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Blue Light Emitting Electrochemical Cells Incorporating Triazole-based Luminophores

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Supporting Information

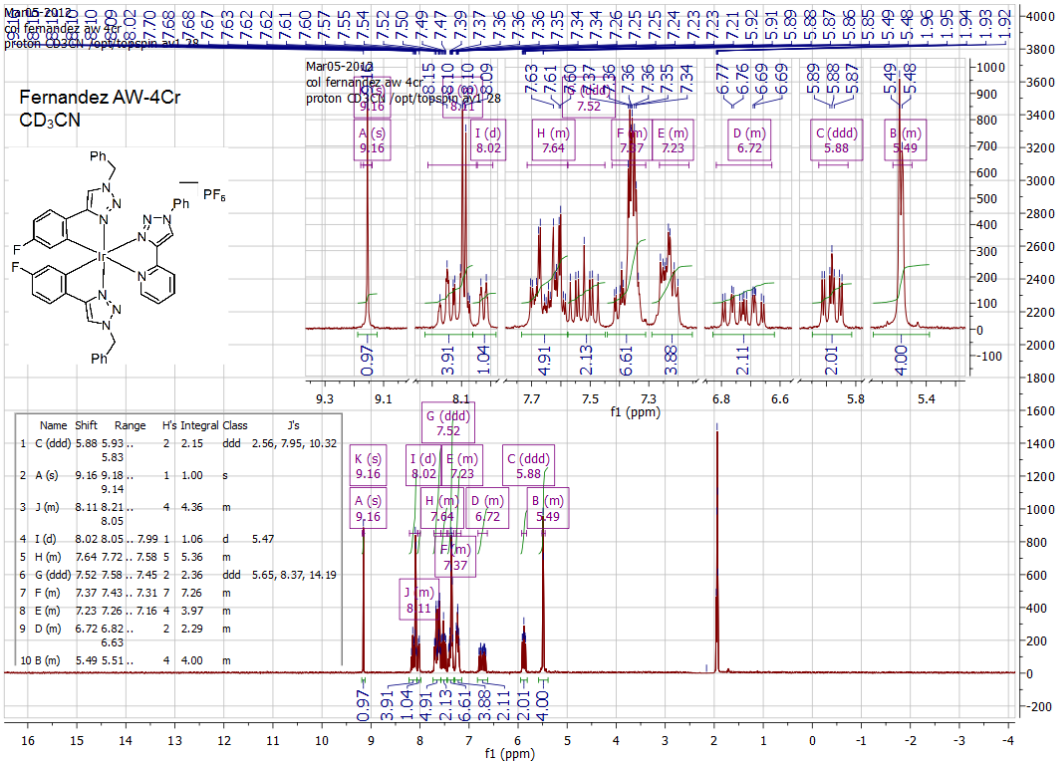
^{1}H and ^{19}F[^{1}H] NMR spectra

Cyclic Voltammetry

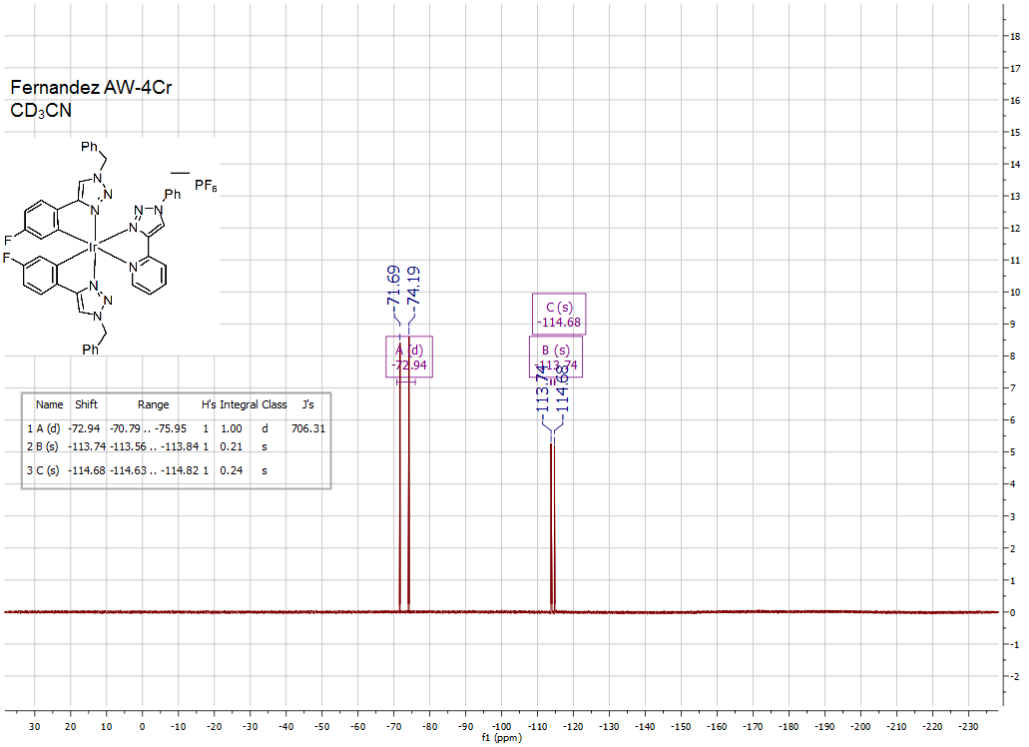
Additional Photophysical Spectra

Calculations

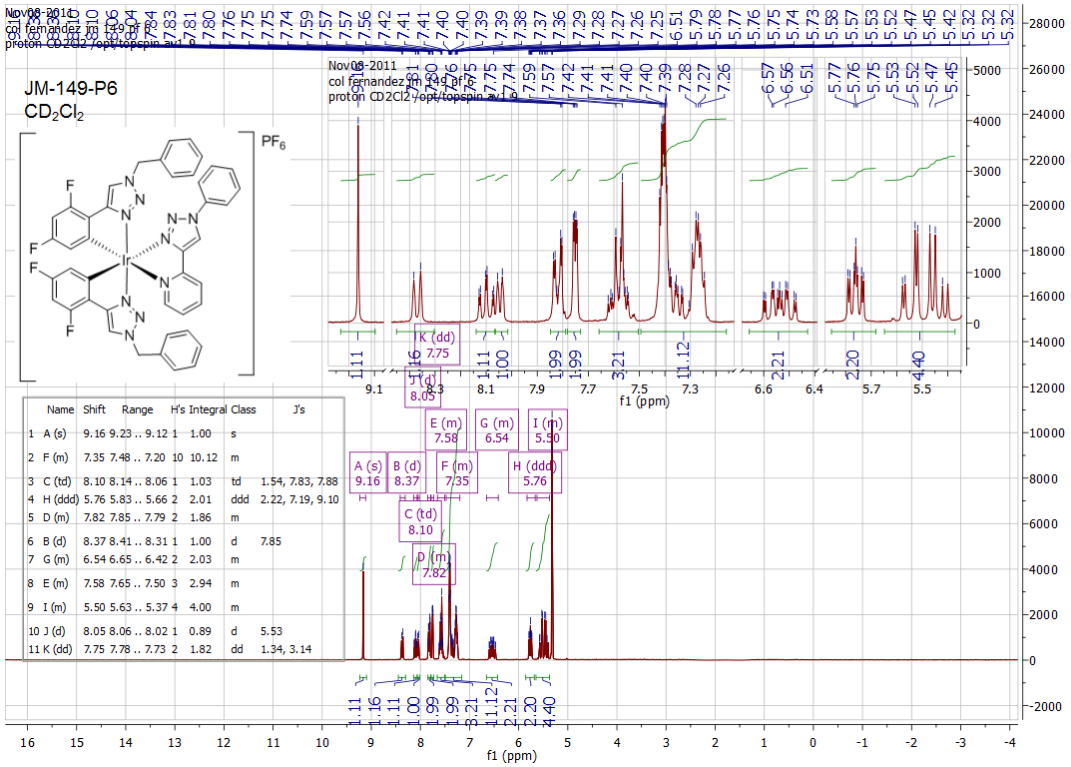
^{1}H NMR spectra Complex 1a [Ir(Fphtl)$_2$(PytlPh)]$^{+}$PF$_6^{-}$



^{19}F{^{1}H} spectra Complex 1a [Ir(Fphtl)$_2$(PytlPh)]$^{+}$PF$_6^{-}$

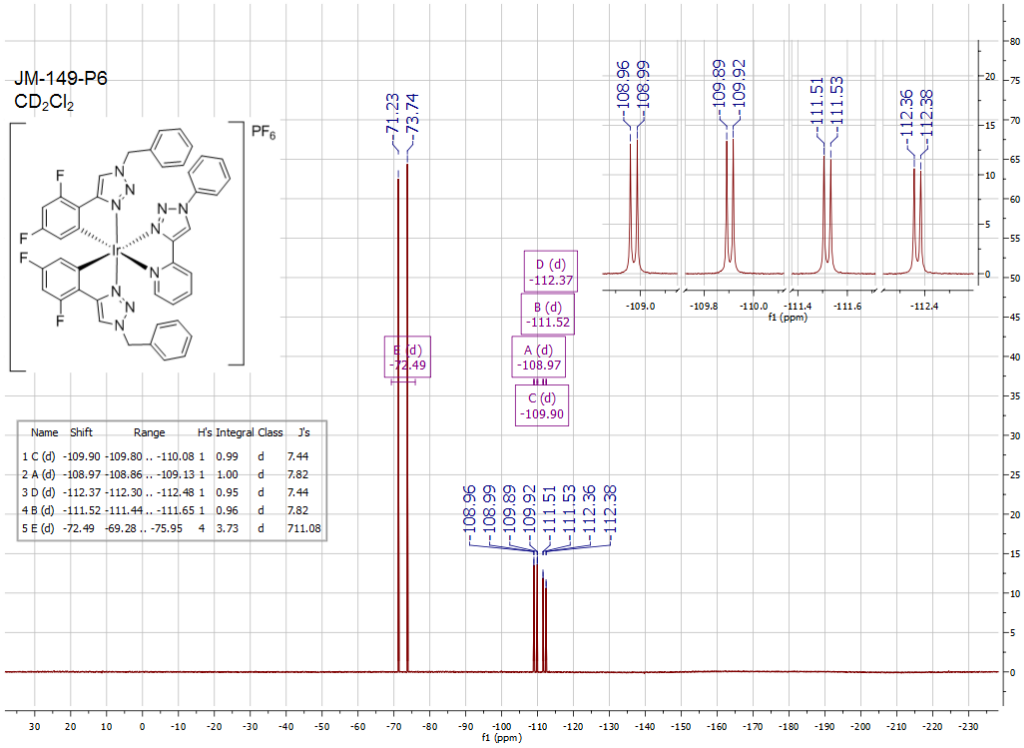


^{1}H NMR spectra Complex 1b [Ir(dFphtl)$_2$(PytlPh)]$^{+}$PF$_6^{-}$



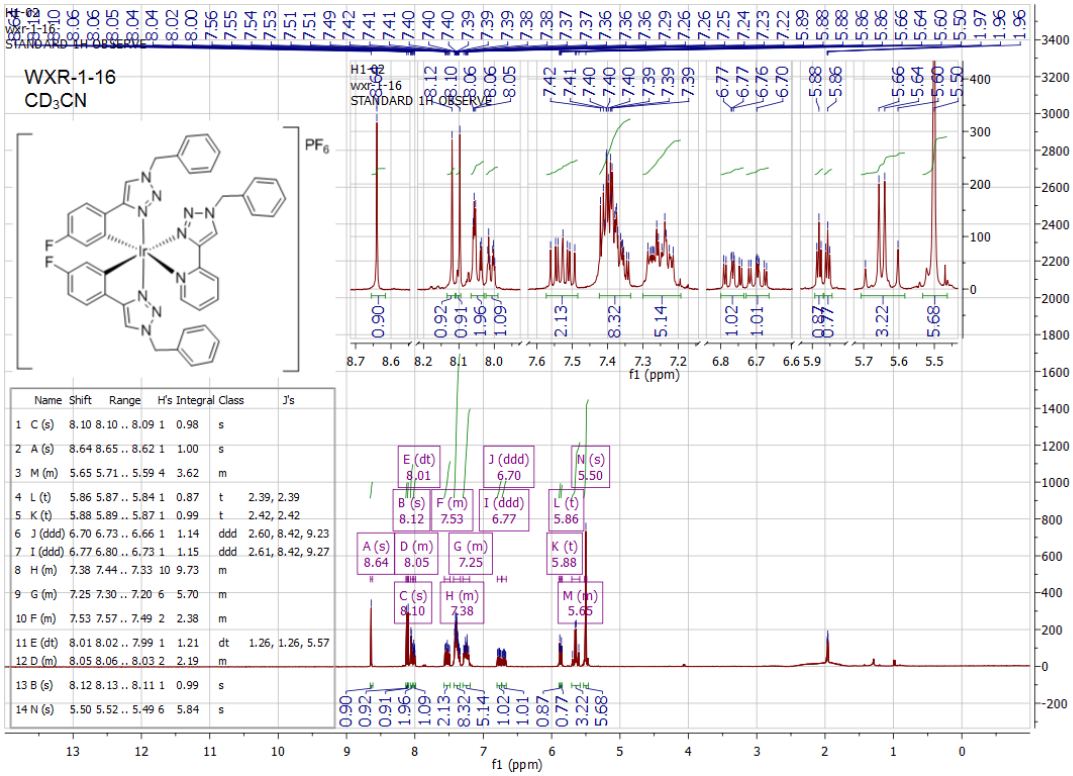
	Name	Shift	Range	H's	Integral	Class	J's
1	A (s)	9.16	9.23 .. 9.12	1	1.00	s	
2	F (m)	7.35	7.48 .. 7.20	10	10.12	m	
3	C (td)	8.10	8.14 .. 8.06	1	1.03	td	1.54, 7.83, 7.88
4	H (ddd)	5.76	5.83 .. 5.66	2	2.01	ddd	2.22, 7.19, 9.10
5	D (m)	7.82	7.85 .. 7.79	2	1.86	m	
6	B (d)	8.37	8.41 .. 8.31	1	1.00	d	7.85
7	G (m)	6.54	6.65 .. 6.42	2	2.03	m	
8	E (m)	7.58	7.65 .. 7.50	3	2.94	m	
9	I (m)	5.50	5.63 .. 5.37	4	4.00	m	
10	J (d)	8.05	8.06 .. 8.02	1	0.89	d	5.53
11	K (dd)	7.75	7.78 .. 7.73	2	1.82	dd	1.34, 3.14

^{19}F{^{1}H} spectra Complex 1b [Ir(dFphtl)$_2$(PytlPh)]$^{+}$PF$_6^{-}$

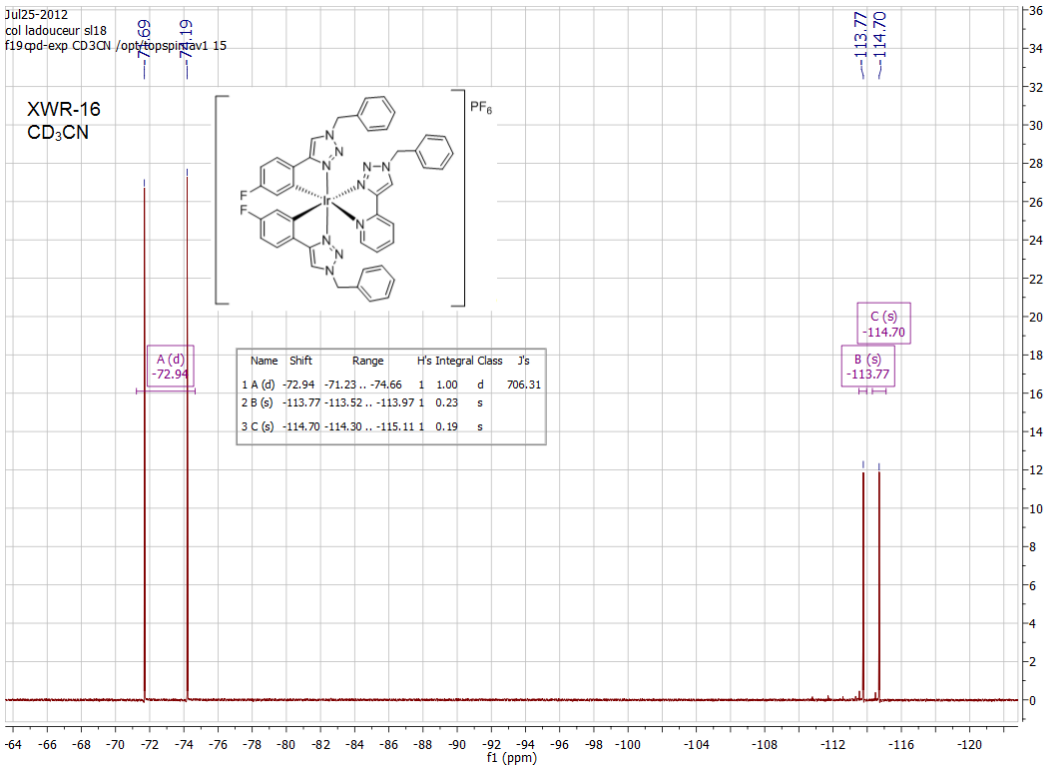


	Name	Shift	Range	H's	Integral	Class	J's
1	C (d)	-109.90	-109.80 .. -110.08	1	0.99	d	7.44
2	A (d)	-108.97	-108.86 .. -109.13	1	1.00	d	7.82
3	D (d)	-112.37	-112.30 .. -112.48	1	0.95	d	7.44
4	B (d)	-111.52	-111.44 .. -111.65	1	0.96	d	7.82
5	E (d)	-72.49	-69.28 .. -75.95	4	3.73	d	711.08

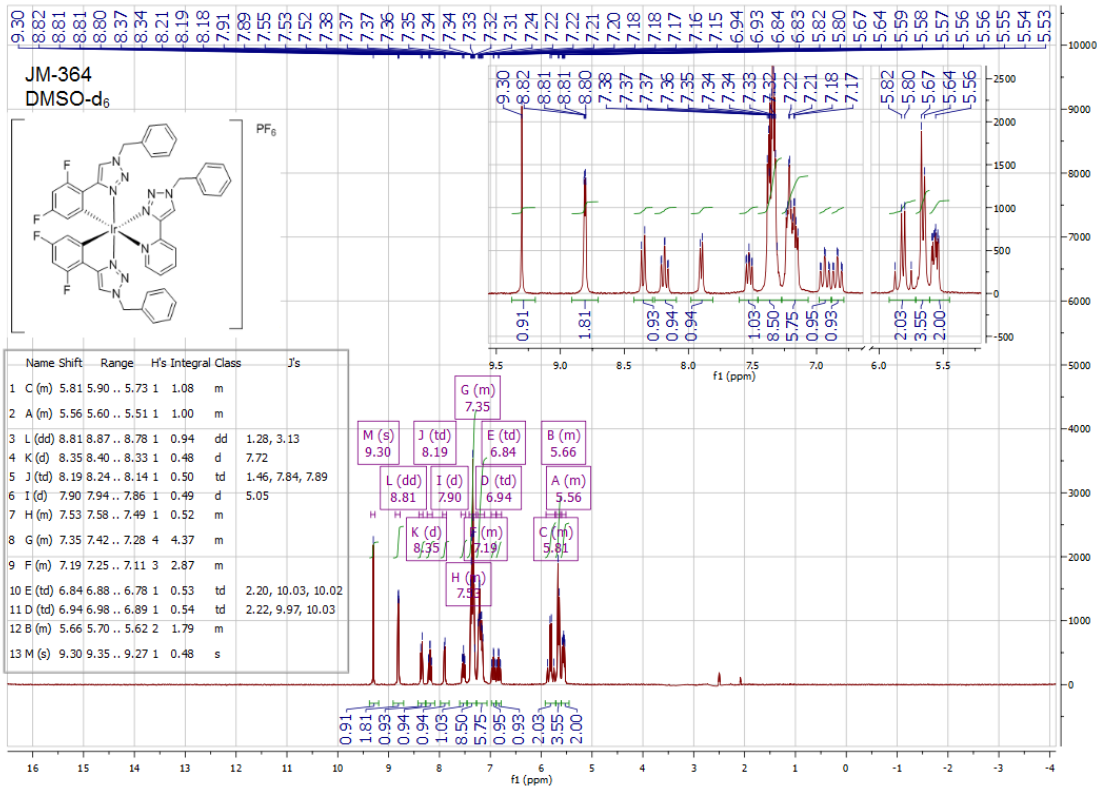
^{1}H NMR spectra Complex 2a [Ir(Fphtl)$_2$(PytlBn)]$^{+}$PF$_6^{-}$



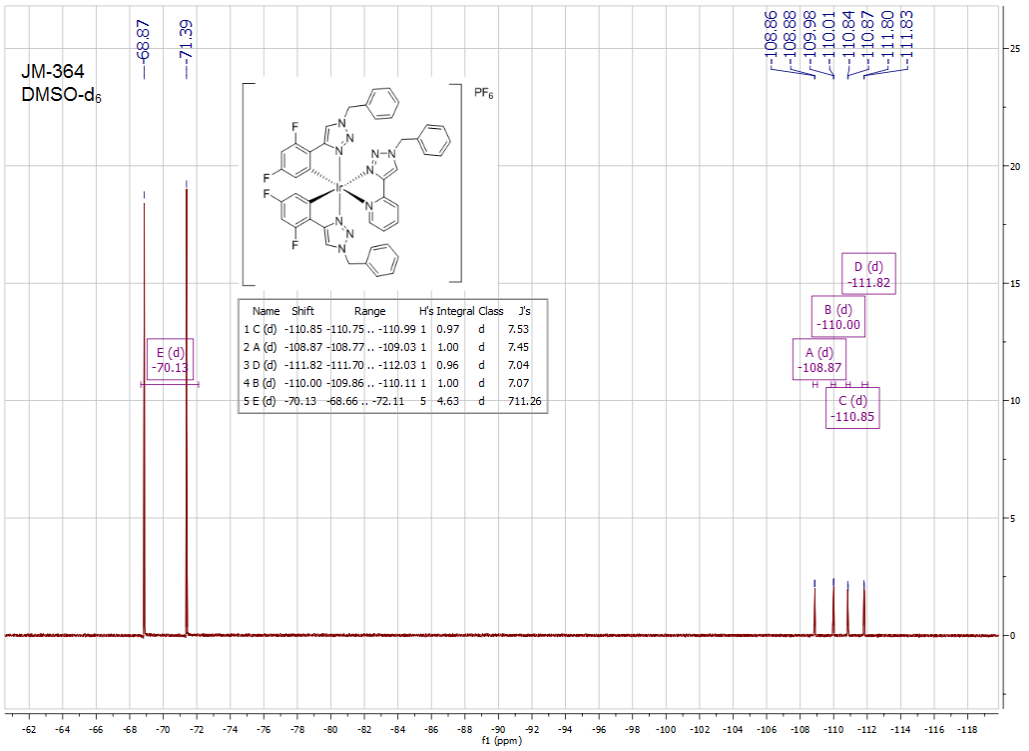
^{19}F {^{1}H} NMR spectra Complex 2a [Ir(Fphtl)$_2$(PytlBn)]$^{+}$PF$_6^{-}$



^{1}H NMR spectra Complex 2b [Ir(dFphtl)$_2$(PytlBn)]$^{+}$PF$_6^{-}$



^{19}F {^{1}H} NMR spectra Complex 2b [Ir(dFphtl)$_2$(PytlBn)]$^{+}$PF$_6^{-}$



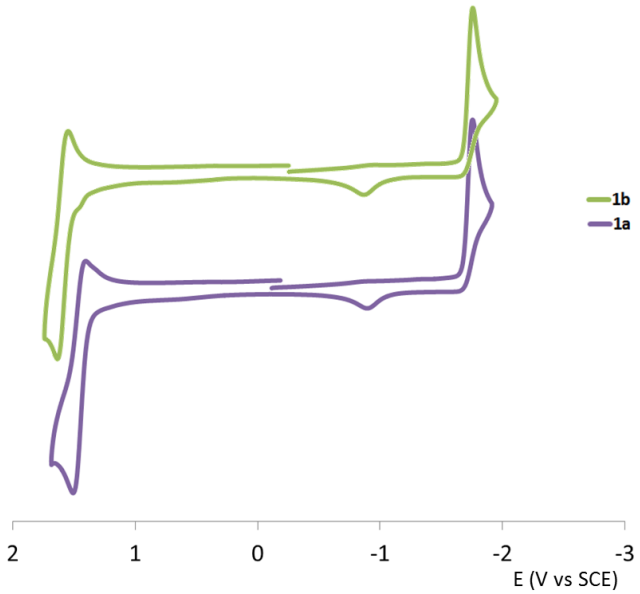


Figure S1: Cyclic Voltammetry of Complexes **1a-b**

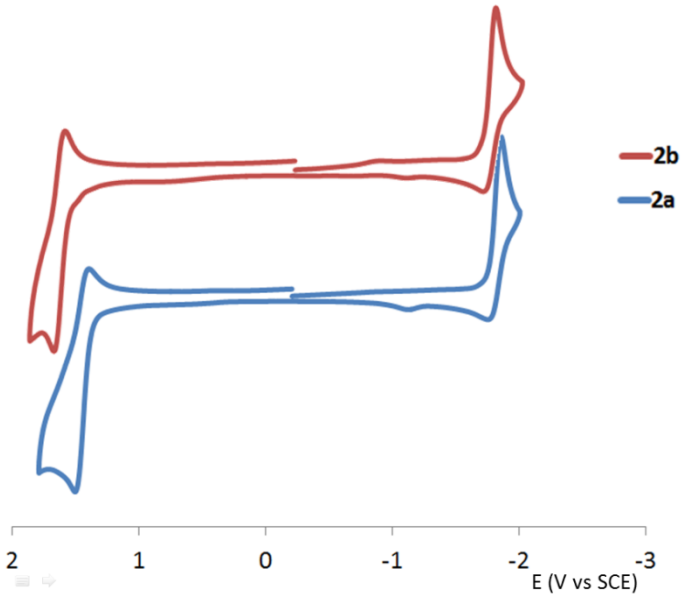


Figure S2: Cyclic Voltammetry of Complexes **2a-b**

Additional Photophysical Data

Figure S3: Photophysical data for Complex **1a** $[Ir(Fphtl)_2(PytlPh)]^+PF_6^-$

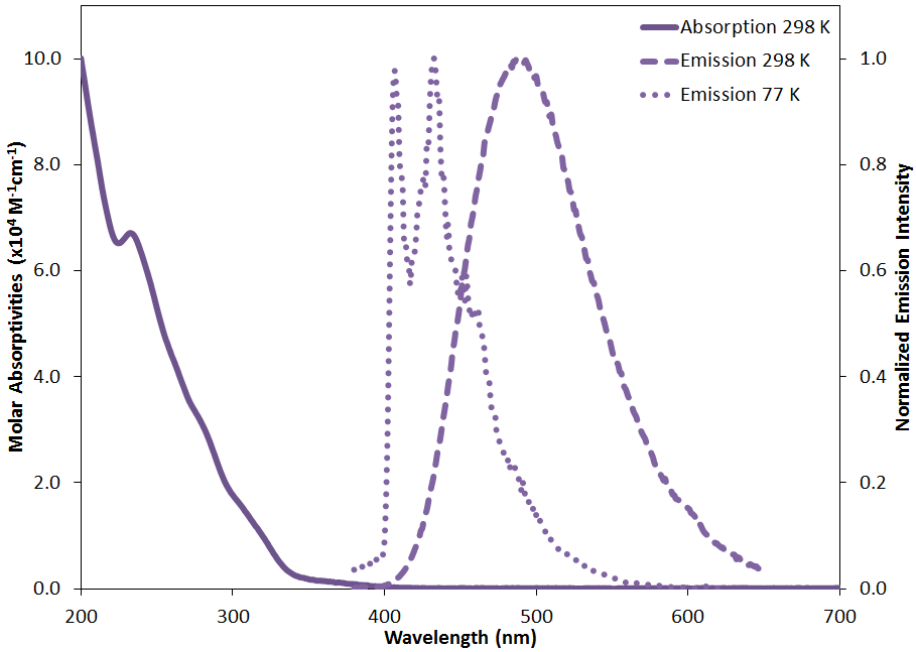


Figure S4: Photophysical data for Complex **1b** $[Ir(dFphtl)_2(PytlPh)]^+PF_6^-$

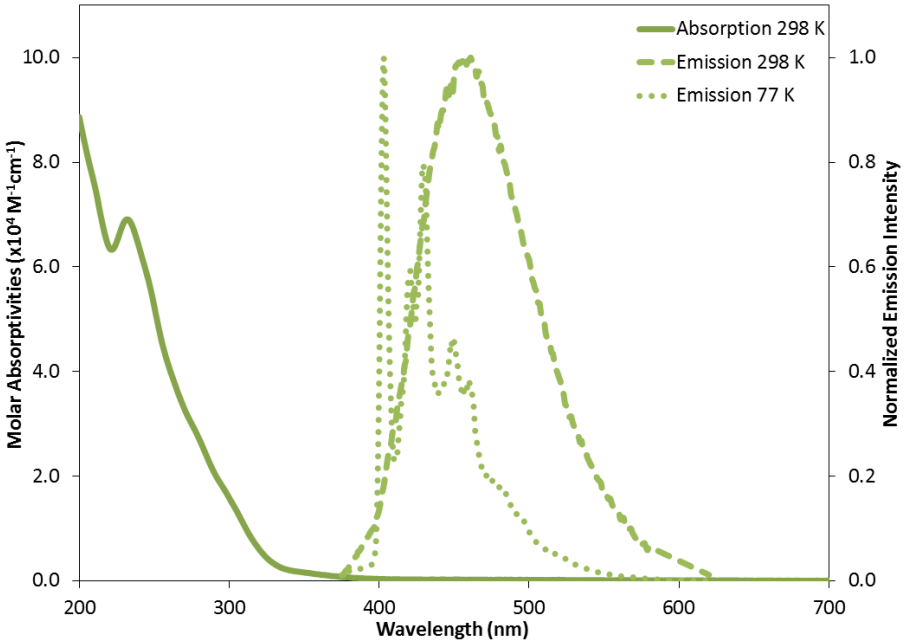


Figure S5: Photophysical data for Complex **2a** $[Ir(Fphtl)_2(PytlBn)]^+PF_6^-$

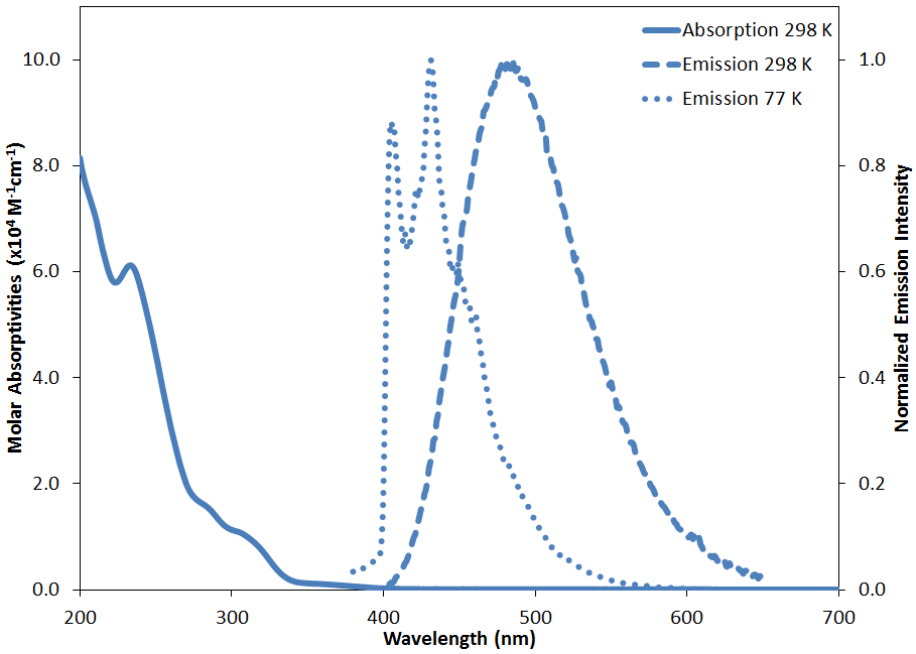


Figure S6: Photophysical data for Complex **2b** $[Ir(dFphtl)_2(PytlBn)]^+PF_6^-$

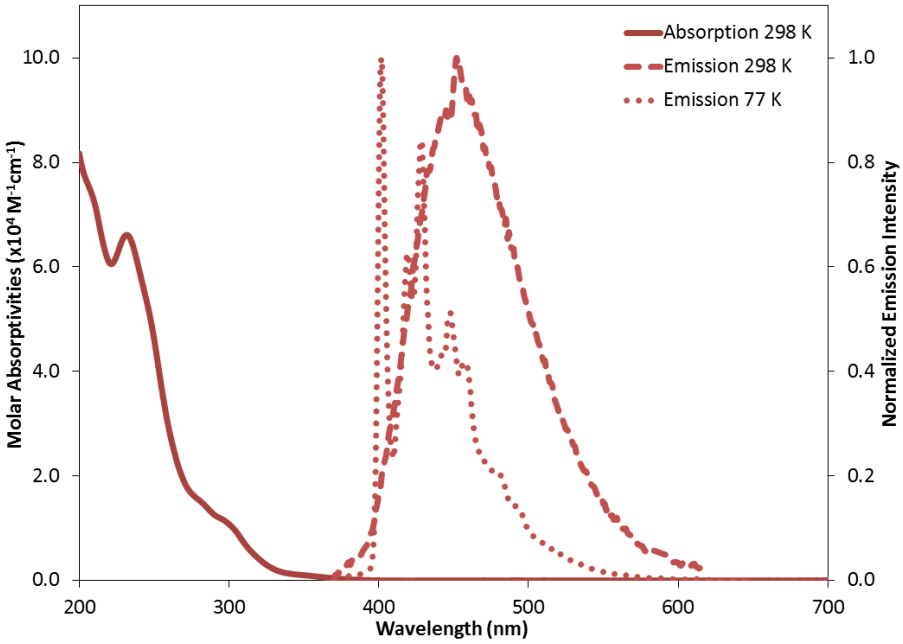


Figure S7: Emission Spectra of Powdered Samples of complexes **1a-b** and **2a-b**

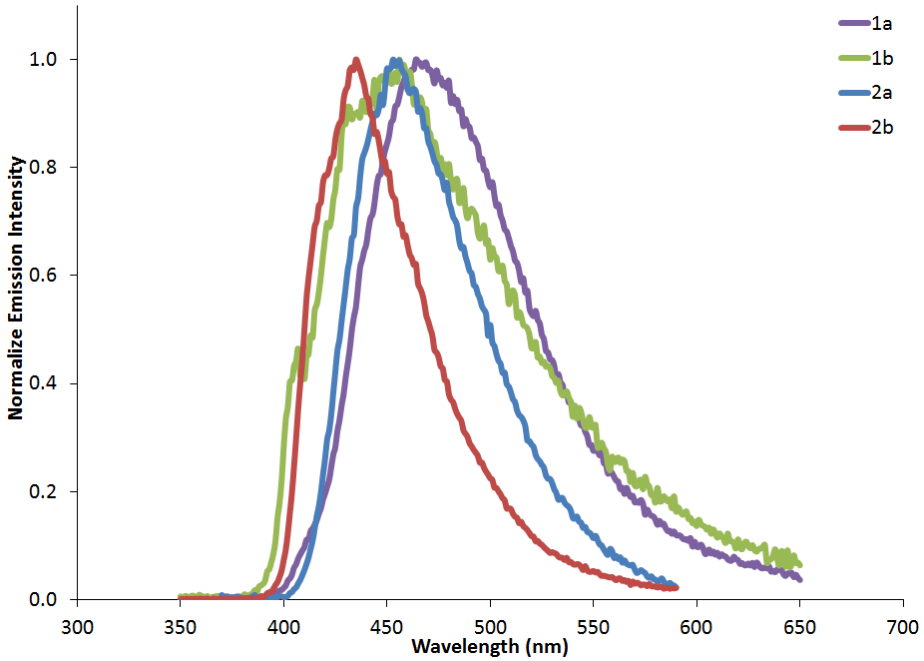


Figure S8: Emission Spectra of Thin films of Complex **1a** $[Ir(Fphtl)_2(PytlPh)]^+PF_6^-$

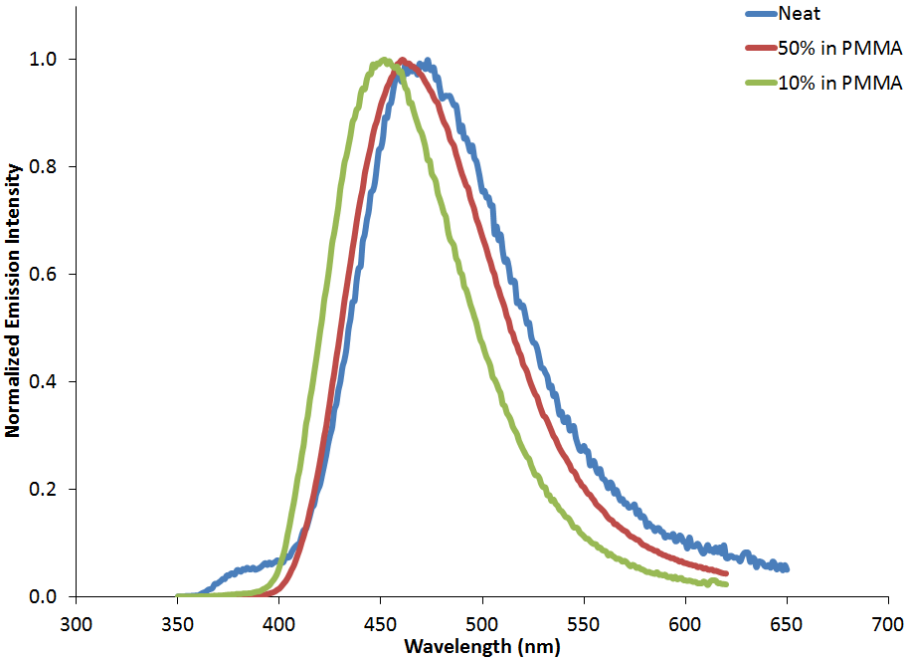


Figure S9: Emission spectra of Thin films of Complex **1b** $[Ir(dFphtl)_2(PytlPh)]^+PF_6^-$

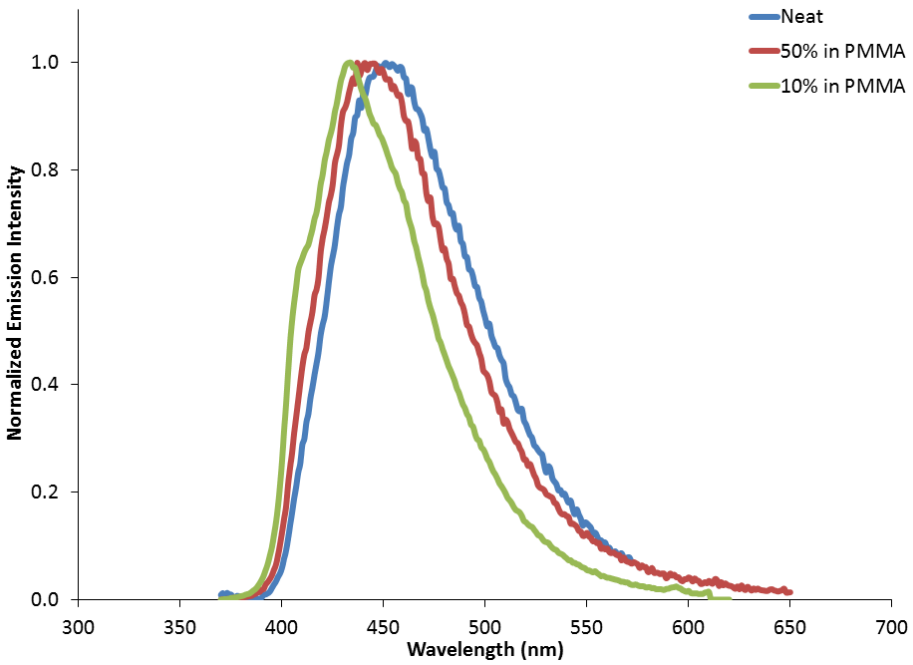


Figure S10: Emission spectra of Thin films of Complex **2a** $[Ir(Fphtl)_2(PytlBn)]^+PF_6^-$

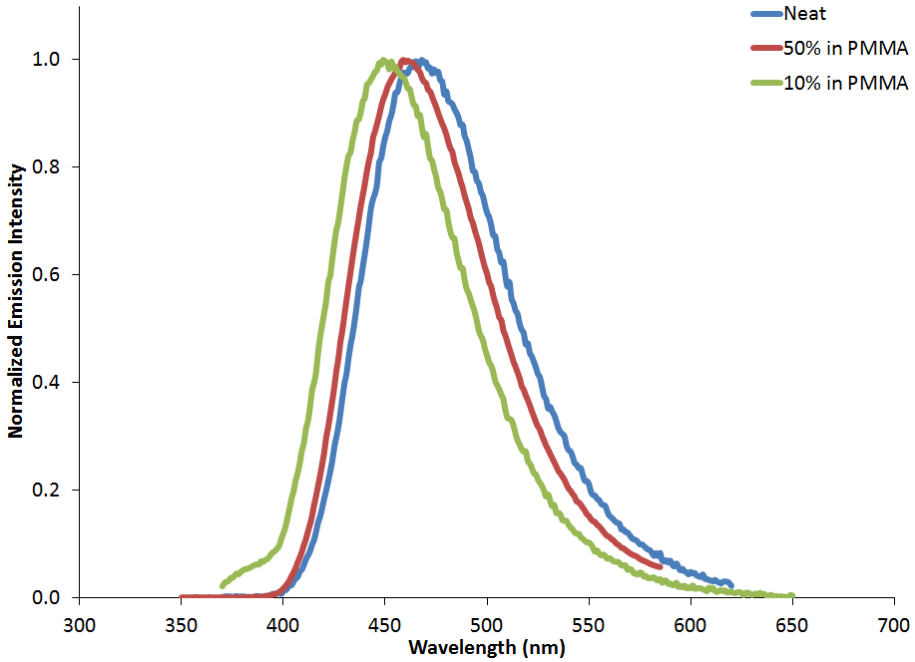
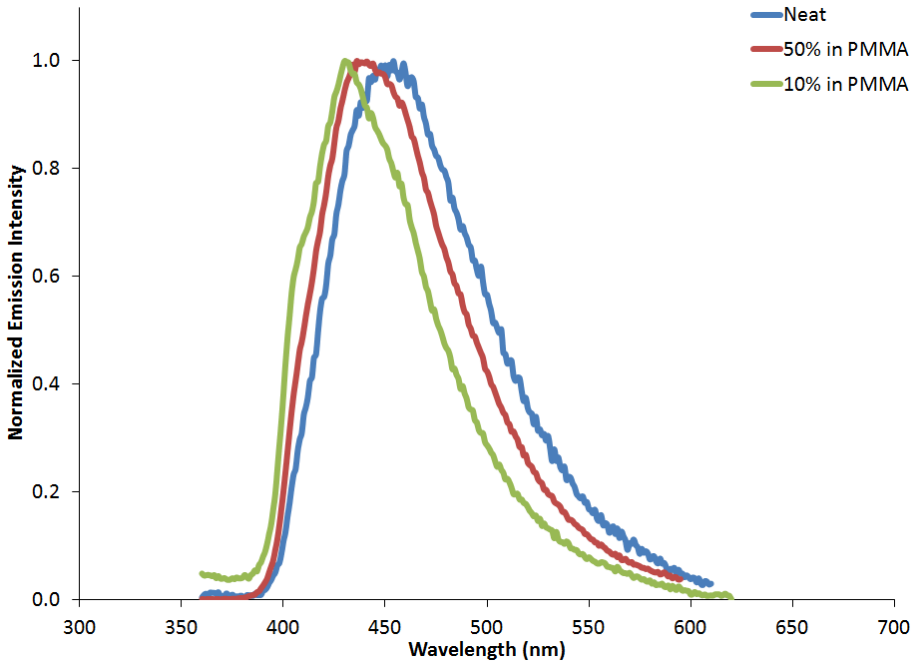


Figure S11: Emission spectra of Thin films of Complex **2b** $[Ir(dFphtl)_2(PytlBn)]^+PF_6^-$



Calculations

Table S1: Selected bond and angle distance in complexes 1a-b

Complexes	1a						1b					
Structural Parameters	HOMO (S_0)			HSOMO (T_1)			HOMO (S_0)			HSOMO (T_1)		
	Bond Distance (Å)		Average (Å)	Bond Distance (Å)		Average (Å)	Bond Distance (Å)		Average (Å)	Bond Distance (Å)		Average (Å)
Ir-N_{py} (pytl)	2.212		2.212	2.177		2.177	2.204		2.204	2.156		2.156
Ir-N_{tl} (pytl)	2.156		2.156	2.151		2.151	2.149		2.149	2.142		2.142
Ir-N (phtl)	2.043	2.042	2.043	2.049	2.041	2.045	2.048	2.048	2.048	2.050	2.045	2.048
Ir-C (phtl)	2.043	2.045	2.044	2.028	2.010	2.019	2.046	2.048	2.047	2.057	2.046	2.051
C_{ph}-C_{tl} (phtl)	1.457	1.458	1.458	1.453	1.452	1.453	1.446	1.446	1.446	1.445	1.446	1.445
	Bond Angle (°)		Average (°)	Bond Angle (°)		Average (°)	Bond Angle (°)		Average (°)	Bond Angle (°)		Average (°)
N-Ir-N (pytl)	75.8		75.8	75.9		75.9	76.0		76.0	77.4		77.4
C-Ir-N (phtl)	79.9	79.8	79.9	80.4	80.6	80.5	80.4	80.3	80.4	80.3	80.4	80.4

Table S2: Selected bond and angle distance in complexes 2a-b

Complexes	2a						2b					
Structural Parameters	HOMO (S_0)			HSOMO (T_1)			HOMO (S_0)			HSOMO (T_1)		
	Bond Distance (Å)		Average (Å)	Bond Distance (Å)		Average (Å)	Bond Distance (Å)		Average (Å)	Bond Distance (Å)		Average (Å)
Ir-N_{py} (pytl)	2.215		2.215	2.178		2.178	2.203		2.203	2.141		2.141
Ir-N_{tl} (pytl)	2.160		2.160	2.148		2.148	2.147		2.147	2.152		2.152
Ir-N (phtl)	2.038	2.040	2.039	2.045	2.041	2.043	2.046	2.048	2.047	2.049	2.044	2.047
Ir-C (phtl)	2.041	2.044	2.042	2.022	2.010	2.016	2.048	2.046	2.047	2.057	2.046	2.051
C_{ph}-C_{tl} (phtl)	1.459	1.458	1.459	1.454	1.453	1.453	1.446	1.446	1.446	1.445	1.444	1.445
	Bond Angle (°)		Average (°)	Bond Angle (°)		Average (°)	Bond Angle (°)		Average (°)	Bond Angle (°)		Average (°)
N-Ir-N (pytl)	75.7		75.7	75.8		75.8	76.0		76.0	77.4		77.4
C-Ir-N (phtl)	79.7	79.6	79.7	80.5	80.3	80.4	80.4	80.3	80.4	80.4	80.4	80.4

Figure S12: Quantification of Selected MOs of Complex **1a**

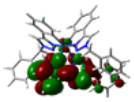
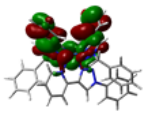
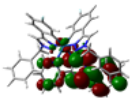
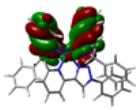
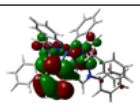
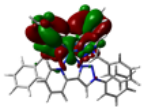
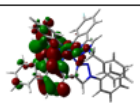
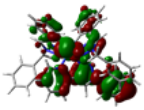
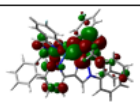
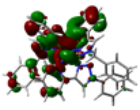
Orbitals Energy (eV)	Molecular sections	Contribution (%)	Visualization	Orbitals Energy (eV)	Molecular sections	Contribution (%)	Visualization
LUMO -2.06	Ir Fphtl pytlPh	1.5% 1.1% 97.3%		HOMO -5.96	Ir Fphtl pytlPh	33.4% 63.3% 3.3%	
LUMO+1 -1.89	Ir Fphtl pytlPh	4.3% 3.6% 92.0%		HOMO-1 -6.29	Ir Fphtl pytlPh	4.3% 94.9% 0.8%	
LUMO+2 -1.37	Ir Fphtl pytlPh	3.0% 24.6% 72.4%		HOMO-2 -6.63	Ir Fphtl pytlPh	23.1% 74.0% 3.0%	
LUMO+3 -1.28	Ir Fphtl pytlPh	7.0% 76.0% 16.9%		HOMO-3 -6.85	Ir Fphtl pytlPh	44.8% 22.9% 32.2%	
LUMO+4 -1.26	Ir Fphtl pytlPh	7.3% 85.9% 6.8%		HOMO-4 -6.94	Ir Fphtl pytlPh	49.2% 42.0% 8.8%	

Figure S13: Quantification of Selected MOs of Complex **1b**

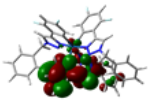
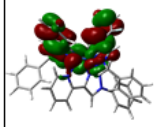
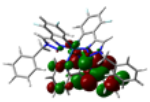
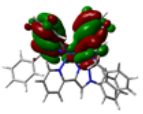
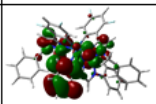
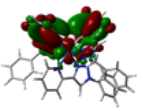
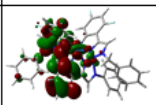
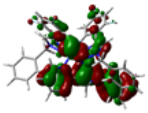
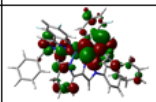
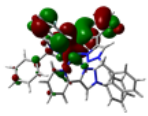
Orbitals Energy (eV)	Molecular sections	Contribution (%)	Visualization	Orbitals Energy (eV)	Molecular sections	Contribution (%)	Visualization
LUMO -2.1	Ir dFphtl pytlPh	1.6% 1.2% 97.1%		HOMO -6.17	Ir dFphtl pytlPh	32.8% 64.1% 3.1%	
LUMO+1 -1.94	Ir dFphtl pytlPh	4.2% 3.8% 92.0%		HOMO-1 -6.44	Ir dFphtl pytlPh	4.6% 94.7% 0.7%	
LUMO+2 -1.41	Ir dFphtl pytlPh	4.0% 40.5% 55.5%		HOMO-2 -6.65	Ir dFphtl pytlPh	17.6% 79.8% 2.6%	
LUMO+3 -1.36	Ir dFphtl pytlPh	6.4% 61.3% 32.3%		HOMO-3 -6.93	Ir dFphtl pytlPh	36.4% 19.8% 43.8%	
LUMO+4 -1.32	Ir dFphtl pytlPh	7.4% 85.1% 7.5%		HOMO-4 -7.03	Ir dFphtl pytlPh	14.6% 80.6% 4.7%	

Figure S14: Quantification of Selected MOs of Complex **2a**

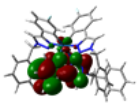
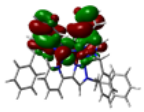
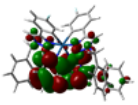
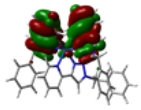
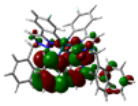
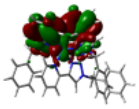
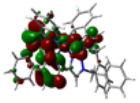
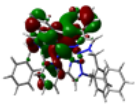
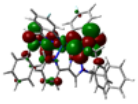
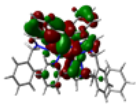
Orbitals Energy (eV)	Molecular sections	Contribution (%)	Visualization	Orbitals Energy (eV)	Molecular sections	Contribution (%)	Visualization
LUMO -1.95	Ir Fphtl pytlBn	2.6% 1.8% 95.6%		HOMO -5.75	Ir Fphtl pytlBn	33.3% 63.5% 3.2%	
LUMO+1 -1.41	Ir Fphtl pytlBn	3.7% 12.0% 84.2%		HOMO-1 -6.09	Ir Fphtl pytlBn	3.5% 95.7% 0.7%	
LUMO+2 -1.23	Ir Fphtl pytlBn	3.2% 11.1% 85.7%		HOMO-2 -6.44	Ir Fphtl pytlBn	21.9% 75.6% 2.5%	
LUMO+3 -1.16	Ir Fphtl pytlBn	6.9% 78.0% 15.2%		HOMO-3 -6.76	Ir Fphtl pytlBn	46.1% 46.1% 7.8%	
LUMO+4 -1.15	Ir Fphtl pytlBn	7.7% 87.7% 4.6%		HOMO-4 -6.78	Ir Fphtl pytlBn	50.4% 38.1% 11.4%	

Figure S15: Quantification of Selected MOs of Complex **2b**

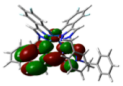
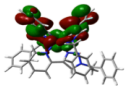
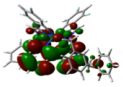
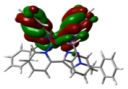
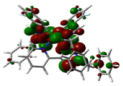
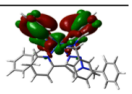
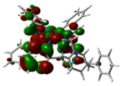
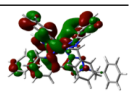
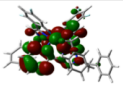
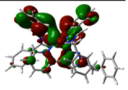
Orbitals Energy (eV)	Molecular sections	Contribution (%)	Visualization	Orbitals Energy (eV)	Molecular sections	Contribution (%)	Visualization
LUMO -2.05	Ir	2.7%		HOMO -6.14	Ir	32.9%	
	dFphtl	1.9%			dFphtl	64.1%	
	pytlBn	95.4%			pytlBn	3.0%	
LUMO+1 -1.49	Ir	3.9%		HOMO-1 -6.42	Ir	4.4%	
	dFphtl	19.7%			dFphtl	95.0%	
	pytlBn	76.4%			pytlBn	0.6%	
LUMO+2 -1.35	Ir	7.1%		HOMO-2 -6.63	Ir	17.6%	
	dFphtl	60.4%			dFphtl	80.4%	
	pytlBn	32.5%			pytlBn	2.0%	
LUMO+3 -1.32	Ir	6.6%		HOMO-3 -6.99	Ir	38.9%	
	dFphtl	58.6%			dFphtl	50.4%	
	pytlBn	34.8%			pytlBn	10.7%	
LUMO+4 -1.29	Ir	4.4%		HOMO-4 -7.01	Ir	31.3%	
	dFphtl	53.4%			dFphtl	55.6%	
	pytlBn	42.2%			pytlBn	13.1%	

Figure S16: Comparison of experimental and calculated absorption spectra of **1a**

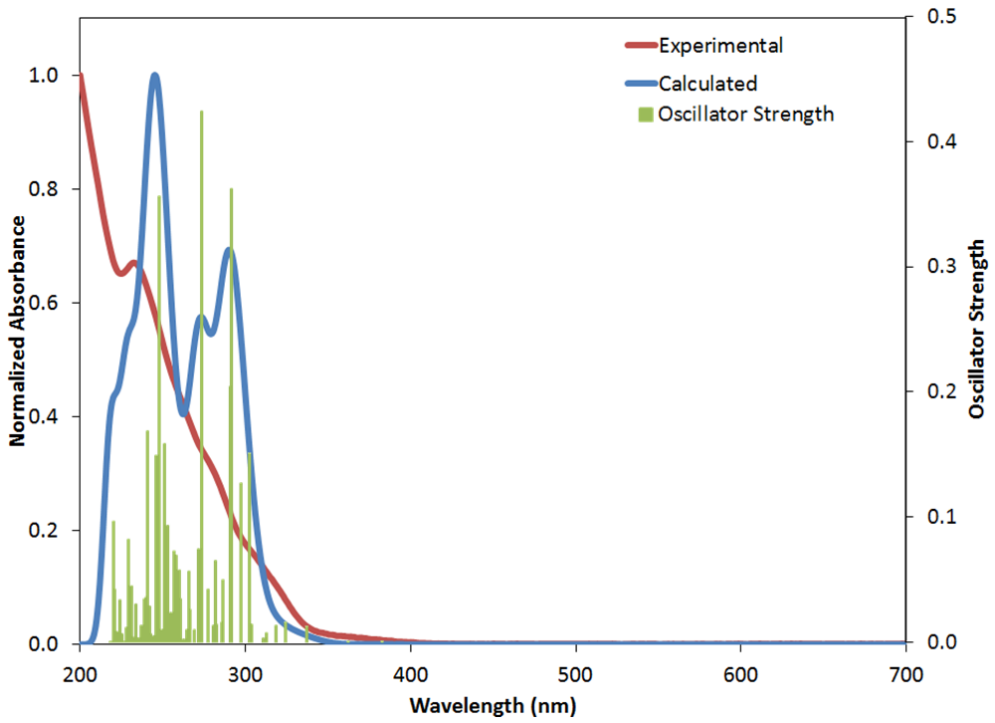


Figure S17: Comparison of experimental and calculated absorption spectra of **b**

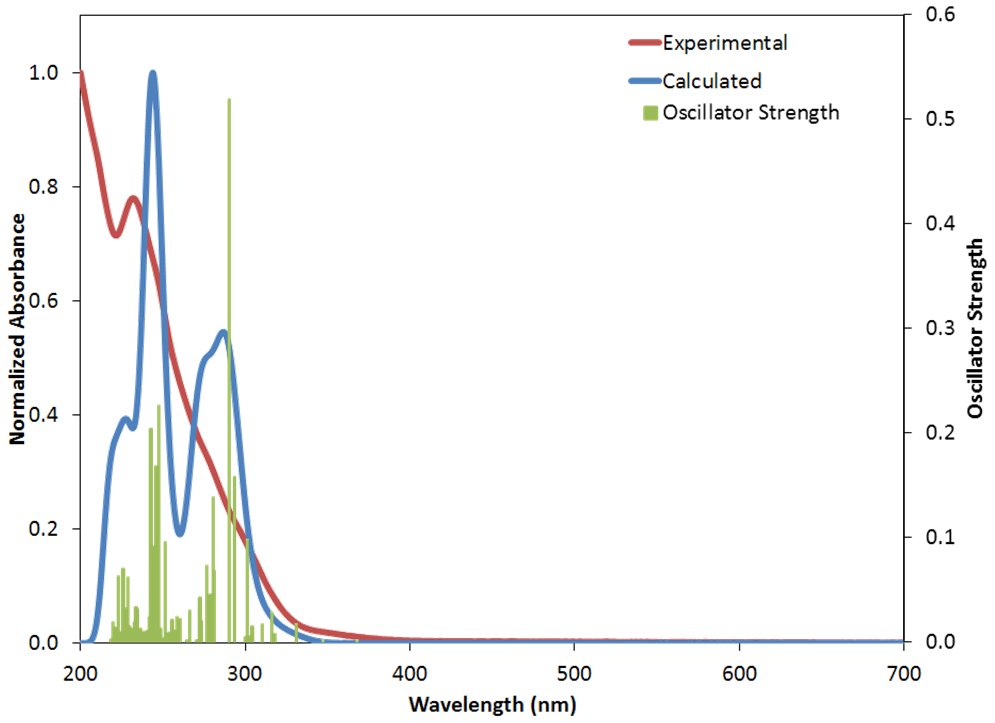


Figure S18: Comparison of experimental and calculated absorption spectra of **2a**

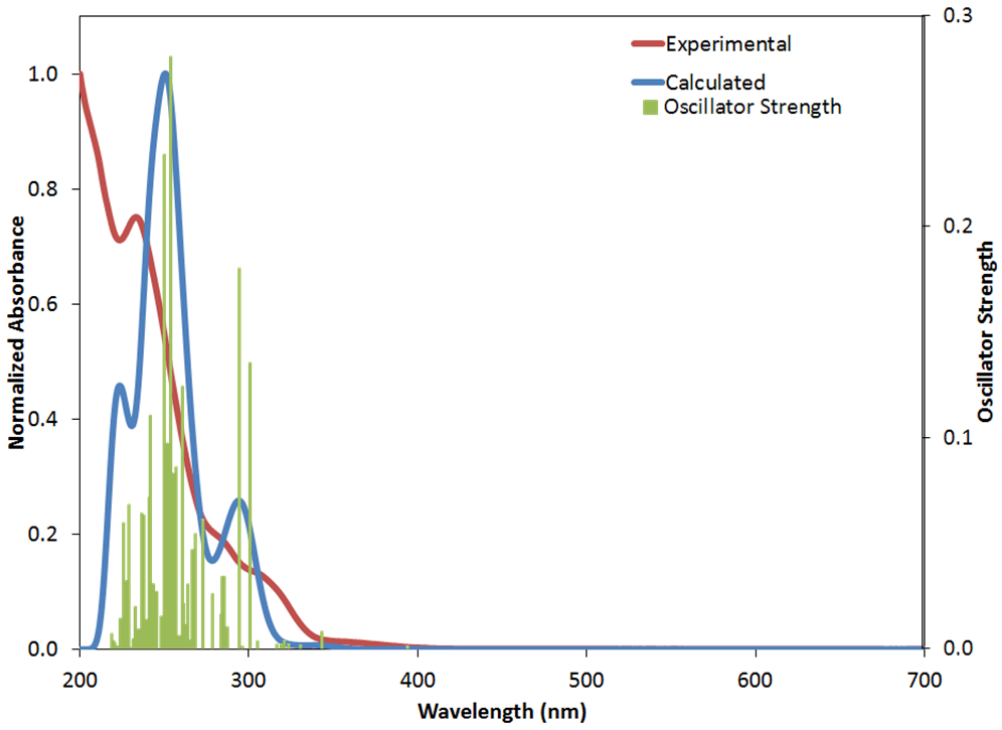


Figure S19: Comparison of experimental and calculated absorption spectra of **2b**

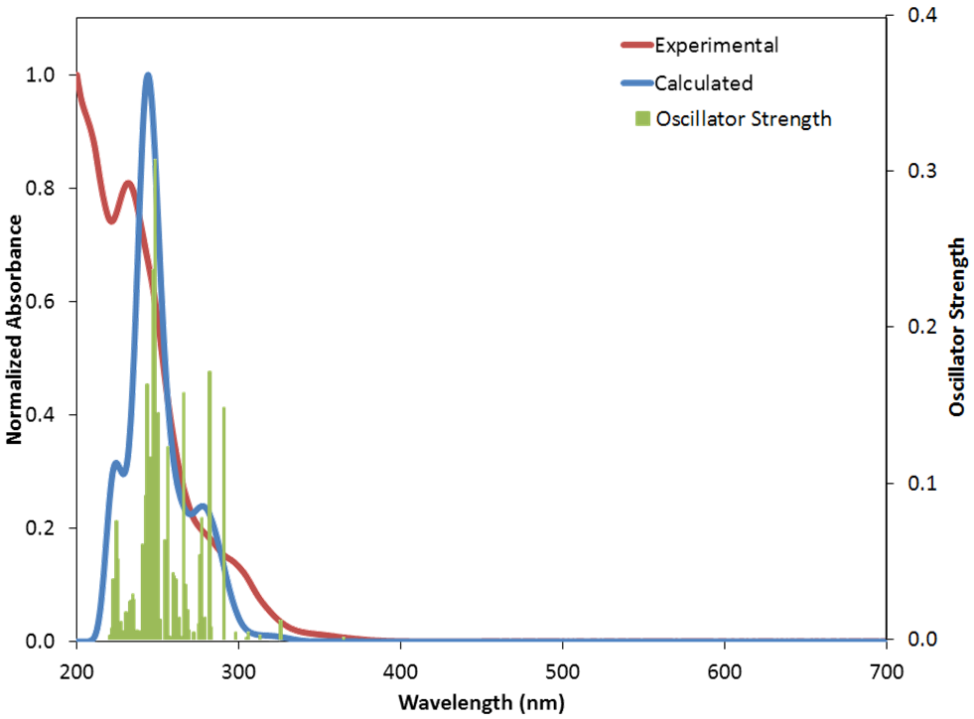


Figure S20: Dipole moment of S_1 and T_1 states of complex **1a**

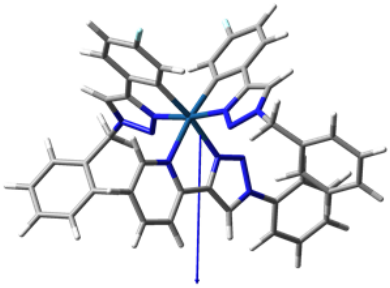
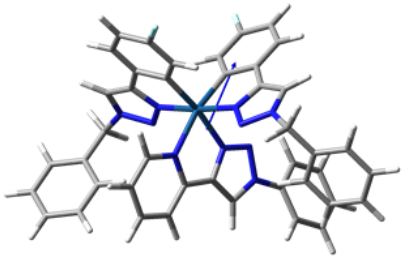
	Singlet State (S_0)	Triplet State (T_1)
		
Scaling Factor	0.5	1.03
Magnitude of dipole (db)	12.3089	3.0078

Figure S21: Dipole moment of S_1 and T_1 states of complex **1b**

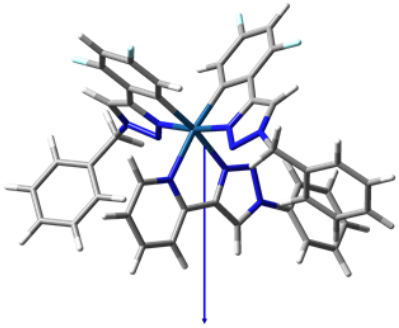
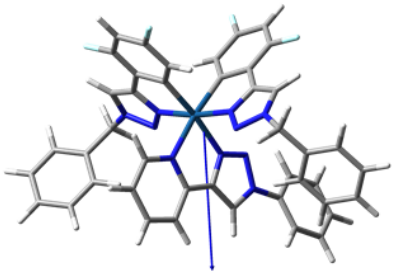
	Singlet State (S_0)	Triplet State (T_1)
		
Scaling Factor	0.5	0.5
Magnitude of dipole (db)	13.8456	11.6705

Figure S22: Dipole moment of S_1 and T_1 states of complex **2a**

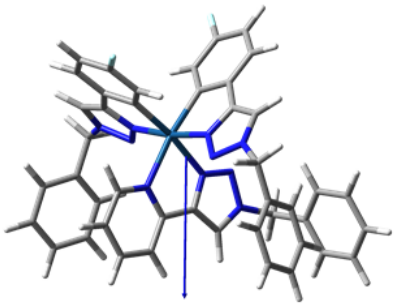
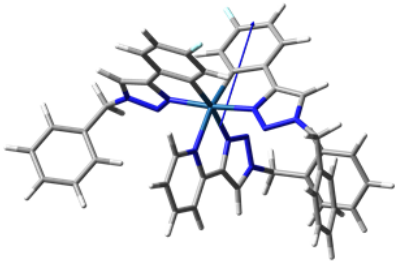
	Singlet State (S_0)	Triplet State (T_1)
		
Scaling Factor	0.5	1
Magnitude of dipole (db)	10.6174	4.9991

Figure S23: Dipole moment of S_1 and T_1 states of complex **2b**

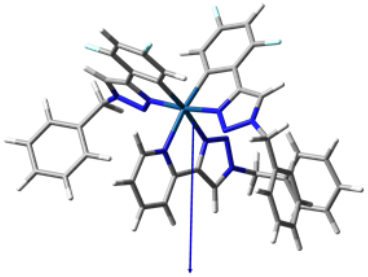
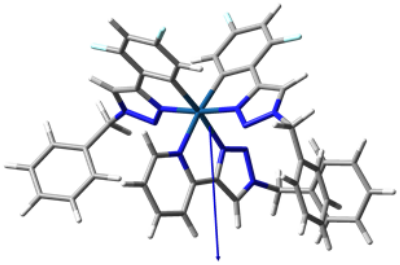
	Singlet State (S_0)	Triplet State (T_1)
		
Scaling Factor	0.5	0.5
Magnitude of dipole (db)	13.7904	11.3898

Table S3: TDDFT 100 lowest vertical singlet transition for complex **1a:**

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	26197.1	381.7	0.0004	Singlet-?Sym	HOMO->LUMO (78%), HOMO->L+1 (19%)
2	27727.9	360.6	0.0002	Singlet-?Sym	HOMO->LUMO (20%), HOMO->L+1 (78%)
3	29745.9	336.2	0.0124	Singlet-?Sym	H-1->LUMO (90%)
4	30996.1	322.6	0.0159	Singlet-?Sym	H-1->L+1 (88%)
5	31498.6	317.5	0.0056	Singlet-?Sym	HOMO->L+2 (36%), HOMO->L+3 (43%), HOMO->L+4 (11%)
6	31593.0	316.5	0.0130	Singlet-?Sym	H-3->LUMO (20%), H-2->LUMO (55%), H-2->L+1 (12%)
7	32136.6	311.2	0.0071	Singlet-?Sym	HOMO->L+2 (27%), HOMO->L+4 (67%)
8	32367.3	309.0	0.0032	Singlet-?Sym	HOMO->L+2 (33%), HOMO->L+3 (47%), HOMO->L+4 (15%)
9	33098.8	302.1	0.0141	Singlet-?Sym	H-3->LUMO (28%), H-3->L+1 (18%), H-2->LUMO (40%)
10	33246.4	300.8	0.1505	Singlet-?Sym	H-3->LUMO (37%), H-2->L+1 (51%)
11	33729.5	296.5	0.1270	Singlet-?Sym	H-4->LUMO (68%), H-2->L+1 (11%)
12	34471.6	290.1	0.3617	Singlet-?Sym	H-3->LUMO (11%), H-3->L+1 (63%), H-2->L+1 (11%)
13	34566.7	289.3	0.2041	Singlet-?Sym	HOMO->L+5 (86%)
14	35078.1	285.1	0.0493	Singlet-?Sym	H-4->LUMO (15%), H-4->L+1 (70%)
15	35230.5	283.8	0.0154	Singlet-?Sym	H-1->L+2 (76%), H-1->L+3 (13%)
16	35611.2	280.8	0.0137	Singlet-?Sym	H-1->L+4 (31%), HOMO->L+6 (49%)
17	35691.9	280.2	0.0652	Singlet-?Sym	H-1->L+3 (24%), H-1->L+4 (50%), HOMO->L+6 (14%)
18	35868.5	278.8	0.0129	Singlet-?Sym	H-1->L+3 (51%), HOMO->L+6 (24%)
19	36250.0	275.9	0.0424	Singlet-?Sym	H-5->LUMO (78%)
20	36709.0	272.4	0.4243	Singlet-?Sym	H-8->LUMO (13%), H-7->LUMO (33%), H-6->LUMO (25%)
21	36985.6	270.4	0.0741	Singlet-?Sym	H-2->L+2 (22%), H-2->L+3 (28%)
22	37492.9	266.7	0.0095	Singlet-?Sym	H-5->LUMO (10%), H-5->L+1 (61%)
23	37705.1	265.2	0.0256	Singlet-?Sym	H-4->L+3 (10%), H-2->L+3 (23%), H-2->L+4 (30%)
24	37826.1	264.4	0.0562	Singlet-?Sym	H-5->L+1 (14%), H-2->L+2 (28%), H-1->L+5 (14%)
25	37954.3	263.5	0.0127	Singlet-?Sym	H-1->L+5 (71%)
26	38060.8	262.7	0.0102	Singlet-?Sym	H-2->L+4 (12%), HOMO->L+7 (35%), HOMO->L+15 (10%)
27	38337.4	260.8	0.0022	Singlet-?Sym	H-7->LUMO (26%), H-6->LUMO (66%)
28	38635.8	258.8	0.0347	Singlet-?Sym	H-4->L+2 (10%), H-4->L+3 (12%), H-3->L+2 (18%), H-3->L+4 (10%)
29	38720.5	258.3	0.0002	Singlet-?Sym	H-8->LUMO (75%), H-7->LUMO (24%)
30	38769.7	257.9	0.0576	Singlet-?Sym	H-4->L+4 (13%), H-1->L+6 (61%)
31	38899.6	257.1	0.0399	Singlet-?Sym	H-6->L+1 (18%), H-3->L+4 (14%)
32	39115.7	255.7	0.0693	Singlet-?Sym	H-3->L+2 (10%), HOMO->L+12 (37%)
33	39220.6	255.0	0.0220	Singlet-?Sym	H-4->L+2 (12%), H-3->L+2 (32%), HOMO->L+12 (20%)
34	39264.1	254.7	0.0726	Singlet-?Sym	H-6->L+1 (22%), H-3->L+2 (14%), H-3->L+4 (25%), H-2->L+4 (10%)
35	39474.7	253.3	0.0027	Singlet-?Sym	H-6->L+1 (36%), H-3->L+3 (12%)
36	39540.0	252.9	0.0232	Singlet-?Sym	H-11->LUMO (26%), H-11->L+1 (42%)
37	39627.1	252.4	0.0037	Singlet-?Sym	H-9->LUMO (57%)
38	39675.5	252.0	0.0136	Singlet-?Sym	H-9->LUMO (33%), H-7->L+1 (15%)
39	39783.6	251.4	0.1046	Singlet-?Sym	H-7->L+1 (18%), H-4->L+2 (17%), H-4->L+4 (12%)
40	39906.2	250.6	0.0927	Singlet-?Sym	H-7->L+1 (18%), H-4->L+2 (10%), H-4->L+4 (10%), H-2->L+5 (21%)
41	39955.4	250.3	0.0036	Singlet-?Sym	H-8->L+1 (82%), H-7->L+1 (13%)
42	40025.5	249.8	0.0002	Singlet-?Sym	H-10->LUMO (96%)
43	40234.4	248.5	0.1580	Singlet-?Sym	H-3->L+3 (12%), HOMO->L+8 (15%), HOMO->L+9 (36%)
44	40249.0	248.5	0.0095	Singlet-?Sym	HOMO->L+8 (81%)
45	40618.4	246.2	0.3558	Singlet-?Sym	H-4->L+4 (10%), H-2->L+5 (31%), HOMO->L+9 (20%)
46	40933.7	244.3	0.0646	Singlet-?Sym	H-12->L+1 (12%), H-9->L+1 (63%)
47	41024.1	243.8	0.1489	Singlet-?Sym	H-12->LUMO (18%), H-12->L+1 (23%), H-9->L+1 (26%)
48	41091.0	243.4	0.0533	Singlet-?Sym	H-5->L+3 (10%), HOMO->L+15 (15%)
49	41168.4	242.9	0.0047	Singlet-?Sym	H-1->L+7 (33%)
50	41274.1	242.3	0.0798	Singlet-?Sym	H-2->L+6 (46%)

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
51	41339.4	241.9	0.0001	Singlet-?Sym	H-10->L+1 (94%)
52	41408.8	241.5	0.0062	Singlet-?Sym	H-11->LUMO (51%), H-11->L+1 (29%)
53	41586.2	240.5	0.0434	Singlet-?Sym	H-4->L+4 (10%), HOMO->L+15 (12%)
54	41670.9	240.0	0.0285	Singlet-?Sym	H-5->L+2 (23%), H-5->L+4 (20%)
55	41868.5	238.8	0.1687	Singlet-?Sym	H-5->L+4 (17%), H-3->L+5 (21%)
56	41983.9	238.2	0.0434	Singlet-?Sym	H-13->LUMO (25%), H-4->L+5 (19%)
57	42061.3	237.7	0.0365	Singlet-?Sym	H-5->L+4 (12%), H-4->L+5 (11%), H-3->L+5 (31%)
58	42120.2	237.4	0.0505	Singlet-?Sym	H-13->LUMO (39%), H-5->L+2 (12%), H-5->L+3 (13%)
59	42168.6	237.1	0.0195	Singlet-?Sym	HOMO->L+10 (58%)
60	42243.6	236.7	0.0342	Singlet-?Sym	H-4->L+5 (18%), HOMO->L+10 (23%)
61	42354.1	236.1	0.0316	Singlet-?Sym	H-4->L+6 (11%), H-1->L+7 (26%)
62	42373.4	236.0	0.0035	Singlet-?Sym	H-12->LUMO (38%), H-12->L+1 (33%)
63	42547.7	235.0	0.0135	Singlet-?Sym	H-6->L+2 (17%), H-6->L+3 (51%), HOMO->L+11 (10%)
64	42667.8	234.4	0.0027	Singlet-?Sym	HOMO->L+11 (78%)
65	42941.3	232.9	0.0018	Singlet-?Sym	H-1->L+8 (90%)
66	42979.2	232.7	0.0033	Singlet-?Sym	H-3->L+6 (36%), H-1->L+9 (22%)
67	43171.1	231.6	0.0300	Singlet-?Sym	H-5->L+5 (18%), H-4->L+6 (15%)
68	43241.3	231.3	0.0538	Singlet-?Sym	H-7->L+2 (24%), H-7->L+3 (10%), H-6->L+2 (10%), H-1->L+9 (14%)
69	43276.8	231.1	0.0544	Singlet-?Sym	H-5->L+5 (16%), H-4->L+6 (22%), H-3->L+6 (12%), H-2->L+6 (12%)
70	43324.4	230.8	0.0153	Singlet-?Sym	H-8->L+3 (21%), H-7->L+2 (16%), H-1->L+9 (18%)
71	43383.2	230.5	0.0043	Singlet-?Sym	H-8->L+2 (20%), H-8->L+3 (25%), H-1->L+9 (18%)
72	43433.3	230.2	0.0008	Singlet-?Sym	H-5->L+5 (11%), H-1->L+12 (41%)
73	43588.1	229.4	0.0902	Singlet-?Sym	H-7->L+3 (11%), H-7->L+4 (21%), H-6->L+4 (11%)
74	43738.1	228.6	0.0450	Singlet-?Sym	HOMO->L+13 (31%), HOMO->L+14 (24%)
75	43841.4	228.1	0.0897	Singlet-?Sym	H-9->L+4 (10%), H-7->L+3 (18%), H-7->L+4 (10%)
76	43897.0	227.8	0.0300	Singlet-?Sym	H-10->L+4 (14%), H-9->L+4 (38%)
77	44021.2	227.2	0.0816	Singlet-?Sym	H-5->L+6 (17%), H-4->L+6 (11%), HOMO->L+13 (17%), HOMO->L+16 (10%)
78	44197.9	226.3	0.0065	Singlet-?Sym	H-14->LUMO (46%), H-14->L+1 (17%), H-13->L+1 (20%)
79	44207.6	226.2	0.0001	Singlet-?Sym	H-14->LUMO (28%), H-13->LUMO (10%), H-13->L+1 (52%)
80	44243.8	226.0	0.0118	Singlet-?Sym	H-7->L+2 (22%), H-7->L+3 (10%), H-6->L+2 (39%)
81	44474.5	224.8	0.0539	Singlet-?Sym	H-1->L+14 (23%), HOMO->L+16 (23%)
82	44533.4	224.6	0.0003	Singlet-?Sym	H-10->L+2 (13%), H-10->L+4 (53%), H-9->L+4 (17%)
83	44602.8	224.2	0.0022	Singlet-?Sym	H-8->L+2 (56%), H-8->L+3 (16%), H-7->L+2 (17%)
84	44672.1	223.9	0.0001	Singlet-?Sym	H-1->L+10 (90%)
85	44880.2	222.8	0.0054	Singlet-?Sym	H-10->L+7 (26%), H-10->L+10 (14%), H-9->L+7 (21%), H-9->L+10 (17%)
86	44907.6	222.7	0.0050	Singlet-?Sym	H-2->L+7 (55%)
87	44939.9	222.5	0.0063	Singlet-?Sym	H-8->L+9 (13%), H-6->L+11 (11%), H-2->L+7 (14%), H-1->L+11 (24%)
88	45125.4	221.6	0.0336	Singlet-?Sym	H-15->LUMO (48%), H-15->L+1 (10%), H-2->L+12 (10%)
89	45362.5	220.4	0.0657	Singlet-?Sym	H-15->LUMO (26%), H-2->L+12 (17%)
90	45394.0	220.3	0.0056	Singlet-?Sym	H-9->L+2 (70%), H-9->L+4 (14%)
91	45534.3	219.6	0.0014	Singlet-?Sym	H-14->L+1 (15%), H-1->L+11 (44%)
92	45544.8	219.6	0.0085	Singlet-?Sym	H-14->L+1 (32%), H-2->L+8 (27%), H-1->L+11 (11%)
93	45629.5	219.2	0.0420	Singlet-?Sym	H-14->L+1 (16%), H-2->L+8 (54%)
94	45767.4	218.5	0.0043	Singlet-?Sym	H-10->L+2 (75%), H-10->L+4 (13%)
95	45814.2	218.3	0.1174	Singlet-?Sym	H-5->L+5 (10%), H-2->L+9 (17%)
96	45874.7	218.0	0.0101	Singlet-?Sym	H-7->L+4 (18%), H-6->L+4 (53%)
97	45966.7	217.5	0.0961	Singlet-?Sym	H-5->L+6 (17%), H-4->L+7 (11%), H-2->L+9 (10%)
98	46221.5	216.3	0.0526	Singlet-?Sym	H-6->L+5 (15%), H-2->L+9 (33%), H-1->L+13 (10%)
99	46245.7	216.2	0.0105	Singlet-?Sym	H-7->L+5 (23%), H-6->L+5 (22%), H-2->L+9 (17%)
100	46342.5	215.8	0.0002	Singlet-?Sym	H-8->L+4 (70%), H-7->L+4 (22%)

Table S4: TDDFT 100 lowest vertical singlet transition for complex **1b:**

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	27331.9	365.9	0.0002	Singlet-?Sym	HOMO->LUMO (80%), HOMO->L+1 (17%)
2	28970.8	345.2	0.0004	Singlet-?Sym	HOMO->LUMO (18%), HOMO->L+1 (80%)
3	30424.2	328.7	0.0171	Singlet-?Sym	H-1->LUMO (91%)
4	31685.7	315.6	0.0075	Singlet-?Sym	H-2->LUMO (20%), H-1->L+1 (58%)
5	31822.0	314.2	0.0287	Singlet-?Sym	H-2->LUMO (48%), H-1->L+1 (30%)
6	32485.8	307.8	0.0167	Singlet-?Sym	HOMO->L+2 (19%), HOMO->L+3 (67%)
7	33156.1	301.6	0.0152	Singlet-?Sym	H-3->LUMO (37%), H-3->L+1 (11%), H-2->LUMO (23%)
8	33231.1	300.9	0.0054	Singlet-?Sym	HOMO->L+2 (18%), HOMO->L+3 (16%), HOMO->L+4 (46%)
9	33396.4	299.4	0.0980	Singlet-?Sym	H-3->LUMO (23%), H-2->L+1 (65%)
10	33545.6	298.1	0.0045	Singlet-?Sym	HOMO->L+2 (51%), HOMO->L+4 (35%)
11	34336.1	291.2	0.1579	Singlet-?Sym	H-5->LUMO (46%), H-4->LUMO (21%)
12	34685.3	288.3	0.5185	Singlet-?Sym	H-3->L+1 (71%)
13	35832.2	279.1	0.0682	Singlet-?Sym	H-5->L+1 (44%), H-4->L+1 (24%)
14	35916.9	278.4	0.0217	Singlet-?Sym	H-1->L+2 (43%), H-1->L+3 (27%), HOMO->L+5 (14%)
15	35946.8	278.2	0.0255	Singlet-?Sym	H-5->LUMO (26%), H-4->LUMO (52%)
16	36007.3	277.7	0.1388	Singlet-?Sym	HOMO->L+5 (66%)
17	36172.6	276.5	0.0455	Singlet-?Sym	H-1->L+2 (21%), H-1->L+3 (28%), H-1->L+4 (38%)
18	36443.6	274.4	0.0730	Singlet-?Sym	H-1->L+2 (14%), H-1->L+3 (18%), H-1->L+4 (47%)
19	36879.1	271.2	0.3164	Singlet-?Sym	H-10->LUMO (22%), H-6->LUMO (24%), H-2->L+3 (19%)
20	36946.1	270.7	0.0199	Singlet-?Sym	H-2->L+3 (11%), HOMO->L+6 (61%)
21	37048.5	269.9	0.0426	Singlet-?Sym	H-10->LUMO (10%), H-6->LUMO (12%), H-2->L+2 (12%), H-2->L+3 (20%), HOMO->L+6 (19%)
22	37274.4	268.3	0.0009	Singlet-?Sym	H-5->L+1 (26%), H-4->L+1 (50%)
23	37809.9	264.5	0.0262	Singlet-?Sym	H-2->L+4 (68%)
24	37903.5	263.8	0.0302	Singlet-?Sym	H-2->L+2 (61%), H-2->L+3 (15%)
25	38134.2	262.2	0.0019	Singlet-?Sym	HOMO->L+7 (42%), HOMO->L+15 (15%)
26	38738.3	258.1	0.0219	Singlet-?Sym	H-3->L+2 (11%), H-3->L+3 (35%), H-1->L+5 (10%)
27	38924.6	256.9	0.0170	Singlet-?Sym	H-1->L+5 (56%)
28	39028.6	256.2	0.0244	Singlet-?Sym	H-10->L+1 (13%), H-6->L+1 (20%), H-3->L+2 (12%), H-3->L+3 (12%)
29	39210.1	255.0	0.0105	Singlet-?Sym	H-7->LUMO (78%)
30	39335.1	254.2	0.0062	Singlet-?Sym	H-11->L+1 (10%), H-3->L+4 (14%), H-1->L+6 (19%)
31	39367.4	254.0	0.0016	Singlet-?Sym	H-10->LUMO (26%), H-6->LUMO (29%), H-1->L+6 (11%)
32	39436.8	253.6	0.0098	Singlet-?Sym	H-11->LUMO (12%), H-11->L+1 (21%)
33	39459.3	253.4	0.0216	Singlet-?Sym	H-11->L+1 (13%), H-5->L+4 (10%), H-3->L+4 (13%)
34	39605.3	252.5	0.0327	Singlet-?Sym	H-8->LUMO (18%), HOMO->L+12 (30%)
35	39608.5	252.5	0.0433	Singlet-?Sym	H-8->LUMO (24%), H-6->L+1 (14%), H-3->L+2 (18%)
36	39614.2	252.4	0.0416	Singlet-?Sym	H-9->LUMO (11%), H-8->LUMO (30%), H-6->L+1 (16%), H-3->L+2 (13%)
37	39718.2	251.8	0.0007	Singlet-?Sym	H-9->LUMO (65%), H-8->LUMO (26%)
38	39888.4	250.7	0.0094	Singlet-?Sym	H-4->L+3 (13%), HOMO->L+7 (12%)
39	40177.2	248.9	0.0960	Singlet-?Sym	H-2->L+5 (31%), H-1->L+6 (27%)
40	40306.2	248.1	0.0038	Singlet-?Sym	H-5->L+2 (18%), H-4->L+3 (10%)
41	40518.3	246.8	0.0009	Singlet-?Sym	H-10->L+1 (19%), H-7->L+1 (49%), H-6->L+1 (14%)
42	40579.6	246.4	0.0690	Singlet-?Sym	H-7->L+1 (12%), H-5->L+3 (13%), H-4->L+3 (10%)
43	40624.0	246.2	0.0131	Singlet-?Sym	H-10->L+1 (31%), H-7->L+1 (30%), H-6->L+1 (12%)
44	40811.9	245.0	0.0149	Singlet-?Sym	H-9->L+1 (25%), H-8->L+1 (62%)
45	40867.6	244.7	0.2263	Singlet-?Sym	H-1->L+7 (19%), HOMO->L+8 (36%)
46	40928.9	244.3	0.4863	Singlet-?Sym	H-2->L+5 (25%), H-1->L+6 (15%), H-1->L+7 (13%)
47	40970.8	244.1	0.1311	Singlet-?Sym	H-12->L+1 (12%), H-11->LUMO (36%), H-11->L+1 (15%)
48	40991.0	244.0	0.0087	Singlet-?Sym	H-9->L+1 (55%), H-8->L+1 (28%)
49	41132.9	243.1	0.0378	Singlet-?Sym	H-4->L+2 (14%), H-4->L+3 (13%), H-2->L+6 (33%)
50	41162.0	242.9	0.1682	Singlet-?Sym	H-12->LUMO (10%), H-12->L+1 (15%), H-11->LUMO (19%), H-11->L+1 (10%)

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
51	41241.0	242.5	0.0038	Singlet-?Sym	H-5->L+2 (10%), H-4->L+4 (42%)
52	41474.1	241.1	0.0920	Singlet-?Sym	H-5->L+4 (14%), H-3->L+4 (11%), HOMO->L+8 (32%)
53	41711.3	239.7	0.0108	Singlet-?Sym	HOMO->L+9 (90%)
54	41737.1	239.6	0.2037	Singlet-?Sym	H-5->L+3 (23%), H-3->L+4 (10%)
55	41799.2	239.2	0.0246	Singlet-?Sym	H-5->L+2 (22%), H-4->L+2 (37%)
56	42086.3	237.6	0.0109	Singlet-?Sym	H-1->L+8 (16%), HOMO->L+7 (21%), HOMO->L+13 (13%), HOMO->L+15 (19%)
57	42317.8	236.3	0.0058	Singlet-?Sym	H-12->LUMO (30%), H-12->L+1 (38%), H-3->L+5 (13%)
58	42388.8	235.9	0.0097	Singlet-?Sym	H-3->L+5 (56%)
59	42749.3	233.9	0.0132	Singlet-?Sym	H-4->L+5 (30%), H-1->L+7 (16%)
60	42867.1	233.3	0.0396	Singlet-?Sym	H-4->L+5 (13%), H-1->L+7 (24%)
61	42938.8	232.9	0.0039	Singlet-?Sym	H-14->LUMO (20%), H-13->LUMO (41%), H-4->L+5 (11%)
62	43146.9	231.8	0.0315	Singlet-?Sym	H-6->L+2 (16%), H-6->L+3 (23%)
63	43261.5	231.2	0.0078	Singlet-?Sym	H-3->L+6 (14%), H-1->L+8 (28%)
64	43296.9	231.0	0.0161	Singlet-?Sym	H-7->L+3 (22%), H-6->L+4 (18%)
65	43347.8	230.7	0.0337	Singlet-?Sym	H-4->L+6 (39%)
66	43405.8	230.4	0.0215	Singlet-?Sym	H-10->L+3 (14%), H-6->L+4 (21%), H-1->L+8 (11%)
67	43513.9	229.8	0.0187	Singlet-?Sym	H-7->L+3 (10%), H-3->L+6 (18%), H-1->L+8 (10%)
68	43574.4	229.5	0.0186	Singlet-?Sym	H-10->L+2 (12%), H-5->L+5 (30%)
69	43605.9	229.3	0.1142	Singlet-?Sym	H-10->L+2 (10%), H-6->L+3 (11%), H-5->L+5 (14%), H-3->L+6 (13%)
70	43652.6	229.1	0.0051	Singlet-?Sym	HOMO->L+10 (14%), HOMO->L+11 (60%)
71	43750.2	228.6	0.0040	Singlet-?Sym	HOMO->L+10 (58%), HOMO->L+11 (24%)
72	43876.9	227.9	0.0129	Singlet-?Sym	H-1->L+9 (58%)
73	43963.2	227.5	0.0919	Singlet-?Sym	H-10->L+4 (28%), H-1->L+9 (28%)
74	44008.3	227.2	0.0040	Singlet-?Sym	H-9->L+3 (23%), H-8->L+3 (27%), H-7->L+3 (10%)
75	44044.6	227.0	0.0153	Singlet-?Sym	H-10->L+4 (13%), H-2->L+7 (11%), H-1->L+9 (11%), H-1->L+12 (15%)
76	44138.2	226.6	0.0149	Singlet-?Sym	H-9->L+4 (29%), H-8->L+4 (24%)
77	44303.5	225.7	0.0621	Singlet-?Sym	H-5->L+6 (48%)
78	44481.8	224.8	0.0031	Singlet-?Sym	H-14->LUMO (44%), H-14->L+1 (12%), H-13->LUMO (24%)
79	44645.5	224.0	0.0320	Singlet-?Sym	H-2->L+7 (35%), HOMO->L+15 (15%)
80	44827.0	223.1	0.0209	Singlet-?Sym	H-7->L+2 (12%)
81	44857.6	222.9	0.0059	Singlet-?Sym	H-9->L+8 (12%), H-8->L+7 (12%), H-6->L+11 (11%)
82	44863.3	222.9	0.0699	Singlet-?Sym	H-1->L+13 (15%), HOMO->L+14 (20%), HOMO->L+16 (11%)
83	45004.4	222.2	0.0099	Singlet-?Sym	H-7->L+2 (61%), H-7->L+3 (17%)
84	45156.1	221.5	0.0423	Singlet-?Sym	H-14->L+1 (11%), H-2->L+12 (13%), HOMO->L+14 (18%)
85	45184.3	221.3	0.0022	Singlet-?Sym	H-14->L+1 (18%), H-13->L+1 (37%), HOMO->L+14 (10%)
86	45264.1	220.9	0.0063	Singlet-?Sym	H-10->L+2 (30%), H-6->L+2 (33%)
87	45289.2	220.8	0.0094	Singlet-?Sym	H-2->L+8 (83%)
88	45399.6	220.3	0.0001	Singlet-?Sym	H-10->L+2 (10%), H-9->L+2 (23%), H-8->L+2 (44%), H-8->L+3 (10%)
89	45523.9	219.7	0.0633	Singlet-?Sym	HOMO->L+14 (16%), HOMO->L+16 (17%)
90	45590.0	219.3	0.0001	Singlet-?Sym	H-9->L+2 (44%), H-8->L+2 (32%)
91	45684.4	218.9	0.0084	Singlet-?Sym	H-16->LUMO (54%), H-1->L+10 (10%)
92	45737.6	218.6	0.0050	Singlet-?Sym	H-2->L+9 (68%), H-1->L+10 (16%)
93	45789.2	218.4	0.0187	Singlet-?Sym	H-1->L+11 (68%)
94	45815.0	218.3	0.0137	Singlet-?Sym	H-2->L+9 (10%), H-1->L+10 (47%), H-1->L+11 (13%)
95	46015.9	217.3	0.0655	Singlet-?Sym	H-10->L+3 (19%), H-6->L+3 (24%)
96	46079.6	217.0	0.0668	Singlet-?Sym	H-10->L+3 (13%), H-6->L+3 (22%)
97	46172.3	216.6	0.0191	Singlet-?Sym	H-7->L+3 (14%), H-7->L+4 (52%)
98	46204.6	216.4	0.0594	Singlet-?Sym	H-1->L+13 (17%), H-1->L+15 (10%)
99	46249.8	216.2	0.0352	Singlet-?Sym	H-14->L+1 (28%), H-13->L+1 (30%), HOMO->L+14 (10%)
100	46380.4	215.6	0.0028	Singlet-?Sym	H-9->L+3 (35%), H-8->L+3 (43%)

Table S5: TDDFT 100 lowest vertical singlet transition for complex **2a:**

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	25380.8	394.0	0.0008	Singlet-?Sym	HOMO->LUMO (97%)
2	29162.0	342.9	0.0080	Singlet-?Sym	H-1->LUMO (98%)
3	30257.3	330.5	0.0014	Singlet-?Sym	HOMO->L+1 (88%)
4	30932.4	323.3	0.0017	Singlet-?Sym	HOMO->L+2 (47%), HOMO->L+3 (35%)
5	31184.0	320.7	0.0033	Singlet-?Sym	H-4->LUMO (11%), H-3->LUMO (11%), H-2->LUMO (73%)
6	31359.1	318.9	0.0018	Singlet-?Sym	HOMO->L+2 (20%), HOMO->L+3 (34%), HOMO->L+4 (37%)
7	31680.9	315.6	0.0017	Singlet-?Sym	HOMO->L+2 (27%), HOMO->L+3 (13%), HOMO->L+4 (55%)
8	32752.8	305.3	0.0032	Singlet-?Sym	H-4->LUMO (52%), H-3->LUMO (22%), H-2->LUMO (22%)
9	33351.3	299.8	0.1351	Singlet-?Sym	H-5->LUMO (29%), H-4->LUMO (19%), H-3->LUMO (44%)
10	33780.3	296.0	0.0006	Singlet-?Sym	H-1->L+1 (94%)
11	34052.2	293.7	0.1802	Singlet-?Sym	HOMO->L+5 (87%)
12	34858.7	286.9	0.0100	Singlet-?Sym	H-1->L+2 (82%)
13	35095.8	284.9	0.0340	Singlet-?Sym	H-1->L+3 (37%), H-1->L+4 (11%), HOMO->L+6 (37%)
14	35181.3	284.2	0.0339	Singlet-?Sym	H-1->L+3 (12%), H-1->L+4 (38%), HOMO->L+6 (38%)
15	35295.1	283.3	0.0288	Singlet-?Sym	H-5->LUMO (11%), H-1->L+3 (23%), H-1->L+4 (35%)
16	35376.5	282.7	0.0161	Singlet-?Sym	H-5->LUMO (52%), H-4->LUMO (10%), H-3->LUMO (12%), H-1->L+3 (13%)
17	35985.5	277.9	0.0255	Singlet-?Sym	H-2->L+1 (69%)
18	36798.5	271.8	0.0609	Singlet-?Sym	H-2->L+1 (13%), H-2->L+2 (26%), H-2->L+3 (35%)
19	37271.9	268.3	0.0054	Singlet-?Sym	H-2->L+3 (12%), H-2->L+4 (50%)
20	37335.7	267.8	0.0544	Singlet-?Sym	H-3->L+1 (15%), H-2->L+2 (15%), H-2->L+3 (11%), H-2->L+4 (17%)
21	37460.7	266.9	0.0293	Singlet-?Sym	H-4->L+1 (17%), H-3->L+1 (12%), H-2->L+2 (28%)
22	37620.4	265.8	0.0465	Singlet-?Sym	H-1->L+5 (71%)
23	37847.8	264.2	0.0039	Singlet-?Sym	HOMO->L+8 (10%)
24	38083.3	262.6	0.0301	Singlet-?Sym	H-6->LUMO (85%)
25	38165.6	262.0	0.0111	Singlet-?Sym	H-5->L+1 (16%), H-4->L+1 (20%), H-3->L+1 (25%)
26	38251.9	261.4	0.1788	Singlet-?Sym	H-12->LUMO (10%), H-9->LUMO (13%), H-4->L+1 (11%)
27	38374.5	260.6	0.0210	Singlet-?Sym	H-4->L+1 (10%), H-4->L+3 (12%), H-3->L+2 (21%)
28	38529.4	259.5	0.1239	Singlet-?Sym	H-1->L+6 (71%)
29	38726.2	258.2	0.0178	Singlet-?Sym	H-7->LUMO (42%), HOMO->L+7 (21%), HOMO->L+13 (17%)
30	38743.9	258.1	0.0057	Singlet-?Sym	H-7->LUMO (43%), HOMO->L+7 (21%), HOMO->L+13 (15%)
31	38914.9	257.0	0.0279	Singlet-?Sym	H-4->L+3 (10%), H-4->L+4 (17%), HOMO->L+8 (10%)
32	38948.8	256.7	0.0041	Singlet-?Sym	H-8->LUMO (86%)
33	39106.1	255.7	0.0859	Singlet-?Sym	H-4->L+2 (35%), H-3->L+4 (15%)
34	39232.7	254.9	0.0215	Singlet-?Sym	H-11->LUMO (13%), H-9->LUMO (52%)
35	39265.8	254.7	0.0000	Singlet-?Sym	H-10->LUMO (100%)
36	39348.0	254.1	0.0214	Singlet-?Sym	HOMO->L+7 (30%), HOMO->L+9 (17%), HOMO->L+13 (16%)
37	39431.9	253.6	0.0826	Singlet-?Sym	H-3->L+3 (16%), HOMO->L+8 (33%)
38	39560.2	252.8	0.2802	Singlet-?Sym	H-4->L+3 (13%), H-4->L+4 (21%)
39	39673.1	252.1	0.0493	Singlet-?Sym	HOMO->L+7 (10%), HOMO->L+9 (32%), HOMO->L+13 (14%)
40	39753.7	251.5	0.0887	Singlet-?Sym	H-11->LUMO (55%)
41	39876.3	250.8	0.0972	Singlet-?Sym	H-12->LUMO (27%), H-5->L+1 (19%), H-3->L+1 (11%)
42	39957.0	250.3	0.0795	Singlet-?Sym	H-12->LUMO (20%), H-5->L+1 (38%)
43	40173.9	248.9	0.2340	Singlet-?Sym	H-3->L+4 (10%), H-2->L+5 (47%)
44	40539.3	246.7	0.0150	Singlet-?Sym	H-3->L+3 (11%), HOMO->L+9 (11%), HOMO->L+15 (22%)
45	40765.2	245.3	0.0519	Singlet-?Sym	H-5->L+2 (13%), H-2->L+6 (32%)
46	40878.1	244.6	0.0266	Singlet-?Sym	HOMO->L+10 (88%)
47	41105.5	243.3	0.2008	Singlet-?Sym	H-5->L+2 (21%), H-5->L+4 (22%), H-2->L+6 (10%)
48	41199.9	242.7	0.1314	Singlet-?Sym	H-5->L+3 (23%), H-5->L+4 (10%), HOMO->L+11 (29%)
49	41224.1	242.6	0.0303	Singlet-?Sym	H-13->LUMO (83%)
50	41358.8	241.8	0.0304	Singlet-?Sym	H-5->L+2 (17%), H-5->L+4 (17%), HOMO->L+11 (32%)

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
51	41412.0	241.5	0.0336	Singlet-?Sym	H-5->L+2 (11%), H-5->L+3 (18%), HOMO->L+11 (19%), HOMO->L+12 (15%)
52	41449.9	241.3	0.1104	Singlet-?Sym	H-1->L+8 (12%)
53	41617.7	240.3	0.0274	Singlet-?Sym	HOMO->L+12 (70%)
54	41714.5	239.7	0.0716	Singlet-?Sym	H-3->L+5 (16%)
55	41800.8	239.2	0.0135	Singlet-?Sym	H-4->L+5 (16%), H-3->L+5 (32%), H-2->L+6 (12%)
56	41940.3	238.4	0.0239	Singlet-?Sym	H-9->L+1 (22%), H-7->L+1 (12%), H-6->L+1 (31%)
57	42001.6	238.1	0.0371	Singlet-?Sym	H-4->L+5 (19%), H-1->L+7 (38%)
58	42058.1	237.8	0.0092	Singlet-?Sym	H-9->L+1 (20%), H-7->L+1 (12%), H-6->L+1 (19%), H-6->L+4 (16%)
59	42121.0	237.4	0.0628	Singlet-?Sym	H-4->L+5 (15%), H-1->L+7 (40%)
60	42291.2	236.5	0.0641	Singlet-?Sym	H-1->L+8 (50%)
61	42588.0	234.8	0.0058	Singlet-?Sym	H-1->L+9 (71%)
62	42702.5	234.2	0.0098	Singlet-?Sym	H-11->L+1 (58%), H-11->L+2 (19%)
63	42795.3	233.7	0.0089	Singlet-?Sym	H-3->L+6 (31%)
64	42884.8	233.2	0.0078	Singlet-?Sym	H-14->LUMO (10%), H-8->L+1 (29%), H-8->L+3 (14%), H-8->L+4 (17%)
65	42903.3	233.1	0.0005	Singlet-?Sym	H-6->L+1 (35%), H-6->L+2 (12%), H-6->L+3 (15%), H-6->L+4 (17%)
66	42917.9	233.0	0.0028	Singlet-?Sym	H-14->LUMO (13%), H-8->L+1 (16%), H-7->L+1 (33%)
67	42930.0	232.9	0.0044	Singlet-?Sym	H-14->LUMO (58%), H-7->L+1 (14%)
68	43047.7	232.3	0.0274	Singlet-?Sym	H-5->L+5 (33%), H-4->L+6 (18%)
69	43184.8	231.6	0.0196	Singlet-?Sym	H-5->L+5 (13%), H-4->L+6 (32%), H-3->L+6 (11%)
70	43319.5	230.8	0.0711	Singlet-?Sym	H-12->L+1 (36%)
71	43339.7	230.7	0.0238	Singlet-?Sym	H-10->L+1 (16%), H-1->L+13 (23%)
72	43373.6	230.6	0.0042	Singlet-?Sym	H-10->L+1 (41%), H-10->L+3 (11%), H-10->L+4 (13%), H-1->L+13 (10%)
73	43703.5	228.8	0.0003	Singlet-?Sym	H-7->L+1 (11%), H-7->L+2 (18%), H-7->L+3 (19%), H-7->L+4 (25%)
74	43768.8	228.5	0.0058	Singlet-?Sym	H-1->L+10 (85%)
75	43826.9	228.2	0.0119	Singlet-?Sym	H-8->L+1 (33%), H-8->L+3 (16%), H-1->L+11 (16%)
76	43921.2	227.7	0.0678	Singlet-?Sym	H-8->L+1 (10%), H-5->L+6 (25%)
77	44020.4	227.2	0.0029	Singlet-?Sym	H-6->L+2 (75%), H-6->L+3 (14%)
78	44040.6	227.1	0.0317	Singlet-?Sym	H-10->L+1 (10%), H-1->L+11 (46%)
79	44203.5	226.2	0.0189	Singlet-?Sym	H-1->L+12 (54%)
80	44264.0	225.9	0.0067	Singlet-?Sym	H-10->L+1 (27%), H-10->L+3 (29%), H-10->L+4 (15%), H-1->L+11 (16%)
81	44340.6	225.5	0.0112	Singlet-?Sym	H-15->LUMO (53%)
82	44409.2	225.2	0.0096	Singlet-?Sym	H-12->L+3 (14%), H-9->L+3 (16%)
83	44434.2	225.1	0.0592	Singlet-?Sym	H-15->LUMO (17%), H-1->L+14 (15%), HOMO->L+16 (11%)
84	44547.1	224.5	0.0327	Singlet-?Sym	H-12->L+3 (16%), H-12->L+4 (10%), H-9->L+4 (12%), H-7->L+2 (10%)
85	44644.7	224.0	0.0054	Singlet-?Sym	H-7->L+2 (55%), H-7->L+4 (13%)
86	44764.1	223.4	0.0160	Singlet-?Sym	H-2->L+7 (69%), HOMO->L+16 (11%)
87	44800.4	223.2	0.1089	Singlet-?Sym	H-12->L+2 (12%), H-12->L+4 (10%), H-9->L+2 (21%), H-8->L+2 (10%)
88	44912.5	222.7	0.0142	Singlet-?Sym	H-2->L+8 (52%)
89	44961.7	222.4	0.0014	Singlet-?Sym	H-9->L+2 (15%), H-8->L+2 (69%)
90	45051.2	222.0	0.0132	Singlet-?Sym	H-12->L+2 (26%), H-11->L+1 (11%), H-11->L+7 (14%)
91	45094.0	221.8	0.0143	Singlet-?Sym	H-12->L+2 (17%), H-11->L+2 (35%), H-9->L+2 (13%)
92	45140.7	221.5	0.0007	Singlet-?Sym	H-7->L+9 (24%), H-6->L+12 (29%), H-1->L+12 (20%)
93	45241.6	221.0	0.0319	Singlet-?Sym	H-2->L+9 (58%)
94	45248.8	221.0	0.0006	Singlet-?Sym	H-10->L+2 (85%), H-10->L+3 (11%)
95	45426.3	220.1	0.0293	Singlet-?Sym	H-10->L+8 (17%), H-8->L+11 (17%), H-2->L+9 (11%)
96	45474.7	219.9	0.0896	Singlet-?Sym	H-2->L+8 (10%), H-2->L+9 (16%)
97	45527.1	219.6	0.0023	Singlet-?Sym	H-6->L+3 (51%), H-6->L+4 (37%)
98	45743.2	218.6	0.0032	Singlet-?Sym	H-12->L+3 (12%), H-12->L+4 (16%), H-11->L+4 (10%), H-9->L+3 (19%), H-9->L+4 (20%)
99	45827.9	218.2	0.1330	Singlet-?Sym	H-2->L+13 (11%), H-1->L+13 (10%)
100	45963.4	217.6	0.0070	Singlet-?Sym	H-12->L+2 (13%), H-11->L+2 (20%), H-11->L+7 (20%)

Table S6: TDDFT 100 lowest vertical singlet transition for complex **2b:**

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	27527.1	363.3	0.0010	Singlet-?Sym	HOMO->LUMO (96%)
2	30905.0	323.6	0.0117	Singlet-?Sym	H-1->LUMO (98%)
3	32105.9	311.5	0.0059	Singlet-?Sym	HOMO->L+1 (40%), HOMO->L+2 (39%)
4	32126.9	311.3	0.0027	Singlet-?Sym	H-2->LUMO (77%)
5	32881.0	304.1	0.0046	Singlet-?Sym	HOMO->L+1 (50%), HOMO->L+2 (42%)
6	33051.2	302.6	0.0012	Singlet-?Sym	HOMO->L+3 (80%), HOMO->L+4 (11%)
7	33740.0	296.4	0.0092	Singlet-?Sym	H-4->LUMO (31%), H-3->LUMO (43%), H-2->LUMO (14%)
8	33818.3	295.7	0.0046	Singlet-?Sym	HOMO->L+4 (76%)
9	34659.5	288.5	0.1482	Singlet-?Sym	H-5->LUMO (44%), H-4->LUMO (16%), H-3->LUMO (20%)
10	35528.2	281.5	0.0080	Singlet-?Sym	H-1->L+1 (82%)
11	35729.8	279.9	0.1714	Singlet-?Sym	HOMO->L+5 (85%)
12	36112.1	276.9	0.0141	Singlet-?Sym	H-5->LUMO (30%), H-4->LUMO (41%), H-3->LUMO (19%)
13	36246.0	275.9	0.0122	Singlet-?Sym	H-1->L+2 (65%)
14	36345.2	275.1	0.0776	Singlet-?Sym	H-1->L+3 (72%), H-1->L+4 (12%)
15	36557.3	273.5	0.0541	Singlet-?Sym	H-2->L+1 (45%), H-2->L+2 (19%)
16	36634.0	273.0	0.0102	Singlet-?Sym	H-1->L+2 (10%), HOMO->L+6 (73%)
17	36992.1	270.3	0.0047	Singlet-?Sym	H-2->L+2 (13%), H-1->L+4 (65%)
18	37515.5	266.6	0.0058	Singlet-?Sym	H-6->LUMO (12%), H-2->L+1 (30%), H-2->L+2 (29%)
19	37588.9	266.0	0.0187	Singlet-?Sym	H-6->LUMO (83%)
20	37688.1	265.3	0.0347	Singlet-?Sym	H-2->L+3 (56%), H-2->L+4 (19%)
21	37813.1	264.5	0.1582	Singlet-?Sym	H-12->LUMO (36%), H-10->LUMO (21%)
22	38130.9	262.3	0.0042	Singlet-?Sym	H-7->LUMO (90%)
23	38235.8	261.5	0.0018	Singlet-?Sym	H-8->LUMO (73%), H-5->LUMO (10%)
24	38355.2	260.7	0.0055	Singlet-?Sym	H-2->L+2 (12%), H-2->L+3 (20%), H-2->L+4 (18%)
25	38386.6	260.5	0.0140	Singlet-?Sym	H-2->L+4 (29%)
26	38638.3	258.8	0.0385	Singlet-?Sym	H-10->LUMO (44%), H-3->L+1 (14%)
27	38769.7	257.9	0.0008	Singlet-?Sym	H-9->LUMO (97%)
28	38823.0	257.6	0.0403	Singlet-?Sym	H-12->LUMO (14%), H-11->LUMO (11%), H-10->LUMO (16%), H-3->L+2 (11%)
29	38939.9	256.8	0.0428	Singlet-?Sym	H-1->L+5 (67%)
30	39216.6	255.0	0.0017	Singlet-?Sym	H-11->LUMO (79%)
31	39367.4	254.0	0.0366	Singlet-?Sym	H-5->L+1 (17%), H-3->L+3 (11%)
32	39420.6	253.7	0.0519	Singlet-?Sym	H-3->L+1 (24%), H-1->L+6 (11%)
33	39447.2	253.5	0.1232	Singlet-?Sym	H-4->L+1 (12%), H-3->L+1 (12%), H-3->L+2 (12%), H-1->L+6 (14%)
34	39609.4	252.5	0.0502	Singlet-?Sym	H-4->L+1 (11%), H-1->L+6 (23%)
35	39737.6	251.7	0.0635	Singlet-?Sym	HOMO->L+13 (19%)
36	40125.6	249.2	0.0968	Singlet-?Sym	H-4->L+2 (14%), H-3->L+4 (15%), H-2->L+5 (13%)
37	40194.9	248.8	0.0128	Singlet-?Sym	H-5->L+1 (14%), H-4->L+2 (11%), H-2->L+5 (13%)
38	40261.1	248.4	0.1453	Singlet-?Sym	H-4->L+4 (17%), H-3->L+2 (11%), H-3->L+4 (14%)
39	40515.9	246.8	0.0657	Singlet-?Sym	H-5->L+2 (10%), H-4->L+1 (17%), H-2->L+6 (18%)
40	40682.1	245.8	0.3072	Singlet-?Sym	H-4->L+3 (16%), H-4->L+4 (10%), H-3->L+3 (24%), H-2->L+5 (20%)
41	40894.2	244.5	0.2368	Singlet-?Sym	H-5->L+2 (18%), H-5->L+4 (11%), H-3->L+4 (15%)
42	41074.9	243.5	0.0655	Singlet-?Sym	H-4->L+4 (14%), H-2->L+6 (16%)
43	41189.4	242.8	0.1427	Singlet-?Sym	H-5->L+1 (11%)
44	41203.1	242.7	0.1165	Singlet-?Sym	H-5->L+3 (16%), H-4->L+3 (10%)
45	41309.6	242.1	0.0612	Singlet-?Sym	H-6->L+1 (21%), H-6->L+4 (12%), H-5->L+3 (11%)
46	41418.5	241.4	0.1409	Singlet-?Sym	H-5->L+15 (11%)
47	41576.6	240.5	0.1632	Singlet-?Sym	H-10->L+1 (19%)
48	41723.3	239.7	0.0921	Singlet-?Sym	H-10->L+1 (28%), H-5->L+2 (10%)
49	41975.0	238.2	0.0498	Singlet-?Sym	HOMO->L+7 (50%)
50	42053.2	237.8	0.0606	Singlet-?Sym	H-8->L+1 (13%), H-8->L+3 (15%), HOMO->L+7 (20%)

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
51	42147.6	237.3	0.1002	Singlet-?Sym	H-5->L+4 (14%), H-4->L+4 (10%)
52	42201.6	237.0	0.0054	Singlet-?Sym	H-7->L+1 (44%), H-7->L+4 (14%)
53	42287.1	236.5	0.0112	Singlet-?Sym	H-11->L+1 (48%), H-11->L+2 (13%)
54	42373.4	236.0	0.0131	Singlet-?Sym	H-6->L+1 (41%), H-6->L+2 (22%)
55	42385.5	235.9	0.0053	Singlet-?Sym	H-3->L+5 (31%), HOMO->L+9 (23%)
56	42485.5	235.4	0.0046	Singlet-?Sym	H-4->L+5 (24%), HOMO->L+9 (24%)
57	42542.8	235.1	0.0331	Singlet-?Sym	H-4->L+5 (29%), H-3->L+5 (11%), HOMO->L+9 (27%)
58	42600.1	234.7	0.0061	Singlet-?Sym	H-9->L+1 (36%), H-9->L+2 (22%), H-9->L+3 (25%)
59	42878.3	233.2	0.0042	Singlet-?Sym	HOMO->L+8 (39%), HOMO->L+14 (15%), HOMO->L+15 (13%)
60	42963.0	232.8	0.0047	Singlet-?Sym	H-7->L+1 (29%), H-7->L+2 (38%), H-7->L+4 (10%)
61	43010.6	232.5	0.0254	Singlet-?Sym	H-3->L+6 (32%)
62	43046.1	232.3	0.0226	Singlet-?Sym	H-14->LUMO (14%), H-13->LUMO (37%)
63	43192.1	231.5	0.0291	Singlet-?Sym	H-13->LUMO (10%), H-8->L+1 (36%), H-8->L+3 (14%)
64	43301.0	230.9	0.0250	Singlet-?Sym	H-12->L+1 (25%), H-12->L+2 (10%), H-10->L+2 (14%), H-8->L+1 (11%)
65	43388.1	230.5	0.0152	Singlet-?Sym	H-4->L+6 (46%), H-3->L+6 (23%)
66	43451.8	230.1	0.0243	Singlet-?Sym	H-5->L+5 (55%)
67	43576.8	229.5	0.0031	Singlet-?Sym	H-6->L+2 (11%), H-6->L+3 (24%), H-6->L+4 (59%)
68	43595.4	229.4	0.0007	Singlet-?Sym	HOMO->L+10 (91%)
69	43730.1	228.7	0.0032	Singlet-?Sym	H-9->L+1 (55%), H-9->L+2 (16%), H-9->L+3 (23%)
70	43779.3	228.4	0.0007	Singlet-?Sym	H-5->L+6 (18%), H-1->L+8 (38%)
71	43905.9	227.8	0.0174	Singlet-?Sym	H-12->L+3 (27%), H-10->L+3 (19%)
72	43963.2	227.5	0.0804	Singlet-?Sym	H-12->L+1 (20%), H-12->L+2 (19%), H-10->L+2 (13%)
73	44101.1	226.8	0.0101	Singlet-?Sym	H-7->L+3 (16%), H-7->L+4 (34%)
74	44124.5	226.6	0.0097	Singlet-?Sym	H-7->L+4 (25%), HOMO->L+12 (11%)
75	44146.3	226.5	0.0054	Singlet-?Sym	H-1->L+7 (21%), HOMO->L+12 (37%)
76	44259.2	225.9	0.0010	Singlet-?Sym	HOMO->L+11 (78%), HOMO->L+13 (10%)
77	44308.4	225.7	0.0049	Singlet-?Sym	H-8->L+2 (25%), H-8->L+3 (31%), H-8->L+4 (22%)
78	44347.9	225.5	0.0017	Singlet-?Sym	H-6->L+2 (30%), H-6->L+3 (44%)
79	44406.8	225.2	0.0459	Singlet-?Sym	H-5->L+6 (23%), H-1->L+7 (18%)
80	44415.6	225.1	0.0112	Singlet-?Sym	H-12->L+4 (10%), H-10->L+2 (21%)
81	44509.2	224.7	0.0019	Singlet-?Sym	H-11->L+1 (19%), H-11->L+2 (36%), H-11->L+3 (14%)
82	44539.9	224.5	0.0111	Singlet-?Sym	H-1->L+7 (26%), H-1->L+8 (10%), H-1->L+13 (10%)
83	44687.5	223.8	0.0028	Singlet-?Sym	H-15->LUMO (11%), H-14->LUMO (57%), H-13->LUMO (24%)
84	44839.9	223.0	0.0304	Singlet-?Sym	H-12->L+2 (20%), H-10->L+4 (17%), H-9->L+3 (10%)
85	44869.7	222.9	0.0086	Singlet-?Sym	H-9->L+2 (21%), H-9->L+3 (26%), H-9->L+4 (19%)
86	44905.2	222.7	0.0143	Singlet-?Sym	H-1->L+9 (48%)
87	44932.7	222.6	0.0510	Singlet-?Sym	H-7->L+2 (11%), H-7->L+3 (14%), HOMO->L+13 (11%)
88	44964.1	222.4	0.0369	Singlet-?Sym	H-7->L+2 (18%), H-7->L+3 (35%)
89	44987.5	222.3	0.0010	Singlet-?Sym	H-8->L+2 (17%), H-8->L+4 (41%)
90	45038.3	222.0	0.0759	Singlet-?Sym	H-7->L+9 (11%), H-6->L+12 (10%), H-1->L+9 (13%), HOMO->L+12 (13%)
91	45180.3	221.3	0.0398	Singlet-?Sym	H-12->L+4 (34%), H-11->L+4 (24%), H-10->L+4 (21%)
92	45323.8	220.6	0.0025	Singlet-?Sym	H-9->L+8 (39%), H-8->L+11 (22%)
93	45358.5	220.5	0.0164	Singlet-?Sym	H-12->L+4 (15%), H-11->L+4 (42%)
94	45438.4	220.1	0.0046	Singlet-?Sym	H-12->L+3 (14%), H-10->L+2 (14%), H-10->L+3 (41%)
95	45472.2	219.9	0.0384	Singlet-?Sym	H-2->L+8 (17%)
96	45581.9	219.4	0.0000	Singlet-?Sym	H-9->L+2 (25%), H-9->L+4 (60%)
97	45628.7	219.2	0.0352	Singlet-?Sym	H-15->LUMO (10%), H-2->L+7 (15%), H-2->L+8 (18%)
98	45756.1	218.5	0.0070	Singlet-?Sym	H-11->L+3 (27%), H-11->L+4 (10%), H-11->L+7 (21%), H-10->L+10 (11%)
99	45788.4	218.4	0.0021	Singlet-?Sym	H-15->LUMO (10%), H-11->L+2 (18%), H-11->L+3 (36%)
100	45807.8	218.3	0.0024	Singlet-?Sym	H-16->LUMO (12%), H-15->LUMO (31%)