159	→	165	-0.19139
				159	→	166	0.12157
				159	→	167	-0.21329
				159	→	168	0.15487
				159	→	172	-0.10695
				160	→	168	0.15239
				160	→	169	0.37641
33	4.3411	285.61	0.0044	154	→	162	-0.11338
				155	→	162	0.28834
				155	→	163	0.38492
				158	→	165	-0.18975
				158	→	166	0.11085
				159	→	166	0.10079
				159	→	167	0.25872
				159	→	168	-0.18416
34	4.3775	283.23	0.0125	155	→	163	0.12064
				158	→	165	-0.18694
				158	→	166	0.24013
				159	→	165	0.12659
				159	→	166	-0.19008
				159	→	167	-0.17543
				159	→	168	0.41578
				160	→	167	0.10275
				160	→	169	-0.23866
				160	→	172	-0.12912
35	4.4289	279.94	0.0209	154	→	162	-0.12431
				158	→	167	0.30484
				158	→	168	-0.29076
				159	→	167	-0.23655
				159	→	168	-0.14405
				159	→	171	-0.1159
				159	→	172	0.17216
				159	→	174	0.11395
				160	→	169	0.12176
				160	→	171	0.1063
				160	→	175	0.18292
36	4.4353	279.54	0.0051	158	→	166	0.14948
				158	→	172	-0.12903
				158	→	173	0.11312
				158	→	175	-0.10619
				159	→	166	-0.10877
				159	→	167	0.36758
				159	→	168	0.25503
				160	→	165	0.10424

				160	→	169	0.19647
				160	→	172	0.14218
				160	→	173	-0.112
				160	→	175	0.15938
37	4.4675	277.53	0.002	158	→	167	0.17233
				158	→	172	-0.12488
				159	→	166	-0.10341
				159	→	167	-0.18207
				159	→	169	-0.14085
				159	→	171	0.22117
				159	→	172	-0.13132
				159	→	173	-0.11482
				159	→	175	0.28701
				159	→	177	-0.10229
				160	→	168	-0.11671
				160	→	171	-0.17627
				160	→	172	0.20124
				160	→	174	0.15158
38	4.4958	275.78	0.0018	152	→	162	-0.10516
				154	→	162	0.12387
				158	→	166	0.18436
				158	→	167	0.10215
				158	→	169	0.14964
				159	→	168	-0.14272
				159	→	169	0.45984
				159	→	172	0.10303
				159	→	175	0.10672
39	4.533	273.51	0.0074	158	→	164	-0.12208
				158	→	165	0.20801
				158	→	166	-0.14696
				158	→	167	0.43486
				158	→	168	0.33264
				158	→	169	-0.13248
				159	→	167	0.16246
				159	→	168	0.11414
40	4.5554	272.17	0.0074	154	→	161	-0.15306
				154	→	163	-0.10706
				158	→	168	-0.31695
				158	→	169	-0.26569
				159	→	165	-0.11163
				159	→	168	0.14359
				159	→	169	0.36773
				160	→	169	0.10574

Table S8. TDDFT calculated transitions for *mer*-$[Ru(Q3PzH)_2(Q3Pz_a)]^+$.

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	2.2748	545.03	0.006	160	→	161	-0.47304
				160	→	162	0.51488
2	2.3697	523.21	0.159	160	→	161	0.51265
				160	→	162	0.46974
3	2.5739	481.69	0.0596	158	→	163	0.13777
				159	→	161	-0.24679
				159	→	162	0.16661
				160	→	163	0.60843
4	2.6251	472.29	0.0055	159	→	161	0.50873
				159	→	162	0.45972
5	2.7364	453.09	0.0228	158	→	161	0.28151
				158	→	162	-0.24477
				159	→	161	0.27756
				159	→	162	-0.233
				159	→	163	0.43362
				160	→	163	0.11066
6	2.7621	448.88	0.0028	158	→	161	-0.37515
				158	→	162	0.44251
				159	→	161	0.15254
				159	→	162	-0.13629
				159	→	163	0.27499
				160	→	163	0.16344
7	2.7963	443.39	0.0722	158	→	161	0.49121
				158	→	162	0.45083
				158	→	163	-0.1389
				159	→	162	0.10698
8	2.8518	434.75	0.0659	158	→	163	-0.28397
				159	→	161	-0.23532
				159	→	162	0.36211
				159	→	163	0.43444
				160	→	163	-0.1311
9	3.0302	409.16	0.0239	157	→	163	-0.10602
				158	→	163	0.57797
				159	→	161	-0.11682
				159	→	162	0.1626
				159	→	163	0.13198
				160	→	163	-0.20321
10	3.2474	381.79	0.0177	157	→	161	0.59474
				157	→	162	0.32942
11	3.3979	364.89	0.0162	157	→	161	-0.285
				157	→	162	0.56611
				157	→	163	-0.20397
				160	→	165	-0.11212
12	3.4304	361.43	0.0122	157	→	161	-0.10765
				157	→	162	0.2048

				157	→	163	0.12451
				160	→	164	-0.21238
				160	→	165	0.4631
				160	→	166	-0.18561
				160	→	167	0.19861
				160	→	169	0.1458
				160	→	173	0.15081
13	3.4836	355.91	0.0351	157	→	161	-0.15648
				157	→	163	0.58993
				160	→	164	0.26709
				160	→	165	-0.14101
14	3.5384	350.39	0.0108	157	→	163	-0.24832
				160	→	164	0.55484
				160	→	165	0.10224
				160	→	166	-0.14573
				160	→	167	0.12267
				160	→	169	0.1032
				160	→	173	0.11868
15	3.6187	342.62	0.0021	160	→	164	0.13165
				160	→	165	0.35371
				160	→	166	0.5398
				160	→	169	-0.14963
16	3.709	334.28	0.0035	159	→	164	0.21081
				159	→	165	0.24819
				159	→	166	-0.11324
				159	→	167	0.20202
				159	→	169	0.19208
				159	→	173	0.2953
				159	→	175	0.11028
				160	→	164	0.12444
				160	→	165	0.17458
				160	→	166	-0.14618
				160	→	167	-0.14984
				160	→	177	0.12117
17	3.7739	328.53	0.0016	158	→	165	-0.11951
				158	→	169	-0.103
				158	→	173	-0.11539
				159	→	164	0.22555
				159	→	173	0.10346
				160	→	164	-0.10591
				160	→	165	-0.25361
				160	→	166	0.21613
				160	→	167	0.36517
				160	→	169	0.13868
				160	→	173	0.14699
18	3.798	326.45	0.001	158	→	165	0.12413

				159	→	164	0.5377
				159	→	165	-0.15812
				159	→	166	0.16311
				159	→	168	0.14049
				160	→	166	-0.13251
19	3.8377	323.06	0.0206	155	→	161	-0.10409
				158	→	165	-0.11302
				160	→	164	-0.11237
				160	→	167	-0.32574
				160	→	168	0.50248
20	3.8842	319.2	0.0817	155	→	161	-0.18446
				155	→	162	0.25958
				156	→	162	0.19844
				158	→	164	0.1083
				159	→	164	-0.18106
				160	→	166	-0.15061
				160	→	167	0.29865
				160	→	168	0.27091
				160	→	169	-0.19553
				160	→	173	-0.13049
21	3.894	318.4	0.031	155	→	161	-0.21767
				155	→	162	0.43464
				156	→	161	-0.30058
				156	→	162	0.1207
				158	→	164	-0.10491
				160	→	167	-0.15197
				160	→	168	-0.26242
22	3.9164	316.58	0.089	155	→	161	-0.18539
				156	→	161	0.43782
				156	→	162	0.44317
				158	→	164	-0.12408
23	3.972	312.15	0.0184	156	→	162	0.14142
				158	→	164	0.24427
				158	→	167	0.10296
				158	→	173	0.11959
				159	→	165	0.43801
				159	→	166	0.21125
				159	→	167	0.1078
				160	→	169	0.1312
				160	→	177	-0.10818
24	3.9923	310.56	0.0117	155	→	161	0.51787
				155	→	162	0.39698
				156	→	161	0.21424
25	4.0153	308.78	0.0155	158	→	164	-0.26054
				158	→	165	-0.25612
				158	→	167	-0.19783

				158	→	169	-0.1007
				158	→	173	-0.10647
				159	→	165	0.24786
				159	→	166	0.32863
				160	→	169	-0.22603
26	4.0249	308.04	0.0068	155	→	161	0.27248
				155	→	162	-0.182
				156	→	161	-0.3091
				156	→	162	0.40241
				158	→	164	0.14088
				158	→	165	-0.23099
27	4.0432	306.65	0.0202	155	→	161	-0.10048
				155	→	162	0.12843
				156	→	161	0.20345
				156	→	162	-0.17009
				158	→	164	0.37564
				158	→	165	-0.32953
				159	→	165	-0.17819
				160	→	168	-0.16176
28	4.0789	303.96	0.0057	159	→	164	-0.17169
				159	→	165	-0.24725
				159	→	166	0.41785
				159	→	167	0.29604
				159	→	168	0.21849
				159	→	173	0.11554
				160	→	169	0.11705
29	4.0901	303.13	0.0032	158	→	164	0.14494
				158	→	166	-0.15645
				158	→	176	-0.16025
				158	→	177	0.25571
				159	→	166	0.12462
				160	→	171	0.11242
				160	→	172	0.13414
				160	→	174	-0.14097
				160	→	176	-0.18463
				160	→	177	0.36003
30	4.1422	299.32	0.0091	156	→	163	0.10487
				158	→	164	0.22056
				158	→	165	0.24521
				158	→	166	0.43834
				158	→	169	-0.10456
				158	→	173	-0.1162
				159	→	166	0.10698
				159	→	167	-0.11979
				159	→	168	-0.20225
31	4.2031	294.98	0.0057	154	→	161	0.18485

				154	→	162	0.10291
				155	→	163	0.10166
				156	→	163	0.59023
				159	→	166	-0.10673
				159	→	167	0.10183
				159	→	168	0.1255
32	4.2148	294.17	0.0112	154	→	161	-0.14101
				155	→	163	0.20703
				156	→	163	-0.13366
				158	→	166	0.3156
				159	→	166	-0.25259
				159	→	167	0.25936
				159	→	168	0.18428
				159	→	169	-0.1563
				159	→	173	-0.16405
33	4.2281	293.24	0.0052	155	→	163	0.20232
				156	→	163	-0.14807
				158	→	164	0.23015
				158	→	165	0.20086
				158	→	166	-0.16435
				158	→	167	-0.14235
				158	→	168	-0.19706
				158	→	169	-0.11199
				158	→	173	-0.14759
				159	→	167	-0.12175
				159	→	168	0.35977
				160	→	169	-0.14361
34	4.2448	292.09	0.0107	154	→	161	0.28675
				154	→	162	0.19235
				155	→	163	-0.30972
				156	→	163	-0.16347
				158	→	165	0.11188
				158	→	167	-0.1096
				159	→	167	0.32019
				159	→	168	-0.10617
				160	→	169	-0.20426
35	4.2619	290.91	0.0139	155	→	163	0.45214
				158	→	165	0.11858
				158	→	166	-0.1767
				159	→	167	0.20087
				159	→	168	-0.359
36	4.2705	290.32	0.0031	154	→	161	0.395
				154	→	162	0.25719
				155	→	163	0.26678
				156	→	163	-0.16768
				158	→	165	-0.17564

				158	→	167	0.30154
				159	→	167	-0.11205
37	4.2998	288.35	0.0214	154	→	161	-0.20413
				154	→	162	-0.12708
				155	→	163	-0.12095
				157	→	166	-0.10348
				158	→	165	-0.11139
				158	→	166	-0.10935
				158	→	167	0.45305
				158	→	168	-0.1079
				160	→	169	-0.23863
				160	→	173	0.13958
38	4.3395	285.71	0.0044	154	→	162	0.1345
				158	→	168	0.54405
				159	→	167	-0.15117
				159	→	168	0.11272
				160	→	169	-0.20638
				160	→	173	0.14541
39	4.3878	282.56	0.0001	152	→	161	-0.13567
				152	→	163	-0.11559
				154	→	161	-0.21581
				154	→	162	0.31773
				154	→	163	-0.17781
				157	→	164	-0.1022
				157	→	166	0.19295
				158	→	168	-0.22686
				158	→	169	0.17262
				159	→	169	0.16109
				160	→	169	-0.10683
				160	→	173	0.11673
40	4.4199	280.51	0.0024	152	→	161	0.15126
				152	→	163	0.12548
				154	→	161	-0.27996
				154	→	162	0.42748
				157	→	164	0.13008
				157	→	165	-0.14223
				157	→	166	-0.25188
				158	→	169	-0.10756
				160	→	173	-0.13683

Table S9. TDDFT calculated transitions for *mer*-$[Ru(Q3PzH)_2(Q3Pz_b)]^+$.

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	2.3575	525.92	0.0222	160	→	161	0.58029
				160	→	162	0.38308
2	2.423	511.61	0.101	159	→	161	0.13462
				160	→	161	-0.36945

				160	→	162	0.57483
3	2.596	477.58	0.0493	159	→	161	0.52499
				159	→	162	0.14472
				160	→	163	0.41073
4	2.641	469.44	0.0069	158	→	161	0.21044
				159	→	161	0.10604
				159	→	162	0.53668
				159	→	163	0.22473
				160	→	163	-0.27168
5	2.647	468.24	0.0302	158	→	162	0.1514
				159	→	161	0.40195
				159	→	162	-0.33789
				160	→	161	0.10894
				160	→	163	-0.40044
6	2.769	447.75	0.0533	157	→	161	0.17373
				157	→	162	-0.1019
				158	→	161	0.55628
				158	→	162	-0.25706
				159	→	162	-0.13406
				159	→	163	-0.19035
7	2.79	444.3	0.0101	158	→	162	-0.1993
				158	→	163	-0.25582
				159	→	162	-0.14409
				159	→	163	0.57984
				160	→	163	0.11066
8	2.889	429.06	0.0786	157	→	162	0.13519
				157	→	163	-0.11762
				158	→	161	0.2118
				158	→	162	0.54224
				158	→	163	-0.27724
				159	→	161	-0.12053
9	3.022	410.22	0.0536	157	→	161	0.22941
				157	→	162	-0.12454
				157	→	163	0.19274
				158	→	161	0.13525
				158	→	162	0.15528
				158	→	163	0.48362
				159	→	163	0.18181
				160	→	163	0.21852
10	3.08	402.48	0.0046	157	→	161	0.57163
				157	→	162	-0.21935
				158	→	161	-0.25349
				158	→	163	-0.16517
				159	→	163	-0.10328
11	3.155	392.93	0.011	157	→	161	0.26215
				157	→	162	0.601

				158	→	162	-0.17177
12	3.285	377.41	0.0707	157	→	162	0.13685
				157	→	163	0.64251
				158	→	163	-0.21074
13	3.429	361.51	0.0116	160	→	164	0.45728
				160	→	165	-0.18542
				160	→	166	0.2852
				160	→	167	0.15382
				160	→	168	-0.1801
				160	→	169	-0.11781
				160	→	173	-0.20334
14	3.593	344.99	0.001	159	→	164	-0.20451
				159	→	166	-0.1564
				159	→	167	-0.10382
				159	→	173	0.13874
				160	→	164	0.32558
				160	→	165	0.46135
				160	→	168	0.15609
15	3.614	343.02	0.001	158	→	173	-0.10254
				160	→	164	-0.33909
				160	→	165	0.3464
				160	→	166	0.3857
				160	→	169	-0.14233
				160	→	173	-0.14937
16	3.701	334.95	0.0028	157	→	173	0.1416
				158	→	164	-0.27037
				158	→	166	-0.21926
				158	→	167	-0.12987
				158	→	168	0.12487
				158	→	169	0.1411
				158	→	173	0.30213
				160	→	166	0.24329
17	3.775	328.4	0.0131	158	→	165	-0.10149
				159	→	164	0.36526
				159	→	166	0.1637
				159	→	173	-0.20222
				160	→	164	0.15439
				160	→	165	0.26949
				160	→	166	-0.28079
18	3.837	323.08	0.0032	159	→	164	0.31477
				159	→	165	0.26196
				159	→	177	-0.11268
				160	→	166	0.25179
				160	→	167	-0.30085
				160	→	168	0.21902
19	3.85	321.99	0.0315	158	→	164	-0.12352

				159	→	164	0.12663
				159	→	165	0.36807
				159	→	168	0.15599
				159	→	173	0.17942
				160	→	166	-0.15635
				160	→	167	0.12864
				160	→	168	-0.26719
				160	→	173	-0.1799
				160	→	176	0.12938
				160	→	177	-0.12635
20	3.866	320.69	0.0078	159	→	164	0.20184
				159	→	166	-0.15599
				159	→	177	-0.11446
				160	→	167	0.52995
				160	→	168	0.11529
				160	→	173	0.13158
21	3.902	317.71	0.0703	155	→	161	-0.10911
				156	→	161	0.5494
				156	→	162	-0.30877
				159	→	164	0.15514
22	3.915	316.68	0.0206	156	→	161	0.13879
				159	→	164	-0.29086
				159	→	165	0.44212
				159	→	166	0.23089
				159	→	173	-0.16521
				160	→	176	-0.10154
				160	→	177	0.13292
23	3.944	314.3	0.0066	156	→	161	0.12956
				159	→	176	-0.10273
				159	→	177	0.13254
				160	→	165	-0.14164
				160	→	167	0.11486
				160	→	168	0.48342
				160	→	169	-0.11692
				160	→	173	-0.21231
				160	→	176	0.11777
24	3.966	312.58	0.0223	157	→	164	0.15842
				157	→	165	0.10255
				158	→	164	0.51576
				158	→	165	0.19411
				158	→	173	0.15671
				159	→	164	0.13447
				159	→	165	0.10462
25	4.004	309.64	0.0774	155	→	161	0.23474
				155	→	162	0.17021
				156	→	161	0.31491

				156	→	162	0.52808
26	4.023	308.17	0.0027	157	→	165	0.182
				158	→	164	-0.19867
				158	→	165	0.5609
				158	→	166	0.14221
				158	→	168	0.13049
				158	→	173	-0.10708
27	4.066	304.9	0.0254	154	→	161	-0.19114
				155	→	161	0.45264
				155	→	162	0.11048
				156	→	162	-0.18206
				158	→	166	0.12321
				159	→	166	0.29107
				160	→	167	0.12447
				160	→	169	0.11045
28	4.093	302.89	0.0044	154	→	162	0.12129
				155	→	161	-0.2362
				155	→	162	-0.35588
				156	→	162	0.17462
				159	→	166	0.35691
				159	→	167	-0.15301
				159	→	168	0.12828
				160	→	169	0.10908
				160	→	177	-0.11159
29	4.124	300.64	0.0214	154	→	161	0.29087
				154	→	162	-0.22205
				155	→	161	-0.21064
				155	→	162	0.42187
				156	→	163	0.1677
				159	→	166	0.18187
				159	→	167	-0.11997
30	4.147	298.96	0.004	155	→	161	-0.12033
				155	→	162	0.14893
				156	→	163	-0.2702
				158	→	166	-0.22872
				158	→	173	-0.1493
				159	→	165	-0.16457
				159	→	166	0.14246
				159	→	167	0.298
				159	→	168	0.23669
31	4.148	298.88	0.0215	154	→	161	0.1302
				154	→	162	-0.14595
				154	→	163	0.10583
				155	→	162	-0.20053
				156	→	163	0.41141
				158	→	166	-0.2063

				158	→	167	-0.10961
				159	→	167	0.28897
				160	→	169	0.14395
32	4.183	296.38	0.0098	154	→	161	-0.22322
				154	→	162	0.10924
				154	→	163	0.11749
				155	→	161	-0.17104
				155	→	162	0.13036
				158	→	166	0.14376
				159	→	167	0.27148
				159	→	168	-0.21674
				159	→	173	-0.10042
				160	→	169	0.30645
				160	→	177	-0.12441
33	4.199	295.27	0.0111	158	→	166	0.42151
				158	→	173	0.16322
				159	→	165	-0.11562
				159	→	167	0.31569
				159	→	168	0.22476
				160	→	169	-0.13123
34	4.21	294.49	0.0055	154	→	161	0.41009
				154	→	162	-0.14385
				155	→	161	0.19657
				155	→	162	-0.16657
				156	→	163	-0.35828
				160	→	169	0.18504
35	4.237	292.59	0.0285	157	→	164	0.33096
				157	→	165	-0.16795
				157	→	166	-0.20836
				158	→	165	0.12157
				158	→	167	-0.30525
				158	→	168	-0.10375
				159	→	168	-0.28702
				160	→	169	-0.13644
36	4.246	291.94	0.0108	153	→	161	-0.16141
				157	→	164	0.28049
				157	→	165	-0.13358
				158	→	167	-0.14883
				159	→	166	-0.17604
				159	→	168	0.30147
				159	→	169	-0.12279
				159	→	173	-0.1138
				159	→	177	0.11233
				160	→	169	0.24552
37	4.278	289.81	0.0168	154	→	161	0.20656
				154	→	162	0.30489

				154	→	163	0.10215
				155	→	163	-0.15934
				157	→	164	0.25492
				157	→	165	-0.15796
				157	→	167	0.11193
				158	→	164	-0.10698
				158	→	166	-0.19152
				158	→	167	0.30768
				159	→	167	0.13082
38	4.292	288.87	0.0043	154	→	161	0.19809
				154	→	162	0.43015
				156	→	162	-0.10199
				157	→	164	-0.14756
				157	→	167	-0.11361
				158	→	164	0.14958
				158	→	166	0.11824
				158	→	167	-0.32201
				158	→	168	0.16638
39	4.307	287.83	0.0012	153	→	161	-0.21483
				153	→	162	0.13286
				154	→	162	-0.2371
				154	→	163	0.13479
				155	→	163	-0.23414
				157	→	166	0.20648
				158	→	168	0.33101
				159	→	168	-0.15825
				160	→	169	-0.13343
40	4.34	285.68	0.0093	153	→	161	-0.22126
				153	→	162	0.14855
				154	→	163	-0.21488
				155	→	163	0.48819
				156	→	163	0.17753
				157	→	166	0.11212
				158	→	167	0.12289
				158	→	168	0.14736
				159	→	169	0.10226

Table S10. TDDFT calculated transitions for *mer*-[Ru(Q3PzH)$_2$(Q3Pz$_c$)]$^+$.

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	2.276	544.74	0.1307	159	→	161	0.10663
				160	→	161	0.69365
2	2.389	518.84	0.0062	160	→	162	0.64174
				160	→	163	-0.27341
3	2.527	490.51	0.025	159	→	163	0.2383
				160	→	162	0.24128
				160	→	163	0.59157

4	2.564	483.55	0.0658	158	→	161	0.17809
				159	→	161	0.66104
5	2.681	462.42	0.0548	158	→	162	0.18888
				158	→	163	0.10337
				159	→	162	0.57084
				159	→	163	0.27341
				160	→	163	-0.13199
6	2.749	450.94	0.0464	157	→	161	-0.10554
				158	→	161	0.67003
				159	→	161	-0.16173
7	2.858	433.78	0.0292	157	→	162	-0.12041
				158	→	162	0.59851
				158	→	163	0.25316
				159	→	162	-0.21021
8	2.907	426.39	0.0146	158	→	162	-0.26312
				158	→	163	0.47378
				159	→	162	-0.20928
				159	→	163	0.371
9	3.048	406.75	0.0622	157	→	163	0.11197
				158	→	162	0.1236
				158	→	163	-0.40848
				159	→	162	-0.22252
				159	→	163	0.43684
				160	→	163	-0.12626
10	3.291	376.73	0.0037	157	→	161	0.68495
11	3.359	369.07	0.0012	160	→	164	-0.3205
				160	→	165	0.42304
				160	→	168	-0.28165
				160	→	173	0.20612
12	3.375	367.3	0.0417	157	→	162	0.66227
				158	→	162	0.10226
				159	→	162	-0.10938
13	3.432	361.25	0.0083	160	→	164	0.55949
				160	→	165	0.35912
				160	→	167	0.16477
14	3.572	347.04	0.0114	157	→	163	0.60802
				159	→	163	-0.11724
				159	→	165	-0.12641
				159	→	168	0.10956
				159	→	173	-0.14884
15	3.616	342.84	0.0068	157	→	162	0.11566
				157	→	163	0.28854
				159	→	164	-0.24034
				159	→	165	0.27503
				159	→	168	-0.2629
				159	→	173	0.29646

				159	→	176	-0.11578
16	3.674	337.43	0.003	160	→	164	-0.147
				160	→	166	0.64715
				160	→	167	0.16243
17	3.732	332.15	0.0046	158	→	165	-0.1148
				158	→	173	-0.10716
				160	→	164	-0.20203
				160	→	165	0.28439
				160	→	166	-0.14977
				160	→	167	0.34209
				160	→	168	0.30284
				160	→	169	0.11205
				160	→	173	-0.19661
18	3.767	329.08	0.0081	155	→	161	-0.12037
				156	→	161	0.54512
				160	→	165	-0.1296
				160	→	166	-0.11061
				160	→	167	0.33466
				160	→	168	-0.10351
19	3.777	328.21	0.0091	156	→	161	-0.3912
				160	→	165	-0.22638
				160	→	167	0.41785
				160	→	168	-0.2111
				160	→	173	0.10004
20	3.821	324.45	0.0035	158	→	165	0.12628
				159	→	164	0.56698
				159	→	165	0.28905
				159	→	167	0.13156
21	3.873	320.1	0.1504	155	→	161	0.64809
				156	→	162	0.13691
				156	→	163	0.13036
				160	→	167	0.10055
22	3.919	316.37	0.0252	158	→	164	0.3512
				158	→	165	-0.202
				158	→	168	0.19491
				158	→	173	-0.21789
				159	→	166	0.22359
				160	→	168	-0.28602
				160	→	177	-0.11719
23	3.965	312.69	0.0042	153	→	162	-0.1163
				158	→	164	-0.12071
				159	→	166	0.60233
				160	→	168	0.1188
24	3.993	310.46	0.0325	158	→	164	0.43386
				158	→	165	0.3348
				158	→	167	0.18793

				159	→	164	-0.11666
				160	→	168	0.19785
				160	→	169	-0.16338
25	4.03	307.62	0.0219	155	→	161	-0.19443
				156	→	162	0.57138
				156	→	163	0.3202
26	4.035	307.22	0.0147	155	→	162	-0.15942
				159	→	164	-0.20977
				159	→	165	0.47057
				159	→	167	0.11464
				159	→	168	0.18329
				159	→	169	0.10797
				159	→	173	-0.21562
				160	→	169	0.11634
27	4.063	305.12	0.0186	158	→	164	0.1535
				158	→	165	0.17419
				158	→	166	0.12697
				158	→	177	-0.16145
				159	→	165	-0.11607
				160	→	168	-0.13498
				160	→	169	0.40349
				160	→	173	-0.18153
				160	→	177	0.21671
28	4.102	302.23	0.0054	155	→	162	0.58269
				155	→	163	0.16772
				156	→	163	-0.2348
				159	→	167	0.10995
29	4.134	299.9	0.0075	156	→	163	0.17198
				158	→	164	-0.15348
				158	→	165	0.12938
				159	→	165	-0.12701
				159	→	167	0.51888
				160	→	169	0.10752
				160	→	177	-0.14661
30	4.143	299.25	0.0047	155	→	162	-0.12623
				156	→	162	0.19609
				156	→	163	-0.25286
				158	→	164	-0.16287
				158	→	165	0.28331
				159	→	167	-0.19709
				160	→	168	-0.13932
				160	→	171	0.10039
				160	→	173	-0.15278
				160	→	174	0.11828
				160	→	177	-0.28211
31	4.158	298.13	0.0167	155	→	162	0.15598

				156	→	162	-0.29233
				156	→	163	0.45236
				158	→	165	0.12491
				159	→	167	-0.24358
				160	→	173	-0.12247
				160	→	177	-0.10698
32	4.196	295.44	0.0034	154	→	162	0.11611
				155	→	163	0.55562
				158	→	177	0.12653
				160	→	169	0.21637
				160	→	173	0.15535
33	4.226	293.38	0.0036	155	→	163	-0.13823
				158	→	164	-0.16469
				158	→	166	0.48525
				158	→	167	0.22285
				160	→	168	0.10628
				160	→	169	0.19405
				160	→	171	-0.11135
				160	→	173	0.19432
34	4.253	291.52	0.0183	155	→	162	-0.17648
				155	→	163	0.31634
				158	→	166	0.30897
				158	→	177	-0.17685
				159	→	167	0.11805
				159	→	168	0.10309
				159	→	169	-0.10923
				160	→	169	-0.31505
				160	→	173	-0.13594
35	4.289	289.02	0.0027	154	→	161	0.14428
				158	→	164	-0.14842
				158	→	166	-0.23434
				158	→	167	0.51947
				158	→	177	-0.11136
				159	→	168	-0.18675
36	4.319	287.06	0.0047	154	→	161	0.64398
				158	→	167	-0.10566
				158	→	168	-0.12374
37	4.334	286.04	0.0294	154	→	161	0.11118
				158	→	166	-0.16974
				158	→	167	0.15422
				158	→	168	0.13488
				159	→	168	0.47773
				159	→	169	-0.21321
				159	→	171	-0.11043
				159	→	173	0.19597
38	4.355	284.68	0.0018	154	→	161	0.12668

				158	→	165	0.32705
				158	→	167	-0.21762
				158	→	168	0.42463
				158	→	173	-0.1543
				160	→	177	0.15837
39	4.486	276.35	0.0294	154	→	162	0.48121
				157	→	164	0.22336
				157	→	166	-0.27809
				159	→	166	-0.10723
				159	→	169	-0.25565
40	4.497	275.69	0.0015	153	→	162	0.22465
				154	→	162	0.1439
				154	→	163	0.19286
				157	→	164	-0.25953
				157	→	166	0.34674
				159	→	168	-0.12256
				159	→	169	-0.23379
				159	→	173	-0.14631

Table S11. TDDFT calculated transitions for *mer*-[Ru(Q3PzH$_a$)(Q3Pz)$_2$].

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	2.1731	570.54	0.1431	158	→	161	0.11888
				159	→	161	-0.13505
				160	→	161	0.67142
2	2.237	554.24	0.0128	159	→	161	0.6819
				160	→	161	0.12848
3	2.2592	548.79	0.0147	160	→	161	0.10009
				160	→	162	0.66423
				160	→	163	-0.17972
4	2.4017	516.24	0.0293	158	→	163	-0.13715
				159	→	162	0.46506
				159	→	163	0.27377
				160	→	162	-0.10361
				160	→	163	-0.39946
5	2.4152	513.34	0.0174	159	→	163	0.61474
				160	→	162	0.13837
				160	→	163	0.25506
6	2.4848	498.97	0.0022	158	→	162	-0.17541
				158	→	163	0.25218
				159	→	162	0.46391
				159	→	163	-0.1074
				160	→	163	0.37897
7	2.5488	486.45	0.077	158	→	161	0.66643
				158	→	163	-0.12213
				160	→	161	-0.1177

8	2.7291	454.31	0.0566	158	→	162	0.56765
				158	→	163	0.34473
				159	→	162	0.10379
				160	→	163	-0.1047
9	2.9005	427.46	0.0792	157	→	161	-0.10591
				158	→	162	-0.33369
				158	→	163	0.4907
				159	→	162	-0.18189
				160	→	163	-0.23057
10	3.0734	403.41	0.0139	157	→	161	0.68263
11	3.1926	388.35	0.0127	156	→	161	0.6842
				157	→	161	-0.10974
12	3.279	378.11	0.0582	157	→	162	0.61006
				157	→	163	0.32249
13	3.309	374.69	0.0339	156	→	162	0.35017
				160	→	164	0.45205
				160	→	165	0.27158
				160	→	166	-0.11926
				160	→	167	0.18747
14	3.3178	373.7	0.0384	156	→	162	0.57001
				157	→	163	0.11098
				160	→	164	-0.31118
				160	→	165	-0.125
				160	→	166	0.11124
				160	→	167	-0.11135
15	3.3668	368.26	0.0242	156	→	162	-0.13991
				157	→	162	-0.34121
				157	→	163	0.55874
				160	→	164	-0.11856
				160	→	165	0.13033
16	3.4027	364.37	0.0063	157	→	163	-0.19662
				160	→	164	-0.35547
				160	→	165	0.49572
				160	→	169	0.15947
17	3.4655	357.77	0.0094	156	→	163	0.64693
				157	→	163	-0.1158
				158	→	163	0.1251
				159	→	164	-0.1032
18	3.5336	350.88	0.0101	156	→	163	0.12542
				159	→	164	0.45269
				159	→	165	0.16616
				160	→	164	-0.11725
				160	→	166	-0.41774
				160	→	167	0.11932
19	3.5548	348.78	0.003	159	→	164	0.4941
				160	→	164	0.15263

				160	→	166	0.42475
				160	→	167	-0.1649
20	3.6343	341.15	0.0057	156	→	163	0.10001
				159	→	164	-0.12391
				159	→	165	0.51311
				159	→	169	0.12039
				160	→	165	-0.16432
				160	→	166	0.24182
				160	→	167	0.1073
				160	→	169	0.12035
21	3.6471	339.95	0.0111	159	→	165	-0.22772
				160	→	165	-0.26915
				160	→	166	0.13342
				160	→	167	0.44171
				160	→	168	-0.10538
				160	→	169	0.15538
				160	→	174	0.10104
				160	→	175	-0.11932
22	3.6958	335.47	0.0141	158	→	164	0.11306
				159	→	166	0.64024
				159	→	167	-0.10092
				159	→	168	-0.10274
				160	→	167	0.13294
23	3.7341	332.03	0.0019	158	→	164	0.23671
				158	→	165	0.25976
				158	→	167	0.17903
				158	→	169	0.127
				158	→	174	0.12433
				158	→	175	-0.14653
				159	→	166	-0.20462
				160	→	166	0.11361
				160	→	167	0.30854
				160	→	169	-0.1477
				160	→	175	0.11462
24	3.79	327.13	0.0024	158	→	164	0.32067
				158	→	165	0.10072
				159	→	165	-0.2366
				159	→	167	0.16925
				160	→	165	-0.10794
				160	→	167	-0.22615
				160	→	168	-0.17609
				160	→	169	0.28555
				160	→	174	0.11155
				160	→	175	-0.11473
25	3.8339	323.39	0.0165	158	→	164	0.47711
				158	→	165	-0.14735

				159	→	165	0.20272
				159	→	167	-0.2103
				159	→	169	-0.14822
				159	→	174	-0.12039
				159	→	175	0.13913
26	3.8639	320.88	0.0256	155	→	161	0.16727
				158	→	164	0.2246
				158	→	165	-0.23193
				158	→	167	-0.12109
				158	→	174	-0.10867
				158	→	175	0.13113
				159	→	167	0.38139
				160	→	168	0.25824
27	3.8871	318.96	0.0547	154	→	161	-0.16351
				155	→	161	0.62267
				160	→	168	-0.14156
28	3.9378	314.86	0.0273	155	→	161	-0.13939
				158	→	165	0.14354
				158	→	166	0.33926
				158	→	167	-0.12669
				159	→	166	0.10158
				159	→	167	0.32266
				159	→	168	0.14617
				159	→	169	-0.209
				159	→	174	-0.11845
				159	→	175	0.15899
				160	→	176	0.12387
29	3.9531	313.64	0.0032	158	→	165	-0.20312
				158	→	166	0.50263
				159	→	166	-0.10669
				159	→	167	-0.27039
				159	→	168	-0.11475
				159	→	169	0.13065
30	3.9805	311.48	0.0235	154	→	161	0.66212
				155	→	161	0.15827
31	4.0191	308.48	0.0089	158	→	165	-0.14445
				158	→	174	0.10803
				158	→	175	-0.14306
				160	→	168	0.44253
				160	→	169	0.3834
32	4.035	307.27	0.0089	158	→	165	0.44612
				158	→	166	0.18909
				158	→	169	-0.15472
				158	→	172	0.1034
				158	→	174	-0.13505
				158	→	175	0.17691

				159	→	167	-0.13549
				160	→	168	0.20851
				160	→	169	0.11724
33	4.077	304.1	0.0179	154	→	162	-0.1302
				158	→	176	-0.12718
				159	→	169	-0.2127
				159	→	176	0.26348
				160	→	168	-0.20746
				160	→	169	0.26085
				160	→	172	0.14924
				160	→	174	-0.16903
				160	→	175	0.23243
				160	→	176	-0.14635
34	4.101	302.33	0.0104	153	→	162	0.12978
				155	→	162	0.16653
				159	→	168	0.56992
				159	→	169	0.23856
35	4.1265	300.46	0.0046	156	→	167	-0.10141
				158	→	166	0.17594
				158	→	167	0.5874
36	4.1483	298.88	0.0061	154	→	162	-0.2583
				154	→	163	-0.1924
				155	→	162	0.43544
				155	→	163	0.36516
37	4.1931	295.68	0.0094	152	→	161	-0.11306
				153	→	161	0.57195
				157	→	164	0.22731
				157	→	165	-0.13977
				158	→	165	0.10644
				159	→	169	0.11139
38	4.1993	295.25	0.0085	154	→	162	0.51088
				155	→	162	0.39059
				159	→	168	-0.11353
				159	→	169	-0.14266
39	4.2152	294.14	0.0019	154	→	162	0.34754
				154	→	163	-0.13827
				155	→	162	-0.29348
				155	→	163	0.46181
				157	→	164	-0.10464
40	4.2429	292.21	0.0154	152	→	161	0.1161
				153	→	161	-0.25031
				155	→	163	0.15479
				157	→	164	0.15815
				157	→	165	-0.13643
				159	→	168	-0.13313
				159	→	169	0.33122

				160	→	168	-0.10803
				160	→	169	0.11074
				160	→	171	0.14329
				160	→	176	0.22993

Table S12. TDDFT calculated transitions for *mer*-[Ru(Q3PzH$_b$)(Q3Pz)$_2$].

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	2.05	604.8	0.0021	160	→	161	0.22522
				160	→	162	0.63855
				160	→	163	-0.18391
2	2.105	589	0.0491	160	→	161	0.65707
				160	→	162	-0.23575
3	2.2279	556.51	0.0687	158	→	163	-0.14256
				159	→	163	0.19692
				160	→	162	0.15977
				160	→	163	0.61792
4	2.4162	513.13	0.0011	159	→	161	0.56041
				159	→	162	-0.28042
				159	→	163	-0.29103
5	2.5253	490.98	0.063	159	→	161	0.39152
				159	→	162	0.26847
				159	→	163	0.48567
				160	→	163	-0.12131
6	2.6339	470.73	0.1475	158	→	161	0.1356
				158	→	163	-0.32897
				159	→	161	0.11248
				159	→	162	0.50287
				159	→	163	-0.28114
7	2.6757	463.37	0.0123	158	→	161	0.19709
				158	→	162	0.64448
				159	→	163	0.10021
8	2.7257	454.87	0.0292	158	→	161	0.62174
				158	→	162	-0.1458
				158	→	163	0.26
9	2.8445	435.87	0.0264	158	→	161	-0.18475
				158	→	162	0.17956
				158	→	163	0.5037
				159	→	162	0.23753
				159	→	163	-0.1693
				160	→	163	0.21045
10	3.1317	395.9	0.0497	156	→	161	-0.18305
				157	→	161	0.649
11	3.1776	390.18	0.0598	156	→	161	0.13066
				156	→	162	0.17954
				157	→	162	0.64185
12	3.2243	384.53	0.0066	156	→	163	0.11219

				157	→	161	0.10106
				157	→	163	-0.38716
				160	→	165	0.49158
				160	→	167	0.16612
13	3.2508	381.4	0.0559	156	→	161	-0.21498
				156	→	162	-0.2083
				157	→	162	0.1192
				157	→	163	0.43618
				160	→	165	0.39221
				160	→	167	0.1073
14	3.2794	378.07	0.0146	156	→	161	0.1399
				156	→	162	0.28107
				156	→	163	-0.11981
				157	→	162	-0.15277
				157	→	163	0.12002
				160	→	164	0.55695
				160	→	165	0.1353
15	3.3153	373.98	0.0273	156	→	161	0.14614
				156	→	162	0.46162
				156	→	163	-0.15214
				157	→	162	-0.12153
				157	→	163	0.23056
				160	→	164	-0.39773
16	3.3215	373.27	0.0029	156	→	161	0.5656
				156	→	162	-0.31876
				156	→	163	-0.14923
				157	→	161	0.16675
				157	→	163	0.10392
17	3.4573	358.62	0.0004	160	→	166	0.67858
18	3.4923	355.02	0.0025	156	→	161	0.14629
				156	→	163	0.62565
				157	→	163	0.23336
19	3.5607	348.21	0.017	160	→	165	-0.2402
				160	→	167	0.63166
20	3.5832	346.02	0.0013	159	→	164	-0.25426
				159	→	165	0.52838
				159	→	167	0.24906
				159	→	175	0.17416
21	3.6196	342.53	0.0035	159	→	164	0.59394
				159	→	165	0.25569
				159	→	166	0.16429
				159	→	167	0.11461
22	3.7742	328.5	0.0034	158	→	164	0.11691
				159	→	166	0.1709
				160	→	167	0.14083
				160	→	168	0.3057

				160	→	169	0.45327
				160	→	175	-0.17804
				160	→	176	0.11962
23	3.8034	325.98	0.0353	158	→	164	-0.15359
				158	→	165	0.46547
				158	→	167	0.2195
				158	→	172	-0.12216
				158	→	175	0.23619
				160	→	168	0.19858
24	3.8348	323.31	0.0445	155	→	161	0.10406
				159	→	164	0.10341
				159	→	166	-0.22806
				160	→	168	0.47279
				160	→	169	-0.32601
				160	→	176	-0.12645
25	3.8392	322.95	0.0075	159	→	164	-0.18923
				159	→	166	0.54007
				159	→	168	0.13538
				159	→	175	-0.11173
				160	→	168	0.12259
				160	→	169	-0.2506
				160	→	176	-0.10461
26	3.8884	318.86	0.0559	155	→	161	0.63949
				155	→	162	-0.11501
				159	→	166	0.13433
				159	→	167	0.10026
27	3.9222	316.11	0.0039	155	→	161	-0.13702
				158	→	164	0.19265
				158	→	165	0.1273
				159	→	165	-0.33388
				159	→	167	0.41604
				159	→	168	-0.14686
				159	→	172	-0.1056
				159	→	175	0.20063
28	3.9574	313.3	0.0037	154	→	162	0.1245
				158	→	164	0.58172
				158	→	165	0.20161
				159	→	168	0.1042
29	4.0002	309.95	0.0187	155	→	162	0.41787
				155	→	163	0.52247
30	4.0089	309.27	0.0017	154	→	162	0.11675
				155	→	162	-0.19497
				158	→	166	0.10067
				159	→	166	-0.16081
				159	→	167	0.41637
				159	→	168	0.25414

				159	→	169	0.10412
				159	→	172	0.11704
				159	→	175	-0.2201
				160	→	175	-0.10648
31	4.0493	306.19	0.0088	154	→	162	0.20165
				155	→	161	0.12539
				155	→	162	0.44287
				155	→	163	-0.4052
				158	→	166	0.18802
32	4.0672	304.84	0.0052	154	→	161	0.35458
				154	→	162	0.3779
				155	→	162	-0.19992
				158	→	164	-0.12792
				158	→	165	0.18357
				158	→	175	-0.11712
				159	→	169	-0.10937
33	4.0878	303.3	0.0004	154	→	161	0.17844
				158	→	164	0.16871
				158	→	165	-0.28177
				158	→	166	0.3033
				158	→	167	0.21157
				158	→	169	-0.13237
				158	→	175	0.14451
				158	→	176	-0.11856
				160	→	168	0.13179
				160	→	175	0.16123
				160	→	176	0.17178
34	4.1004	302.37	0.0045	154	→	161	0.49631
				154	→	162	-0.17227
				155	→	163	-0.10929
				158	→	165	-0.10143
				158	→	166	-0.33086
				159	→	167	0.10557
35	4.1209	300.87	0.0175	154	→	161	-0.18127
				154	→	162	0.43808
				158	→	165	-0.13408
				158	→	166	-0.3914
				158	→	167	0.17441
36	4.1802	296.6	0.0047	153	→	161	-0.11884
				154	→	163	0.18928
				158	→	166	-0.14617
				158	→	167	-0.13833
				158	→	176	-0.14075
				159	→	168	0.25628
				159	→	169	-0.20578
				160	→	169	-0.17505

				160	→	174	0.10666
				160	→	176	0.37194
37	4.2051	294.84	0.0059	153	→	162	-0.12595
				153	→	163	-0.17732
				154	→	162	-0.11043
				154	→	163	0.14896
				157	→	164	-0.12992
				158	→	167	0.39431
				159	→	169	-0.12575
				160	→	168	-0.19048
				160	→	171	0.13674
				160	→	172	0.14893
				160	→	175	-0.24299
38	4.2356	292.72	0.0029	153	→	161	0.11901
				154	→	163	-0.25261
				156	→	164	0.13911
				156	→	166	0.16013
				157	→	164	0.37388
				158	→	166	-0.13031
				158	→	167	0.11021
				159	→	168	-0.23717
				160	→	169	-0.11427
				160	→	172	0.10002
				160	→	175	-0.15614
				160	→	176	0.16002
39	4.2558	291.33	0.0101	153	→	161	-0.17751
				153	→	163	-0.11374
				154	→	161	0.105
				154	→	163	0.46414
				156	→	164	0.10098
				157	→	164	0.18721
				158	→	167	-0.16289
				159	→	168	-0.27594
40	4.2659	290.64	0.0147	150	→	163	-0.11217
				153	→	161	0.10127
				154	→	163	0.15786
				156	→	166	0.12042
				157	→	164	0.35248
				157	→	166	-0.11845
				158	→	167	0.1557
				158	→	169	0.10993
				158	→	176	0.12004
				159	→	168	0.29835
				159	→	175	0.15786
				160	→	175	0.10362

Table S13. TDDFT calculated transitions for *mer*-[Ru(Q3PzH$_c$)(Q3Pz)$_2$].

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	1.9785	626.65	0.0066	160	→	161	0.69684
2	2.1641	572.9	0.1234	158	→	162	-0.10213
				160	→	162	0.69115
3	2.3491	527.78	0.0419	158	→	161	-0.20997
				158	→	163	-0.1464
				159	→	161	0.18997
				160	→	163	0.6112
4	2.4337	509.45	0.0161	158	→	161	0.62668
				159	→	161	0.27198
				160	→	163	0.13446
5	2.4998	495.99	0.0197	158	→	162	-0.25727
				159	→	161	-0.17761
				159	→	162	0.61769
6	2.5234	491.34	0.0457	158	→	161	-0.21062
				159	→	161	0.4726
				159	→	162	0.21067
				159	→	163	0.36998
				160	→	163	-0.17196
7	2.6194	473.33	0.1175	158	→	162	0.62621
				158	→	163	-0.12143
				159	→	162	0.2316
				160	→	162	0.11687
8	2.6768	463.18	0.0342	158	→	162	0.13717
				158	→	163	0.45775
				159	→	161	0.23798
				159	→	163	-0.4337
9	2.8517	434.77	0.0069	157	→	162	-0.11114
				158	→	163	0.46693
				159	→	161	-0.21458
				159	→	163	0.35056
				160	→	163	0.2259
10	3.0785	402.74	0.0164	157	→	161	0.60551
				157	→	162	-0.33711
11	3.1077	398.96	0.0018	157	→	161	0.33405
				157	→	162	0.59528
				160	→	164	-0.10918
12	3.2283	384.06	0.0086	160	→	164	0.66472
13	3.3406	371.14	0.1166	156	→	162	-0.1597
				157	→	163	0.65593
				160	→	165	0.12129
14	3.3933	365.38	0.0095	157	→	163	-0.1337
				160	→	165	0.54129
				160	→	166	-0.3238
				160	→	169	-0.17162

15	3.4206	362.46	0.0123	156	→	162	0.47992
				157	→	163	0.13772
				160	→	165	-0.27543
				160	→	166	-0.37773
16	3.4526	359.1	0.0144	156	→	162	0.45944
				157	→	163	0.10474
				160	→	165	0.24521
				160	→	166	0.44118
17	3.4657	357.75	0.003	156	→	161	0.68059
				156	→	162	-0.10273
18	3.5379	350.45	0.0033	159	→	164	-0.39898
				159	→	167	-0.13182
				160	→	164	-0.1394
				160	→	167	0.48197
19	3.5663	347.66	0.0113	158	→	164	-0.15887
				159	→	164	0.49672
				159	→	167	0.13663
				160	→	167	0.33868
20	3.6635	338.43	0.006	156	→	163	0.57433
				158	→	164	-0.12835
				160	→	166	0.1157
				160	→	167	0.16376
				160	→	169	-0.15766
21	3.7155	333.7	0.0181	156	→	163	0.35181
				159	→	165	-0.12474
				159	→	169	0.13805
				159	→	173	-0.10913
				159	→	175	0.14009
				160	→	166	-0.12049
				160	→	167	-0.16659
				160	→	169	0.34823
				160	→	173	-0.15731
				160	→	175	0.18872
22	3.7233	333	0.0487	158	→	164	0.60188
				158	→	167	0.14759
				160	→	167	0.20395
23	3.7733	328.58	0.0012	158	→	165	-0.11198
				158	→	166	0.11092
				158	→	169	0.12909
				159	→	165	0.27458
				159	→	166	-0.20375
				159	→	169	-0.21918
				159	→	173	0.16722
				159	→	175	-0.20102
				160	→	168	-0.24969
				160	→	169	0.18012

				160	→	177	0.11936
24	3.8156	324.94	0.0192	155	→	161	0.38368
				155	→	162	-0.1201
				159	→	166	-0.12658
				160	→	168	0.50882
25	3.8293	323.78	0.0559	155	→	161	0.52716
				158	→	165	0.10007
				159	→	167	0.1193
				160	→	168	-0.32136
26	3.8673	320.6	0.0122	154	→	162	0.12397
				155	→	162	0.59288
				159	→	165	0.23614
				159	→	167	0.11768
				160	→	168	0.15737
27	3.8794	319.59	0.0109	155	→	161	-0.11715
				155	→	162	-0.26252
				159	→	164	-0.11613
				159	→	165	0.48669
				159	→	166	0.26918
				159	→	167	0.19886
28	3.8962	318.22	0.0112	158	→	165	0.15885
				159	→	164	0.15723
				159	→	166	0.48043
				159	→	167	-0.3354
				159	→	175	-0.118
				160	→	169	0.10869
29	3.9326	315.27	0.0031	155	→	162	-0.12353
				158	→	165	0.51648
				158	→	166	-0.12732
				158	→	169	-0.10026
				159	→	165	0.15153
				159	→	166	-0.23399
				160	→	169	0.14443
30	3.9556	313.44	0.0053	158	→	164	-0.126
				158	→	165	0.33549
				158	→	166	0.47456
				158	→	167	0.19808
				158	→	169	0.12256
				158	→	175	0.10587
				159	→	165	-0.12209
31	3.9675	312.5	0.0117	158	→	164	-0.19415
				158	→	166	-0.3809
				158	→	167	0.47549
				158	→	169	0.13125
				158	→	175	0.11439
32	4.032	307.5	0.0243	154	→	161	0.28871

				155	→	163	0.12822
				158	→	166	-0.11211
				158	→	167	-0.1457
				159	→	165	-0.17582
				159	→	166	0.17711
				159	→	167	0.42723
				159	→	169	-0.17684
				159	→	173	0.11882
				159	→	175	-0.14388
				160	→	169	0.10799
33	4.0558	305.69	0.0225	154	→	161	0.54376
				155	→	161	0.10366
				158	→	165	-0.10476
				159	→	167	-0.13104
				160	→	176	-0.12529
				160	→	177	-0.19239
34	4.096	302.7	0.005	154	→	161	0.24835
				158	→	167	-0.21998
				158	→	175	0.1178
				158	→	176	-0.10452
				158	→	177	-0.18598
				159	→	167	-0.18614
				159	→	169	0.10611
				159	→	175	0.12018
				160	→	171	0.10735
				160	→	175	-0.13141
				160	→	176	0.17318
				160	→	177	0.30158
				160	→	179	0.11518
35	4.1241	300.64	0.0005	154	→	161	-0.10649
				154	→	163	0.14134
				155	→	163	0.66693
36	4.1455	299.08	0.0017	157	→	165	-0.12413
				158	→	165	0.11138
				158	→	166	-0.18231
				158	→	167	-0.28542
				158	→	169	0.2987
				158	→	173	-0.14584
				158	→	175	0.15327
				158	→	176	0.10699
				158	→	177	0.17642
				160	→	169	-0.27465
				160	→	173	-0.12168
				160	→	175	0.13937
37	4.2009	295.14	0.0042	154	→	162	0.67733
				155	→	162	-0.14715

38	4.2611	290.97	0.0036	152	→	162	-0.11243
				153	→	162	-0.14844
				157	→	164	0.19522
				157	→	165	0.28069
				157	→	166	0.10748
				159	→	168	0.51169
39	4.2811	289.61	0.0082	152	→	162	-0.11365
				157	→	164	0.2867
				157	→	165	0.39913
				158	→	168	-0.19707
				159	→	168	-0.34666
40	4.3057	287.95	0.0043	152	→	162	0.10428
				153	→	162	-0.18162
				157	→	164	0.41715
				157	→	165	-0.30078
				157	→	166	0.17478
				157	→	167	0.11418
				158	→	168	-0.27242

Table S14. TDDFT calculated transitions for *mer*-$[Ru(Q3Pz)_3]^-$.

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	1.9128	648.19	0.0425	158	→	161	-0.11438
				159	→	161	-0.10268
				160	→	161	0.67766
2	1.9663	630.54	0.0234	159	→	161	0.13227
				160	→	162	0.67406
3	2.0862	594.3	0.0042	159	→	161	0.45802
				159	→	162	0.29278
				159	→	163	-0.29943
				160	→	163	0.30971
4	2.1036	589.38	0.014	159	→	161	-0.32783
				159	→	162	-0.22413
				159	→	163	-0.14866
				160	→	162	0.10005
				160	→	163	0.53577
5	2.2089	561.29	0.0926	158	→	161	0.16303
				159	→	161	-0.32122
				159	→	162	0.5689
				160	→	162	0.12544
6	2.3787	521.22	0.1362	158	→	161	0.48143
				158	→	163	-0.12466
				159	→	161	0.16206
				159	→	163	0.42057
				160	→	161	0.12266
				160	→	163	0.11115
7	2.4012	516.35	0.0172	158	→	161	-0.35088

				158	→	162	0.40927
				158	→	163	-0.32398
				159	→	162	0.10428
				159	→	163	0.25686
				160	→	163	0.1133
8	2.4887	498.19	0.0507	158	→	161	0.16216
				158	→	162	0.51664
				158	→	163	0.41489
				159	→	161	-0.1003
9	2.6729	463.85	0.0209	158	→	161	-0.23608
				158	→	162	-0.17502
				158	→	163	0.41739
				159	→	163	0.33632
				160	→	163	0.25745
10	3.0187	410.71	0.0046	157	→	161	0.60107
				157	→	162	-0.33389
11	3.1017	399.73	0.0039	157	→	162	0.11392
				160	→	164	0.67884
12	3.1264	396.57	0.0158	157	→	161	0.34012
				157	→	162	0.59993
13	3.2438	382.22	0.1292	156	→	161	0.10392
				156	→	162	-0.10187
				157	→	163	0.60144
				160	→	165	0.28
14	3.2501	381.48	0.0369	156	→	162	0.13852
				157	→	163	-0.24744
				159	→	164	-0.10608
				160	→	165	0.60435
15	3.2706	379.09	0.0785	155	→	161	-0.16167
				155	→	162	-0.15264
				156	→	161	0.61138
				156	→	162	0.23077
16	3.2968	376.08	0.0009	156	→	161	-0.20262
				156	→	162	0.2619
				157	→	163	0.21273
				159	→	164	-0.38807
				160	→	165	-0.10073
				160	→	166	0.40336
17	3.3157	373.94	0.0362	155	→	161	-0.16396
				156	→	161	-0.19506
				156	→	162	0.5149
				157	→	163	0.11492
				159	→	164	0.26899
				160	→	166	-0.26786
18	3.3292	372.41	0.0046	159	→	164	0.49636
				160	→	166	0.47746

19	3.4015	364.49	0.0114	155	→	161	0.58536
				155	→	162	-0.31501
				156	→	162	0.20017
20	3.4504	359.34	0.0059	155	→	161	0.2241
				155	→	162	0.52343
				156	→	161	0.14608
				156	→	162	0.16306
				156	→	163	0.14022
				159	→	165	0.26165
21	3.4755	356.73	0.0029	155	→	161	-0.12038
				155	→	162	-0.24679
				159	→	165	0.54908
				159	→	166	-0.19876
				159	→	174	-0.12134
				160	→	169	0.10871
22	3.5316	351.07	0.0059	155	→	162	-0.12695
				156	→	163	0.37589
				158	→	164	-0.23135
				159	→	165	0.10526
				159	→	166	0.49569
23	3.5341	350.82	0.007	155	→	163	0.18114
				156	→	163	0.52556
				158	→	164	0.27153
				159	→	165	-0.12725
				159	→	166	-0.24627
24	3.5498	349.27	0.0044	156	→	163	-0.14461
				158	→	164	0.53085
				159	→	165	0.13776
				159	→	166	0.35559
				160	→	167	-0.11758
25	3.588	345.55	0.0006	155	→	163	-0.14997
				158	→	164	0.25578
				160	→	165	0.13241
				160	→	167	0.46115
				160	→	168	0.20609
				160	→	169	-0.21944
				160	→	174	0.17645
26	3.6379	340.81	0.0063	155	→	163	0.60403
				156	→	163	-0.14371
				160	→	167	0.29728
27	3.6655	338.25	0.0108	155	→	163	0.19543
				158	→	165	-0.23476
				158	→	174	0.10175
				160	→	167	-0.3048
				160	→	168	0.49086
28	3.6899	336.01	0.0137	155	→	163	-0.10414

				158	→	165	0.3777
				158	→	174	-0.16433
				160	→	168	0.41644
				160	→	169	0.20868
29	3.7222	333.09	0.0272	158	→	165	0.32698
				159	→	165	0.20587
				159	→	167	0.22333
				159	→	168	0.11954
				159	→	169	-0.2776
				159	→	174	0.23451
				159	→	175	0.11621
				160	→	169	-0.22822
30	3.7848	327.58	0.0014	158	→	165	0.1517
				158	→	166	0.46637
				159	→	168	-0.1118
				159	→	169	0.18271
				159	→	174	-0.20582
				160	→	169	-0.31479
31	3.7913	327.03	0.0052	154	→	161	0.60292
				154	→	162	-0.34179
32	3.8008	326.2	0.0175	158	→	165	-0.13917
				158	→	166	0.505
				159	→	168	0.12462
				159	→	169	-0.15701
				159	→	174	0.18878
				160	→	167	0.10051
				160	→	169	0.2797
33	3.874	320.04	0.0272	158	→	165	-0.10332
				159	→	167	0.59139
				159	→	168	0.10838
				159	→	169	0.20237
				160	→	169	0.119
34	3.8976	318.1	0.0032	158	→	165	0.32845
				158	→	167	0.17774
				158	→	168	0.1055
				158	→	169	-0.26546
				158	→	172	0.13753
				158	→	174	0.392
				160	→	169	0.18461
				160	→	174	0.10747
35	3.9103	317.07	0.0056	154	→	161	0.2841
				154	→	162	0.46634
				159	→	167	0.18175
				159	→	168	-0.34691
36	3.922	316.12	0.0127	154	→	161	0.15322
				154	→	162	0.36675

				159	→	168	0.53938
37	3.9712	312.21	0.0012	158	→	175	-0.13643
				160	→	167	0.11601
				160	→	169	-0.10681
				160	→	174	-0.28979
				160	→	175	0.38255
				160	→	177	0.17553
				160	→	178	0.26876
38	4.0333	307.4	0.0004	154	→	163	0.68149
39	4.1089	301.74	0.0098	157	→	164	-0.23374
				157	→	166	0.13383
				158	→	167	0.56334
				158	→	168	-0.16393
				158	→	169	0.12566
				158	→	174	-0.12546
40	4.1378	299.64	0.0015	157	→	164	0.4839
				157	→	166	-0.28471
				158	→	167	0.27653
				158	→	168	-0.14195

Table S15. TDDFT calculated transitions for *fac*-$[Ru(Q1Pz)_3]^{2+}$.

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	2.6579	466.47	0.0397	160	→	161	0.61016
				160	→	162	0.30257
				160	→	163	-0.11447
2	2.7384	452.76	0.057	160	→	161	-0.27803
				160	→	162	0.61761
				160	→	163	0.14906
3	2.7957	443.48	0.0195	159	→	161	-0.44303
				159	→	163	0.14653
				160	→	161	0.17672
				160	→	163	0.47806
4	2.8713	431.8	0.0365	159	→	161	0.49076
				159	→	162	0.19132
				159	→	163	0.29721
				160	→	162	-0.10441
				160	→	163	0.30856
5	2.8843	429.85	0.0144	159	→	162	0.50451
				159	→	163	-0.4586
				160	→	163	0.12661
6	2.9321	422.85	0.0125	158	→	162	-0.22788
				159	→	161	-0.19492
				159	→	162	0.42159
				159	→	163	0.36902
				160	→	163	-0.26509
7	3.0549	405.85	0.013	158	→	161	0.64756

				158	→	162	-0.10007
				158	→	163	0.21463
8	3.1478	393.88	0.1004	158	→	161	-0.18567
				158	→	162	0.13484
				158	→	163	0.6397
9	3.1991	387.56	0.0323	158	→	161	0.10724
				158	→	162	0.61772
				159	→	163	0.10759
				160	→	163	-0.17095
10	3.6405	340.57	0.0006	159	→	170	0.12994
				159	→	175	-0.10693
				160	→	164	0.31012
				160	→	165	0.10986
				160	→	166	0.15838
				160	→	167	0.23609
				160	→	168	-0.15146
				160	→	170	0.19329
				160	→	171	0.19798
				160	→	174	0.23589
				160	→	175	-0.15015
11	3.7125	333.97	0.0073	158	→	170	-0.13728
				158	→	175	0.11155
				159	→	165	-0.13656
				159	→	167	0.15968
				159	→	168	-0.12698
				159	→	170	0.2866
				159	→	175	-0.2097
				160	→	165	0.22492
				160	→	167	-0.11417
				160	→	169	0.10522
				160	→	170	-0.16919
				160	→	171	0.12447
				160	→	174	0.12034
				160	→	175	0.12094
12	3.7815	327.87	0.0039	158	→	171	-0.15949
				158	→	174	-0.17568
				159	→	164	-0.15754
				159	→	167	-0.18447
				159	→	168	0.10074
				159	→	170	-0.22837
				159	→	175	0.16815
				160	→	164	0.1593
				160	→	165	0.32465
				160	→	170	-0.14442
				160	→	171	0.11234
				160	→	174	0.12203

				160	→	175	0.10266
13	3.8194	324.61	0.0691	155	→	161	0.14179
				156	→	161	0.10239
				157	→	161	0.64399
				160	→	164	0.10168
14	3.8655	320.75	0.0507	155	→	161	-0.16224
				156	→	161	0.39733
				156	→	162	0.2017
				156	→	163	-0.21445
				157	→	162	0.2549
				157	→	163	-0.26084
				159	→	165	-0.10184
				160	→	166	-0.15562
15	3.8933	318.45	0.0215	156	→	161	-0.22883
				160	→	164	0.46698
				160	→	165	-0.31117
				160	→	166	-0.18795
16	3.9137	316.8	0.0305	155	→	161	0.14085
				155	→	163	-0.18871
				156	→	161	-0.16672
				156	→	162	-0.21881
				157	→	162	0.48096
				157	→	163	-0.26699
				160	→	166	0.15219
17	3.9306	315.43	0.061	155	→	162	-0.21659
				156	→	162	-0.32725
				156	→	163	-0.1027
				157	→	162	0.17639
				157	→	163	0.35887
				160	→	164	-0.16801
				160	→	165	-0.12275
				160	→	166	-0.20037
				160	→	167	0.10632
18	3.9451	314.28	0.0867	155	→	162	-0.16706
				156	→	161	0.18878
				156	→	163	-0.12638
				157	→	163	0.2715
				160	→	164	0.22041
				160	→	165	0.1454
				160	→	166	0.32426
				160	→	167	-0.14347
				160	→	169	-0.11716
				160	→	171	-0.15095
				160	→	174	-0.13645
19	4.012	309.03	0.0038	156	→	161	0.19883
				156	→	162	-0.20777

				158	→	170	0.10578
				159	→	164	0.3496
				159	→	165	0.1504
				159	→	171	0.116
				159	→	174	0.11325
				160	→	164	0.15217
				160	→	166	-0.14431
				160	→	167	-0.25379
				160	→	168	0.17474
20	4.0228	308.2	0.0061	156	→	161	0.11915
				156	→	162	-0.18645
				157	→	162	-0.14396
				157	→	163	-0.11728
				158	→	167	-0.10917
				158	→	171	-0.12178
				158	→	174	-0.13276
				160	→	165	-0.35956
				160	→	166	0.36219
				160	→	171	0.11189
				160	→	174	0.10127
21	4.0378	307.06	0.0179	155	→	161	0.13012
				155	→	162	0.11833
				156	→	161	0.29954
				156	→	162	-0.27679
				156	→	163	0.32809
				157	→	162	-0.11558
				159	→	164	-0.22884
				159	→	165	-0.16937
22	4.0738	304.35	0.0104	155	→	161	0.267
				156	→	161	0.14501
				156	→	162	0.3001
				156	→	163	0.34353
				157	→	161	-0.12349
				157	→	162	0.182
				157	→	163	0.14414
				159	→	165	0.19987
23	4.1003	302.37	0.0099	156	→	163	0.2324
				157	→	162	0.12518
				158	→	164	-0.1031
				159	→	164	0.39534
				159	→	165	-0.20303
				159	→	166	-0.29856
				159	→	170	-0.12038
				160	→	167	0.2086
24	4.1201	300.93	0.0056	155	→	161	0.47553
				155	→	162	-0.11118

				155	→	163	0.1551
				156	→	163	-0.22957
				157	→	162	-0.11138
				157	→	163	-0.12075
				158	→	167	-0.10747
				158	→	170	-0.1145
				160	→	166	-0.11697
				160	→	167	0.19301
25	4.1238	300.66	0.0024	155	→	161	-0.2627
				156	→	162	-0.11904
				156	→	163	0.17602
				158	→	164	-0.19788
				158	→	167	-0.15919
				158	→	170	-0.13402
				159	→	164	0.10877
				159	→	165	0.27142
				159	→	166	0.2278
				160	→	166	-0.15361
				160	→	168	-0.22911
				160	→	169	-0.12036
26	4.1738	297.06	0.0087	155	→	162	-0.30734
				156	→	163	0.10397
				157	→	163	-0.15765
				159	→	164	0.15332
				159	→	165	-0.19345
				159	→	166	0.36711
				159	→	167	-0.20836
				160	→	166	0.12049
				160	→	168	0.18647
27	4.177	296.82	0.004	155	→	162	0.50264
				157	→	162	0.12314
				157	→	163	0.18288
				159	→	164	0.13098
				159	→	166	0.29552
				159	→	167	-0.19889
				160	→	167	0.10888
28	4.1869	296.13	0.0031	155	→	161	-0.10973
				155	→	163	0.142
				158	→	165	0.20304
				158	→	171	0.10502
				159	→	165	0.21311
				160	→	167	0.26921
				160	→	168	0.33877
				160	→	169	0.27267
29	4.2124	294.33	0.0062	155	→	163	0.43768
				157	→	162	0.13864

				158	→	164	-0.29281
				159	→	164	-0.12724
				159	→	165	-0.19744
				160	→	167	-0.14056
30	4.2233	293.57	0.0006	155	→	163	-0.31126
				158	→	164	-0.31093
				158	→	165	0.13952
				158	→	166	0.16237
				158	→	167	-0.11563
				159	→	165	-0.11342
				160	→	167	-0.10788
				160	→	169	0.34358
				160	→	170	0.12714
31	4.2471	291.93	0.0071	154	→	163	-0.10958
				155	→	163	0.29804
				158	→	164	0.19017
				159	→	164	0.10682
				159	→	167	-0.10519
				159	→	169	-0.10876
				160	→	168	-0.28634
				160	→	169	0.3897
32	4.3008	288.28	0.0126	154	→	161	-0.10948
				158	→	165	0.49328
				158	→	166	0.11516
				159	→	165	0.10822
				159	→	167	-0.20375
				160	→	168	-0.17255
				160	→	169	-0.12116
				160	→	170	-0.10509
				160	→	171	0.14525
				160	→	174	0.13249
33	4.3386	285.77	0.0202	158	→	164	0.12344
				158	→	166	-0.14076
				158	→	169	0.10246
				159	→	165	-0.19143
				159	→	166	0.20199
				159	→	167	0.17886
				159	→	168	0.30096
				159	→	169	0.32839
				159	→	171	0.10809
				160	→	170	-0.17793
34	4.3549	284.7	0.0103	153	→	162	-0.11232
				154	→	161	0.1134
				158	→	164	0.18997
				158	→	166	0.50654
				158	→	167	-0.19821

				158	→	168	-0.11927
				159	→	167	0.20428
				159	→	168	0.11067
35	4.4099	281.15	0.0028	158	→	164	0.16942
				158	→	165	0.23257
				158	→	166	-0.25886
				158	→	169	-0.14261
				158	→	171	-0.10102
				159	→	166	0.15795
				159	→	167	0.27196
				159	→	169	-0.19497
				159	→	170	-0.16783
				160	→	170	0.20597
				160	→	175	-0.10372
36	4.4177	280.65	0.0113	158	→	164	-0.19568
				158	→	167	0.37166
				158	→	168	-0.12875
				158	→	169	-0.10079
				159	→	165	0.16571
				159	→	167	0.25906
				159	→	169	-0.10897
				160	→	167	0.16266
				160	→	168	-0.11807
				160	→	169	0.11246
				160	→	170	-0.1913
				160	→	171	-0.11034
				160	→	175	0.11297
37	4.4467	278.82	0.0389	154	→	161	-0.12169
				158	→	164	0.14658
				158	→	168	-0.10116
				158	→	169	-0.2178
				158	→	171	-0.14731
				158	→	174	-0.12854
				159	→	168	-0.25353
				159	→	169	0.44419
				160	→	171	-0.14949
				160	→	174	-0.12471
38	4.5049	275.22	0.0215	154	→	161	0.13419
				158	→	166	-0.12615
				158	→	168	-0.23755
				159	→	168	0.41132
				159	→	170	0.20792
				159	→	171	-0.14328
				159	→	174	-0.12893
				160	→	170	0.15502
39	4.5365	273.31	0.0094	153	→	162	-0.1185

				153	→	163	-0.10032
				154	→	161	-0.20885
				158	→	167	0.17287
				158	→	168	0.32773
				159	→	168	0.18064
				159	→	171	-0.23452
				159	→	174	-0.18883
				160	→	167	-0.11943
				160	→	170	0.17333
40	4.5551	272.19	0.0212	152	→	161	0.18764
				152	→	163	0.11388
				154	→	161	0.31825
				154	→	162	-0.14142
				154	→	163	0.19737
				155	→	164	0.12767
				157	→	164	0.27488
				157	→	166	0.15675
				158	→	167	0.12311
				158	→	168	0.12356
				159	→	168	-0.10598
				159	→	169	0.13691
				160	→	168	-0.10528

Table S16. TDDFT calculated transitions for *mer*-$[Ru(Q1Pz)_3]^{2+}$.

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	2.7322	453.8	0.1456	159	→	161	0.12057
				160	→	161	0.68977
2	2.758	449.54	0.0186	160	→	162	0.69195
3	2.8662	432.57	0.0369	159	→	161	0.6602
				160	→	161	-0.11424
				160	→	163	0.17636
4	2.9116	425.82	0.015	159	→	162	0.63799
				160	→	163	0.23489
5	2.9233	424.12	0.0077	158	→	161	0.1609
				158	→	162	0.17165
				159	→	161	-0.16821
				159	→	162	-0.14067
				159	→	163	0.36482
				160	→	163	0.48767
6	2.982	415.77	0.0139	158	→	161	-0.23777
				158	→	162	-0.11
				159	→	162	0.16003
				159	→	163	0.5676
				160	→	163	-0.22435
7	3.017	410.95	0.0066	158	→	161	0.62115
				158	→	162	-0.1452

				158	→	163	0.17863
				159	→	163	0.10099
				160	→	163	-0.1818
8	3.1107	398.58	0.0158	158	→	162	0.28322
				158	→	163	0.61117
9	3.1874	388.98	0.0687	158	→	161	0.10392
				158	→	162	0.57056
				158	→	163	-0.20743
				159	→	162	0.1628
				160	→	163	-0.22748
10	3.5977	344.62	0.0049	159	→	170	-0.10885
				159	→	175	-0.10609
				160	→	165	0.3733
				160	→	168	-0.15303
				160	→	169	-0.21777
				160	→	170	0.1672
				160	→	171	0.24796
				160	→	174	-0.20542
				160	→	175	0.16892
11	3.7011	334.99	0.0054	158	→	165	-0.12632
				158	→	170	-0.14211
				158	→	175	-0.13268
				159	→	170	0.12047
				159	→	171	-0.15677
				159	→	174	0.14586
				160	→	164	-0.18189
				160	→	166	0.28757
				160	→	167	0.15902
				160	→	170	0.23048
				160	→	171	-0.18635
				160	→	174	0.17521
				160	→	175	0.16218
12	3.7679	329.05	0.0063	157	→	161	0.66216
13	3.772	328.69	0.008	157	→	161	0.14856
				158	→	165	0.12656
				158	→	166	-0.10319
				158	→	171	0.22854
				158	→	174	-0.19689
				159	→	164	-0.10931
				159	→	165	0.19693
				159	→	167	0.14226
				159	→	168	-0.15234
				159	→	170	0.31204
				159	→	175	0.25258
14	3.82	324.57	0.0017	156	→	161	-0.14381
				160	→	164	0.56479

				160	→	166	-0.17329
15	3.8893	318.78	0.2	155	→	161	-0.12863
				156	→	161	0.47108
				157	→	162	0.17905
				157	→	163	0.38522
				160	→	164	0.20959
16	3.9498	313.9	0.1198	155	→	162	0.20255
				156	→	162	0.61127
				157	→	162	0.21873
17	3.9638	312.79	0.0111	156	→	161	-0.35834
				156	→	162	-0.16474
				157	→	162	0.54616
				157	→	163	0.14888
18	3.9754	311.88	0.0144	157	→	163	-0.16138
				158	→	165	0.15267
				158	→	166	-0.1186
				158	→	171	0.20799
				158	→	174	-0.1686
				159	→	164	0.11922
				159	→	165	-0.22741
				159	→	166	0.10694
				159	→	168	0.11172
				159	→	171	-0.1366
				159	→	174	0.11795
				160	→	165	-0.25541
				160	→	166	0.26571
				160	→	168	0.12302
				160	→	171	0.11389
19	3.9889	310.82	0.0169	156	→	162	-0.10846
				157	→	162	0.22163
				157	→	163	-0.25161
				159	→	164	0.12505
				159	→	165	0.11657
				159	→	166	-0.15813
				159	→	171	0.11371
				160	→	164	0.17265
				160	→	165	0.2897
				160	→	166	0.33154
20	4.0013	309.86	0.0128	155	→	161	-0.1073
				156	→	161	-0.31458
				156	→	162	0.14113
				157	→	162	-0.2259
				157	→	163	0.38991
				160	→	164	0.10494
				160	→	165	0.17171
				160	→	166	0.26569

				160	→	168	0.11113
21	4.0375	307.08	0.009	157	→	163	0.11678
				159	→	164	0.30105
				159	→	165	0.17117
				159	→	166	-0.29989
				159	→	167	-0.13756
				160	→	165	-0.21725
				160	→	167	0.23538
				160	→	168	-0.22481
				160	→	170	0.1155
22	4.0674	304.82	0.0096	159	→	164	0.52045
				160	→	165	0.13298
				160	→	166	-0.12973
				160	→	167	-0.29219
				160	→	168	0.13719
23	4.121	300.86	0.0139	156	→	163	0.63677
				157	→	161	-0.10561
				160	→	169	-0.14414
24	4.1327	300	0.0088	158	→	164	0.38062
				158	→	165	-0.14701
				158	→	166	-0.1558
				158	→	167	-0.20859
				158	→	168	0.11114
				158	→	170	-0.14073
				159	→	164	-0.17317
				159	→	165	0.16708
				159	→	166	-0.14876
				160	→	166	0.15293
				160	→	167	-0.23778
25	4.1406	299.43	0.0023	154	→	161	0.12266
				154	→	163	-0.1098
				155	→	161	-0.18126
				156	→	163	0.1528
				157	→	163	-0.10328
				158	→	166	-0.14016
				160	→	165	0.1239
				160	→	166	-0.17727
				160	→	167	0.3497
				160	→	168	0.3478
				160	→	169	0.18947
26	4.1599	298.05	0.0159	155	→	161	0.63391
				157	→	163	0.17318
				160	→	167	0.12774
				160	→	168	0.13269
27	4.1745	297	0.0054	156	→	163	-0.13413
				158	→	164	0.23095

				158	→	166	0.10112
				158	→	171	-0.10577
				159	→	164	0.18005
				159	→	165	0.16332
				159	→	166	0.29404
				160	→	167	0.25044
				160	→	169	-0.26707
				160	→	170	-0.11838
				160	→	171	0.10486
				160	→	174	-0.10008
28	4.1995	295.23	0.0028	158	→	164	0.17379
				159	→	166	0.2773
				159	→	168	0.10089
				160	→	165	0.10766
				160	→	168	-0.31298
				160	→	169	0.44879
29	4.2438	292.15	0.0043	155	→	162	-0.14705
				158	→	164	0.40403
				158	→	165	0.18318
				158	→	170	0.11492
				159	→	165	-0.29728
				159	→	166	-0.17251
				159	→	168	-0.16784
				160	→	168	-0.14956
				160	→	169	-0.14574
				160	→	171	-0.11835
30	4.2589	291.12	0.0039	155	→	162	0.55035
				156	→	162	-0.16351
				158	→	166	0.1159
				159	→	165	-0.13882
				159	→	167	0.1687
				159	→	168	-0.14075
31	4.2841	289.41	0.002	155	→	162	0.31075
				155	→	163	0.14905
				158	→	164	0.11853
				158	→	165	0.19788
				158	→	166	-0.16916
				158	→	168	-0.14178
				159	→	165	0.14941
				159	→	166	0.11348
				159	→	167	-0.27568
				159	→	168	0.15944
				160	→	169	-0.13137
				160	→	170	0.12799
				160	→	171	-0.15528
				160	→	174	0.10558

32	4.3162	287.25	0.0064	158	→	165	0.13119
				158	→	166	0.50491
				158	→	168	0.11429
				158	→	169	-0.13233
				159	→	165	0.12908
				159	→	167	-0.22656
				160	→	168	0.13316
33	4.3338	286.09	0.0008	155	→	162	-0.10767
				155	→	163	0.6345
34	4.3645	284.07	0.011	158	→	165	0.13892
				158	→	168	-0.13937
				159	→	165	0.2916
				159	→	166	-0.10798
				159	→	167	0.40084
				159	→	169	0.31783
35	4.4003	281.76	0.0152	158	→	166	0.13648
				158	→	168	0.10726
				159	→	166	-0.18731
				159	→	167	0.18146
				159	→	168	0.53594
				159	→	169	-0.21833
36	4.4361	279.49	0.0024	155	→	163	0.16153
				158	→	165	-0.10674
				158	→	168	-0.13203
				158	→	171	0.11192
				159	→	165	-0.1034
				159	→	166	0.11023
				159	→	167	0.1362
				159	→	168	-0.10811
				159	→	171	0.3077
				159	→	174	-0.1864
				160	→	168	0.19514
				160	→	170	0.28254
				160	→	175	0.16217
37	4.4378	279.38	0.004	158	→	164	-0.1123
				158	→	165	0.4331
				158	→	167	-0.23423
				158	→	168	0.22277
				158	→	170	-0.10023
				159	→	167	0.16601
				159	→	168	-0.11606
				159	→	169	-0.20751
				159	→	170	-0.15117
38	4.4843	276.48	0.0083	152	→	162	0.14347
				154	→	161	0.10403
				158	→	167	0.24176

				158	→	168	0.44267
				158	→	171	0.12446
				159	→	169	0.26203
				159	→	171	0.16145
39	4.4983	275.63	0.0017	158	→	165	0.11264
				158	→	167	0.29137
				158	→	171	-0.25782
				158	→	174	0.14261
				159	→	169	-0.17646
				159	→	170	0.15783
				159	→	175	0.11734
				160	→	165	-0.10295
				160	→	171	0.29363
				160	→	174	-0.12121
40	4.5674	271.46	0.0292	153	→	163	-0.10447
				154	→	161	0.12446
				157	→	164	-0.13285
				158	→	169	0.50166
				159	→	167	-0.12732
				159	→	169	0.1793
				159	→	170	0.15004

Table S17. TDDFT calculated transitions for *cis-fac*-$[Ru(DQPz)_2]^{2+}$.

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	2.5239	491.24	0.0214	175	→	176	0.68051
				175	→	178	-0.15364
2	2.578	480.93	0.0204	175	→	177	0.66938
				175	→	179	-0.17212
3	2.6846	461.83	0.0358	174	→	176	-0.17112
				175	→	176	0.14066
				175	→	178	0.65541
4	2.7572	449.67	0.0868	174	→	176	0.65132
				174	→	178	-0.18347
				175	→	178	0.1281
5	2.7753	446.75	0.0898	174	→	177	0.66026
				174	→	179	0.17921
6	2.8755	431.18	0.0152	174	→	176	0.17132
				174	→	178	0.64558
				174	→	186	0.10165
				175	→	178	0.11477
7	2.8787	430.7	0.1011	174	→	179	-0.28052
				175	→	177	0.12147
				175	→	179	0.61664
8	3.0822	402.26	0.0039	172	→	177	0.24866
				173	→	177	0.65476
9	3.1104	398.61	0.0315	172	→	176	0.25232

				173	→	176	0.63454
				174	→	179	-0.13205
10	3.2662	379.6	0.0128	172	→	178	0.23171
				173	→	178	0.63987
11	3.2913	376.7	0.0011	173	→	176	0.13629
				174	→	177	-0.14444
				174	→	179	0.58003
				175	→	177	0.12415
				175	→	179	0.24948
12	3.4167	362.88	0.0017	172	→	179	0.24361
				173	→	179	0.64105
13	3.5113	353.1	0.335	172	→	176	0.64162
				173	→	176	-0.24562
14	3.517	352.53	0.0831	171	→	176	-0.15073
				172	→	177	0.63183
				173	→	177	-0.24286
15	3.6056	343.86	0.0186	175	→	180	0.66452
				175	→	183	0.13726
16	3.672	337.64	0.0118	171	→	176	0.59797
				171	→	178	-0.13329
				172	→	177	0.14301
				174	→	186	-0.14567
				174	→	189	-0.12558
				175	→	180	-0.10111
17	3.6803	336.89	0.0269	171	→	177	-0.12096
				172	→	178	0.4382
				173	→	178	-0.19023
				175	→	181	-0.43505
				175	→	182	0.18774
18	3.7145	333.78	0.0578	171	→	177	0.67152
				175	→	181	-0.10504
19	3.7168	333.58	0.0096	172	→	178	0.47488
				173	→	178	-0.13516
				175	→	181	0.42026
				175	→	182	-0.18715
20	3.7403	331.48	0.0034	171	→	176	0.27324
				171	→	178	0.22739
				171	→	186	0.12369
				174	→	178	-0.1389
				174	→	180	-0.19958
				174	→	186	0.26297
				174	→	189	0.21469
				174	→	191	0.13138
				175	→	186	0.22371
				175	→	189	0.16616
				175	→	191	0.10195

21	3.7974	326.5	0.0088	171	→	176	0.12755
				174	→	180	0.59936
				174	→	186	0.17831
				174	→	189	0.14023
22	3.8654	320.76	0.0018	174	→	182	-0.1499
				175	→	181	0.22114
				175	→	182	0.61506
				175	→	193	-0.11872
23	3.9013	317.81	0.0042	171	→	178	0.41096
				172	→	179	-0.3925
				173	→	179	0.19629
				174	→	180	-0.13929
				175	→	183	0.11196
				175	→	186	-0.21226
				175	→	189	-0.12516
24	3.9202	316.27	0.0128	171	→	178	0.3844
				173	→	179	-0.11629
				174	→	180	0.21572
				174	→	183	0.12734
				174	→	186	-0.26961
				174	→	189	-0.19886
				174	→	191	-0.11146
				175	→	183	-0.13843
				175	→	186	0.21733
				175	→	189	0.13729
25	3.9336	315.19	0.0071	171	→	178	0.27575
				172	→	179	0.51177
				173	→	179	-0.14064
				175	→	180	-0.11415
				175	→	183	0.15885
				175	→	186	-0.20656
				175	→	189	-0.13095
26	3.9379	314.85	0.0579	174	→	181	0.49635
				174	→	182	-0.46272
27	4.0143	308.85	0.0025	175	→	183	0.62124
				175	→	186	0.19382
				175	→	189	0.12391
28	4.0268	307.9	0.0001	165	→	177	-0.10335
				166	→	176	0.134
				171	→	179	0.10948
				174	→	181	0.41348
				174	→	182	0.46101
				175	→	182	0.15349
29	4.0867	303.39	0.0002	168	→	176	-0.1321
				168	→	178	-0.15558
				174	→	181	0.10869

				175	→	184	0.61922
30	4.1069	301.89	0.004	167	→	178	-0.13729
				168	→	177	-0.12754
				168	→	179	-0.11498
				170	→	176	-0.12116
				174	→	183	-0.30427
				175	→	185	0.53023
31	4.1183	301.05	0.0036	170	→	177	0.10341
				171	→	179	0.63689
				173	→	180	0.19083
32	4.1537	298.49	0.0055	165	→	176	-0.13211
				166	→	177	0.14679
				174	→	183	0.5141
				174	→	185	0.10751
				175	→	183	0.13117
				175	→	185	0.32237
33	4.2076	294.67	0.0034	172	→	186	0.13022
				172	→	189	0.11364
				173	→	186	0.2654
				173	→	189	0.21077
				173	→	191	0.13192
				174	→	184	-0.11439
				174	→	193	-0.13383
				175	→	181	0.1861
				175	→	187	0.11952
				175	→	188	0.11844
				175	→	190	-0.17481
				175	→	193	0.33713
34	4.3017	288.22	0.0167	172	→	181	0.22001
				172	→	182	-0.12274
				173	→	181	0.54102
				173	→	182	-0.2699
				175	→	186	0.13302
35	4.3154	287.31	0.0012	169	→	176	-0.25953
				171	→	179	-0.1773
				172	→	180	0.18453
				173	→	180	0.46577
				174	→	184	-0.26211
36	4.3387	285.76	0.017	166	→	176	0.12983
				168	→	176	-0.114
				168	→	178	-0.10036
				169	→	176	-0.25793
				173	→	180	0.1781
				174	→	184	0.52247
				175	→	184	-0.13207
37	4.3551	284.69	0.0266	169	→	177	-0.11701

				170	→	176	0.64123
				174	→	183	-0.10575
				174	→	185	-0.12926
				175	→	185	0.11252
38	4.3847	282.77	0.0002	169	→	176	0.41724
				170	→	177	0.42387
				171	→	179	-0.13404
				173	→	180	0.24994
39	4.3873	282.6	0.0093	168	→	177	-0.10429
				169	→	177	0.23362
				170	→	176	0.14591
				170	→	178	-0.10884
				173	→	182	-0.11699
				174	→	183	-0.1083
				174	→	185	0.5352
				175	→	185	-0.15798
40	4.3925	282.26	0.0004	169	→	176	-0.38261
				170	→	177	0.52228
				173	→	180	-0.15848

Table S18. TDDFT calculated transitions for *trans-fac*-$[Ru(DQPz)_2]^{2+}$.

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	2.4483	506.42	0.0857	175	→	176	0.69657
2	2.5288	490.28	0.0011	174	→	177	0.24198
				175	→	177	0.63377
				175	→	178	-0.14427
3	2.6351	470.51	0.1097	174	→	177	0.14497
				174	→	178	0.10024
				175	→	178	0.67201
4	2.6923	460.51	0.0147	175	→	179	0.68245
				175	→	186	-0.11093
5	2.8531	434.56	0.0019	173	→	179	0.10621
				174	→	177	0.61984
				175	→	177	-0.24778
				175	→	178	-0.11273
6	2.8885	429.23	0.0194	174	→	176	0.68108
				174	→	179	-0.10013
7	3.0387	408.01	0.0023	171	→	177	0.25966
				173	→	177	0.54703
				174	→	176	0.1272
				174	→	179	0.28621
8	3.0629	404.8	0.0048	173	→	176	0.29807
				174	→	178	0.62263
9	3.1366	395.29	0.0006	171	→	177	-0.13879
				173	→	177	-0.29166
				174	→	179	0.57001

				174	→	186	-0.14784
10	3.1854	389.23	0.2184	171	→	176	0.23419
				173	→	176	0.57874
				174	→	178	-0.2893
11	3.3252	372.86	0.0261	171	→	178	0.23104
				173	→	178	0.65225
12	3.4597	358.36	0.0016	171	→	177	0.15242
				172	→	176	0.67137
13	3.4642	357.9	0.0404	171	→	179	0.21667
				172	→	177	-0.19002
				173	→	179	0.48134
				175	→	181	0.2435
				175	→	183	0.15839
				175	→	185	0.11308
				175	→	192	0.16653
14	3.4968	354.56	0.024	175	→	180	0.67433
				175	→	182	-0.11241
15	3.5149	352.74	0.3068	171	→	176	0.1672
				172	→	177	0.62555
				175	→	183	0.12757
16	3.5317	351.06	0.0014	171	→	176	-0.16867
				171	→	179	-0.10493
				173	→	179	-0.36666
				175	→	181	0.46207
				175	→	183	0.22365
				175	→	185	0.12713
				175	→	192	0.13902
17	3.5648	347.8	0.0009	171	→	177	0.57743
				172	→	176	-0.17058
				173	→	177	-0.2945
18	3.5939	344.99	0.0633	171	→	176	0.6042
				172	→	177	-0.21535
				173	→	176	-0.21926
				175	→	181	0.11455
19	3.6321	341.36	0.0007	171	→	177	0.13475
				174	→	179	-0.19034
				174	→	186	-0.16431
				174	→	189	-0.12391
				174	→	190	-0.11963
				175	→	179	0.12739
				175	→	180	0.13455
				175	→	182	0.17668
				175	→	184	0.11533
				175	→	186	0.39496
				175	→	189	0.24124
				175	→	190	0.22777

20	3.6878	336.2	0.008	172	→	178	0.69391
21	3.7524	330.41	0.0038	171	→	178	0.61965
				172	→	179	0.11524
				173	→	178	-0.22009
22	3.7861	327.47	0.0031	171	→	177	0.11926
				171	→	178	0.1943
				172	→	179	-0.2968
				174	→	179	0.18118
				174	→	186	0.32784
				174	→	189	0.23548
				174	→	190	0.22498
				175	→	182	0.15659
				175	→	186	0.11199
23	3.8344	323.35	0.0026	172	→	179	0.58882
				174	→	186	0.19029
				174	→	189	0.13301
				174	→	190	0.13094
				175	→	184	0.11566
24	3.8577	321.4	0.0064	171	→	179	0.12732
				173	→	179	-0.10775
				175	→	181	-0.36505
				175	→	183	0.54944
25	3.8852	319.12	0.0138	171	→	179	0.57911
				171	→	186	-0.10723
				173	→	179	-0.26707
				175	→	183	-0.1815
26	3.9187	316.39	0.0081	175	→	182	0.61772
				175	→	184	-0.18015
				175	→	186	-0.15661
27	3.9918	310.6	0.0108	168	→	178	-0.10866
				172	→	179	-0.1273
				174	→	180	0.29274
				175	→	182	0.12223
				175	→	184	0.53391
				175	→	186	-0.14618
28	4.011	309.11	0.0299	174	→	180	0.61194
				175	→	184	-0.28147
29	4.0111	309.1	0.0032	170	→	176	-0.13266
				175	→	181	-0.15091
				175	→	183	-0.16767
				175	→	185	0.59498
				175	→	192	0.1064
30	4.0882	303.28	0.0018	170	→	176	-0.11627
				171	→	179	-0.15924
				171	→	186	-0.10288
				173	→	186	-0.11332

				174	→	181	0.42345
				174	→	192	0.19
				175	→	181	-0.12327
				175	→	185	-0.15087
				175	→	188	-0.13084
				175	→	192	0.26398
31	4.1689	297.4	0.0014	170	→	176	-0.15383
				171	→	179	0.15783
				171	→	186	0.15302
				171	→	189	0.11431
				171	→	190	0.10832
				173	→	180	-0.19135
				173	→	182	0.12682
				173	→	186	0.16957
				173	→	189	0.12177
				173	→	190	0.1091
				174	→	181	0.41197
				175	→	188	0.10166
				175	→	192	-0.20154
32	4.1984	295.31	0.0028	171	→	180	0.20694
				173	→	180	0.60581
				175	→	192	-0.11852
33	4.2454	292.04	0.0077	167	→	177	-0.14584
				168	→	177	0.15219
				170	→	177	-0.26051
				171	→	181	0.11231
				172	→	180	-0.10671
				173	→	181	0.44224
				174	→	182	0.21427
34	4.2859	289.29	0.026	168	→	178	0.1187
				170	→	177	0.47616
				171	→	181	0.12857
				171	→	192	0.10029
				173	→	181	0.23622
				173	→	183	0.25172
				174	→	182	-0.11205
				175	→	184	0.13435
35	4.2879	289.15	0.0002	169	→	177	-0.12159
				170	→	176	0.61179
				174	→	181	0.18694
				175	→	185	0.13149
36	4.3201	286.99	0.0006	167	→	176	0.20756
				167	→	179	-0.1072
				168	→	176	-0.28769
				170	→	179	-0.13149
				172	→	181	0.13823

				173	→	182	-0.14969
				173	→	184	0.10346
				174	→	183	0.4274
37	4.3443	285.39	0.0048	167	→	177	-0.11687
				168	→	177	0.18653
				170	→	177	0.20861
				170	→	178	0.37162
				173	→	181	-0.12006
				173	→	183	-0.10293
				173	→	185	-0.17743
				174	→	182	0.31579
				175	→	184	0.13946
				175	→	186	-0.10128
38	4.4035	281.56	0.0116	168	→	177	-0.10827
				169	→	176	-0.25852
				170	→	177	0.26456
				170	→	178	-0.34439
				174	→	182	0.38365
				174	→	184	-0.18461
39	4.4072	281.32	0.0037	167	→	176	-0.14821
				168	→	176	0.27733
				169	→	177	-0.15174
				170	→	179	0.12952
				173	→	182	0.22368
				174	→	181	-0.24246
				174	→	183	0.32957
				174	→	185	0.13243
				175	→	192	0.14335
40	4.4483	278.72	0.0058	165	→	177	-0.11717
				166	→	178	0.13034
				167	→	176	0.24413
				168	→	176	0.23372
				168	→	179	0.14565
				169	→	177	0.29449
				170	→	179	0.16169
				172	→	181	0.10068
				173	→	182	-0.21138
				173	→	184	-0.17896
				174	→	185	0.13166
				175	→	185	0.16009
				175	→	187	-0.13029

Table S19. TDDFT calculated transitions for C-R_a-*mer*-$[Ru(DQPz)_2]^{2+}$.

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	2.5239	491.24	0.0214	175	→	176	0.68051
				175	→	178	-0.15364

2	2.578	480.93	0.0204	175	→	177	0.66938
				175	→	179	-0.17212
3	2.6846	461.83	0.0358	174	→	176	-0.17112
				175	→	176	0.14066
				175	→	178	0.65541
4	2.7572	449.67	0.0868	174	→	176	0.65132
				174	→	178	-0.18347
				175	→	178	0.1281
5	2.7753	446.75	0.0898	174	→	177	0.66026
				174	→	179	0.17921
6	2.8755	431.18	0.0152	174	→	176	0.17132
				174	→	178	0.64558
				174	→	186	0.10165
				175	→	178	0.11477
7	2.8787	430.7	0.1011	174	→	179	-0.28052
				175	→	177	0.12147
				175	→	179	0.61664
8	3.0822	402.26	0.0039	172	→	177	0.24866
				173	→	177	0.65476
9	3.1104	398.61	0.0315	172	→	176	0.25232
				173	→	176	0.63454
				174	→	179	-0.13205
10	3.2662	379.6	0.0128	172	→	178	0.23171
				173	→	178	0.63987
11	3.2913	376.7	0.0011	173	→	176	0.13629
				174	→	177	-0.14444
				174	→	179	0.58003
				175	→	177	0.12415
				175	→	179	0.24948
12	3.4167	362.88	0.0017	172	→	179	0.24361
				173	→	179	0.64105
13	3.5113	353.1	0.335	172	→	176	0.64162
				173	→	176	-0.24562
14	3.517	352.53	0.0831	171	→	176	-0.15073
				172	→	177	0.63183
				173	→	177	-0.24286
15	3.6056	343.86	0.0186	175	→	180	0.66452
				175	→	183	0.13726
16	3.672	337.64	0.0118	171	→	176	0.59797
				171	→	178	-0.13329
				172	→	177	0.14301
				174	→	186	-0.14567
				174	→	189	-0.12558
				175	→	180	-0.10111
17	3.6803	336.89	0.0269	171	→	177	-0.12096
				172	→	178	0.4382

				173	→	178	-0.19023
				175	→	181	-0.43505
				175	→	182	0.18774
18	3.7145	333.78	0.0578	171	→	177	0.67152
				175	→	181	-0.10504
19	3.7168	333.58	0.0096	172	→	178	0.47488
				173	→	178	-0.13516
				175	→	181	0.42026
				175	→	182	-0.18715
20	3.7403	331.48	0.0034	171	→	176	0.27324
				171	→	178	0.22739
				171	→	186	0.12369
				174	→	178	-0.1389
				174	→	180	-0.19958
				174	→	186	0.26297
				174	→	189	0.21469
				174	→	191	0.13138
				175	→	186	0.22371
				175	→	189	0.16616
				175	→	191	0.10195
21	3.7974	326.5	0.0088	171	→	176	0.12755
				174	→	180	0.59936
				174	→	186	0.17831
				174	→	189	0.14023
22	3.8654	320.76	0.0018	174	→	182	-0.1499
				175	→	181	0.22114
				175	→	182	0.61506
				175	→	193	-0.11872
23	3.9013	317.81	0.0042	171	→	178	0.41096
				172	→	179	-0.3925
				173	→	179	0.19629
				174	→	180	-0.13929
				175	→	183	0.11196
				175	→	186	-0.21226
				175	→	189	-0.12516
24	3.9202	316.27	0.0128	171	→	178	0.3844
				173	→	179	-0.11629
				174	→	180	0.21572
				174	→	183	0.12734
				174	→	186	-0.26961
				174	→	189	-0.19886
				174	→	191	-0.11146
				175	→	183	-0.13843
				175	→	186	0.21733
				175	→	189	0.13729
25	3.9336	315.19	0.0071	171	→	178	0.27575

				172	→	179	0.51177
				173	→	179	-0.14064
				175	→	180	-0.11415
				175	→	183	0.15885
				175	→	186	-0.20656
				175	→	189	-0.13095
26	3.9379	314.85	0.0579	174	→	181	0.49635
				174	→	182	-0.46272
27	4.0143	308.85	0.0025	175	→	183	0.62124
				175	→	186	0.19382
				175	→	189	0.12391
28	4.0268	307.9	0.0001	165	→	177	-0.10335
				166	→	176	0.134
				171	→	179	0.10948
				174	→	181	0.41348
				174	→	182	0.46101
				175	→	182	0.15349
29	4.0867	303.39	0.0002	168	→	176	-0.1321
				168	→	178	-0.15558
				174	→	181	0.10869
				175	→	184	0.61922
30	4.1069	301.89	0.004	167	→	178	-0.13729
				168	→	177	-0.12754
				168	→	179	-0.11498
				170	→	176	-0.12116
				174	→	183	-0.30427
				175	→	185	0.53023
31	4.1183	301.05	0.0036	170	→	177	0.10341
				171	→	179	0.63689
				173	→	180	0.19083
32	4.1537	298.49	0.0055	165	→	176	-0.13211
				166	→	177	0.14679
				174	→	183	0.5141
				174	→	185	0.10751
				175	→	183	0.13117
				175	→	185	0.32237
33	4.2076	294.67	0.0034	172	→	186	0.13022
				172	→	189	0.11364
				173	→	186	0.2654
				173	→	189	0.21077
				173	→	191	0.13192
				174	→	184	-0.11439
				174	→	193	-0.13383
				175	→	181	0.1861
				175	→	187	0.11952
				175	→	188	0.11844

				175	→	190	-0.17481
				175	→	193	0.33713
34	4.3017	288.22	0.0167	172	→	181	0.22001
				172	→	182	-0.12274
				173	→	181	0.54102
				173	→	182	-0.2699
				175	→	186	0.13302
35	4.3154	287.31	0.0012	169	→	176	-0.25953
				171	→	179	-0.1773
				172	→	180	0.18453
				173	→	180	0.46577
				174	→	184	-0.26211
36	4.3387	285.76	0.017	166	→	176	0.12983
				168	→	176	-0.114
				168	→	178	-0.10036
				169	→	176	-0.25793
				173	→	180	0.1781
				174	→	184	0.52247
				175	→	184	-0.13207
37	4.3551	284.69	0.0266	169	→	177	-0.11701
				170	→	176	0.64123
				174	→	183	-0.10575
				174	→	185	-0.12926
				175	→	185	0.11252
38	4.3847	282.77	0.0002	169	→	176	0.41724
				170	→	177	0.42387
				171	→	179	-0.13404
				173	→	180	0.24994
39	4.3873	282.6	0.0093	168	→	177	-0.10429
				169	→	177	0.23362
				170	→	176	0.14591
				170	→	178	-0.10884
				173	→	182	-0.11699
				174	→	183	-0.1083
				174	→	185	0.5352
				175	→	185	-0.15798
40	4.3925	282.26	0.0004	169	→	176	-0.38261
				170	→	177	0.52228
				173	→	180	-0.15848

Table S20. TDDFT calculated transitions for C-S_a-*mer*-$[Ru(DQPz)_2]^{2+}$.

Excited State	Energy (eV)	Wavelength (nm)	f	Transitions			
1	2.5609	484.14	0.0393	175	→	176	0.70108
2	2.5837	479.86	0.0028	174	→	179	-0.11643
				175	→	177	0.65509
				175	→	178	-0.20702

3	2.7008	459.06	0.0814	171	→	177	0.11345
				174	→	177	0.65404
				175	→	179	-0.20869
4	2.7277	454.53	0.0003	174	→	176	-0.36106
				174	→	179	-0.14567
				175	→	177	0.17741
				175	→	178	0.54913
5	2.7655	448.32	0.117	174	→	176	0.59438
				175	→	178	0.35087
6	2.8312	437.92	0.0363	174	→	177	0.15324
				174	→	178	-0.40905
				175	→	179	0.5303
7	2.8842	429.88	0.1108	174	→	177	0.12788
				174	→	178	0.53744
				175	→	179	0.39873
8	3.0739	403.34	0.0113	173	→	177	0.69483
9	3.1214	397.21	0	173	→	176	0.68615
				174	→	179	0.15186
10	3.278	378.23	0.0013	172	→	177	-0.12019
				173	→	176	-0.14694
				174	→	179	0.62677
				175	→	177	0.14715
				175	→	178	0.11292
11	3.2871	377.19	0.0191	173	→	178	0.68563
12	3.4129	363.28	0.0018	173	→	179	0.68405
13	3.5226	351.97	0.0838	171	→	176	0.16151
				172	→	177	0.66457
				174	→	179	0.10798
14	3.5272	351.51	0.3704	171	→	177	0.10032
				172	→	176	0.67968
15	3.6145	343.02	0.0287	175	→	180	0.66674
				175	→	182	-0.14316
16	3.677	337.19	0.0235	171	→	177	0.59372
				172	→	176	-0.11943
				174	→	177	-0.12471
				174	→	186	0.18581
				174	→	189	0.17113
17	3.6879	336.19	0.0199	171	→	176	0.62466
				172	→	177	-0.17644
				172	→	178	0.15368
				174	→	180	0.13918
18	3.7195	333.34	0	171	→	176	-0.21833
				172	→	178	0.61795
				174	→	180	0.17601
				175	→	181	-0.12546
19	3.7527	330.39	0.0043	174	→	180	0.47826

				174	→	182	-0.1104
				175	→	181	0.44025
				175	→	183	-0.10886
				175	→	186	-0.11434
20	3.7536	330.3	0.0336	171	→	177	-0.32319
				171	→	178	-0.26243
				171	→	186	0.11958
				171	→	189	0.11332
				174	→	178	0.17036
				174	→	186	0.33241
				174	→	189	0.29786
				174	→	191	0.12533
				174	→	194	-0.12244
21	3.7786	328.12	0.0079	172	→	178	0.25697
				174	→	180	-0.35794
				175	→	181	0.4924
				175	→	186	0.10396
22	3.8649	320.8	0.0087	171	→	178	-0.11081
				174	→	181	-0.27195
				175	→	180	0.16427
				175	→	182	0.56122
				175	→	192	-0.12977
23	3.9062	317.41	0.007	171	→	178	0.49821
				172	→	179	0.37929
				174	→	186	0.14381
				174	→	189	0.11175
				175	→	182	0.16444
24	3.9193	316.34	0.0139	173	→	179	-0.12229
				173	→	180	0.10154
				173	→	192	0.13071
				174	→	180	0.2512
				175	→	183	0.30123
				175	→	186	0.39655
				175	→	189	0.28302
				175	→	191	0.1068
				175	→	194	-0.10548
25	3.9215	316.17	0.0142	171	→	178	0.18088
				172	→	179	-0.42616
				174	→	181	0.47747
				175	→	182	0.1515
26	3.9334	315.21	0.0305	171	→	178	-0.30329
				172	→	179	0.37224
				174	→	181	0.3881
				174	→	183	-0.12594
				174	→	186	-0.14559
				174	→	189	-0.11244

				175	→	182	0.18933
27	4.0155	308.76	0.0009	171	→	179	-0.15409
				174	→	182	-0.34593
				175	→	183	0.48749
				175	→	186	-0.19183
				175	→	189	-0.1308
28	4.0546	305.79	0.0018	167	→	178	0.10383
				168	→	176	-0.12215
				174	→	182	0.48221
				175	→	183	0.33229
				175	→	184	-0.23716
				175	→	186	-0.12347
29	4.093	302.92	0.0005	171	→	179	0.6114
				173	→	180	0.13555
				174	→	182	-0.19864
				175	→	184	-0.15242
30	4.1084	301.78	0.0044	165	→	176	-0.12391
				166	→	177	-0.10234
				167	→	179	0.10225
				168	→	177	-0.11796
				170	→	176	0.12175
				174	→	183	0.44021
				174	→	184	-0.12216
				175	→	185	0.39914
31	4.1283	300.33	0.0025	167	→	178	-0.10358
				168	→	176	0.11051
				171	→	179	0.19125
				173	→	180	0.1446
				174	→	182	0.18208
				174	→	185	-0.1295
				175	→	183	0.14875
				175	→	184	0.5476
32	4.1519	298.62	0.0007	166	→	177	0.10016
				167	→	176	0.16207
				168	→	178	-0.12622
				173	→	186	0.10432
				174	→	183	-0.38908
				174	→	184	-0.22981
				175	→	185	0.39
				175	→	192	0.1231
33	4.2031	294.98	0.0043	173	→	186	0.26134
				173	→	189	0.23689
				174	→	183	0.17519
				175	→	182	0.21895
				175	→	185	-0.22305
				175	→	187	0.11251

				175	→	188	0.11048
				175	→	190	-0.12898
				175	→	192	0.32446
				175	→	193	-0.13902
34	4.2916	288.9	0.0091	167	→	176	-0.13905
				168	→	178	0.11351
				173	→	186	0.10167
				174	→	184	0.53708
				175	→	182	0.10565
				175	→	185	0.30154
35	4.2988	288.42	0.0006	166	→	176	0.10314
				167	→	177	0.10142
				167	→	178	0.10324
				169	→	176	0.14823
				173	→	180	0.27717
				173	→	182	-0.11723
				174	→	185	0.488
				175	→	184	0.1793
36	4.3202	286.99	0.0053	169	→	176	0.23872
				171	→	179	-0.12845
				173	→	180	0.47684
				174	→	185	-0.31384
				175	→	184	-0.16851
37	4.3396	285.7	0.0233	173	→	181	0.67619
38	4.3675	283.88	0.0265	169	→	177	0.10588
				170	→	176	0.65211
				174	→	183	-0.11063
39	4.3785	283.17	0.0004	170	→	177	0.66725
				171	→	179	-0.12834
40	4.3872	282.61	0.0095	169	→	177	0.6691
				170	→	176	-0.12461