

Systematic Manipulation of the Light- Harvesting Properties for Tridentate Cyclometalated Ruthenium(II) Complexes

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The Institute for Sustainable Energy, Environment and Economy

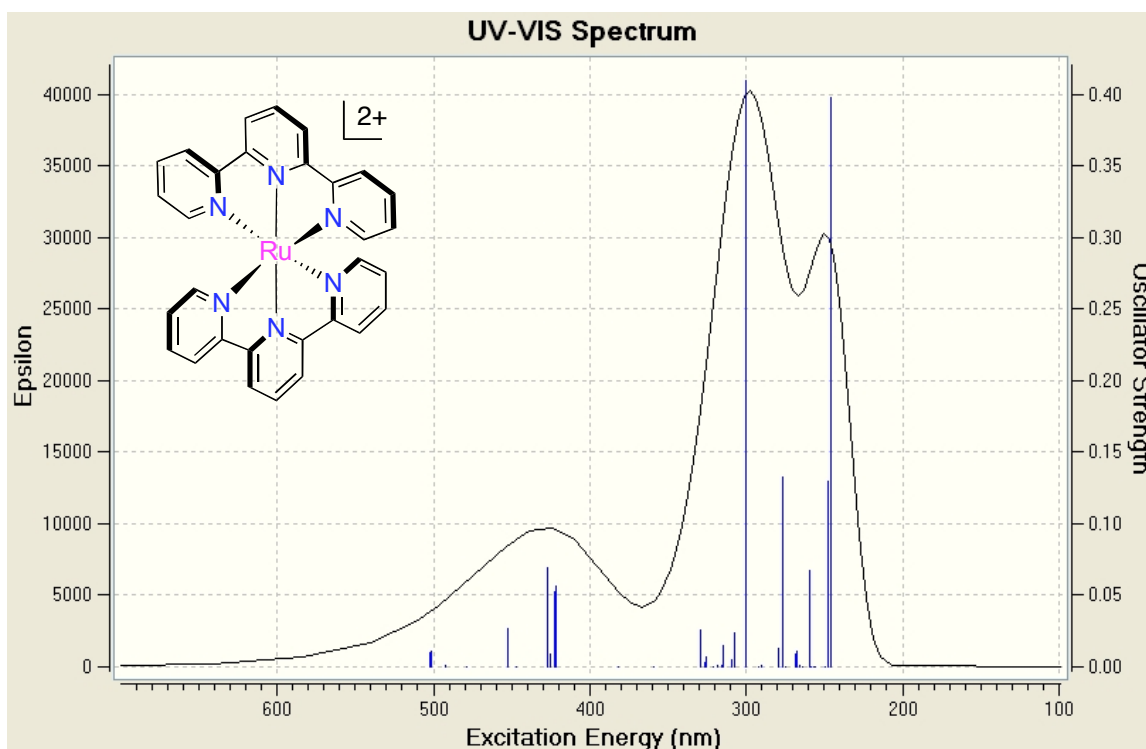
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TD-DFT calculated electronic transitions for $[Ru(tpy)_2](PF_6)_2$ (**1**)



Excitation energies and oscillator strengths:

Excited State 1: Singlet-A" 2.4707 eV 501.82 nm f=0.0098
129 ->131 0.68395

Excited State 2: Singlet-A' 2.4742 eV 501.10 nm f=0.0105
129 ->130 0.68303

Excited State 3: Singlet-A" 2.5206 eV 491.88 nm f=0.0004
127 ->131 0.46879
128 ->130 0.49735

Excited State 4: Singlet-A" 2.5917 eV 478.40 nm f=0.0001
127 ->131 0.51413
128 ->130 -0.48412

Excited State 5: Singlet-A' 2.7408 eV 452.36 nm f=0.0265
127 ->130 0.39343
128 ->131 0.40378
129 ->132 0.40254

Excited State 6: Singlet-A' 2.7744 eV 446.88 nm f=0.0003

127 ->130	-0.32735				
128 ->131	0.31696				
129 ->133	0.52447				
129 ->137	-0.10066				
Excited State 7:	Singlet-A'	2.9041 eV	426.92 nm	f=0.0688	
127 ->130	0.19275				
127 ->132	0.46168				
128 ->131	0.18544				
129 ->132	-0.43050				
Excited State 8:	Singlet-A''	2.9153 eV	425.29 nm	f=0.0086	
128 ->132	0.68128				
128 ->133	-0.16224				
Excited State 9:	Singlet-A'	2.9348 eV	422.46 nm	f=0.0518	
127 ->130	-0.14239				
127 ->132	0.36705				
127 ->133	0.46184				
128 ->131	-0.12865				
129 ->132	0.29543				
Excited State 10:	Singlet-A''	2.9359 eV	422.31 nm	f=0.0257	
128 ->132	0.15253				
128 ->133	0.66992				
Excited State 11:	Singlet-A'	2.9398 eV	421.74 nm	f=0.0558	
127 ->132	-0.37176				
127 ->133	0.50185				
128 ->131	0.13777				
129 ->132	-0.21955				
Excited State 12:	Singlet-A'	3.2503 eV	381.45 nm	f=0.0000	
127 ->130	0.28984				
128 ->131	-0.29101				
129 ->133	0.43144				
129 ->137	0.24777				
Excited State 13:	Singlet-A''	3.4560 eV	358.75 nm	f=0.0000	
127 ->140	0.10603				
129 ->140	0.67483				
Excited State 14:	Singlet-A'	3.7660 eV	329.22 nm	f=0.0252	
127 ->134	-0.22339				
129 ->134	0.64218				

Excited State 15: Singlet-A" 3.7942 eV 326.77 nm f=0.0001
 125 ->131 0.14547
 126 ->131 0.16433
 128 ->134 0.49564
 129 ->135 -0.43189

Excited State 16: Singlet-A' 3.8004 eV 326.24 nm f=0.0025
 125 ->130 -0.21407
 126 ->130 0.23606
 127 ->134 -0.21056
 129 ->134 -0.16143
 129 ->136 0.56251

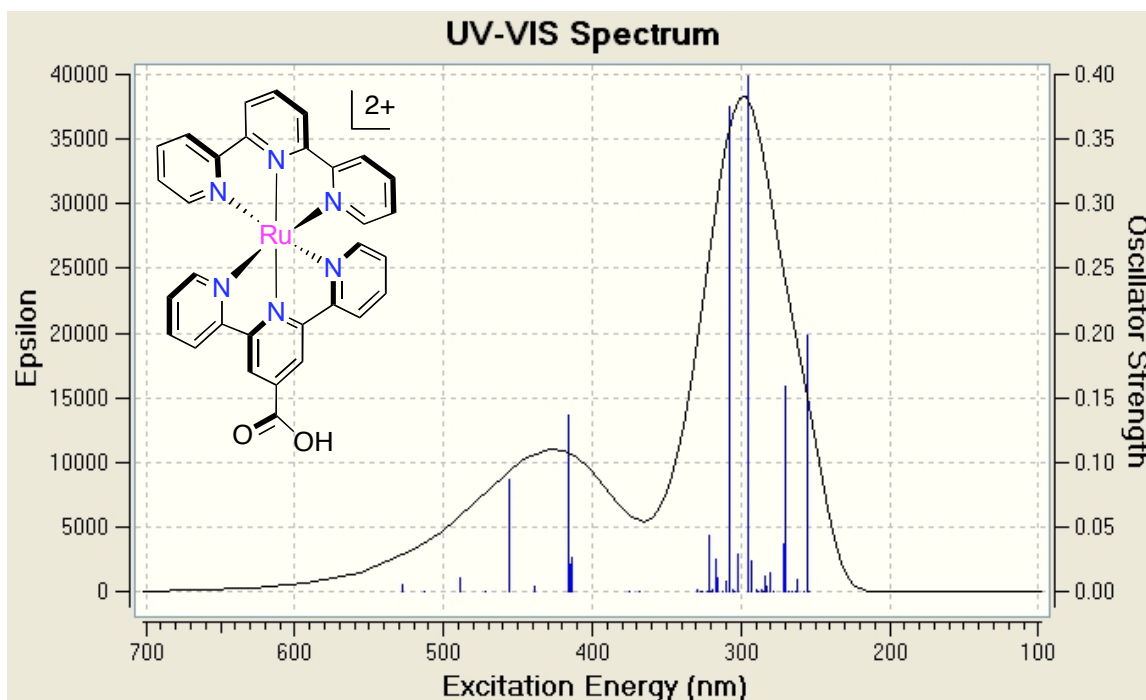
Excited State 17: Singlet-A" 3.8059 eV 325.77 nm f=0.0009
 125 ->131 -0.19414
 126 ->131 -0.20267
 127 ->140 -0.10819
 128 ->134 0.45808
 129 ->135 0.42471

Excited State 18: Singlet-A' 3.8127 eV 325.19 nm f=0.0063
 125 ->130 -0.11561
 126 ->130 0.12118
 127 ->134 0.59824
 127 ->137 -0.11032
 128 ->140 -0.12840
 129 ->134 0.17967
 129 ->136 0.20014

Excited State 19: Singlet-A" 3.8596 eV 321.23 nm f=0.0000
 126 ->131 -0.11578
 127 ->135 0.21609
 127 ->140 0.51281
 127 ->142 0.23857
 128 ->134 0.17442
 128 ->137 -0.20316

Excited State 20: Singlet-A' 3.8611 eV 321.11 nm f=0.0001
 127 ->134 0.18331
 127 ->137 0.21165
 128 ->140 0.54512
 128 ->142 -0.25037

*TD-DFT calculated electronic transitions for [Ru(tpy)(tpy-CO₂H)](PF₆)₂ (**2**)*



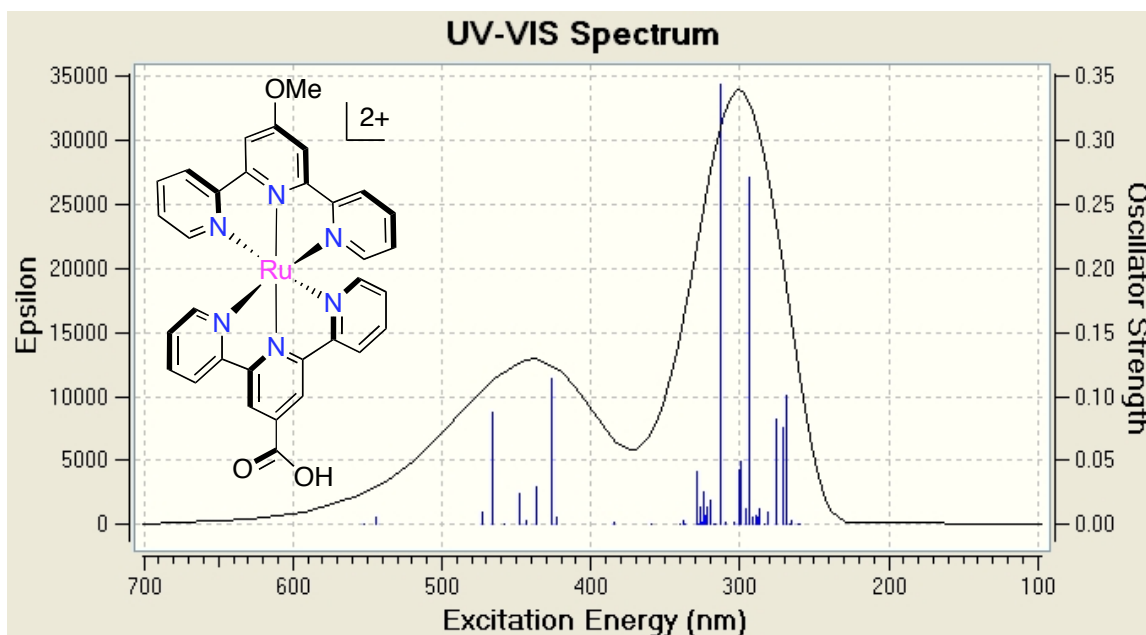
Excitation energies and oscillator strengths:

Excited State 1:	Singlet-A	2.3488 eV	527.87 nm	f=0.0059
140 ->141	0.69101			
Excited State 2:	Singlet-A	2.4182 eV	512.71 nm	f=0.0000
138 ->142	0.11989			
139 ->141	0.68196			
Excited State 3:	Singlet-A	2.5363 eV	488.85 nm	f=0.0104
140 ->142	0.69030			
Excited State 4:	Singlet-A	2.6252 eV	472.28 nm	f=0.0000
138 ->142	0.68794			
139 ->141	-0.13834			
Excited State 5:	Singlet-A	2.7232 eV	455.29 nm	f=0.0867
138 ->141	0.55041			
139 ->142	0.24521			
140 ->143	0.24279			
140 ->144	0.21297			

Excited State	6: Singlet-A	2.8251 eV	438.87 nm	f=0.0043
	138 ->141	-0.11683		
	139 ->142	0.48022		
	140 ->143	0.18283		
	140 ->144	-0.45235		
Excited State	7: Singlet-A	2.9814 eV	415.86 nm	f=0.1363
	138 ->141	-0.15807		
	139 ->142	-0.20855		
	140 ->143	0.61848		
Excited State	8: Singlet-A	2.9818 eV	415.80 nm	f=0.0077
	139 ->143	0.66887		
	139 ->144	0.20397		
Excited State	9: Singlet-A	2.9860 eV	415.22 nm	f=0.0208
	138 ->143	0.67633		
	138 ->144	0.13036		
Excited State	10: Singlet-A	2.9961 eV	413.81 nm	f=0.0267
	139 ->143	-0.19615		
	139 ->144	0.65940		
Excited State	11: Singlet-A	2.9987 eV	413.46 nm	f=0.0094
	138 ->143	-0.14777		
	138 ->144	0.67612		
Excited State	12: Singlet-A	3.3022 eV	375.45 nm	f=0.0004
	138 ->141	-0.24835		
	139 ->142	0.29343		
	140 ->144	0.46455		
	140 ->148	-0.23669		
Excited State	13: Singlet-A	3.3650 eV	368.45 nm	f=0.0000
	140 ->151	0.68572		
Excited State	14: Singlet-A	3.7648 eV	329.32 nm	f=0.0022
	136 ->141	0.28073		
	137 ->141	-0.32770		
	139 ->151	-0.12398		
	140 ->145	0.51795		
Excited State	15: Singlet-A	3.7929 eV	326.89 nm	f=0.0001
	138 ->146	-0.10670		
	138 ->148	0.13509		
	139 ->151	0.56590		

139 ->152	0.27062	
140 ->145	0.15953	
Excited State 16:	Singlet-A	3.8016 eV 326.14 nm f=0.0001
138 ->151	0.59053	
138 ->152	-0.26923	
139 ->148	-0.14040	
Excited State 17:	Singlet-A	3.8494 eV 322.09 nm f=0.0000
135 ->141	0.11275	
139 ->145	0.68490	
Excited State 18:	Singlet-A	3.8578 eV 321.38 nm f=0.0433
140 ->146	0.68017	
Excited State 19:	Singlet-A	3.8761 eV 319.87 nm f=0.0003
135 ->141	0.56694	
135 ->145	-0.14289	
135 ->149	-0.10332	
139 ->146	-0.25300	
140 ->147	0.21863	
Excited State 20:	Singlet-A	3.8777 eV 319.73 nm f=0.0003
135 ->141	-0.31908	
136 ->142	-0.14776	
137 ->142	-0.17199	
139 ->146	-0.36638	
140 ->147	0.42495	

*TD-DFT calculated electronic transitions for [Ru(tpy-OMe)(tpy-CO₂H)](PF₆)₂ (**3**)*



Excitation energies and oscillator strengths:

Excited State 1:	Singlet-A	2.2441 eV	552.50 nm	f=0.0002
148 ->149	0.68948			
Excited State 2:	Singlet-A	2.2780 eV	544.27 nm	f=0.0053
147 ->149	0.68982			
Excited State 3:	Singlet-A	2.6216 eV	472.94 nm	f=0.0101
147 ->150	0.54555			
147 ->151	-0.24607			
148 ->150	-0.29745			
148 ->151	0.11799			
Excited State 4:	Singlet-A	2.6619 eV	465.77 nm	f=0.0880
146 ->149	0.53641			
147 ->151	0.32253			
147 ->152	-0.18645			
148 ->150	-0.17492			
Excited State 5:	Singlet-A	2.7046 eV	458.41 nm	f=0.0000
146 ->150	0.61404			
146 ->151	-0.32001			

Excited State 6: Singlet-A 2.7675 eV 448.00 nm f=0.0237
 147 ->150 0.13252
 147 ->151 -0.12523
 147 ->152 -0.42286
 148 ->150 0.50400

Excited State 7: Singlet-A 2.7975 eV 443.20 nm f=0.0034
 147 ->151 0.16464
 148 ->150 0.13785
 148 ->151 0.58817
 148 ->152 -0.30036

Excited State 8: Singlet-A 2.8384 eV 436.81 nm f=0.0297
 147 ->150 0.20574
 147 ->151 0.11042
 147 ->152 0.24069
 148 ->150 0.13544
 148 ->151 0.18876
 148 ->152 0.55346

Excited State 9: Singlet-A 2.9068 eV 426.53 nm f=0.0682
 146 ->150 0.23252
 146 ->151 0.48490
 146 ->152 -0.14839
 147 ->150 -0.19060
 147 ->151 -0.29459
 148 ->151 0.13566

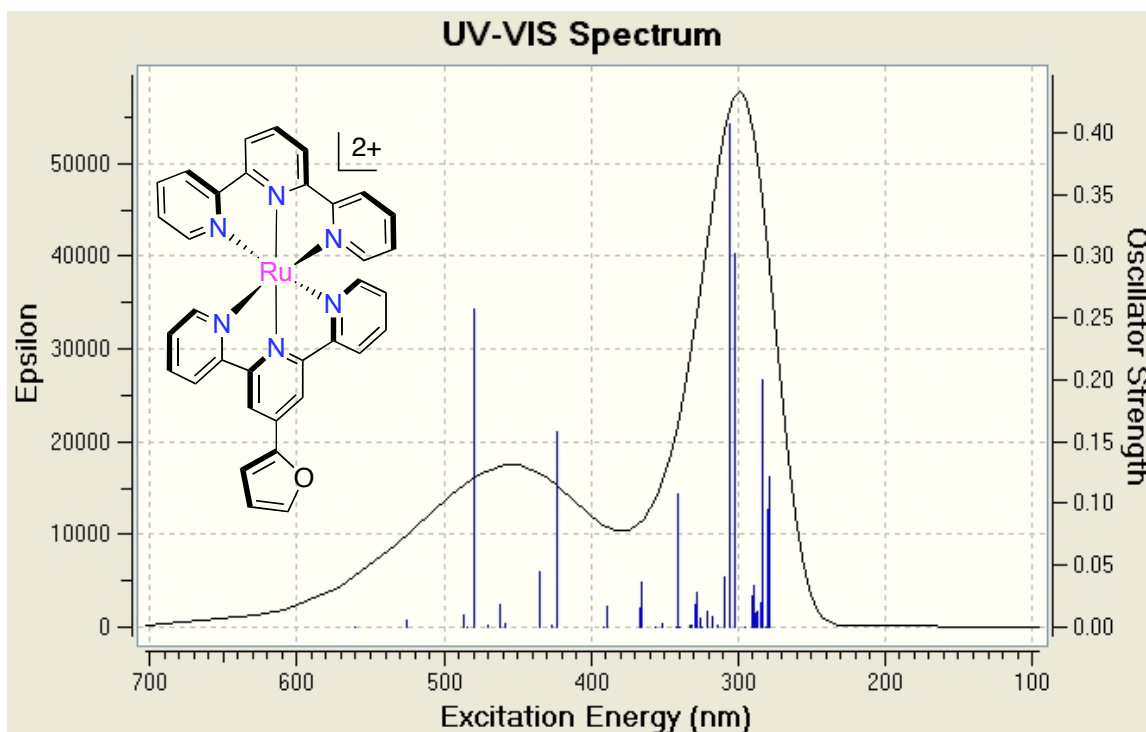
Excited State 10: Singlet-A 2.9094 eV 426.16 nm f=0.1134
 146 ->149 -0.13201
 146 ->150 0.17822
 146 ->151 0.36136
 147 ->150 0.26232
 147 ->151 0.39501
 148 ->151 -0.18838
 148 ->152 -0.13705

Excited State 11: Singlet-A 2.9306 eV 423.07 nm f=0.0052
 146 ->150 0.15908
 146 ->151 0.12189
 146 ->152 0.66458

Excited State 12: Singlet-A 3.2256 eV 384.38 nm f=0.0013
 146 ->149 0.26220
 147 ->150 0.10104
 147 ->151 -0.13773

147 ->152	0.42753	
147 ->156	0.22542	
148 ->150	0.18693	
148 ->151	-0.14405	
148 ->152	-0.16793	
Excited State 13: Singlet-A	3.4481 eV	359.58 nm f=0.0000
147 ->158	0.66930	
148 ->158	-0.13990	
Excited State 14: Singlet-A	3.6407 eV	340.55 nm f=0.0002
148 ->153	0.68847	
Excited State 15: Singlet-A	3.6707 eV	337.77 nm f=0.0029
148 ->154	0.69088	
Excited State 16: Singlet-A	3.6844 eV	336.51 nm f=0.0004
144 ->149	0.21148	
145 ->149	0.35089	
147 ->153	0.55644	
147 ->157	-0.10065	
Excited State 17: Singlet-A	3.7653 eV	329.28 nm f=0.0408
147 ->154	0.66059	
148 ->155	0.13806	
Excited State 18: Singlet-A	3.7689 eV	328.97 nm f=0.0001
146 ->154	0.49464	
146 ->156	-0.16273	
148 ->158	-0.38662	
148 ->161	-0.15008	
Excited State 19: Singlet-A	3.7783 eV	328.15 nm f=0.0000
143 ->149	0.65472	
143 ->153	-0.17600	
143 ->157	-0.11968	
Excited State 20: Singlet-A	3.8009 eV	326.20 nm f=0.0132
146 ->158	0.26598	
148 ->155	0.53203	
148 ->156	-0.28563	

*TD-DFT calculated electronic transitions for [Ru(tpy)(tpy-2-furyl)](PF₆)₂ (**4**)*



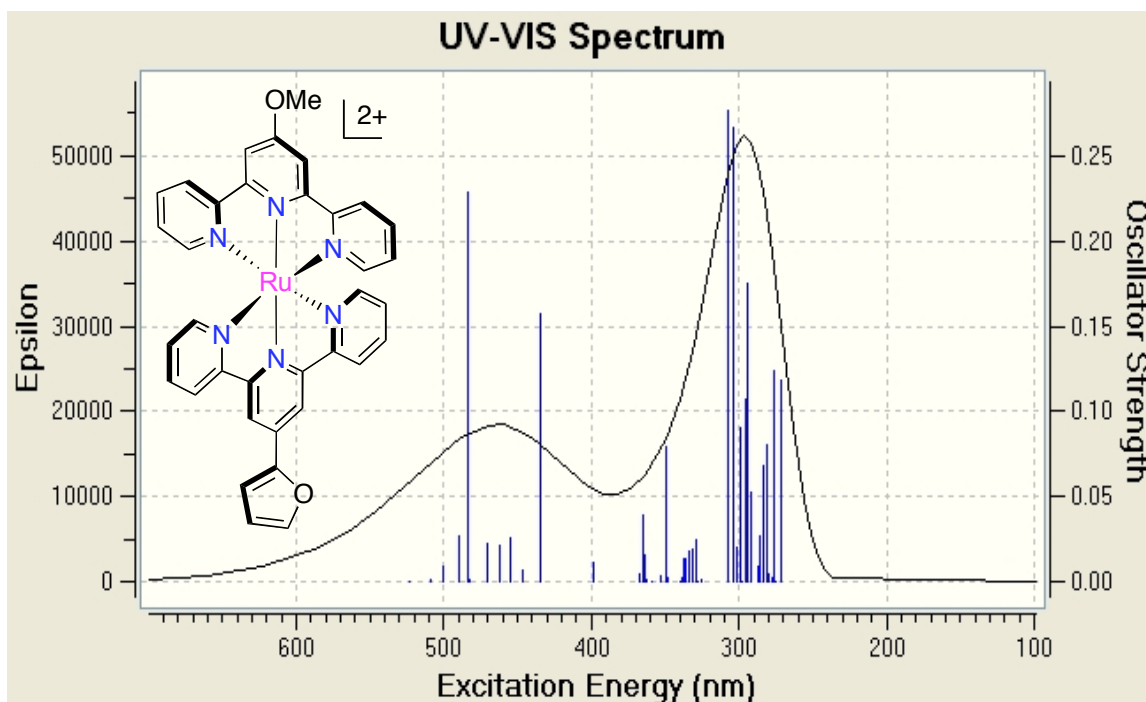
Excitation energies and oscillator strengths:

Excited State 1:	Singlet-A	2.2131 eV	560.23 nm	f=0.0000
143 ->147		0.25815		
146 ->147		0.64275		
Excited State 2:	Singlet-A	2.3589 eV	525.61 nm	f=0.0063
145 ->147		0.68702		
Excited State 3:	Singlet-A	2.5484 eV	486.52 nm	f=0.0102
145 ->148		0.68072		
Excited State 4:	Singlet-A	2.5611 eV	484.10 nm	f=0.0001
144 ->148		0.69471		
Excited State 5:	Singlet-A	2.5872 eV	479.22 nm	f=0.2572
143 ->148		0.15260		
144 ->147		0.33086		
145 ->149		-0.13774		
145 ->150		0.10150		
146 ->148		0.54409		

Excited State	6:	Singlet-A	2.6385 eV	469.91 nm	f=0.0013
143 ->149		0.17788			
146 ->149		0.67400			
Excited State	7:	Singlet-A	2.6871 eV	461.40 nm	f=0.0188
143 ->150		0.12525			
146 ->150		0.66968			
Excited State	8:	Singlet-A	2.7059 eV	458.20 nm	f=0.0026
144 ->147		0.42875			
145 ->149		-0.31975			
145 ->150		-0.33983			
145 ->154		0.11229			
146 ->148		-0.24633			
Excited State	9:	Singlet-A	2.8480 eV	435.34 nm	f=0.0445
144 ->149		0.65996			
144 ->150		0.17921			
Excited State	10:	Singlet-A	2.9101 eV	426.06 nm	f=0.0010
144 ->149		-0.19220			
144 ->150		0.66714			
Excited State	11:	Singlet-A	2.9316 eV	422.92 nm	f=0.1575
144 ->147		0.18615			
145 ->149		0.57191			
145 ->150		-0.31338			
Excited State	12:	Singlet-A	3.1634 eV	391.94 nm	f=0.0000
143 ->147		0.64867			
146 ->147		-0.26954			
Excited State	13:	Singlet-A	3.1861 eV	389.14 nm	f=0.0174
143 ->148		0.25382			
144 ->147		0.25578			
145 ->149		0.16920			
145 ->150		0.43275			
145 ->154		0.14279			
146 ->148		-0.23699			
Excited State	14:	Singlet-A	3.3809 eV	366.72 nm	f=0.0152
143 ->148		-0.14949			
143 ->149		-0.38501			
143 ->150		0.51838			

Excited State 15:	Singlet-A	3.3826 eV	366.54 nm	f=0.0003
145 ->157	0.67568			
Excited State 16:	Singlet-A	3.3887 eV	365.87 nm	f=0.0367
143 ->148	0.56382			
143 ->149	-0.10964			
143 ->150	0.13857			
145 ->150	-0.21829			
145 ->154	-0.18097			
Excited State 17:	Singlet-A	3.4790 eV	356.38 nm	f=0.0006
143 ->149	0.50830			
143 ->150	0.38554			
146 ->149	-0.17434			
146 ->150	-0.12017			
146 ->151	0.13896			
146 ->154	-0.10494			
Excited State 18:	Singlet-A	3.5291 eV	351.32 nm	f=0.0026
143 ->149	-0.18083			
143 ->151	0.15373			
146 ->151	0.66009			
Excited State 19:	Singlet-A	3.6261 eV	341.93 nm	f=0.0004
143 ->153	0.19043			
146 ->153	0.67764			
Excited State 20:	Singlet-A	3.6324 eV	341.33 nm	f=0.1081
143 ->152	0.14944			
146 ->152	0.65889			
146 ->155	-0.11500			

TD-DFT calculated electronic transitions for [Ru(tpy-OMe)(tpy-2-furyl)](PF₆)₂ (5)



Excitation energies and oscillator strengths:

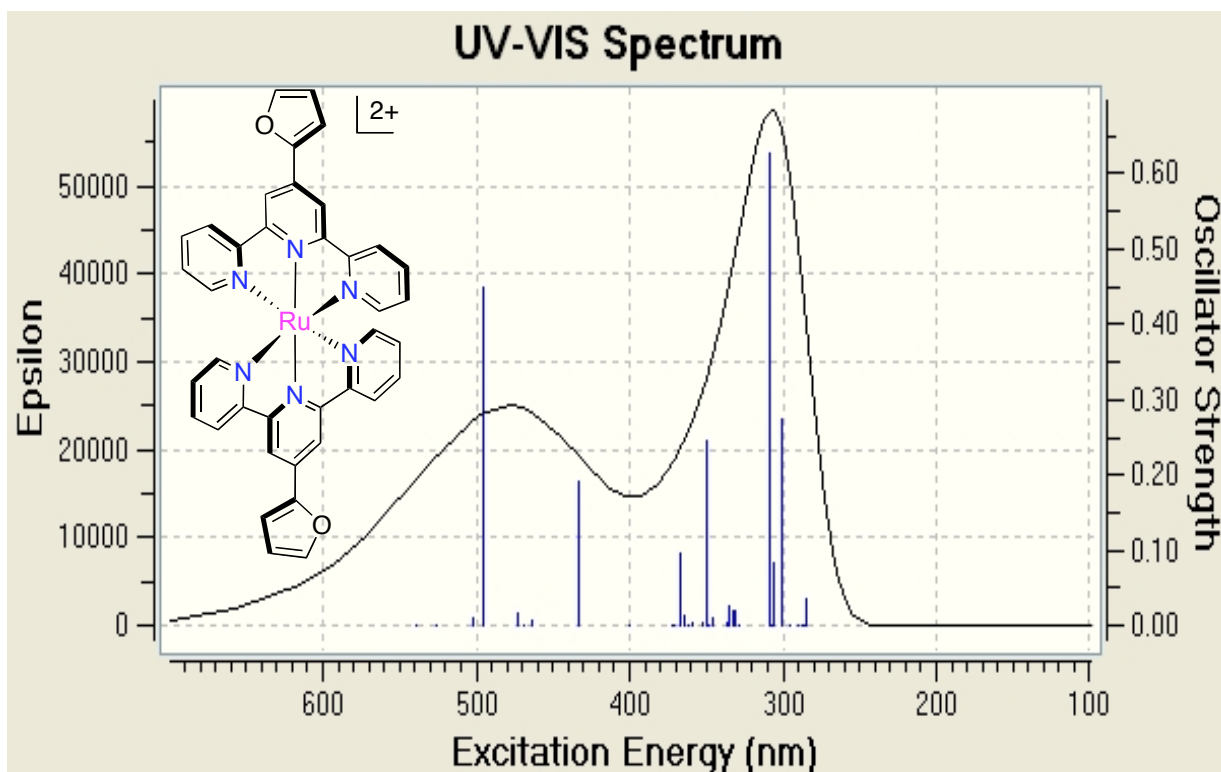
Excited State 1:	Singlet-A	2.3683 eV	523.52 nm	f=0.0000
151 ->156	0.16663			
153 ->155	-0.32289			
154 ->156	0.51672			
154 ->157	0.26088			
Excited State 2:	Singlet-A	2.4350 eV	509.18 nm	f=0.0007
153 ->155	0.61299			
154 ->156	0.30442			
154 ->157	0.11175			
Excited State 3:	Singlet-A	2.4786 eV	500.21 nm	f=0.0093
152 ->155	0.67636			
Excited State 4:	Singlet-A	2.5339 eV	489.30 nm	f=0.0268
152 ->156	0.51725			
152 ->157	0.23267			
153 ->156	-0.34547			
154 ->155	0.14970			

Excited State	5: Singlet-A	2.5608 eV	484.17 nm	f=0.2289
	151 ->155	0.13886		
	152 ->156	-0.19051		
	152 ->157	-0.18947		
	152 ->158	-0.17379		
	153 ->156	-0.11734		
	154 ->155	0.55461		
Excited State	6: Singlet-A	2.5704 eV	482.35 nm	f=0.0013
	151 ->157	0.14951		
	154 ->156	-0.29976		
	154 ->157	0.60664		
Excited State	7: Singlet-A	2.6361 eV	470.34 nm	f=0.0229
	151 ->158	0.11409		
	152 ->155	0.10041		
	154 ->158	0.66740		
Excited State	8: Singlet-A	2.6827 eV	462.15 nm	f=0.0218
	152 ->157	0.37815		
	152 ->158	-0.27901		
	153 ->156	0.47352		
	154 ->155	0.13765		
Excited State	9: Singlet-A	2.7277 eV	454.54 nm	f=0.0261
	152 ->156	-0.20778		
	152 ->157	0.23494		
	152 ->158	-0.12443		
	153 ->156	-0.19368		
	153 ->157	0.56359		
Excited State	10: Singlet-A	2.7795 eV	446.06 nm	f=0.0062
	152 ->156	0.10025		
	153 ->157	0.15855		
	153 ->158	0.66622		
Excited State	11: Singlet-A	2.8506 eV	434.94 nm	f=0.1575
	152 ->156	-0.29745		
	152 ->157	0.43805		
	152 ->158	0.32098		
	153 ->156	-0.12977		
	153 ->157	-0.24892		
Excited State	12: Singlet-A	3.1114 eV	398.48 nm	f=0.0117
	151 ->155	-0.14205		
	152 ->156	0.14343		

152 ->158	0.46494				
152 ->162	0.16508				
153 ->156	0.18180				
153 ->157	0.19919				
154 ->155	0.23052				
Excited State 13:	Singlet-A	3.3787 eV	366.96 nm	f=0.0043	
151 ->156	0.59437				
151 ->158	-0.23443				
154 ->156	-0.17954				
154 ->159	0.19878				
Excited State 14:	Singlet-A	3.3987 eV	364.80 nm	f=0.0392	
151 ->155	0.56823				
151 ->156	-0.13643				
151 ->157	-0.15655				
151 ->158	-0.12506				
152 ->158	0.12913				
152 ->162	0.16274				
Excited State 15:	Singlet-A	3.4046 eV	364.16 nm	f=0.0153	
151 ->155	0.22963				
151 ->156	0.18440				
151 ->157	0.39883				
151 ->158	0.35735				
154 ->157	-0.10434				
154 ->159	-0.25098				
Excited State 16:	Singlet-A	3.4241 eV	362.09 nm	f=0.0013	
151 ->157	0.10084				
151 ->158	0.31213				
151 ->159	0.13380				
154 ->159	0.58391				
Excited State 17:	Singlet-A	3.4549 eV	358.87 nm	f=0.0000	
152 ->165	0.66756				
153 ->165	-0.11493				
Excited State 18:	Singlet-A	3.5113 eV	353.10 nm	f=0.0032	
151 ->156	-0.16756				
151 ->157	0.49898				
151 ->158	-0.32618				
154 ->157	-0.14403				
154 ->158	0.10863				
154 ->159	0.13812				

154 ->162	0.18327			
Excited State 19:	Singlet-A	3.5458 eV	349.66 nm	f=0.0789
151 ->160	0.11528			
154 ->160	0.55563			
154 ->161	-0.34929			
154 ->163	-0.10078			
Excited State 20:	Singlet-A	3.5531 eV	348.95 nm	f=0.0417
151 ->161	0.13856			
154 ->160	0.33606			
154 ->161	0.58395			

TD-DFT calculated electronic transitions for [Ru(tpy-2-furyl)₂](PF₆)₂ (6)



Excitation energies and oscillator strengths:

Excited State 1:	Singlet-A	2.2987 eV	539.37 nm	f=0.0000
159 ->164	0.11918			
160 ->165	-0.11926			
162 ->164	-0.13739			
162 ->165	-0.44050			
163 ->164	0.44183			
163 ->165	-0.13794			
Excited State 2:	Singlet-A	2.3575 eV	525.91 nm	f=0.0000
159 ->165	-0.12918			
160 ->164	0.12918			
162 ->164	0.42374			
162 ->165	0.22720			
163 ->164	0.22635			
163 ->165	-0.42281			
Excited State 3:	Singlet-A	2.4709 eV	501.78 nm	f=0.0106
161 ->164	0.64338			

161 ->165	0.23301				
Excited State 4:	Singlet-A	2.4713 eV	501.69 nm	f=0.0102	
161 ->164	-0.23415				
161 ->165	0.64331				
Excited State 5:	Singlet-A	2.5062 eV	494.71 nm	f=0.4489	
159 ->164	0.10145				
160 ->165	0.10164				
161 ->166	-0.13957				
162 ->164	-0.21435				
162 ->165	0.40033				
163 ->164	0.39959				
163 ->165	0.21441				
Excited State 6:	Singlet-A	2.6218 eV	472.89 nm	f=0.0177	
160 ->166	0.10267				
162 ->166	0.15075				
162 ->167	0.10560				
163 ->166	0.63228				
163 ->167	0.17708				
Excited State 7:	Singlet-A	2.6222 eV	472.82 nm	f=0.0174	
159 ->166	-0.10310				
162 ->166	0.63250				
162 ->167	-0.17476				
163 ->166	-0.15017				
163 ->167	0.10424				
Excited State 8:	Singlet-A	2.6426 eV	469.18 nm	f=0.0002	
161 ->167	-0.39121				
161 ->171	-0.12075				
162 ->164	0.35426				
162 ->165	-0.11110				
163 ->164	0.11003				
163 ->165	0.35517				
Excited State 9:	Singlet-A	2.6729 eV	463.85 nm	f=0.0066	
159 ->167	-0.14168				
162 ->166	0.18085				
162 ->167	0.61840				
163 ->166	-0.10601				
163 ->167	-0.15490				
Excited State 10:	Singlet-A	2.6731 eV	463.82 nm	f=0.0065	
160 ->167	0.14165				

162 ->166	-0.10705	
162 ->167	0.15550	
163 ->166	-0.18136	
163 ->167	0.61634	
Excited State 11: Singlet-A	2.8640 eV	432.91 nm f=0.1902
161 ->166	0.67932	
Excited State 12: Singlet-A	3.0965 eV	400.40 nm f=0.0000
161 ->167	0.52914	
161 ->171	-0.12882	
162 ->164	0.21420	
163 ->165	0.21428	
Excited State 13: Singlet-A	3.3307 eV	372.24 nm f=0.0000
159 ->164	-0.36134	
159 ->165	-0.28181	
160 ->164	-0.30254	
160 ->165	0.36927	
162 ->165	-0.15397	
163 ->164	0.15763	
Excited State 14: Singlet-A	3.3434 eV	370.83 nm f=0.0000
159 ->164	0.22989	
159 ->165	0.42461	
160 ->164	-0.41412	
160 ->165	0.21030	
162 ->164	0.13283	
163 ->165	-0.13020	
Excited State 15: Singlet-A	3.3807 eV	366.75 nm f=0.0972
159 ->164	0.39017	
159 ->165	-0.20415	
160 ->164	0.20766	
160 ->165	0.39728	
161 ->168	-0.14096	
Excited State 16: Singlet-A	3.4051 eV	364.12 nm f=0.0136
159 ->166	0.24891	
160 ->166	0.45279	
160 ->167	0.35687	
163 ->168	0.23067	
Excited State 17: Singlet-A	3.4062 eV	364.00 nm f=0.0147
159 ->166	0.45369	
159 ->167	-0.35938	

160 ->166	-0.24940
162 ->168	-0.22925

Excited State 18: Singlet-A 3.4245 eV 362.05 nm f=0.0006

159 ->164	-0.26562
159 ->165	0.33413
160 ->164	0.32990
160 ->165	0.26481
161 ->167	0.17051
161 ->171	-0.22797

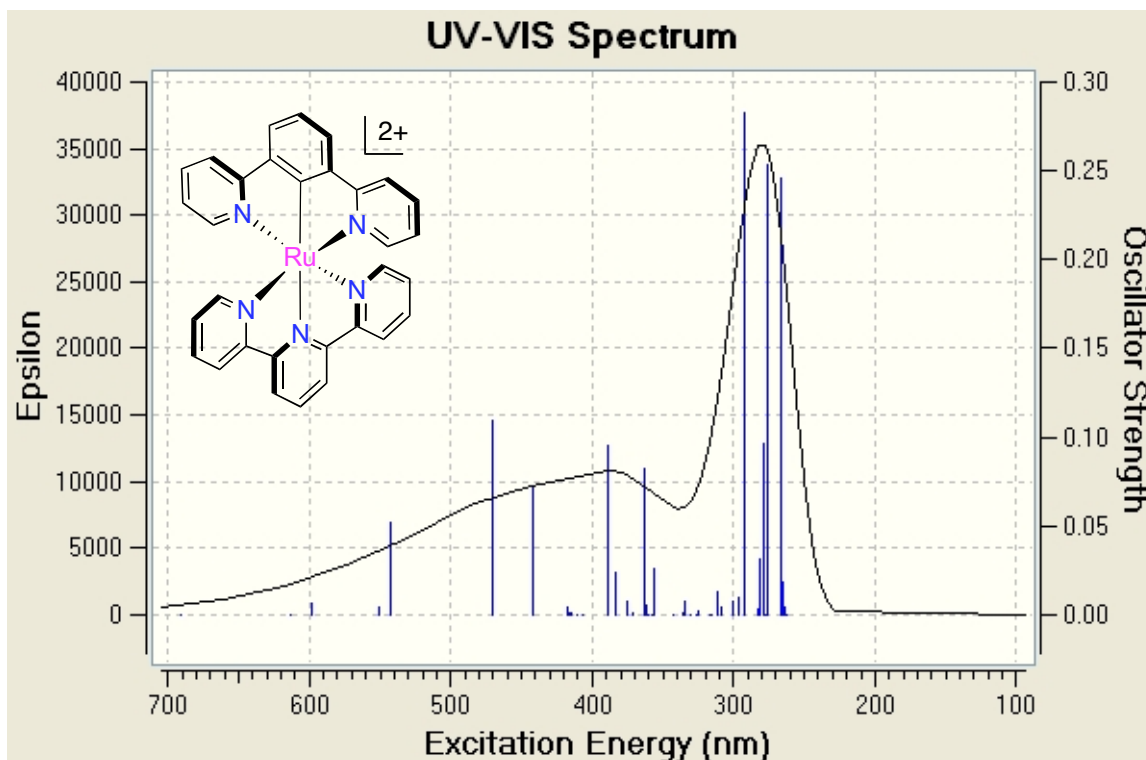
Excited State 19: Singlet-A 3.4504 eV 359.33 nm f=0.0023

160 ->166	-0.15131
160 ->167	-0.17018
160 ->168	0.13929
162 ->168	0.29757
163 ->168	0.56215

Excited State 20: Singlet-A 3.4508 eV 359.29 nm f=0.0016

159 ->166	0.15367
159 ->167	-0.17274
159 ->168	-0.13877
162 ->168	0.56034
163 ->168	-0.29674

TD-DFT calculated electronic transitions for [Ru(tpy)(dpb)]PF₆ (7)



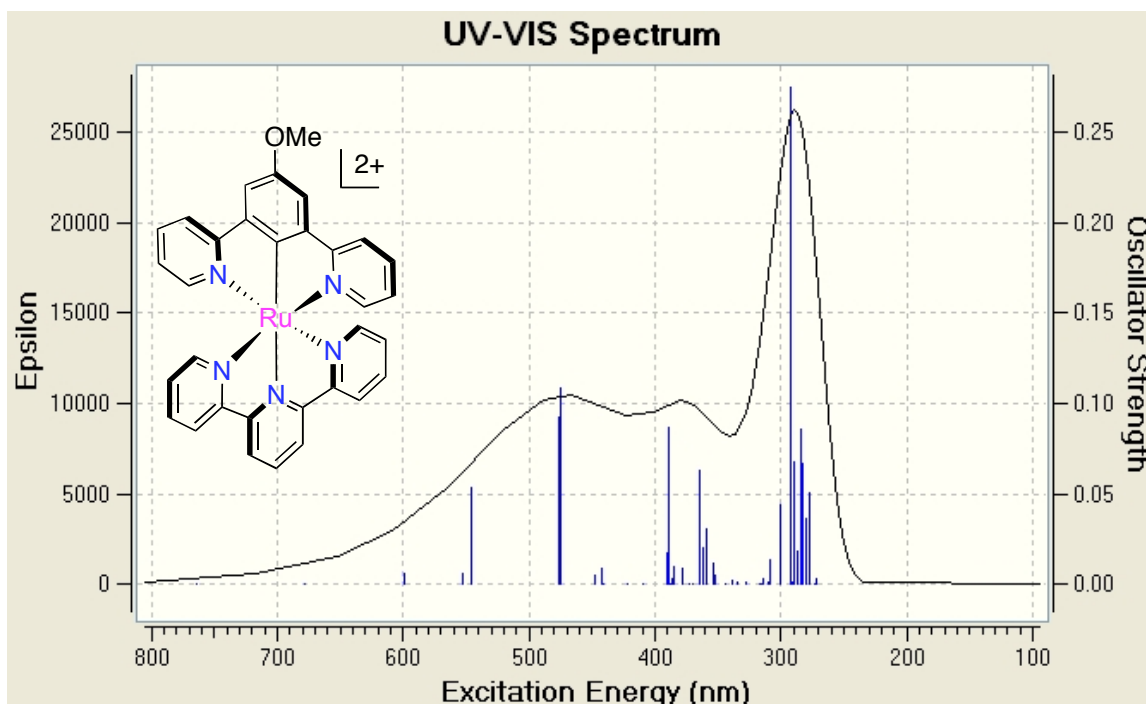
Excitation energies and oscillator strengths:

Excited State 1:	Singlet-A	1.7961 eV	690.31 nm	f=0.0000
129 ->130	0.68922			
Excited State 2:	Singlet-A	2.0226 eV	612.99 nm	f=0.0002
129 ->131	0.69763			
Excited State 3:	Singlet-A	2.0733 eV	598.01 nm	f=0.0063
127 ->130	0.64971			
128 ->131	-0.19524			
Excited State 4:	Singlet-A	2.2496 eV	551.13 nm	f=0.0045
127 ->131	0.52388			
128 ->130	-0.45704			
Excited State 5:	Singlet-A	2.2852 eV	542.54 nm	f=0.0523
127 ->130	0.20139			
128 ->131	0.65811			
Excited State 6:	Singlet-A	2.6350 eV	470.53 nm	f=0.1094
127 ->131	0.43915			

127 ->134	0.15421				
128 ->130	0.41188				
129 ->133	0.17282				
Excited State 7:	Singlet-A	2.8029 eV	442.35 nm	f=0.0721	
127 ->133	0.18286				
129 ->132	0.64295				
129 ->134	-0.11751				
Excited State 8:	Singlet-A	2.9722 eV	417.14 nm	f=0.0044	
129 ->132	0.11642				
129 ->134	0.68527				
Excited State 9:	Singlet-A	2.9810 eV	415.91 nm	f=0.0008	
127 ->132	0.30744				
127 ->136	-0.12881				
129 ->133	0.59698				
Excited State 10:	Singlet-A	2.9881 eV	414.93 nm	f=0.0005	
128 ->132	0.68858				
Excited State 11:	Singlet-A	3.0185 eV	410.75 nm	f=0.0000	
129 ->135	0.70418				
Excited State 12:	Singlet-A	3.0498 eV	406.53 nm	f=0.0000	
128 ->133	0.69806				
Excited State 13:	Singlet-A	3.1932 eV	388.28 nm	f=0.0951	
127 ->133	0.64759				
128 ->139	-0.13993				
129 ->132	-0.16556				
Excited State 14:	Singlet-A	3.2354 eV	383.21 nm	f=0.0240	
127 ->132	0.58061				
127 ->134	0.20942				
127 ->136	0.10577				
129 ->133	-0.24039				
Excited State 15:	Singlet-A	3.2368 eV	383.04 nm	f=0.0086	
127 ->135	-0.13682				
128 ->134	0.67995				
Excited State 16:	Singlet-A	3.2984 eV	375.89 nm	f=0.0078	
128 ->135	0.69091				
Excited State 17:	Singlet-A	3.3345 eV	371.82 nm	f=0.0000	

126 ->139	0.10991	
127 ->139	0.67043	
127 ->142	-0.12920	
Excited State 18: Singlet-A 3.3381 eV 371.42 nm f=0.0004		
126 ->130	0.68286	
129 ->139	-0.12437	
Excited State 19: Singlet-A 3.4124 eV 363.33 nm f=0.0825		
123 ->130	-0.13547	
127 ->135	0.66526	
128 ->134	0.11784	
Excited State 20: Singlet-A 3.4327 eV 361.19 nm f=0.0050		
126 ->131	0.55595	
127 ->134	0.40248	

TD-DFT calculated electronic transitions for [Ru(tpy)(dpb-OMe)]PF₆ (8)



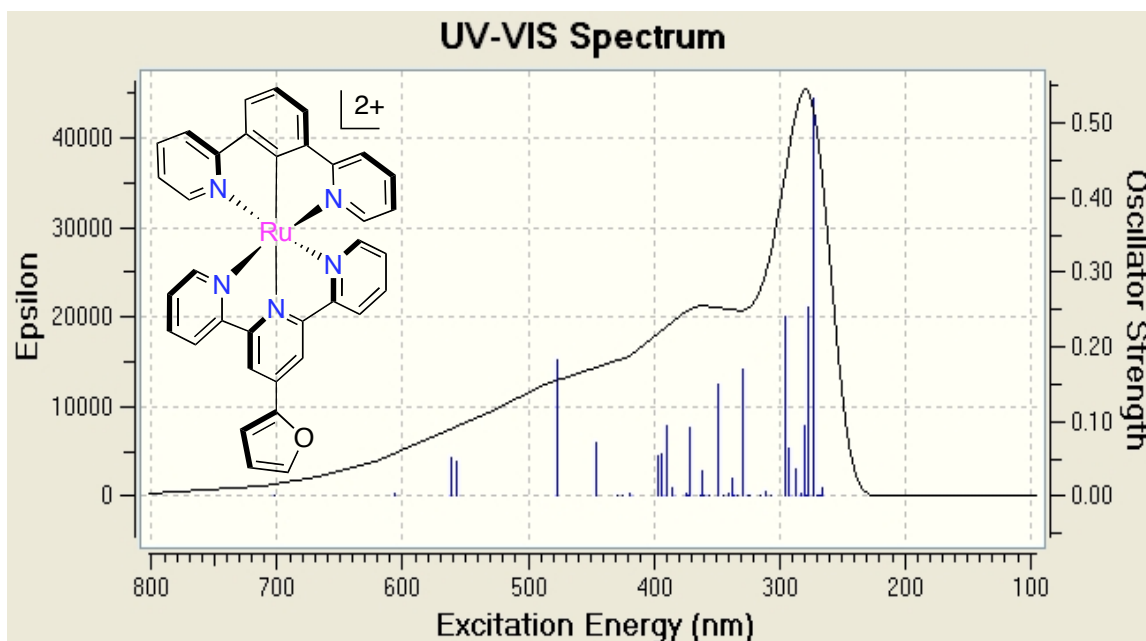
Excitation energies and oscillator strengths:

Excited State 1:	Singlet-A	1.6228 eV	764.03 nm	f=0.0000
137 ->138	0.68533			
Excited State 2:	Singlet-A	1.8266 eV	678.77 nm	f=0.0002
137 ->139	0.69624			
Excited State 3:	Singlet-A	2.0687 eV	599.32 nm	f=0.0055
135 ->138	0.64527			
136 ->139	0.20825			
Excited State 4:	Singlet-A	2.2425 eV	552.89 nm	f=0.0054
135 ->139	0.51993			
136 ->138	0.46040			
Excited State 5:	Singlet-A	2.2708 eV	546.00 nm	f=0.0534
135 ->138	-0.21411			
136 ->139	0.65364			
Excited State 6:	Singlet-A	2.6050 eV	475.95 nm	f=0.0919
135 ->141	0.13420			

137 ->140	0.64466				
Excited State 7:	Singlet-A	2.6108 eV	474.90 nm	f=0.1085	
135 ->139	0.41877				
135 ->142	-0.13633				
136 ->138	-0.37791				
137 ->141	-0.30715				
Excited State 8:	Singlet-A	2.7669 eV	448.10 nm	f=0.0045	
137 ->140	0.10352				
137 ->142	0.68601				
Excited State 9:	Singlet-A	2.7998 eV	442.82 nm	f=0.0091	
135 ->139	0.15851				
135 ->140	0.21171				
135 ->144	0.13223				
136 ->138	-0.15732				
137 ->141	0.58239				
Excited State 10:	Singlet-A	2.8144 eV	440.53 nm	f=0.0000	
137 ->143	0.70252				
Excited State 11:	Singlet-A	2.9363 eV	422.25 nm	f=0.0004	
136 ->140	0.68595				
Excited State 12:	Singlet-A	3.0286 eV	409.38 nm	f=0.0000	
136 ->141	0.68906				
Excited State 13:	Singlet-A	3.1750 eV	390.50 nm	f=0.0177	
135 ->140	0.61112				
135 ->142	0.15835				
137 ->141	-0.13104				
137 ->144	0.14192				
137 ->145	0.13083				
Excited State 14:	Singlet-A	3.1864 eV	389.11 nm	f=0.0862	
135 ->141	0.65513				
136 ->147	0.13846				
137 ->140	-0.10359				
Excited State 15:	Singlet-A	3.1939 eV	388.19 nm	f=0.0000	
133 ->138	0.26385				
134 ->138	0.61813				
136 ->141	-0.10701				
137 ->138	-0.11639				

Excited State 16:	Singlet-A	3.2115 eV	386.07 nm	f=0.0027
135 ->140	-0.11898			
137 ->144	0.65802			
Excited State 17:	Singlet-A	3.2174 eV	385.36 nm	f=0.0094
135 ->143	-0.12807			
136 ->142	0.67314			
137 ->147	-0.11462			
Excited State 18:	Singlet-A	3.2818 eV	377.79 nm	f=0.0089
136 ->143	0.69134			
Excited State 19:	Singlet-A	3.3296 eV	372.37 nm	f=0.0000
134 ->147	-0.11825			
135 ->147	0.61163			
135 ->149	0.12202			
137 ->147	-0.22914			
Excited State 20:	Singlet-A	3.3461 eV	370.54 nm	f=0.0001
133 ->139	0.21983			
134 ->139	0.64388			
137 ->144	0.12295			

TD-DFT calculated electronic transitions for [Ru(tpy-2-furyl)(dpb)]PF₆ (9)



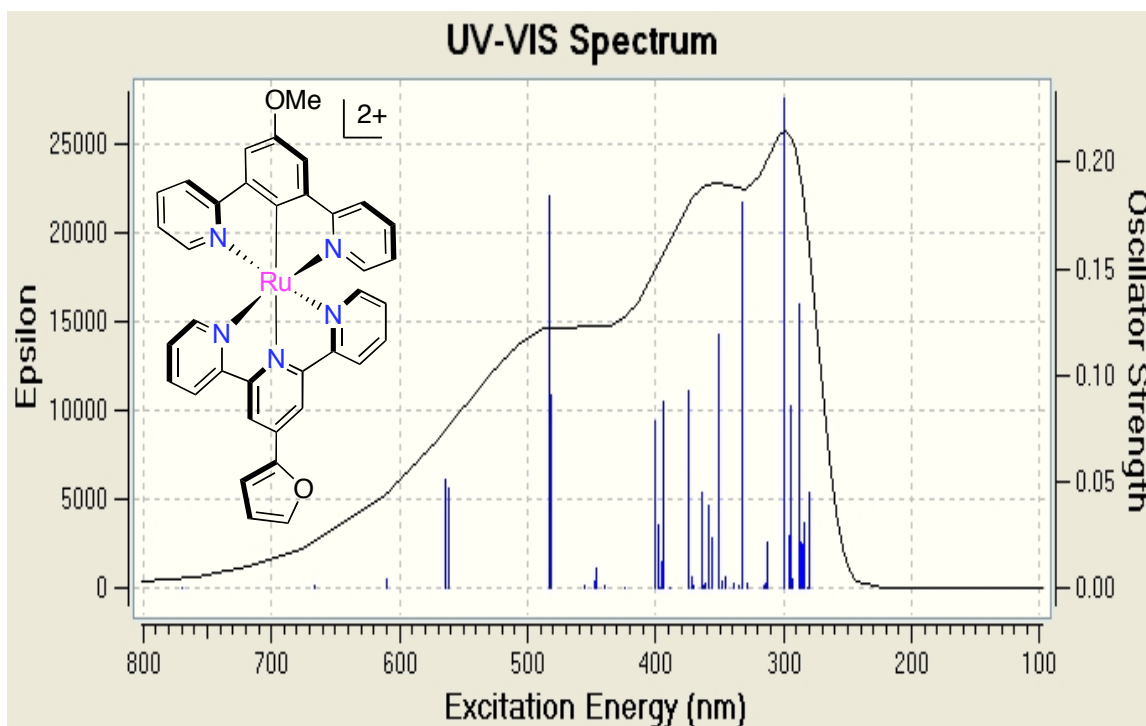
Excitation energies and oscillator strengths:

Excited State 1:	Singlet-A	1.7645 eV	702.65 nm	f=0.0000
146 ->147	0.68753			
Excited State 2:	Singlet-A	2.0443 eV	606.49 nm	f=0.0046
144 ->147	0.63948			
145 ->148	0.19200			
146 ->148	0.11823			
Excited State 3:	Singlet-A	2.0450 eV	606.27 nm	f=0.0003
144 ->147	-0.11052			
146 ->148	0.68670			
Excited State 4:	Singlet-A	2.2104 eV	560.91 nm	f=0.0514
144 ->148	0.44662			
145 ->147	0.51038			
Excited State 5:	Singlet-A	2.2275 eV	556.60 nm	f=0.0456
144 ->147	-0.20694			
145 ->148	0.65422			
Excited State 6:	Singlet-A	2.6010 eV	476.67 nm	f=0.1819
144 ->148	0.51499			

144 ->152	0.12502				
145 ->147	-0.33076				
146 ->151	-0.16784				
Excited State 7:	Singlet-A	2.7802 eV	445.96 nm	f=0.0716	
144 ->151	-0.18151				
146 ->149	0.64332				
146 ->152	-0.11315				
Excited State 8:	Singlet-A	2.8905 eV	428.93 nm	f=0.0004	
145 ->149	0.68886				
Excited State 9:	Singlet-A	2.9181 eV	424.88 nm	f=0.0010	
146 ->150	0.67008				
146 ->152	-0.16676				
146 ->153	-0.11328				
Excited State 10:	Singlet-A	2.9595 eV	418.94 nm	f=0.0004	
144 ->149	-0.11388				
145 ->151	0.60999				
146 ->151	0.22942				
146 ->152	0.19533				
Excited State 11:	Singlet-A	2.9604 eV	418.82 nm	f=0.0028	
145 ->151	-0.23959				
146 ->150	0.15950				
146 ->152	0.62211				
Excited State 12:	Singlet-A	2.9634 eV	418.38 nm	f=0.0002	
144 ->149	-0.28606				
144 ->154	0.11815				
145 ->151	-0.23265				
146 ->151	0.54741				
146 ->152	-0.12876				
Excited State 13:	Singlet-A	3.1230 eV	397.01 nm	f=0.0553	
145 ->150	0.52935				
145 ->152	-0.41493				
145 ->153	-0.11101				
Excited State 14:	Singlet-A	3.1537 eV	393.14 nm	f=0.0571	
144 ->149	-0.12199				
145 ->150	0.38282				
145 ->152	0.54252				
145 ->153	-0.12102				

Excited State 15:	Singlet-A	3.1776 eV	390.18 nm	f=0.0955
144 ->151	0.64461			
145 ->156	0.15014			
146 ->149	0.16331			
Excited State 16:	Singlet-A	3.2203 eV	385.01 nm	f=0.0100
144 ->149	0.55860			
144 ->152	0.20034			
144 ->154	0.10785			
145 ->150	0.10590			
145 ->153	-0.12587			
146 ->151	0.23964			
Excited State 17:	Singlet-A	3.3128 eV	374.26 nm	f=0.0048
143 ->147	0.66377			
144 ->150	0.18091			
146 ->156	-0.11515			
Excited State 18:	Singlet-A	3.3257 eV	372.81 nm	f=0.0001
143 ->156	-0.10555			
144 ->156	0.66046			
144 ->160	0.12234			
146 ->153	-0.12310			
Excited State 19:	Singlet-A	3.3345 eV	371.82 nm	f=0.0924
139 ->147	0.12121			
143 ->147	-0.18545			
144 ->150	0.63486			
144 ->153	-0.11273			
Excited State 20:	Singlet-A	3.3412 eV	371.08 nm	f=0.0000
144 ->156	0.11956			
146 ->150	0.11986			
146 ->153	0.68102			

*TD-DFT calculated electronic transitions for [Ru(tpy-2-furyl)(dpb-OMe)]PF₆ (**10**)*



Excitation energies and oscillator strengths:

Excited State 1:	Singlet-A	1.6095 eV	770.31 nm	f=0.0000
154 ->155	0.68339			
Excited State 2:	Singlet-A	1.8606 eV	666.35 nm	f=0.0003
154 ->156	0.69516			
Excited State 3:	Singlet-A	2.0312 eV	610.41 nm	f=0.0038
152 ->155	0.64347			
153 ->156	-0.20738			
Excited State 4:	Singlet-A	2.1980 eV	564.09 nm	f=0.0507
152 ->156	-0.45431			
153 ->155	0.50223			
Excited State 5:	Singlet-A	2.2061 eV	562.02 nm	f=0.0471
152 ->155	0.22107			
153 ->156	0.64763			
Excited State 6:	Singlet-A	2.5692 eV	482.57 nm	f=0.1838

152 ->156	0.48661				
152 ->160	0.11543				
153 ->155	0.31581				
154 ->159	0.26933				
Excited State 7:	Singlet-A	2.5749 eV	481.52 nm	f=0.0908	
152 ->159	0.13816				
154 ->157	0.64161				
Excited State 8:	Singlet-A	2.7216 eV	455.55 nm	f=0.0007	
154 ->158	0.67516				
154 ->160	-0.14280				
154 ->161	-0.11427				
Excited State 9:	Singlet-A	2.7680 eV	447.91 nm	f=0.0032	
154 ->158	0.14145				
154 ->160	0.67412				
Excited State 10:	Singlet-A	2.7749 eV	446.80 nm	f=0.0093	
152 ->156	-0.14738				
152 ->157	0.21611				
152 ->162	0.12943				
153 ->155	-0.11891				
154 ->159	0.59691				
Excited State 11:	Singlet-A	2.8171 eV	440.11 nm	f=0.0003	
153 ->157	0.68951				
Excited State 12:	Singlet-A	2.9252 eV	423.85 nm	f=0.0000	
153 ->159	0.69104				
Excited State 13:	Singlet-A	3.0951 eV	400.58 nm	f=0.0782	
152 ->157	0.25376				
153 ->158	0.54667				
153 ->160	-0.30943				
153 ->161	-0.10790				
Excited State 14:	Singlet-A	3.1204 eV	397.33 nm	f=0.0291	
152 ->157	0.38038				
153 ->158	0.11196				
153 ->160	0.53906				
Excited State 15:	Singlet-A	3.1303 eV	396.08 nm	f=0.0001	
151 ->155	0.11217				
154 ->158	0.11628				
154 ->161	0.67811				

Excited State 16:	Singlet-A	3.1410 eV	394.73 nm	f=0.0118
152 ->157	0.41370			
152 ->159	0.11559			
152 ->160	0.11402			
153 ->158	-0.34613			
153 ->160	-0.28108			
153 ->161	0.17323			
154 ->159	-0.10492			
Excited State 17:	Singlet-A	3.1487 eV	393.76 nm	f=0.0003
150 ->155	0.29894			
151 ->155	0.59782			
154 ->155	-0.10923			
154 ->161	-0.12862			
Excited State 18:	Singlet-A	3.1516 eV	393.40 nm	f=0.0875
152 ->159	0.65153			
153 ->164	-0.11456			
154 ->157	-0.10990			
Excited State 19:	Singlet-A	3.1947 eV	388.09 nm	f=0.0002
154 ->162	0.67167			
Excited State 20:	Singlet-A	3.3098 eV	374.59 nm	f=0.0926
147 ->155	0.12747			
150 ->155	-0.11435			
152 ->158	0.64762			
152 ->161	-0.11447			
153 ->160	-0.10498			