

Enhanced Luminescent Iridium(III) Complexes Bearing Aryltriazole Cyclometallated Ligands

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SUPPORTING INFORMATION

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Table S1: Crystallographic data for complexes **2a**, **3b** and **4a**

	2a	3b	4a
Identification code	sI03169fI	sI06191fI	sI03169fI
Empirical formula	C40 H32 F6 Ir N8 P	C43 H41 Cl3 F10 Ir N4 P	C41 H30 Cl2 F10 Ir N8 P
Formula weight	961.91	1133.32	1118.8
Temperature	293(2) K	293(2) K	198(2) K
Wavelength	1.54176 Å	1.54176 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	P21/c	P21/n	P21/C
Unit cell dimensions	a = 15.837(4) Å b = 15.516(4) Å c = 18.061(4) Å	a = 12.106(8) Å b = 24.022(14) Å c = 15.686(11) Å	a = 15.248(7) Å b = 16.489(7) Å c = 18.317(7) Å
	α = 90°. β = 115.297(19)°. γ = 90°.	α = 90°. β = 94.88(6)°. γ = 90°.	α = 90°. β = 111.89(4)°. γ = 90°.
Volume	4012.6(17) Å ³	4545(5) Å ³	4273(3) Å ³
Z	4	4	4
Density (calculated)	1.592 Mg/m ³	1.656 Mg/m ³	1.739 Mg/m ³
Absorption coefficient	7.404 mm ⁻¹	8.322 mm ⁻¹	3.373 mm ⁻¹
F(000)	1896	2240	2192
Crystal size	0.30 x 0.20 x 0.05 mm ³	0.7 x 0.3 x 0.2 mm ³	0.50 x 0.30 x 0.20 mm ³
Theta range for data collection	3.93 to 70.04°.	3.37 to 70.02°.	1.44 to 25.55°.
Index ranges	-19<= <i>h</i> <=17, 0<= <i>k</i> <=18, 0<= <i>l</i> <=22	-14<= <i>h</i> <=14, 0<= <i>k</i> <=29, 0<= <i>l</i> <=19	-18<= <i>h</i> <=17, 0<= <i>k</i> <=20, 0<= <i>l</i> <=22
Reflections collected	7448	8192	7685
Independent reflections	7448 [R(int) = 0.0000]	8192 [R(int) = 0.0000]	7685 [R(int) = 0.0000]
Completeness to theta = 25.03°	98.10%	95.00%	96.10%
Absorption correction	Psi-Scan	Psi-Scan	Psi-Scan
Max. and min. transmission	0.7085 and 0.2148	0.19 and 0.10	0.5519 and 0.2834
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	7448 / 54 / 483	8192 / 1 / 542	7685 / 0 / 316
Goodness-of-fit on F ²	0.942	0.958	0.86
Final R indices [I>2sigma(I)]	R1 = 0.0850, wR2 = 0.1749	R1 = 0.0950, wR2 = 0.2322	R1 = 0.0848, wR2 = 0.1432
R indices (all data)	R1 = 0.2207, wR2 = 0.2222	R1 = 0.1509, wR2 = 0.2656	R1 = 0.2464, wR2 = 0.1807
Extinction coefficient	0.00138(11)	0.0025(2)	
Largest diff. peak and hole	1.103 and -1.904 e.Å ⁻³	1.904 and -1.577 e.Å ⁻³	1.855 and -2.210 e.Å ⁻³

Figure S1: Ortep representation of complex **2a** (ellipsoids at 30% probability)

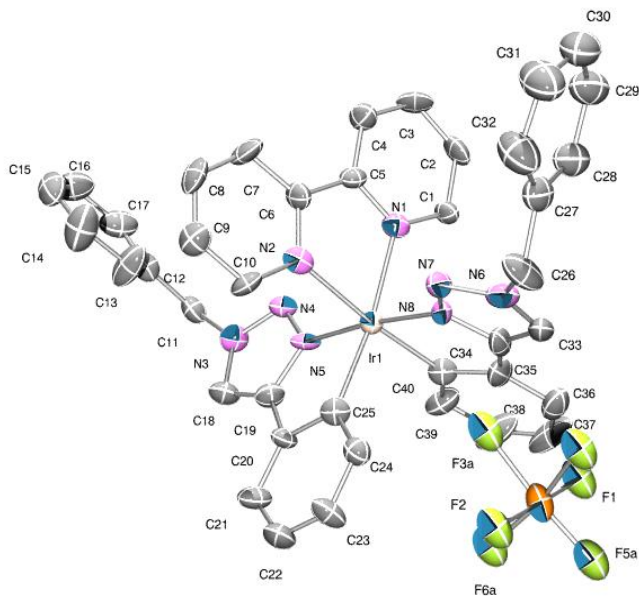


Figure S2: Ortep representation of complex **3b** (ellipsoids at 30% probability)

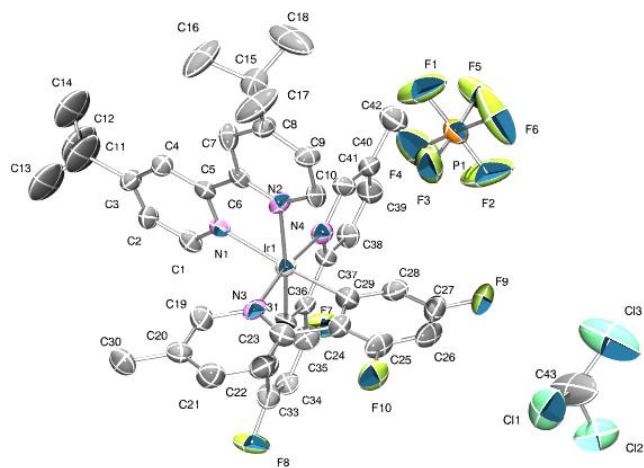
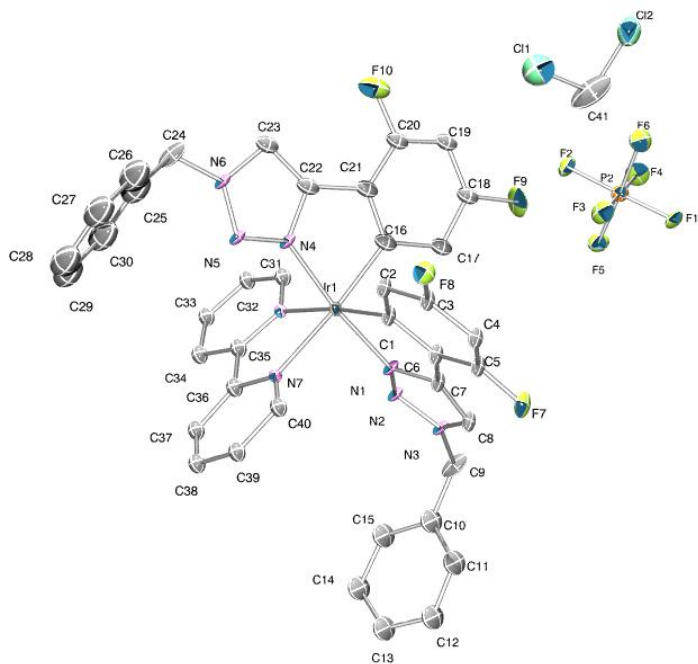
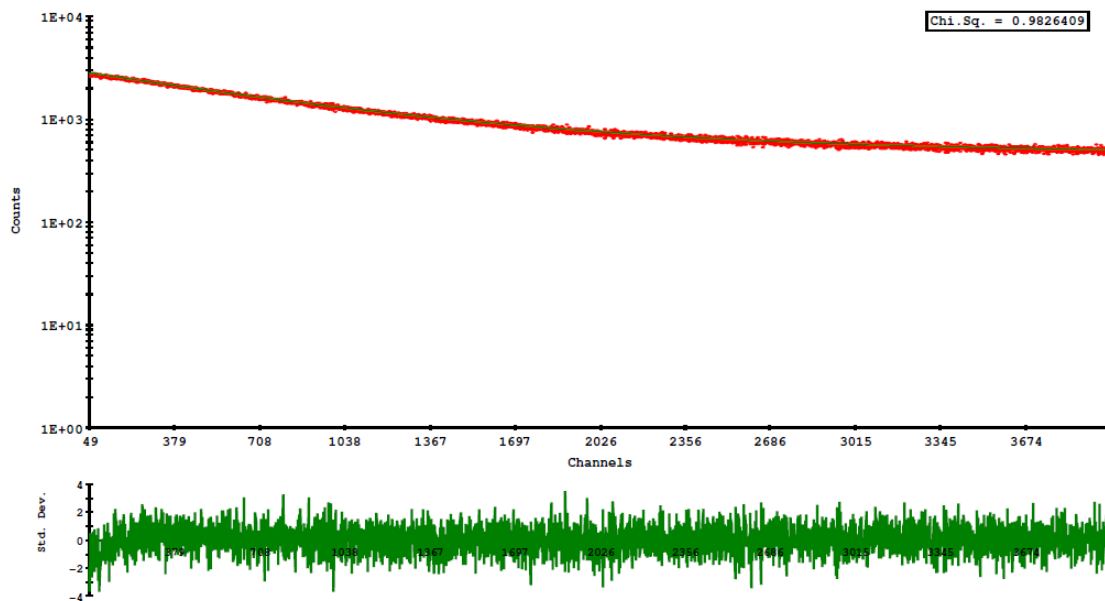


Figure S3: Ortep representation of complex **4a** (ellipsoids at 30% probability)



Figures S4: Example of the lifetime measurement of a sample of **3a** [Ir(dFMeppy)₂bpy]PF₆ in MeOH/EtOH at 77 K. The decay curve is in red and the standard deviation after modeling with a mono-exponential regression is in green.



Calculated using 1 exponential

Prompt data : (none)
Decay data : Decay

The initial paramters are:

Shift Value = Fixed @ 0 ch; 0 sec

T1 Estimate = 824.4095 ch; 5.790092E-06 sec

A Free
B1 Free

Prompt and decay LO = 49 ch; 3.441427E-07 sec
Prompt and decay HI = 4004 ch; 2.812137E-05 sec

Background on prompt = 0
Time calibration = 7.02332E-09 sec/ch

The fitted parameters are:

SHIFT = 0 ch

T1 = 933.9063 ch; 6.559123E-06 sec S.Dev = 1.524536E-08 sec
A = 474.9897 S.Dev = 0.5658206
B1 = 2372.941 [100.00 Rel.Ampl] S.Dev = 2.503846
CHISQ = 0.9826409 [3953 degrees of freedom]

Chi-squared Probability = 77.89504 percent
Durbin-Watson Parameter = 1.952557
Negative residuals = 49.14054 percent
Residuals < 1 s.dev = 67.77048 percent
Residuals < 2 s.dev = 95.8544 percent
Residuals < 3 s.dev = 99.67139 percent
Residuals < 4 s.dev = 100 percent

Figure S5: Absorption and emission spectra for **1a** [Ir(ppy)₂bpy]PF₆:

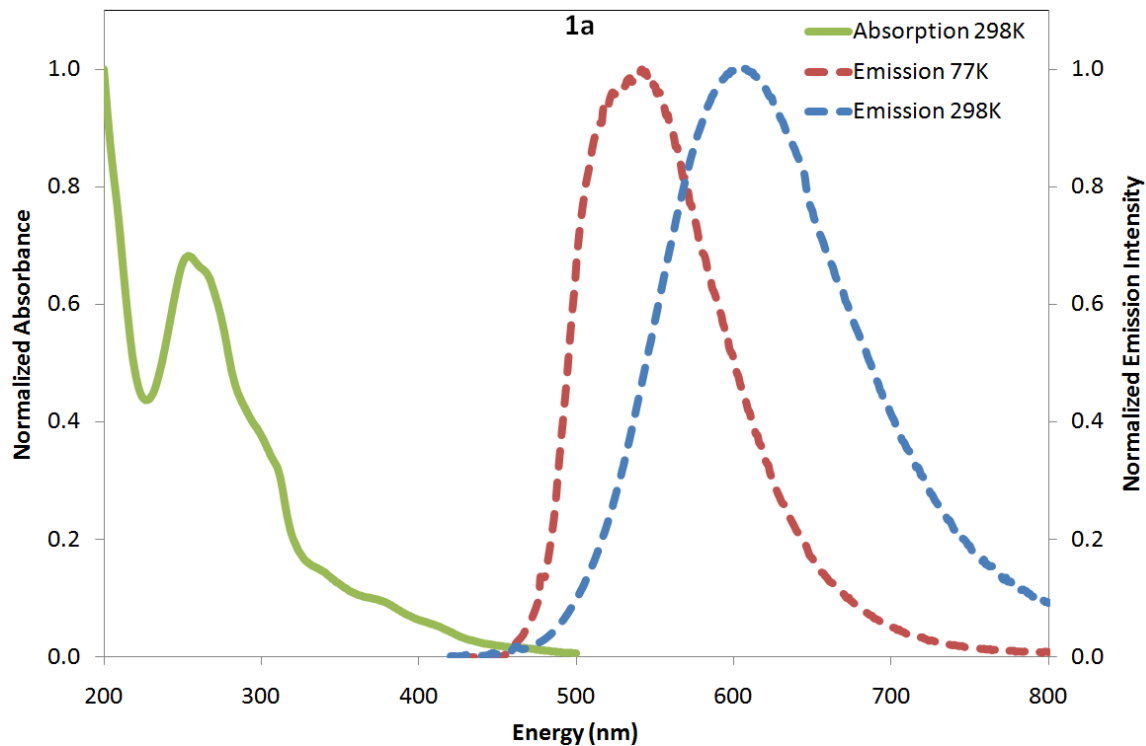


Figure S6: Absorption and emission spectra for **1b** [Ir(ppy)₂dtBubpy]PF₆:

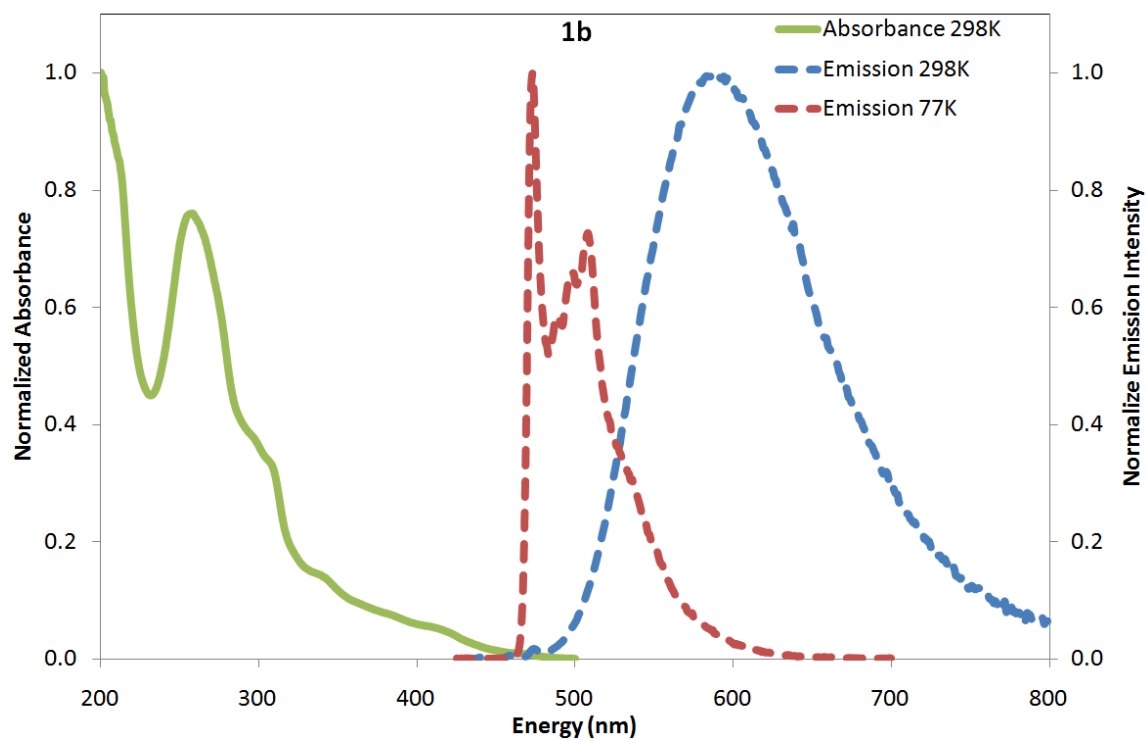


Figure S7: Absorption and emission spectra for **2a** [Ir(phtl)₂bpy]PF₆:

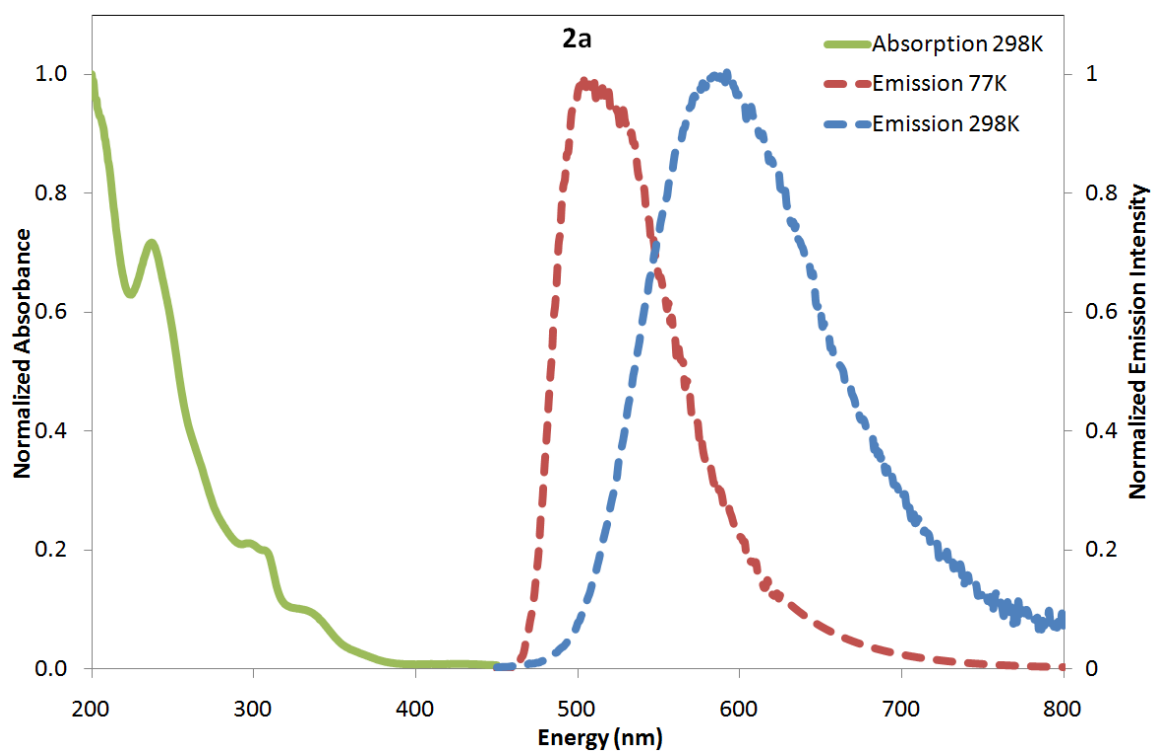


Figure S8: Absorption and emission spectra for **2b** [Ir(phtl)₂dtBubpy]PF₆:

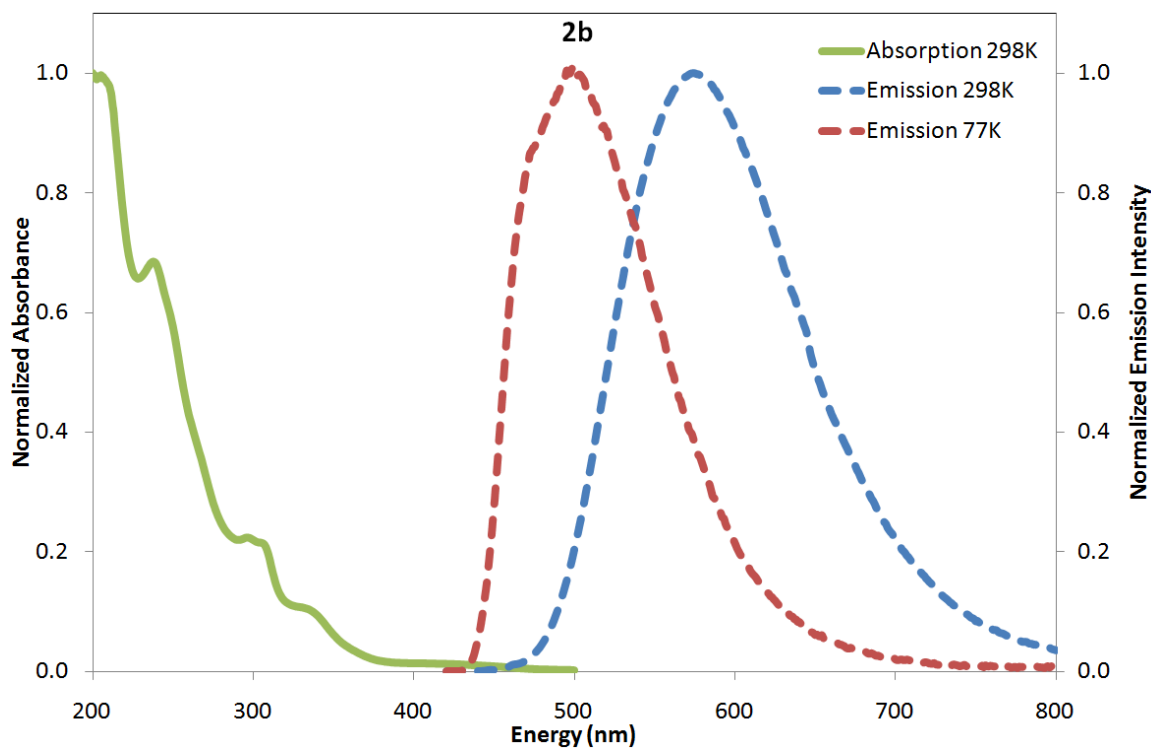


Figure S9: Absorption and emission spectra for **3a** [Ir(dFMeppy)₂bpy]PF₆:

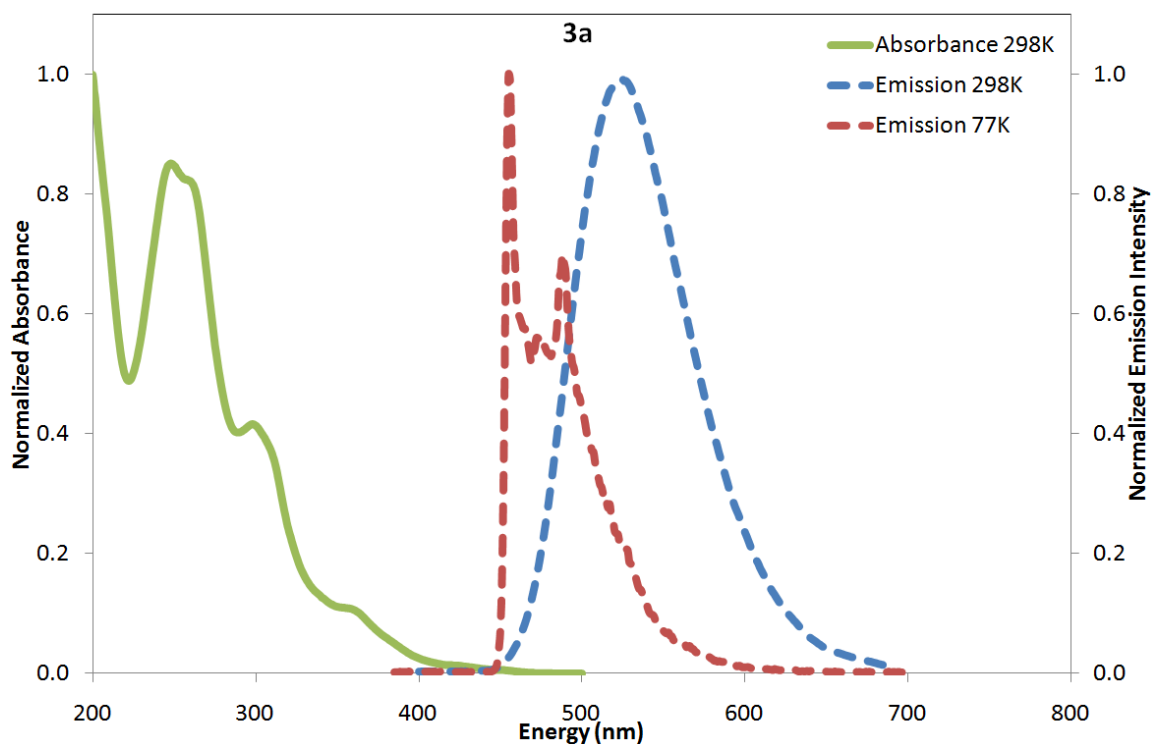


Figure S10: Absorption and emission spectra for **3b** [Ir(dFMeppy)₂dtBubpy]PF₆:

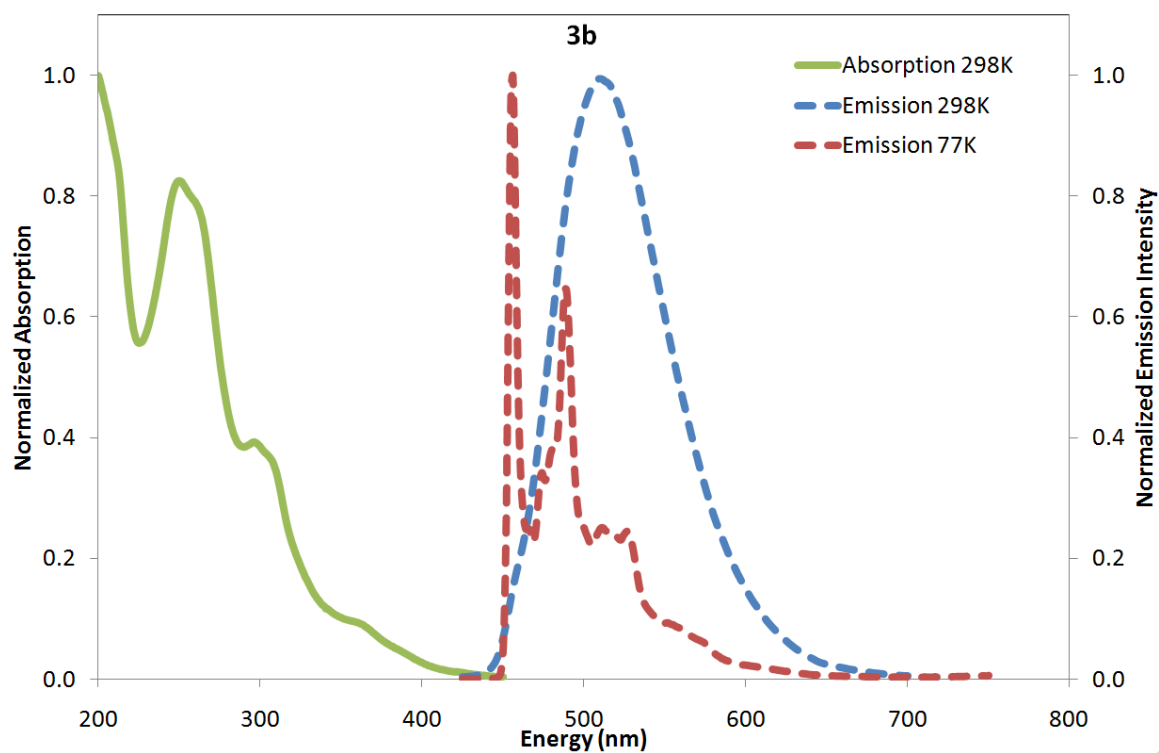


Figure S11: Absorption and emission spectra for **4a** [Ir(dFphtl)₂bpy]PF₆:

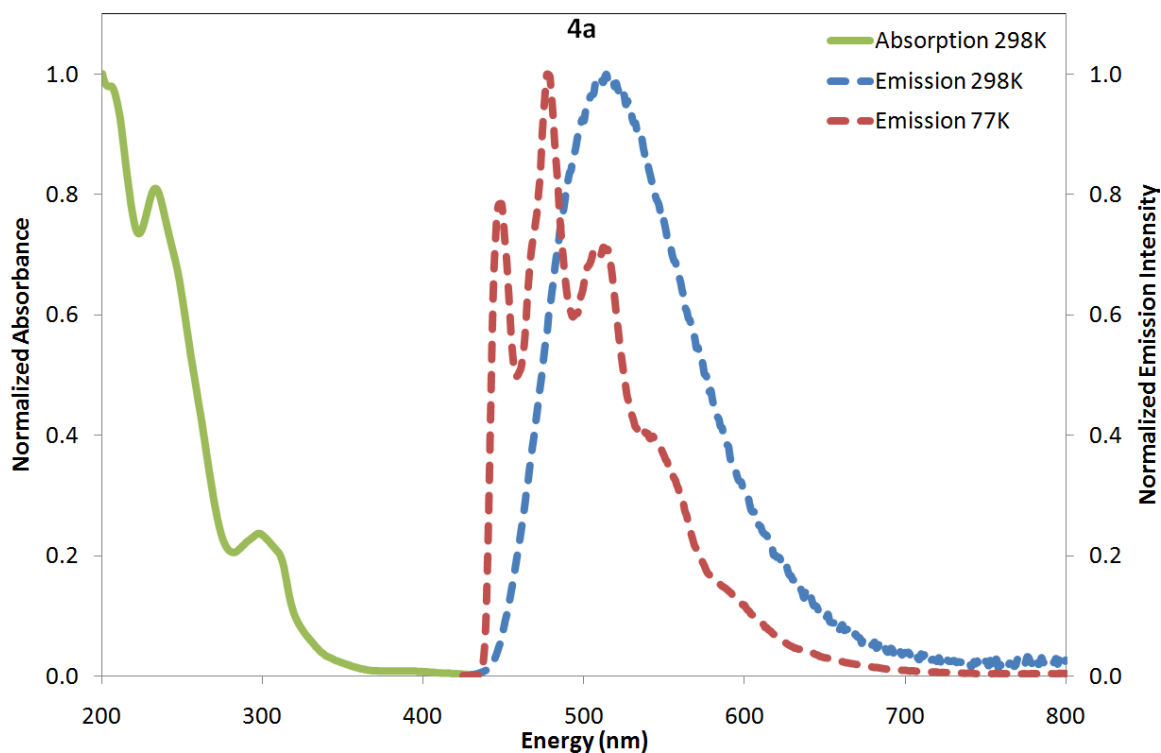


Figure S12 : Absorption and emission spectra for **4b** [Ir(dFphtl)₂dtBubpy]PF₆:

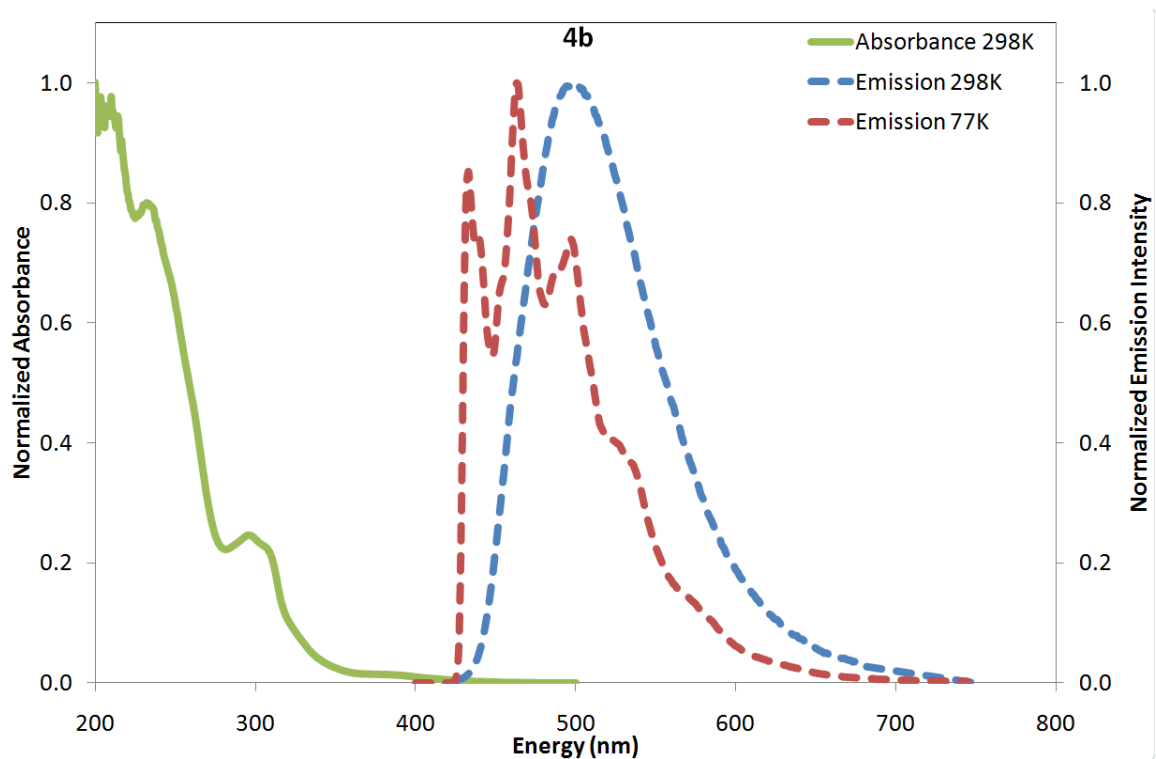


Figure S13 : Calculated and experimental absorption spectra of **1a**

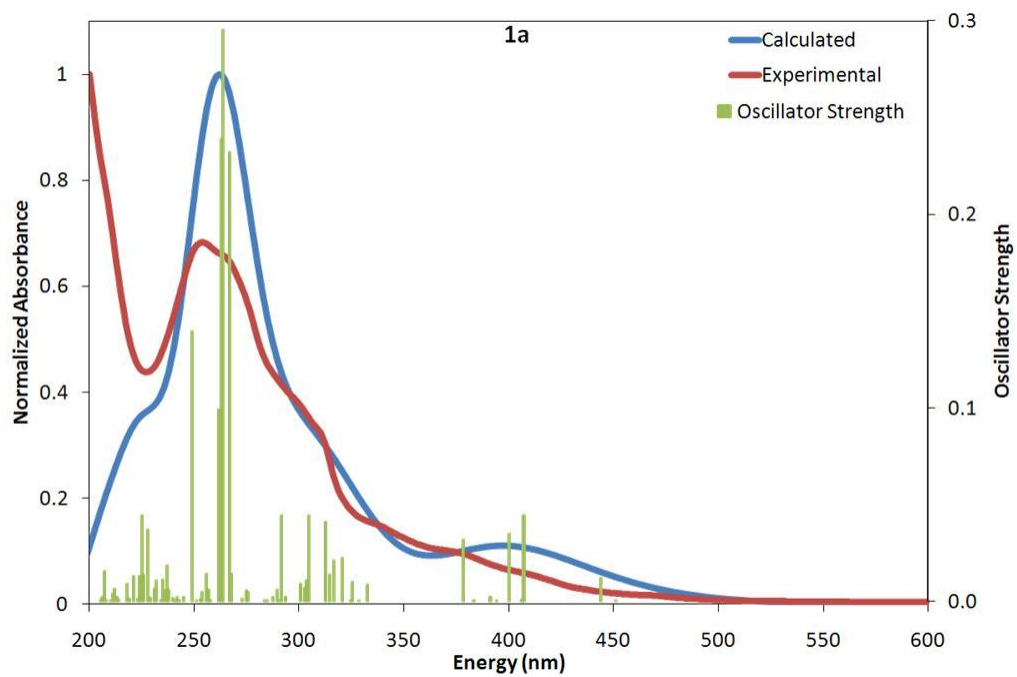


Figure S14 : Calculated and experimental absorption spectra of **1b**

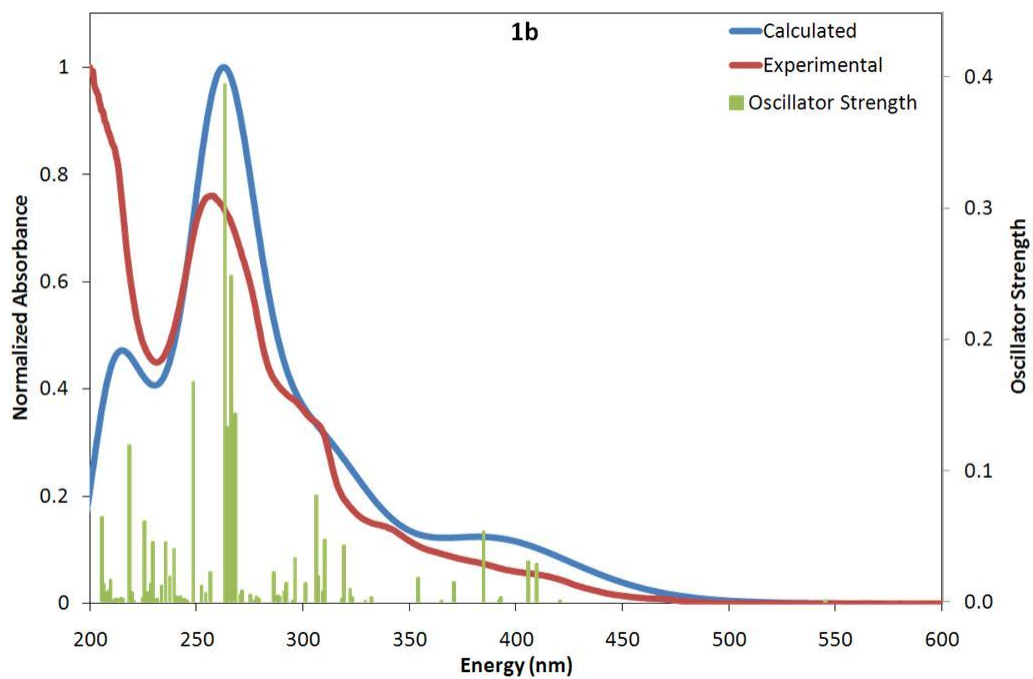


Figure S15 : Calculated and experimental absorption spectra of **3a**

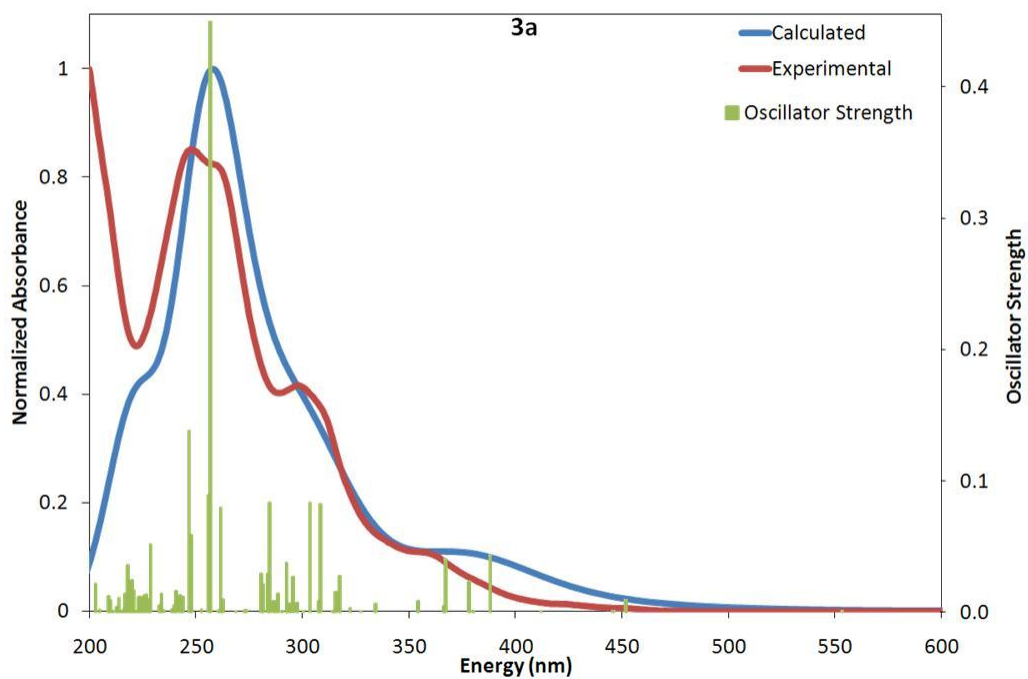


Figure S16 : Calculated and experimental absorption spectra of **3b**

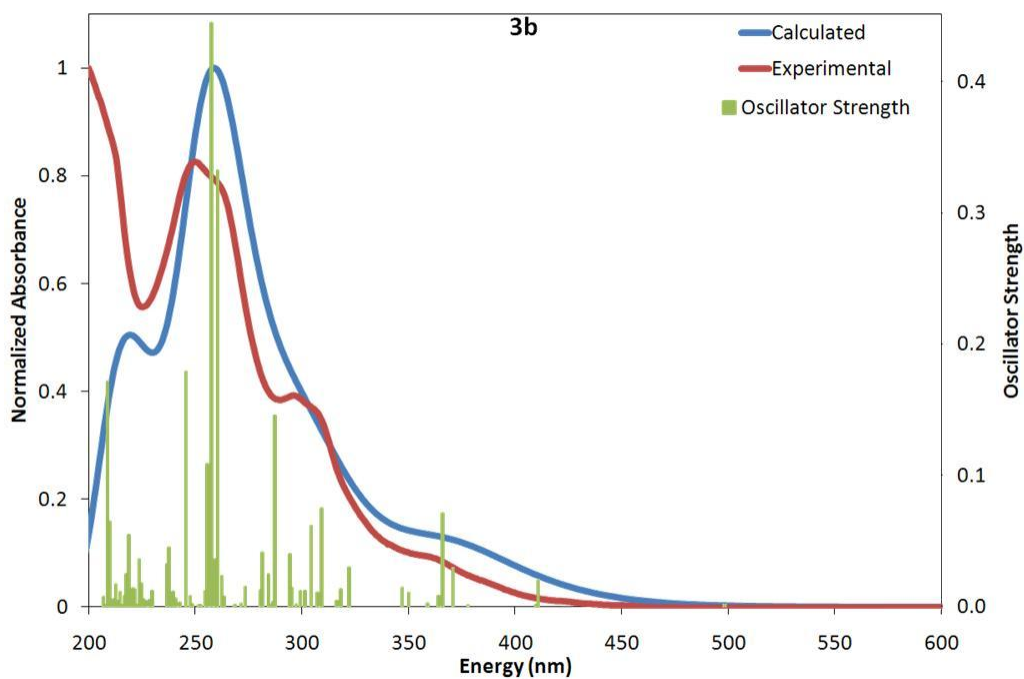


Figure S17: Jablonski diagram for complex **1a**

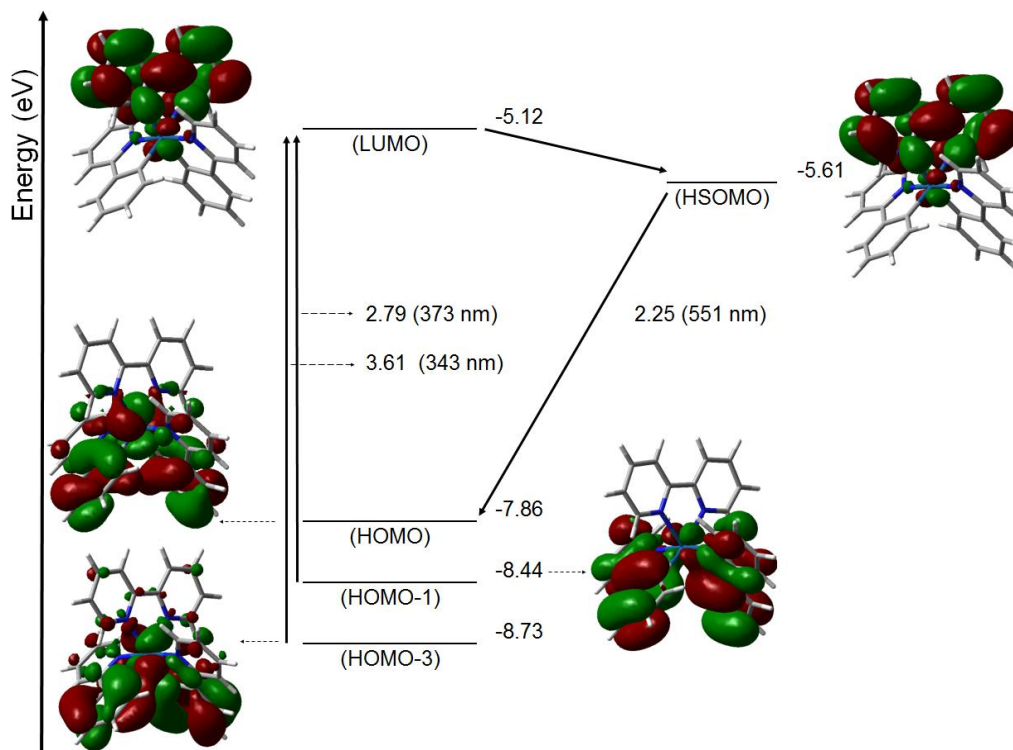


Figure S18: Jablonski diagram for complex **1b**

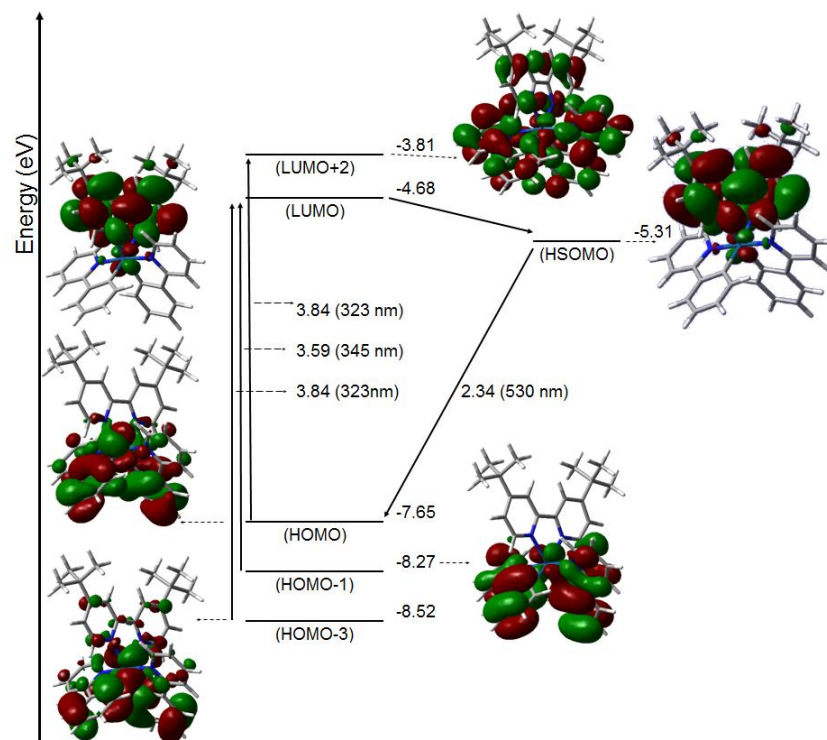


Figure S19: Jablonski diagram for complex **2a**

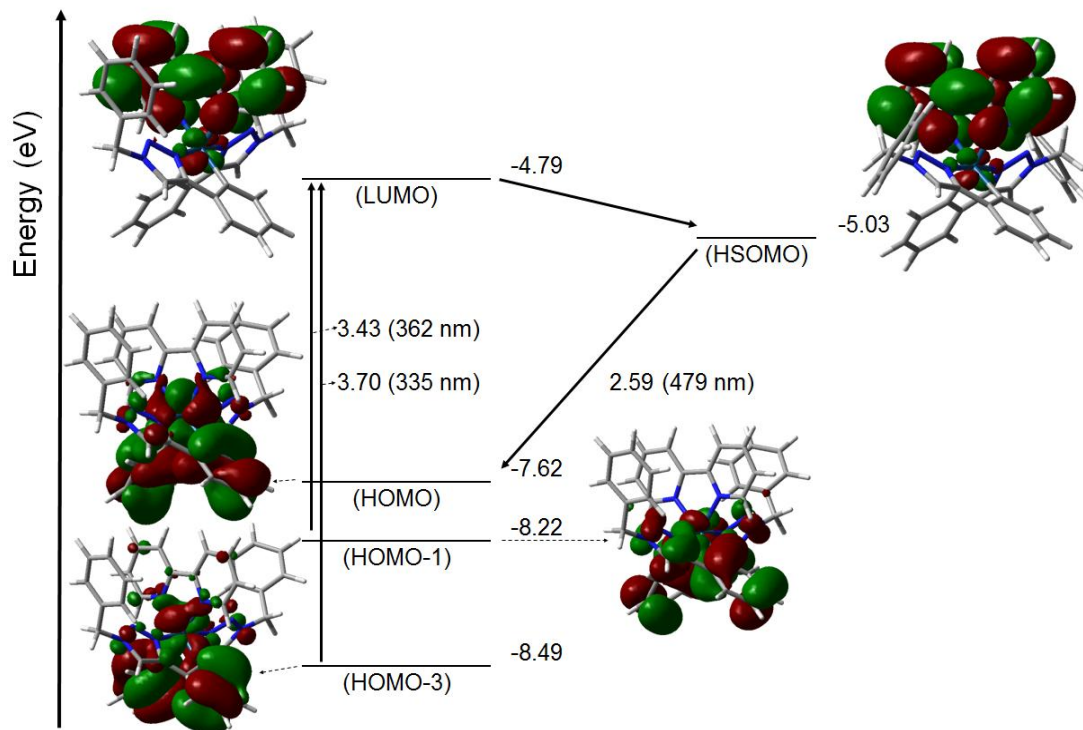


Figure S20: Jablonski diagram for complex **2b**

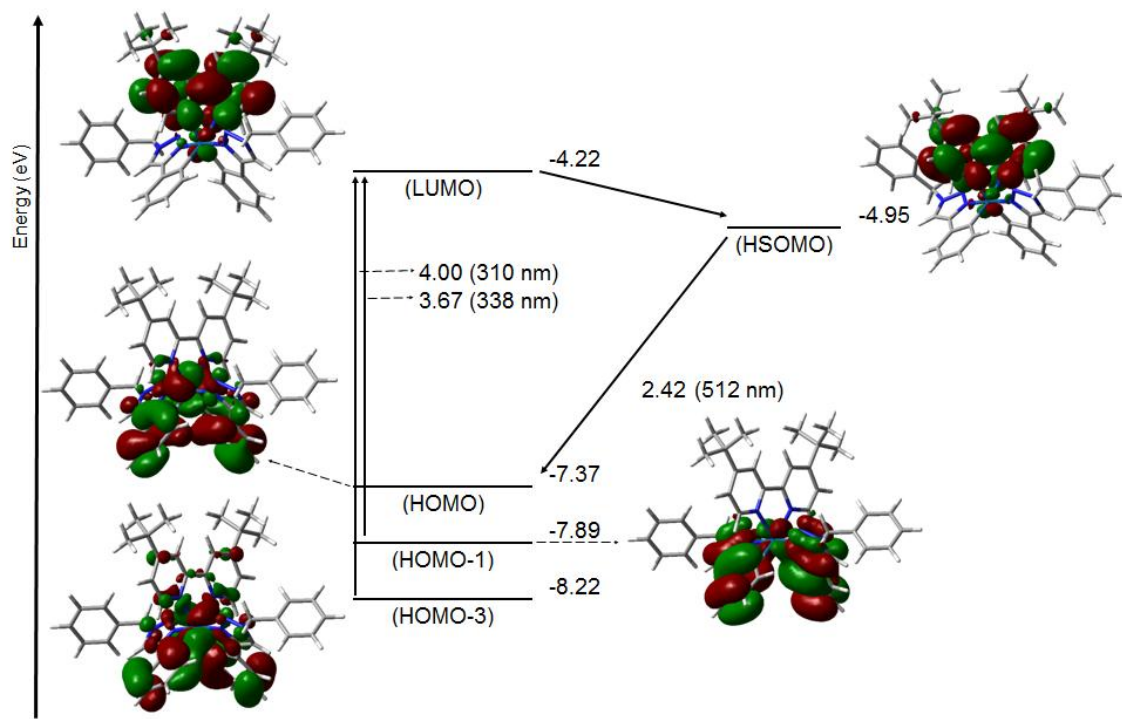


Figure S21: Jablonski diagram for complex **3a**

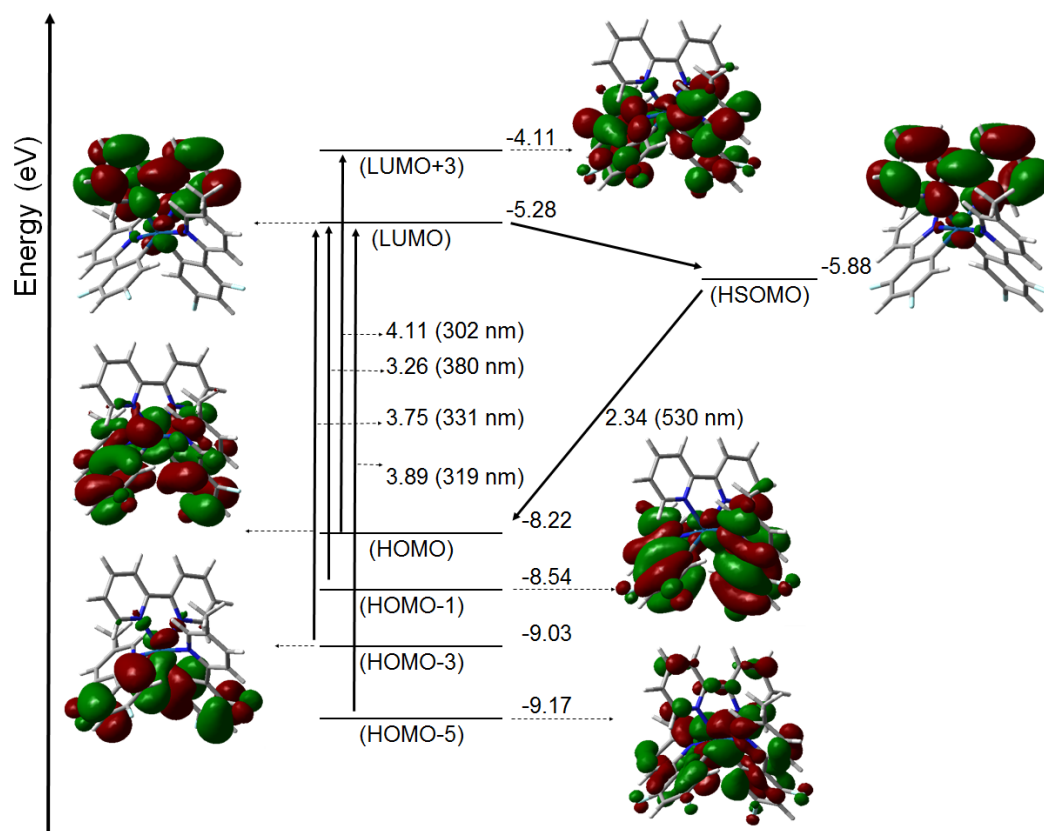


Figure S22: Jablonski diagram for complex **3b**

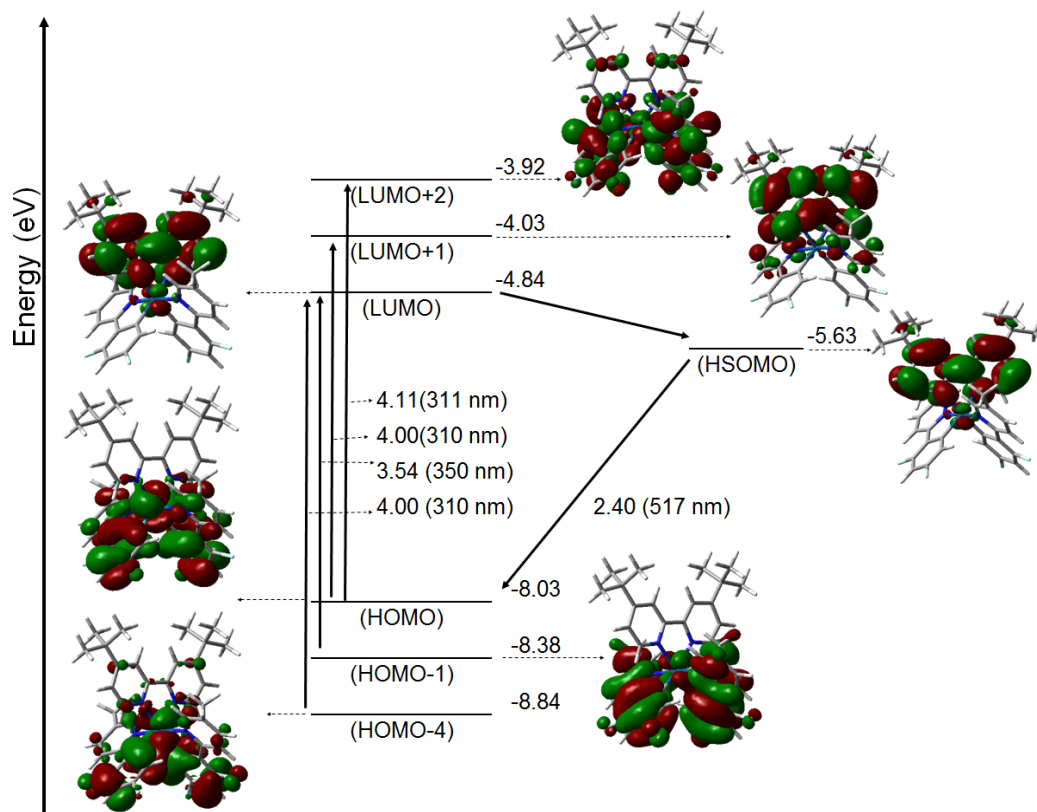


Figure S23: Jablonski diagram for complex **4a**

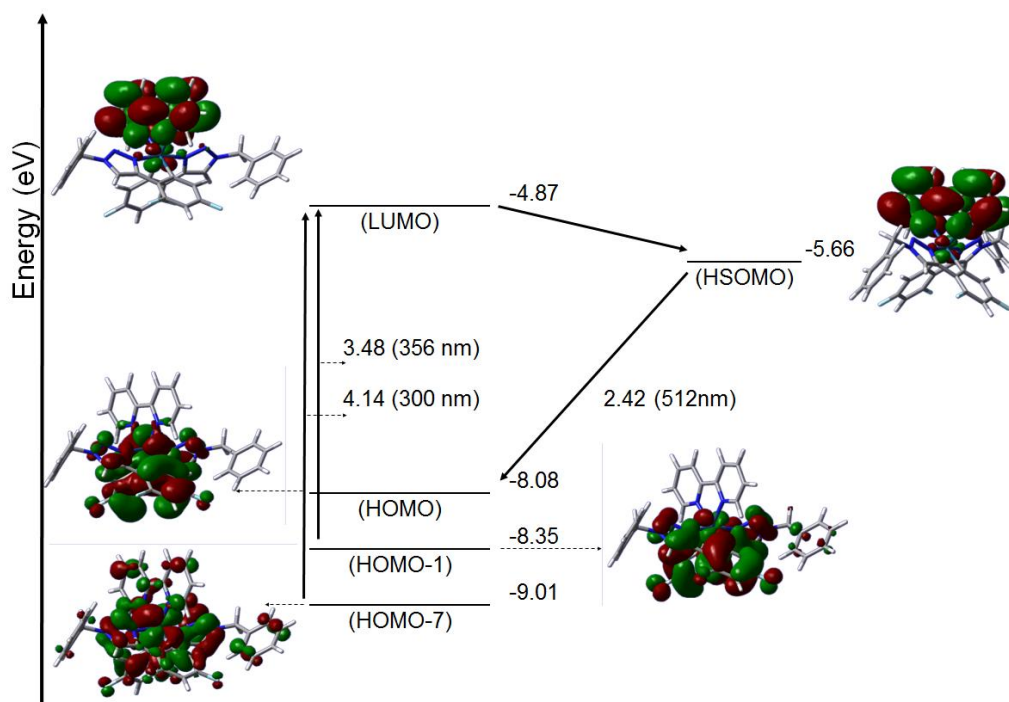
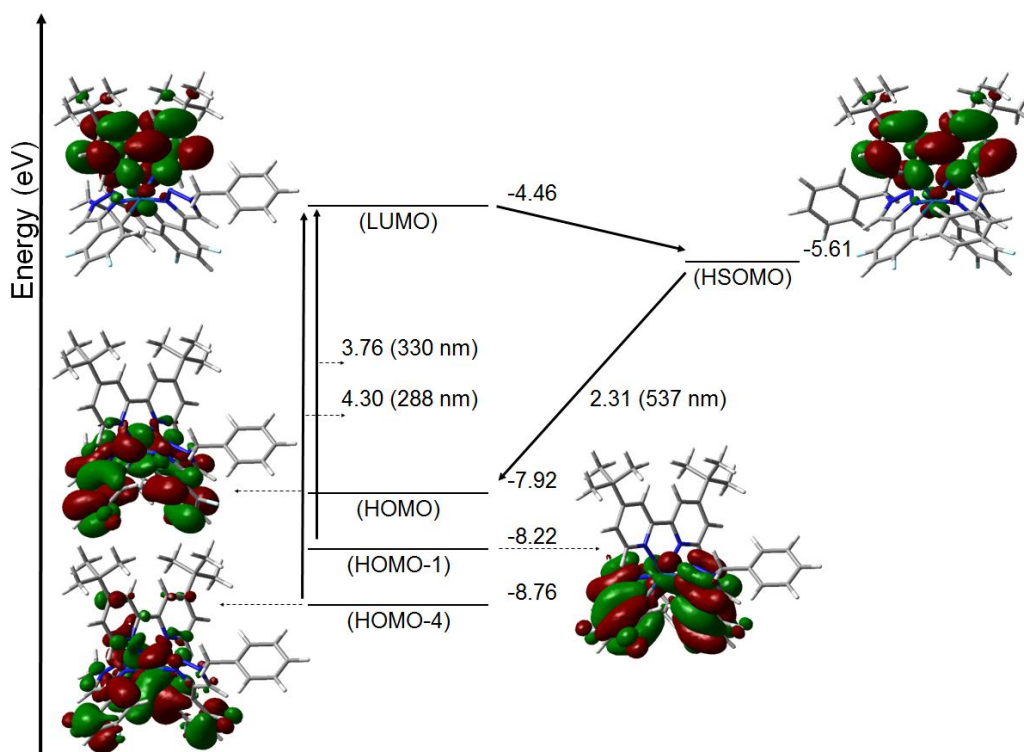


Figure S24: Jablonski diagram for complex **4b**



Cyclic voltammetry: General section

All cyclic voltammograms shown below were measured in ACN (with ca. 0.1M TBAPF₆ as the supporting electrolyte) at a scan rate of 50 mV/sec. Potential windows of either -2 to 1.5 V or -2 V to 2 V were used during voltammogram acquisition. The reversibility and the potentials were found to be independent of the scan rate (from 50 to 200 mV/sec).

Figure S25: Cyclic voltammogram of complex **1a**

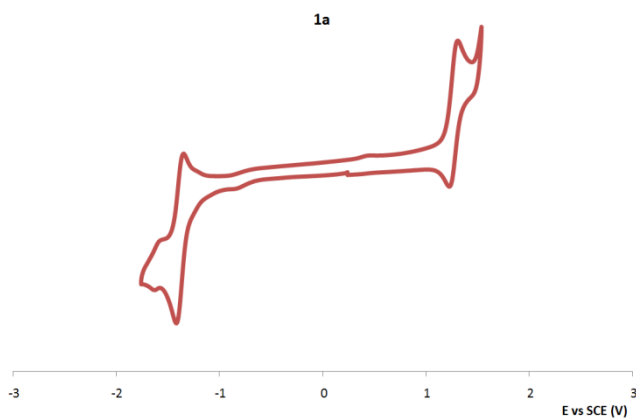


Figure S26: Cyclic voltammogram of complex **1b**

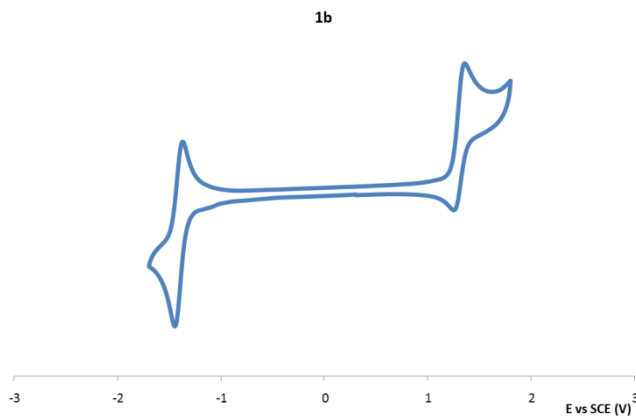


Figure S27: Cyclic v voltammogram of complex **2a**

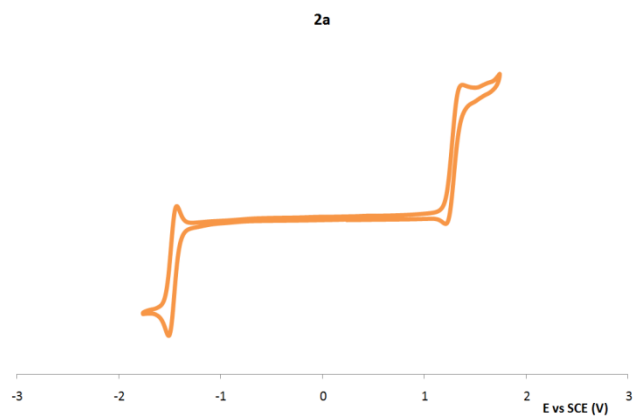


Figure S28: Cyclic voltammogram of complex **2b**

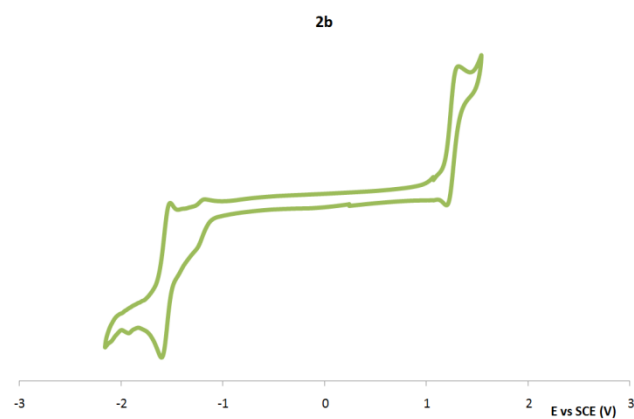


Figure S29: Cyclic voltammogram of complex **3a**

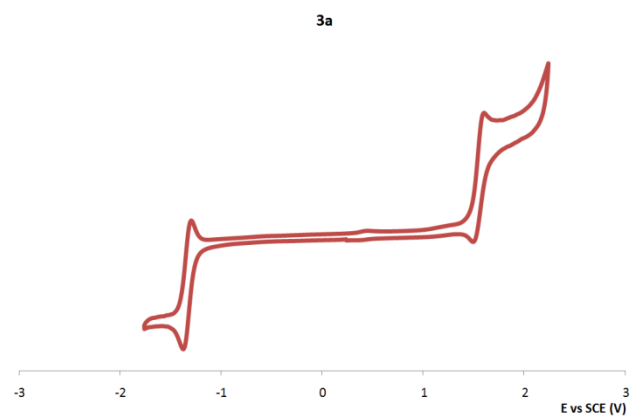


Figure S30: Cyclic voltammogram of complex **3b**

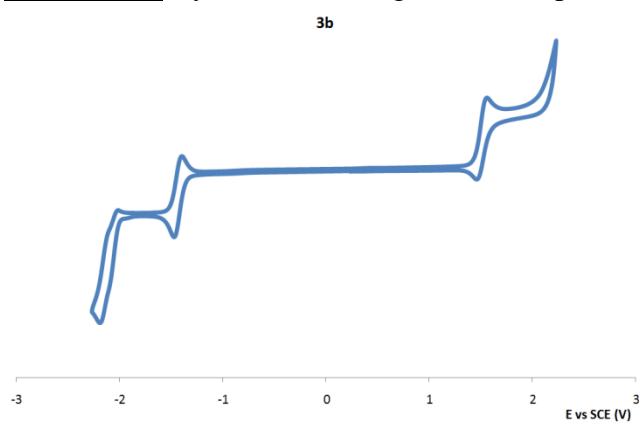


Figure S31: Cyclic voltammogram of complex **4a**

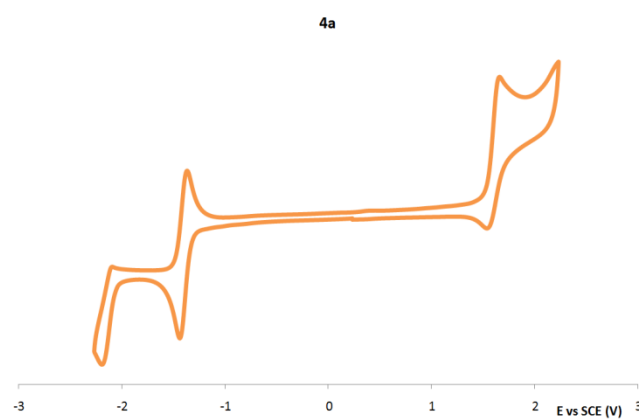


Figure S32: Cyclic voltammogram of complex **4b**

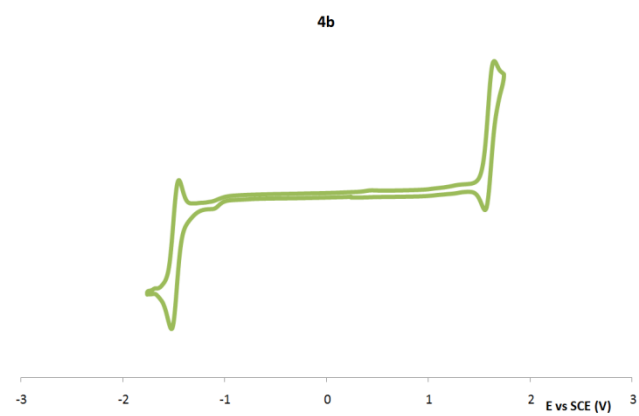


Figure S 33: ^1H and ^{13}C NMRs data of **1a** $[\text{Ir}(\text{ppy})_2\text{bpy}]\text{PF}_6$

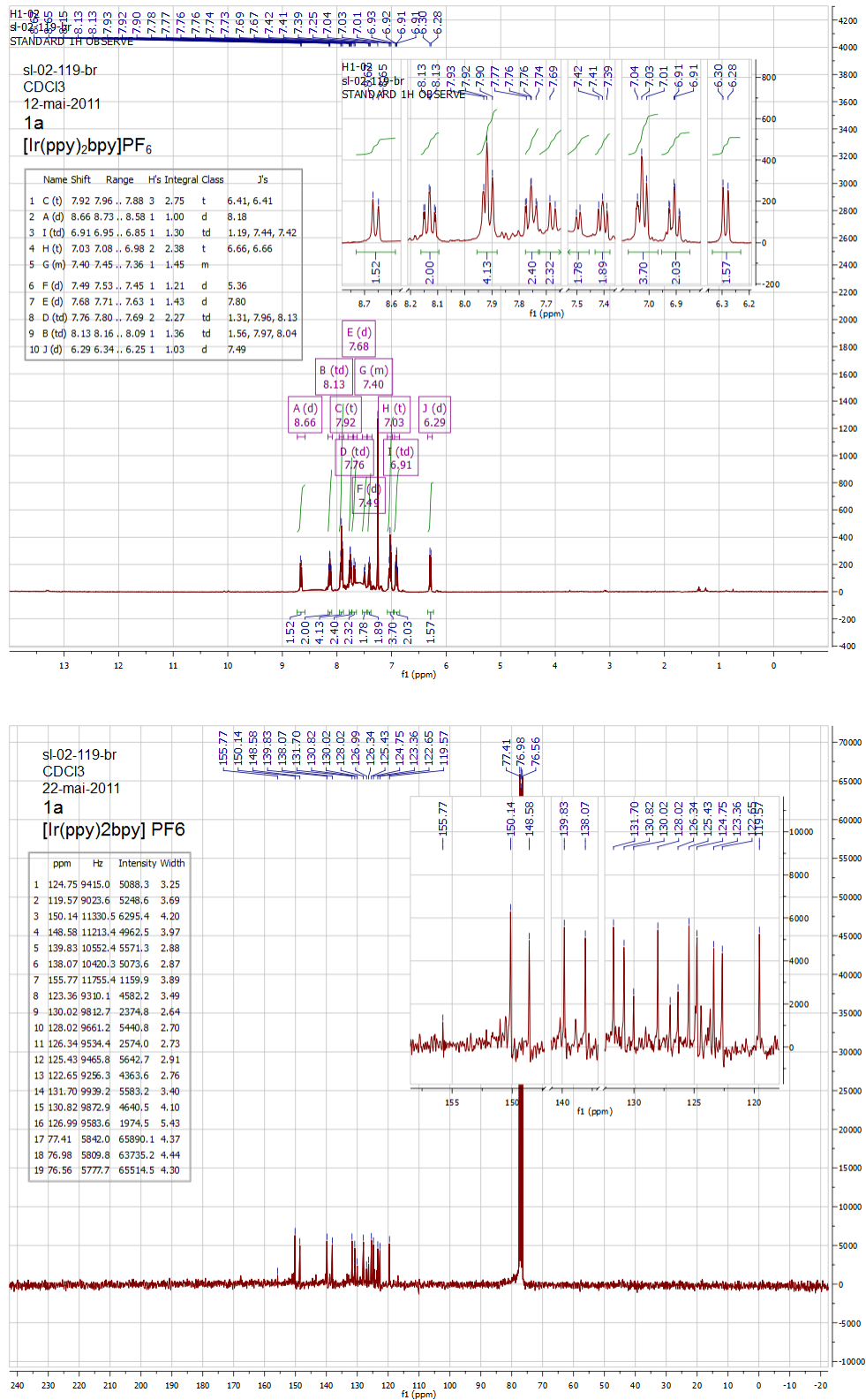


Figure S 34: ^1H and ^{13}C NMRs data of **1b** $[\text{Ir}(\text{ppy})_2\text{di-}t\text{-Bu-bpy}]\text{PF}_6$

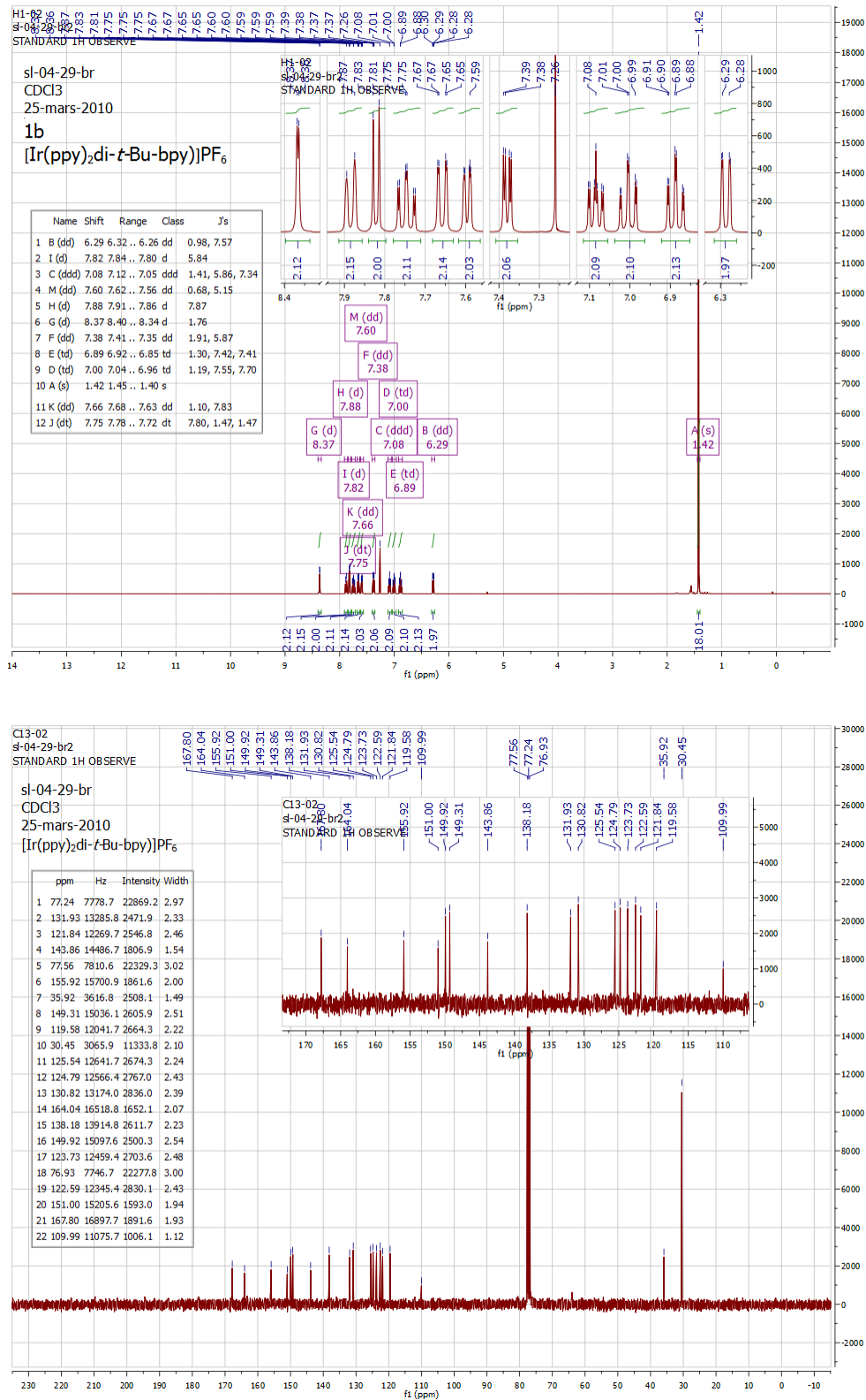


Figure S 35: ^1H and ^{13}C NMRs data of **2a** $[\text{Ir}(\text{phtl})_2\text{bpy}]\text{PF}_6$

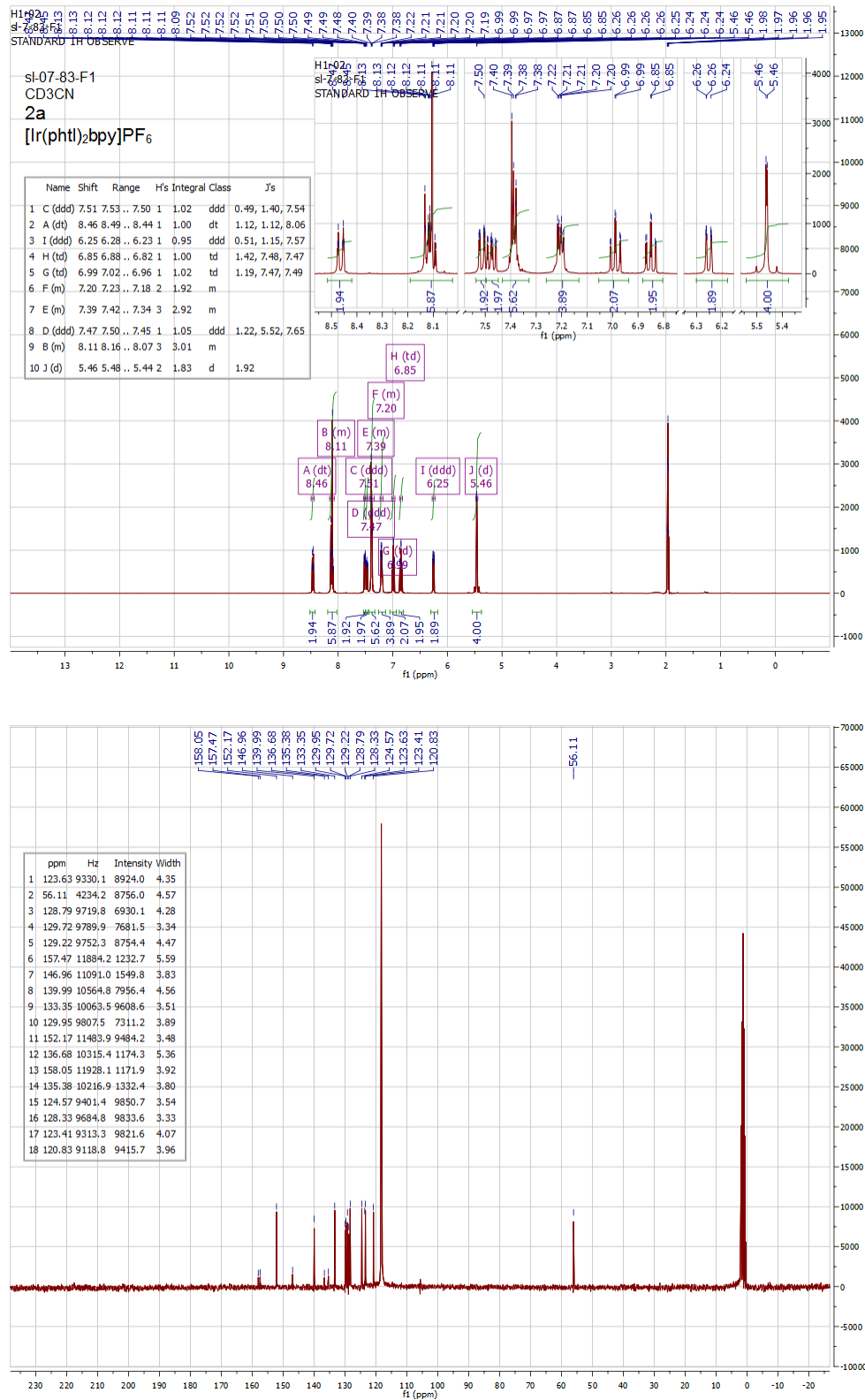


Figure S 36: ^1H and ^{13}C NMRs data of **2b** $[\text{Ir}(\text{phtl})_2\text{dtBubpy}]\text{PF}_6$

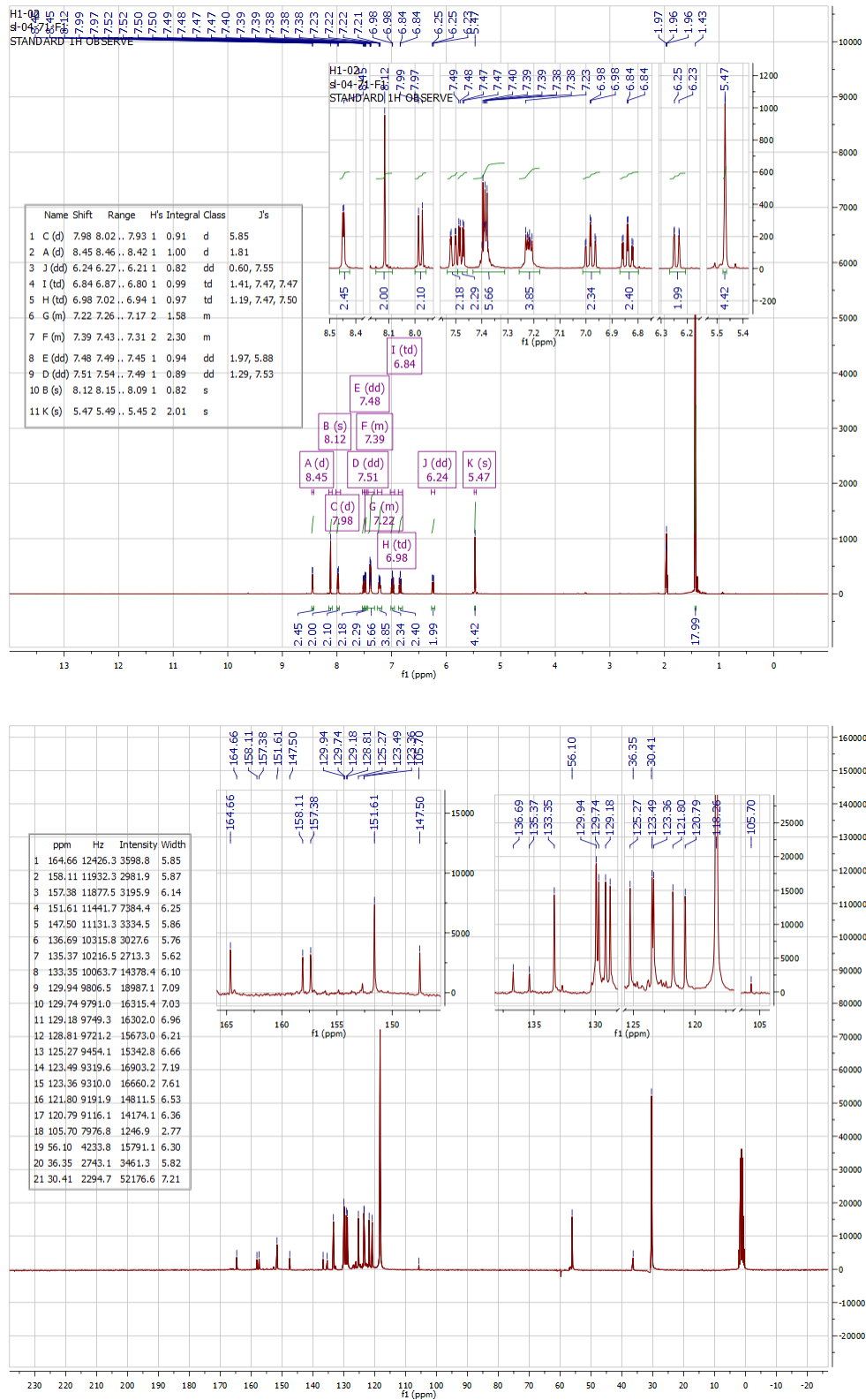


Figure S 37: ^1H and ^{13}C NMRs data of **3a** $[\text{Ir}(\text{dFMeppy})_2\text{bpy}]\text{PF}_6$

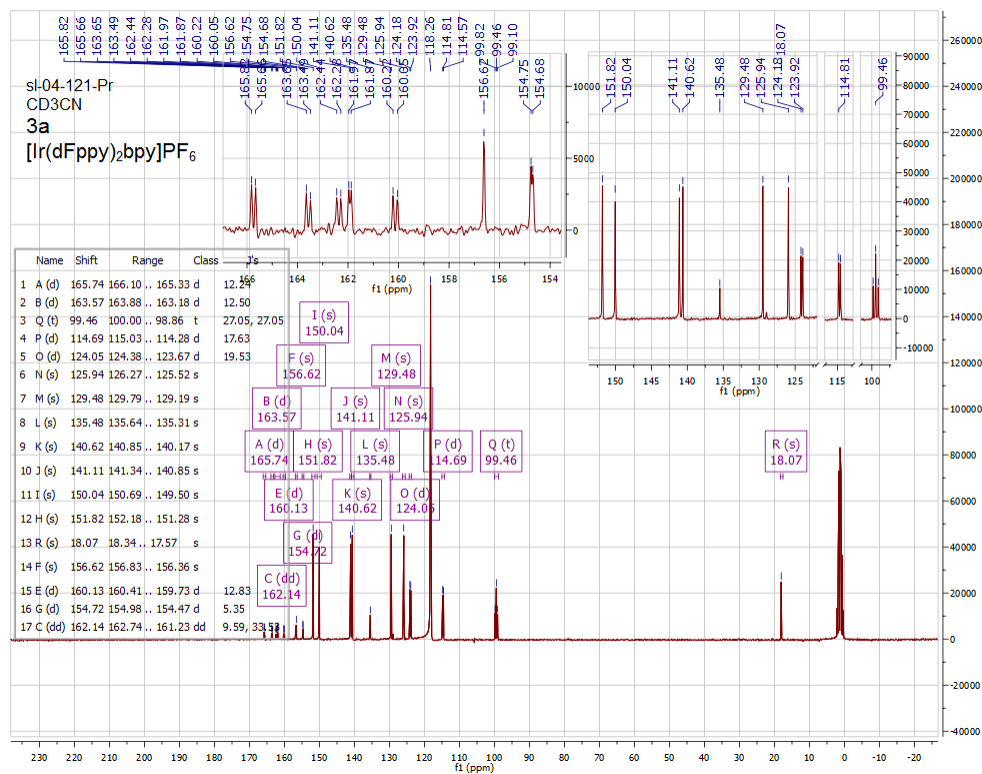
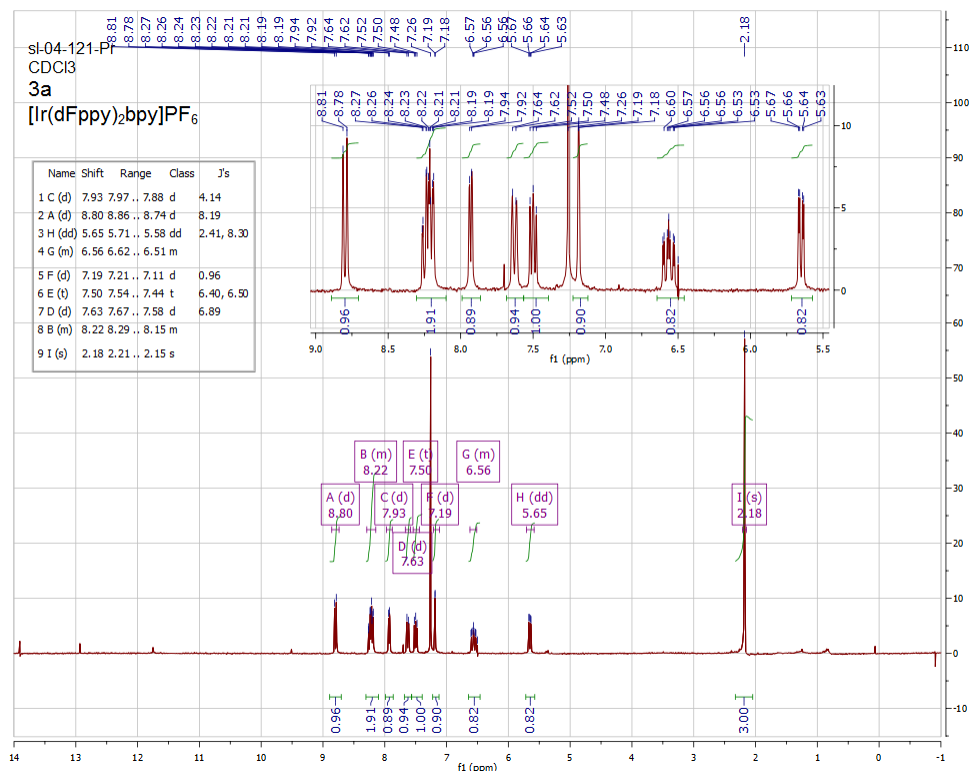


Figure S 38: ^1H and ^{13}C NMRs data of **3b** $[\text{Ir}(\text{dFMeppy})_2\text{dtBubpy}]\text{PF}_6$

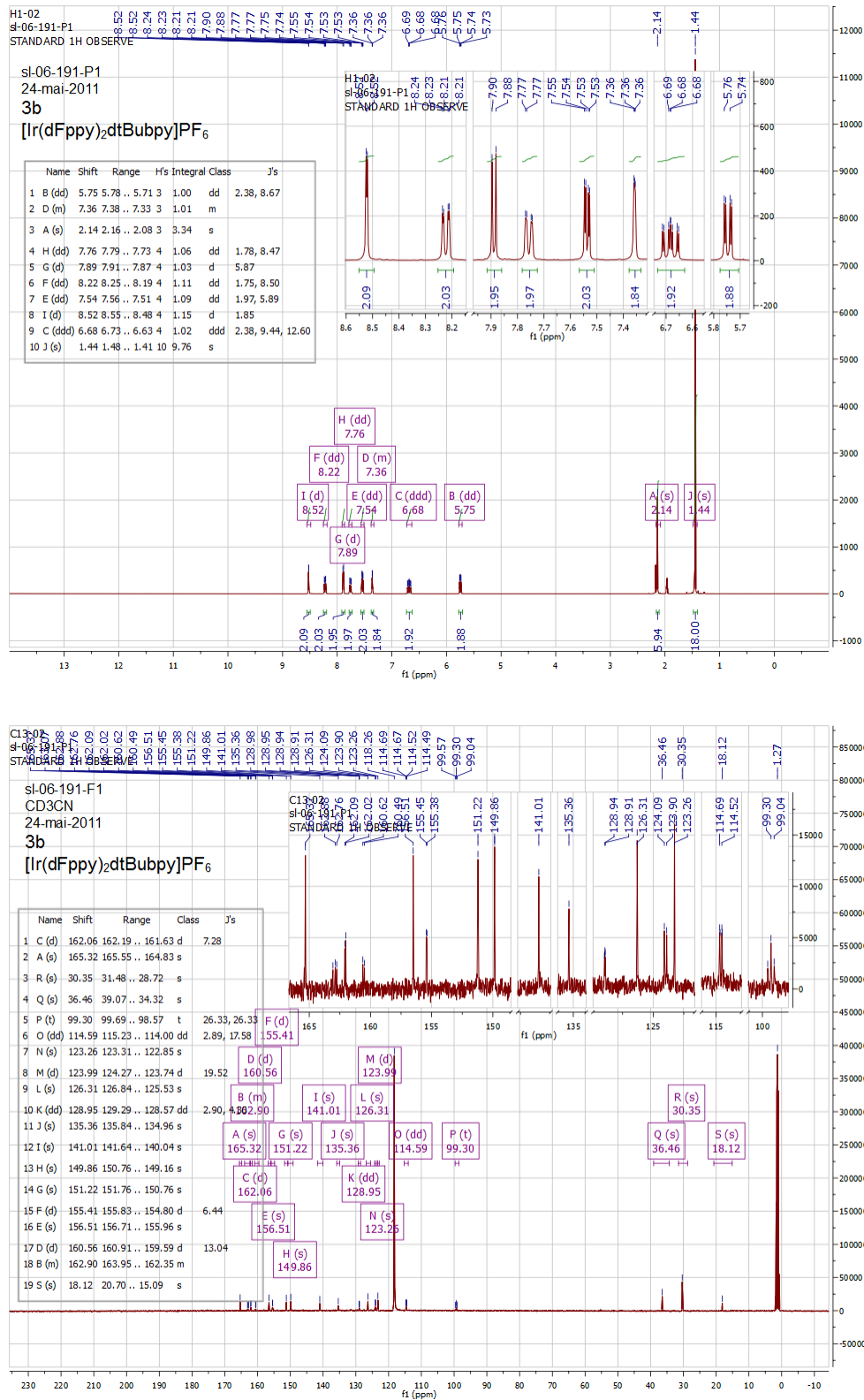


Figure S 39: ^1H and ^{13}C NMRs data of **4a** $[\text{Ir}(\text{dFphtl})_2\text{dtBubpy}]\text{PF}_6$

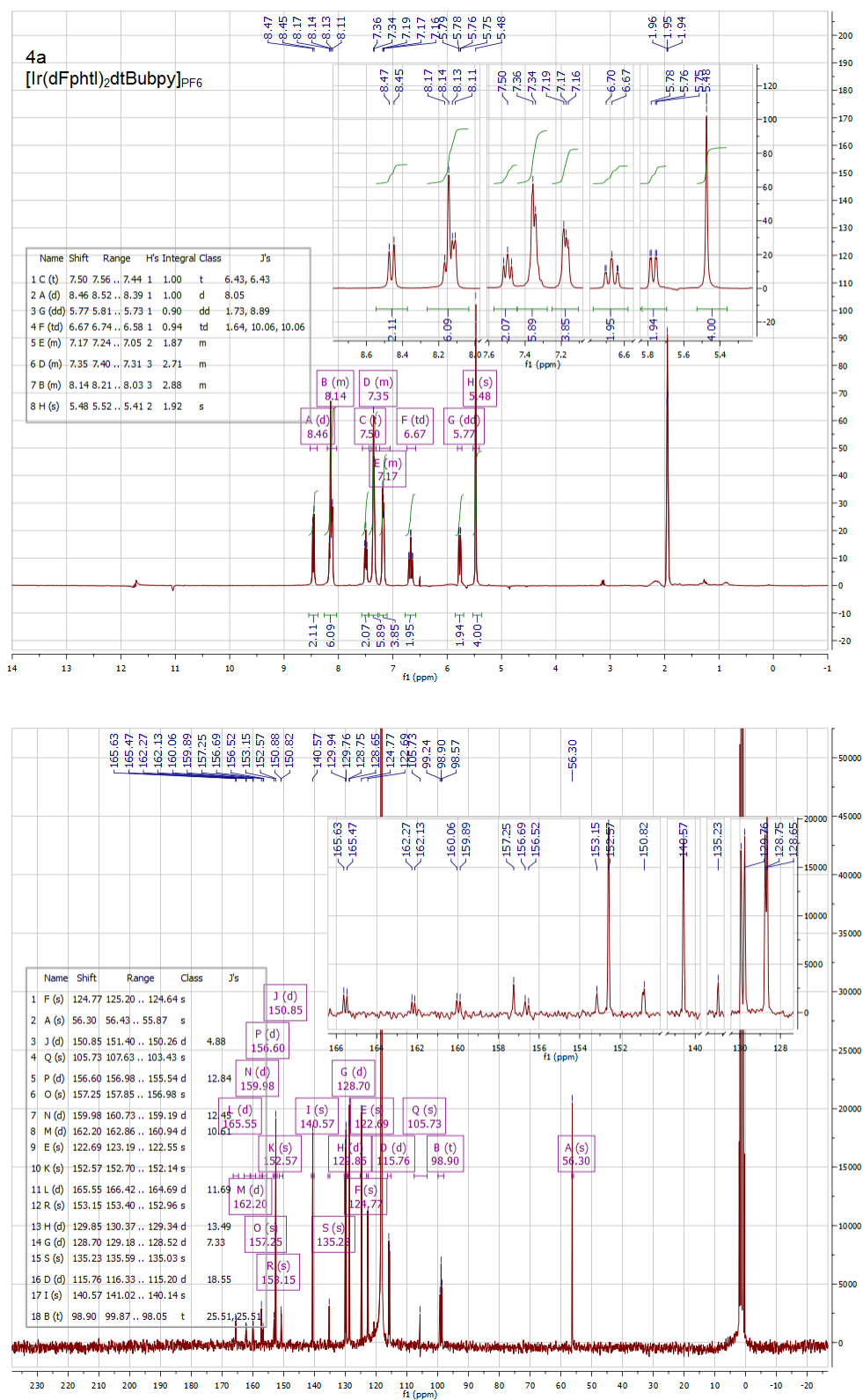


Figure S 40: ^1H and ^{13}C NMRs data of **4b** $[\text{Ir}(\text{dFphtl})_2\text{dtBupy}]\text{PF}_6$

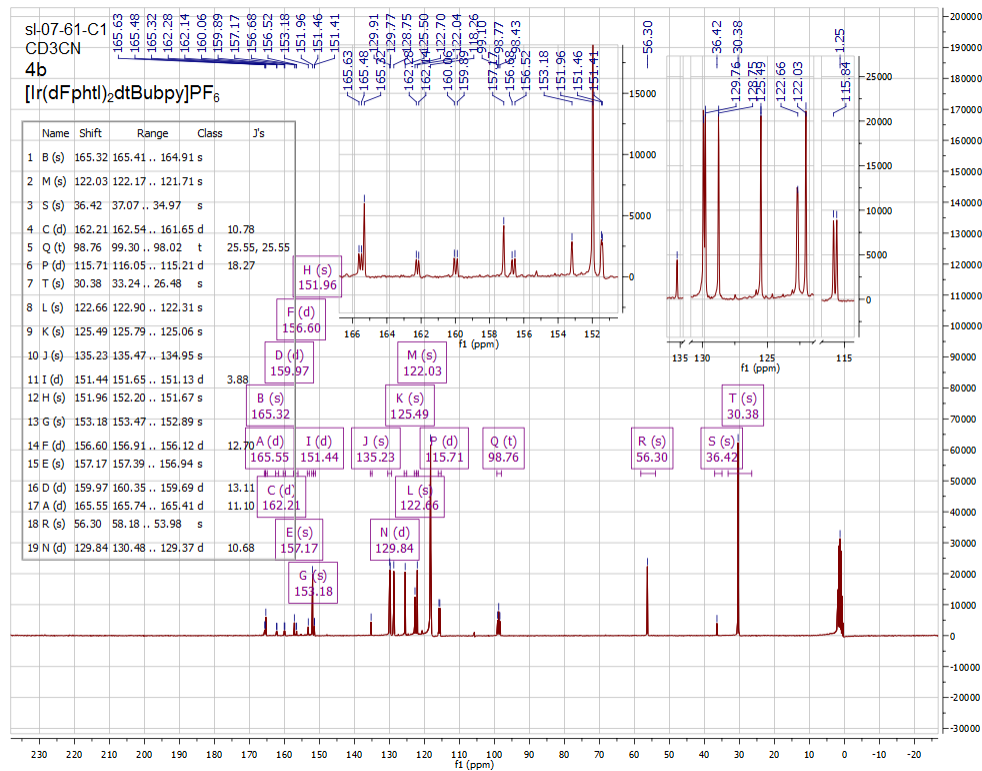
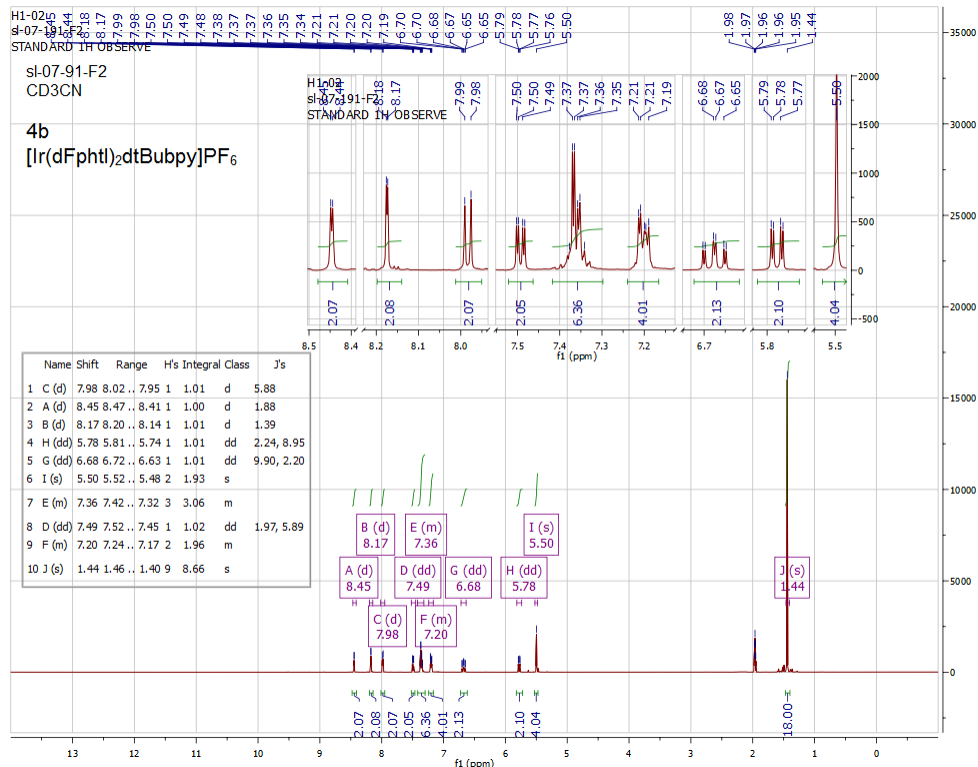


Table S2: Visualisation of MOs of **1a** [Ir(ppy)₂bpy]PF₆

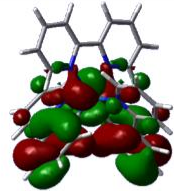
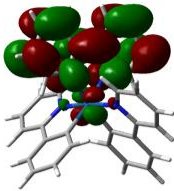
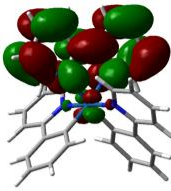
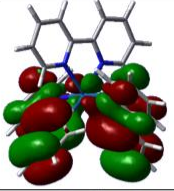
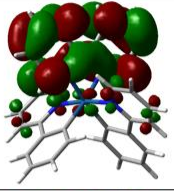
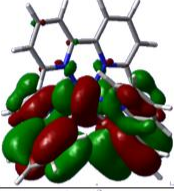
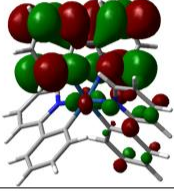
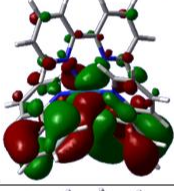
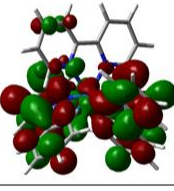
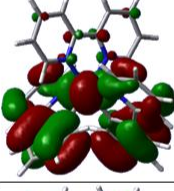
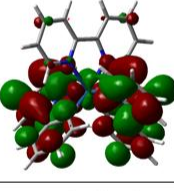
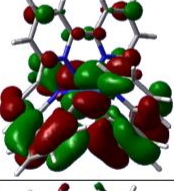
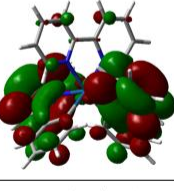
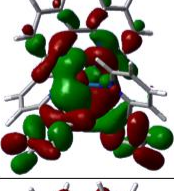
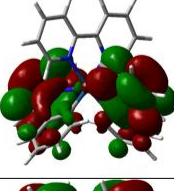
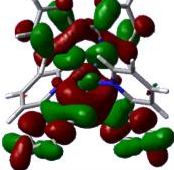
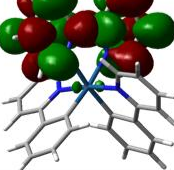
Orbital Energy (eV)	Image	Orbital Energy (eV)	Image	Orbital Energy (eV)	Image
HOMO -7.86		LUMO -5.12		HSOMO -5.61	
HOMO-1 -8.44		LUMO+1 -4.16			
HOMO-2 -8.60		LUMO+2 -4.00			
HOMO-3 -8.73		LUMO+3 -4.00			
HOMO-4 -8.84		LUMO+4 -3.92			
HOMO-5 -8.95		LUMO+5 -3.40			
HOMO-6 -9.99		LUMO+6 -3.35			
HOMO-7 -10.1		LUMO+7 -2.67			

Table S3: Visualisation of MOs of **1b** [Ir(ppy)₂dtBubpy]PF₆

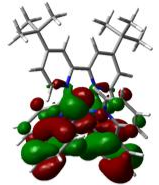
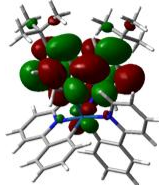
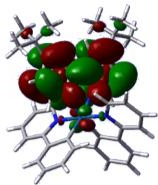
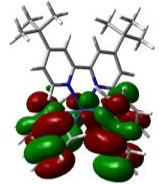
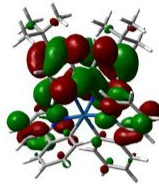
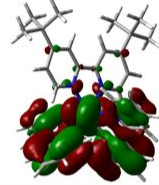
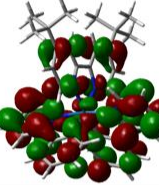
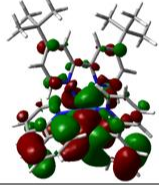
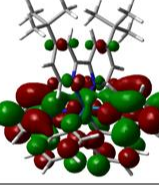
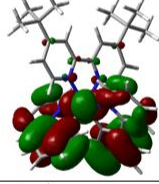
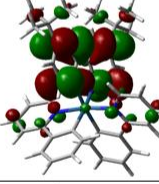
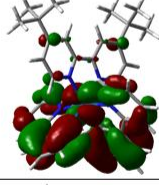
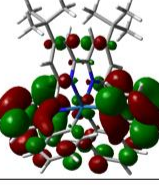
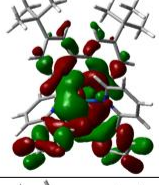
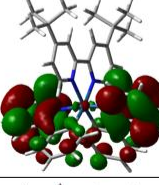
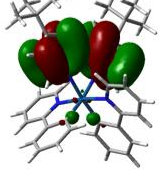
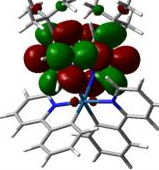
Orbital Energy (eV)	Image	Orbital Energy (eV)	Image	Orbital Energy (eV)	Image
HOMO -7.65		LUMO -4.68		HSOMO -5.31	
HOMO-1 -8.27		LUMO+1 -3.86			
HOMO-2 -8.41		LUMO+2 -3.81			
HOMO-3 -8.52		LUMO+3 -3.73			
HOMO-4 -8.65		LUMO+4 -3.65			
HOMO-5 -8.73		LUMO+5 -3.24			
HOMO-6 -9.77		LUMO+6 -3.18			
HOMO-7 -9.80		LUMO+7 -2.29			

Table S4: Visualisation of MOs of **2a** [Ir(phtl)₂bpy]PF₆

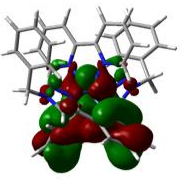
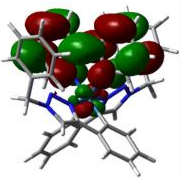
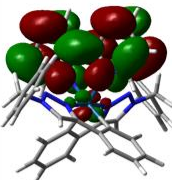
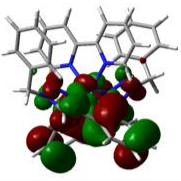
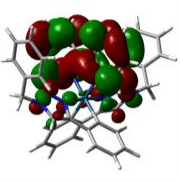
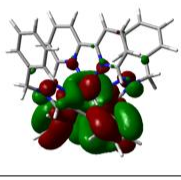
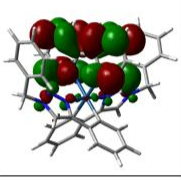
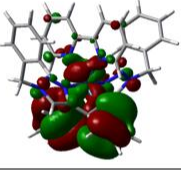
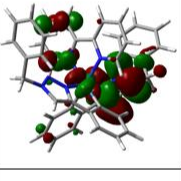
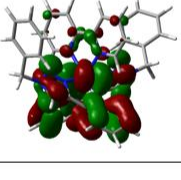
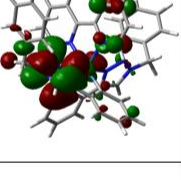
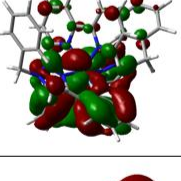
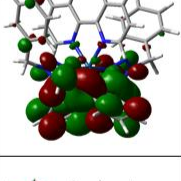
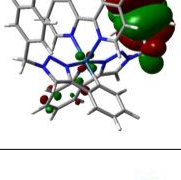
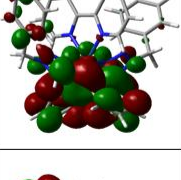
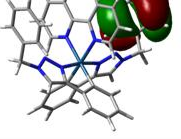
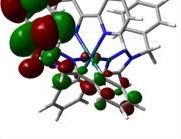
Orbital Energy (eV)	Image	Orbital Energy (eV)	Image	Orbital Energy (eV)	Image
HOMO -7.62		LUMO -4.63		HSOMO -5.03	
HOMO-1 -8.11		LUMO+1 -3.70			
HOMO-2 -8.33		LUMO+2 -3.54			
HOMO-3 -8.49		LUMO+3 -3.40			
HOMO-4 -8.63		LUMO+4 -3.37			
HOMO-5 -8.71		LUMO+5 -2.91			
HOMO-6 -8.93		LUMO+6 -2.75			
HOMO-7 -9.03		LUMO+7 -2.37			

Table S5: Visualisation of MOs of **2b** [Ir(phtl)₂dtBubpy]PF₆

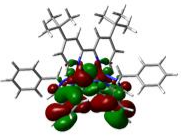
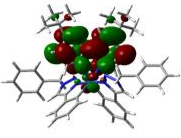
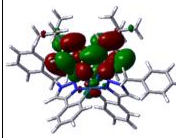
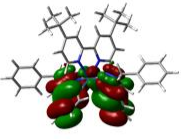
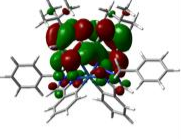
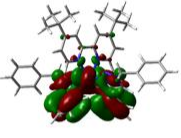
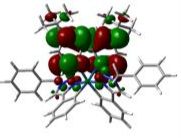
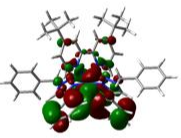
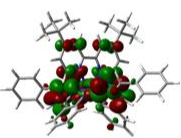
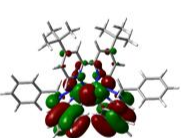
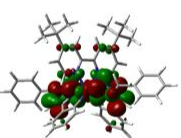
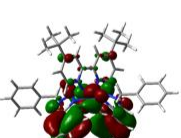
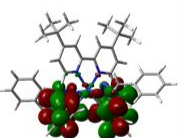
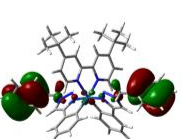
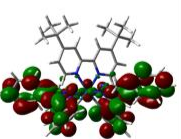
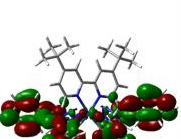
Orbital Energy (eV)	Image	Orbital Energy (eV)	Image	Orbital Energy (eV)	Image
HOMO -7.37		LUMO -4.22		HSOMO -4.95	
HOMO-1 -7.89		LUMO+1 -3.40			
HOMO-2 -8.08		LUMO+2 -3.21			
HOMO-3 -8.22		LUMO+3 -3.10			
HOMO-4 -8.35		LUMO+4 -3.10			
HOMO-5 -8.44		LUMO+5 -2.61			
HOMO-6 -9.09		LUMO+6 -2.50			
HOMO-7 -9.09		LUMO+7 -2.45			

Table S6: Visualisation of MOs of **3a** [Ir(dFppy)₂bpy]PF₆

Orbital Energy (eV)	Image	Orbital Energy (eV)	Image	Orbital Energy (eV)	Image
HOMO -8.22		LUMO -5.28		HSOMO -5.88	
HOMO-1 -8.54		LUMO+1 -4.33			
HOMO-2 -8.68		LUMO+2 -4.19			
HOMO-3 -9.03		LUMO+3 -4.11			
HOMO-4 -9.03		LUMO+4 -4.00			
HOMO-5 -9.17		LUMO+5 -3.37			
HOMO-6 -10.26		LUMO+6 -3.32			
HOMO-7 -10.31		LUMO+7 -2.86			

Table S7: Visualisation of MOs of **3b** [Ir(dFppy)₂dtBubpy]PF₆

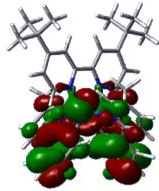
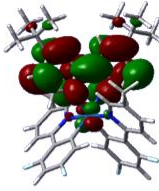
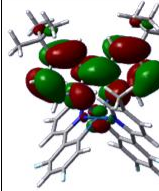
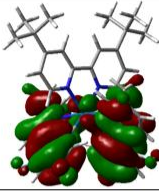
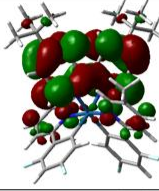
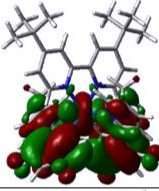
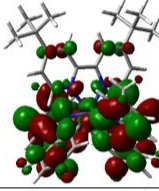
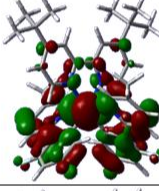
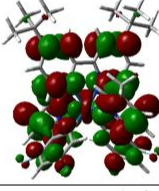
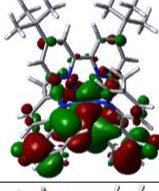
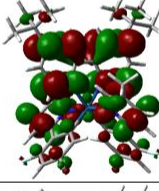
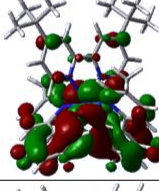
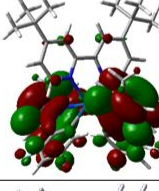
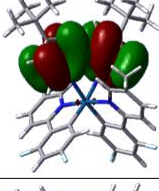
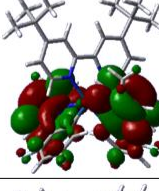
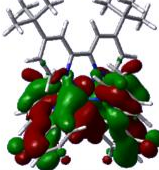
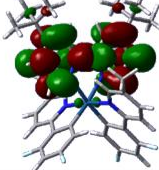
Orbital Energy (eV)	Image	Orbital Energy (eV)	Image	Orbital Energy (eV)	Image
HOMO -8.03		LUMO -4.84		HSOMO -5.63	
HOMO-1 -8.38		LUMO+1 -4.03			
HOMO-2 -8.49		LUMO+2 -3.92			
HOMO-3 -8.82		LUMO+3 -3.86			
HOMO-4 -8.84		LUMO+4 -3.81			
HOMO-5 -8.93		LUMO+5 -3.18			
HOMO-6 -9.96		LUMO+6 -3.16			
HOMO-7 -10.1		LUMO+7 -2.45			

Table S8: Visualisation of MOs of **4a** [Ir(dFphtl)₂bpy]PF₆

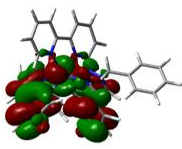
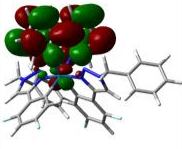
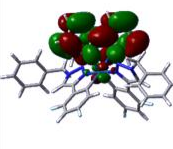
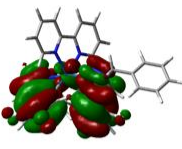
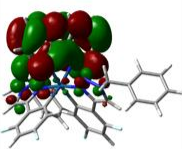
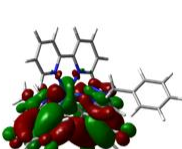
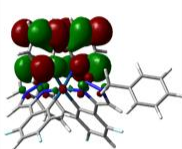
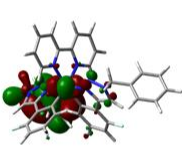
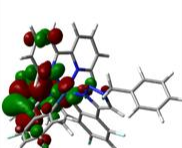
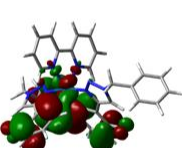
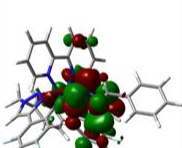
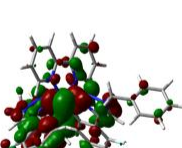
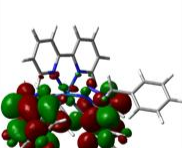
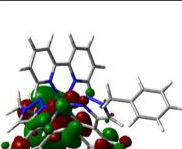
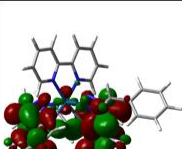
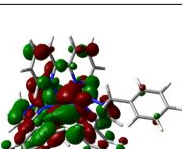
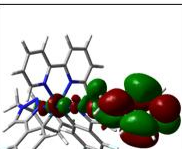
Orbital Energy (eV)	Image	Orbital Energy (eV)	Image	Orbital Energy (eV)	Image
HOMO -8.08		LUMO -4.87		HSOMO -5.66	
HOMO-1 -8.35		LUMO+1 -3.92			
HOMO-2 -8.52		LUMO+2 -3.76			
HOMO-3 -8.90		LUMO+3 -3.62			
HOMO-4 -8.90		LUMO+4 -3.54			
HOMO-5 -8.93		LUMO+5 -3.02			
HOMO-6 -8.98		LUMO+6 -2.88			
HOMO-7 -9.01		LUMO+7 -2.64			

Table S9: Visualisation of MOs of **4b** [Ir(dFphtl)₂dtBubpy]PF₆

Orbital Energy (eV)	Image	Orbital Energy (eV)	Image	Orbital Energy (eV)	Image
HOMO -7.92		LUMO -4.46		HSOMO -5.61	
HOMO-1 -8.22		LUMO+1 -3.65			
HOMO-2 -8.38		LUMO+2 -3.48			
HOMO-3 -8.71		LUMO+3 -3.43			
HOMO-4 -8.76		LUMO+4 -3.37			
HOMO-5 -8.82		LUMO+5 -2.91			
HOMO-6 -8.82		LUMO+6 -2.78			
HOMO-7 -8.87		LUMO+7 -2.53			

Table S10: Energy and composition of TD-DFT calculated transitions of **1a**

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	16464.3093	607.374402	0.0002	Singlet-A	HOMO->LUMO (99%)
2	22152.977	451.4066	0.0005	Singlet-A	H-4->LUMO (21%), H-2->LUMO (78%)
3	22517.5421	444.098204	0.0121	Singlet-A	H-1->LUMO (99%)
4	24567.8176	407.036562	0.0445	Singlet-A	H-3->LUMO (85%)
5	24619.4374	406.183124	0.001	Singlet-A	HOMO->L+1 (96%)
6	25004.9731	399.920446	0.035	Singlet-A	HOMO->L+3 (94%)
7	25403.4138	393.647881	0.0002	Singlet-A	H-4->LUMO (76%), H-2->LUMO (-21%)
8	25546.9814	391.435678	0.0023	Singlet-A	HOMO->L+2 (76%), HOMO->L+4 (-21%)
9	26112.38	382.960113	0.0001	Singlet-A	H-5->LUMO (11%), HOMO->L+2 (15%), HOMO->L+4 (64%)
10	26460.0074	377.928844	0.032	Singlet-A	H-5->LUMO (77%), HOMO->L+4 (-12%)
11	30127.4357	331.923371	0.0085	Singlet-A	H-1->L+1 (91%)
12	30468.6106	328.20663	0.0004	Singlet-A	H-4->L+1 (11%), H-2->L+1 (66%), HOMO-> L+5 (-19%)
13	30533.1354	327.513041	0.0092	Singlet-A	H-2->L+1 (16%), HOMO->L+5 (72%)
14	30814.6248	324.521232	0.0098	Singlet-A	H-1->L+3 (81%)
15	30874.3102	323.893876	0.0001	Singlet-A	HOMO->L+6 (94%)
16	30906.5726	323.555773	0.0287	Singlet-A	H-2->L+3 (49%), H-1->L+2 (11%), H-1->L+4 (- 11%)
17	31263.0722	319.866197	0.0225	Singlet-A	H-2->L+3 (-15%), H-1->L+2 (74%)
18	31619.5717	316.259818	0.0212	Singlet-A	H-1->L+4 (76%)
19	31786.5296	314.598672	0	Singlet-A	H-3->L+3 (21%), H-2->L+2 (32%), H-2->L+4 (- 18%)
20	31892.9955	313.548472	0.0139	Singlet-A	H-3->L+1 (11%), H-2->L+2 (29%), H-2->L+4 (32%)
21	32079.3109	311.727395	0.041	Singlet-A	H-3->L+1 (63%), H-2->L+2 (-12%)
22	32900.389	303.947774	0.0442	Singlet-A	H-5->L+2 (13%), H-3->L+2 (59%), H-3->L+4 (- 11%)
23	33045.5698	302.612425	0.011	Singlet-A	H-6->LUMO (92%)
24	33146.3898	301.691981	0.0068	Singlet-A	H-4->L+1 (71%), H-2->L+1 (-12%)
25	33298.023	300.31813	0.0093	Singlet-A	H-3->L+1 (10%), H-3->L+3 (39%), H-2->L+4 (14%)
26	33337.5445	299.962104	0.0345	Singlet-A	H-3->L+4 (55%)
27	34093.2912	293.312838	0.002	Singlet-A	H-5->L+1 (66%), H-3->L+3 (11%)
28	34177.98	292.586045	0.0514	Singlet-A	H-4->L+3 (64%), H-2->L+3 (-12%)
29	34405.4299	290.651796	0.0443	Singlet-A	H-4->L+2 (31%), H-4->L+4 (-28%), H-1->L+5 (- 18%)
30	34446.5645	290.304713	0.0001	Singlet-A	H-9->LUMO (-11%), H-7->LUMO (78%)
31	34560.2894	289.349429	0.0063	Singlet-A	H-5->L+1 (10%), H-5->L+3 (50%), H-4->L+2 (10%)
32	34820.8083	287.184603	0.0022	Singlet-A	H-4->L+2 (38%), H-4->L+4 (35%), H-2->L+4 (- 12%)
33	34879.6872	286.699819	0.0069	Singlet-A	H-5->L+2 (-31%), H-5->L+4 (32%), H-3->L+2 (10%)
34	35185.3734	284.209006	0.0002	Singlet-A	H-9->LUMO (42%), H-5->L+2 (-19%), H-5-> L+4 (-17%)
35	35392.6594	282.544465	0.0003	Singlet-A	H-9->LUMO (44%), H-5->L+2 (19%), H-5-> L+4 (11%)
36	36386.3413	274.828401	0.005	Singlet-A	H-2->L+6 (-38%), H-1->L+5 (50%)
37	36432.3152	274.481595	0.0056	Singlet-A	H-2->L+5 (48%), H-1->L+6 (-40%)
38	36732.3555	272.239552	0.0012	Singlet-A	HOMO->L+7 (98%)
39	37384.8626	267.487943	0.0143	Singlet-A	H-3->L+5 (46%), H-2->L+6 (-22%), H-1->L+5 (- 13%)
40	37623.6043	265.79059	0.2322	Singlet-A	H-5->L+4 (-10%), H-3->L+6 (-26%), H-2->L+5 (14%), H-1->L+6 (33%)
41	37987.3629	263.245439	0.2955	Singlet-A	H-8->LUMO (65%)
42	38207.5538	261.72835	0.2391	Singlet-A	H-3->L+6 (53%)
43	38357.5739	260.704705	0.099	Singlet-A	H-3->L+5 (35%), H-2->L+6 (14%)
44	38984.271	256.51371	0.0006	Singlet-A	HOMO->L+9 (42%), HOMO->L+10 (-33%)
45	39137.5174	255.509308	0.006	Singlet-A	H-10->LUMO (99%)
46	39281.8917	254.570225	0.0142	Singlet-A	H-4->L+5 (79%), H-2->L+5 (-11%)
47	39602.9026	252.506745	0.0046	Singlet-A	H-4->L+6 (75%), H-2->L+6 (-14%)
48	39706.9488	251.845088	0.0013	Singlet-A	H-11->LUMO (97%)
49	39982.7923	250.107594	0.0001	Singlet-A	H-5->L+5 (78%)
50	40036.0253	249.775045	0.0327	Singlet-A	H-5->L+6 (53%), HOMO->L+8 (29%) H-5->L+6 (32%), HOMO->L+8 (-25%), HOMO-

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
51	40386.8789	247.60517	0.1395	Singlet-A	>L+13 (-10%)
52	41047.4515	243.620484	0.002	Singlet-A	H-6->L+1 (94%)
53	41363.623	241.75832	0.0002	Singlet-A	H-6->L+3 (68%)
54	41501.5448	240.954886	0.0021	Singlet-A	H-6->L+3 (-15%), H-4->L+9 (-11%), H-4->L+10 (10%), H-2->L+9 (-17%), H-2->L+10 (18%)
55	41598.332	240.394254	0.0002	Singlet-A	H-7->L+3 (29%), H-6->L+2 (-20%), H-6->L+4 (35%)
56	41820.136	239.119261	0.0016	Singlet-A	H-5->L+9 (14%), H-5->L+10 (-11%), H-3->L+9 (10%), H-1->L+7 (22%)
57	42155.665	237.216042	0.0061	Singlet-A	H-7->L+3 (11%), H-6->L+2 (49%), H-6->L+4 (10%)
58	42170.9896	237.12984	0.0148	Singlet-A	H-7->L+1 (-13%), H-6->L+2 (-11%), H-1->L+7 (44%)
59	42402.4723	235.835305	0.0187	Singlet-A	H-12->LUMO (29%), H-8->L+2 (-17%), H-2->L+7 (-25%)
60	42474.2562	235.43673	0.0058	Singlet-A	H-7->L+1 (63%), H-1->L+7 (11%)
61	42740.421	233.970555	0.0112	Singlet-A	H-13->LUMO (34%), H-8->L+1 (-28%)
62	42873.5034	233.244293	0.0004	Singlet-A	H-12->LUMO (40%), H-2->L+7 (44%)
63	43200.9667	231.476302	0.011	Singlet-A	H-7->L+3 (-39%), H-6->L+4 (41%)
64	43270.3309	231.105235	0.0174	Singlet-A	H-7->L+2 (40%), H-7->L+4 (-33%), H-6->L+3 (10%)
65	43441.3216	230.195575	0.0066	Singlet-A	H-9->L+1 (75%)
66	43779.2702	228.418609	0.0016	Singlet-A	H-7->L+2 (38%), H-7->L+4 (39%)
67	43805.8867	228.279821	0.0007	Singlet-A	H-13->LUMO (-21%), H-5->L+7 (13%), H-3->L+7 (42%)
68	43867.9918	227.956639	0.0077	Singlet-A	H-9->L+3 (81%)
69	44093.0221	226.793255	0.037	Singlet-A	H-9->L+2 (27%), H-9->L+4 (-15%), HOMO->L+9 (-15%), HOMO->L+10 (-24%)
70	44392.2558	225.264515	0.014	Singlet-A	H-9->L+2 (38%), HOMO->L+9 (15%), HOMO->L+10 (20%)
71	44720.5258	223.610967	0.0446	Singlet-A	H-15->LUMO (10%), H-13->LUMO (19%), H-8->L+1 (30%), H-3->L+7 (27%)
72	44722.1389	223.602901	0.0235	Singlet-A	H-12->LUMO (14%), H-9->L+4 (-16%), H-8->L+2 (25%)
73	44794.7293	223.24055	0.013	Singlet-A	H-9->L+2 (15%), H-9->L+4 (46%)
74	44880.2246	222.815284	0.0729	Singlet-A	HOMO->L+8 (-19%), HOMO->L+12 (49%), HOMO->L+13 (14%)
75	45112.5139	221.667984	0.0014	Singlet-A	H-8->L+3 (90%)
76	45412.5542	220.203425	0.0131	Singlet-A	H-4->L+7 (69%)
77	45839.2245	218.153778	0.0012	Singlet-A	H-8->L+4 (84%)
78	45931.1723	217.717064	0.0073	Singlet-A	H-4->L+8 (22%), H-2->L+8 (45%)
79	45945.6904	217.648269	0.0019	Singlet-A	H-14->LUMO (-12%), H-1->L+8 (37%), HOMO->L+11 (-30%)
80	45999.7299	217.392581	0.0092	Singlet-A	H-14->LUMO (72%), H-1->L+8 (11%)
81	46048.9301	217.160311	0.0073	Singlet-A	H-5->L+7 (78%), H-3->L+7 (-16%)
82	46907.1099	213.187298	0.0008	Singlet-A	H-10->L+1 (92%)
83	47078.1006	212.412987	0.0022	Singlet-A	H-1->L+9 (43%), HOMO->L+13 (23%)
84	47080.5203	212.402071	0.0001	Singlet-A	H-6->L+5 (71%)
85	47111.1696	212.263887	0.0007	Singlet-A	H-6->L+5 (13%), H-5->L+8 (20%), H-3->L+8 (22%), HOMO->L+11 (17%)
86	47278.1275	211.514299	0.0023	Singlet-A	H-10->L+3 (-12%), H-6->L+6 (50%), H-1->L+10 (-11%)
87	47412.0165	210.916994	0.0065	Singlet-A	H-10->L+3 (-24%), H-1->L+10 (27%)
88	47433.7936	210.820161	0.0002	Singlet-A	H-11->L+1 (76%)
89	47625.7549	209.970425	0.0038	Singlet-A	H-10->L+3 (18%), H-7->L+5 (35%), H-6->L+6 (21%)
90	47654.791	209.84249	0.0455	Singlet-A	H-16->LUMO (61%)
91	47761.257	209.374724	0.0006	Singlet-A	H-11->L+3 (23%), H-10->L+2 (15%), H-10->L+4 (-18%), H-7->L+6 (-15%)
92	47933.8608	208.620792	0.0019	Singlet-A	H-18->LUMO (11%), H-15->LUMO (73%)
93	48233.0946	207.326527	0.0001	Singlet-A	H-11->L+1 (-10%), H-10->L+2 (75%)
94	48449.2526	206.401533	0.0155	Singlet-A	H-10->L+3 (-11%), H-7->L+5 (47%), H-6->L+6 (-23%)
95	48683.9616	205.406456	0.0023	Singlet-A	H-11->L+2 (89%)
96	48711.3846	205.290818	0.0101	Singlet-A	H-7->L+6 (30%), H-2->L+9 (-18%), H-2->L+10 (-10%)
97	48727.5158	205.222857	0.0122	Singlet-A	H-7->L+6 (33%), H-2->L+9 (13%)
98	48879.9557	204.582837	0.0157	Singlet-A	H-19->LUMO (10%), H-17->LUMO (62%)
99	48999.3266	204.084438	0.0005	Singlet-A	H-11->L+3 (42%), H-10->L+4 (55%)
100	49090.4678	203.705535	0.0268	Singlet-A	H-11->L+4 (-26%), H-10->L+3 (-18%), H-9->L+5 (29%)

Table S11: Energy and composition of TD-DFT calculated transitions of **1b**

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	18338.7547	545.293296	0.0003	Singlet-A	HOMO->LUMO (99%)
2	23836.2677	419.528767	0.0009	Singlet-A	H-4->LUMO (13%), H-2->LUMO (86%)
3	24471.0304	408.646462	0.0292	Singlet-A	H-1->LUMO (96%)
4	24697.6738	404.896433	0.0305	Singlet-A	HOMO->L+1 (34%), HOMO->L+2 (63%)
5	25490.5222	392.302673	0.0035	Singlet-A	HOMO->L+1 (64%), HOMO->L+2 (-34%)
6	25579.2438	390.941971	0.0011	Singlet-A	HOMO->L+3 (94%)
7	26054.3077	383.813691	0.054	Singlet-A	H-3->LUMO (79%)
8	26999.596	370.375912	0.0152	Singlet-A	HOMO->L+4 (90%)
9	27505.3091	363.566174	0.0001	Singlet-A	H-4->LUMO (86%), H-2->LUMO (-14%)
10	28326.3872	353.027724	0.0179	Singlet-A	H-5->LUMO (90%)
11	30221.8032	330.886941	0.0036	Singlet-A	HOMO->L+5 (82%)
12	30447.64	328.43268	0.0165	Singlet-A	H-1->L+1 (39%), H-1->L+2 (35%)
13	30471.0302	328.180568	0.0336	Singlet-A	H-2->L+1 (16%), H-2->L+2 (41%), HOMO->L+5 (-15%)
14	30533.9419	327.504389	0.0004	Singlet-A	HOMO->L+6 (90%)
15	31034.8157	322.218766	0.0037	Singlet-A	H-2->L+1 (61%), H-1->L+3 (23%)
16	31150.1538	321.025703	0.0097	Singlet-A	H-2->L+3 (17%), H-1->L+1 (47%), H-1->L+2 (-22%)
17	31416.3186	318.305914	0.0426	Singlet-A	H-2->L+2 (28%), H-1->L+3 (53%)
18	31514.7189	317.312048	0.0022	Singlet-A	H-3->L+2 (-16%), H-2->L+3 (29%), H-1->L+2 (34%)
19	32401.9349	308.623545	0.0476	Singlet-A	H-3->L+1 (61%), H-2->L+3 (12%)
20	32484.204	307.841928	0.0077	Singlet-A	H-1->L+4 (80%)
21	32690.6834	305.897552	0.0196	Singlet-A	H-3->L+2 (-13%), H-2->L+4 (64%)
22	32804.4083	304.837079	0.081	Singlet-A	H-3->L+3 (73%)
23	33381.0987	299.570727	0.014	Singlet-A	H-3->L+2 (42%), H-2->L+3 (15%), H-2->L+4 (17%)
24	33943.271	294.609202	0.0331	Singlet-A	H-4->L+1 (61%), H-4->L+2 (12%)
25	34026.3467	293.889911	0.0008	Singlet-A	H-3->L+4 (72%), H-1->L+4 (-15%)
26	34336.8723	291.232117	0.0216	Singlet-A	H-5->L+1 (25%), H-5->L+2 (28%), H-1->L+5 (14%)
27	34413.4955	290.583675	0.0146	Singlet-A	H-4->L+1 (-19%), H-4->L+2 (59%)
28	34537.7058	289.53863	0.0078	Singlet-A	H-5->L+1 (-12%), H-4->L+3 (59%), H-2->L+3 (-10%)
29	34718.3752	288.031912	0.004	Singlet-A	H-6->LUMO (91%)
30	34893.3987	286.587159	0.005	Singlet-A	H-5->L+3 (65%), H-2->L+5 (12%)
31	35083.7469	285.03227	0.0224	Singlet-A	H-5->L+1 (47%), H-5->L+2 (-32%)
32	36020.9696	277.61607	0.0061	Singlet-A	H-4->L+4 (78%)
33	36033.068	277.522858	0.002	Singlet-A	H-2->L+5 (53%), H-1->L+6 (-32%)
34	36073.396	277.212603	0.0042	Singlet-A	H-2->L+6 (49%), H-1->L+5 (-37%)
35	36241.967	275.923213	0.0006	Singlet-A	H-9->LUMO (10%), H-8->LUMO (81%)
36	36518.6171	273.832932	0.0051	Singlet-A	H-5->L+4 (71%), H-3->L+4 (-14%)
37	37083.2091	269.663825	0.0087	Singlet-A	H-3->L+5 (56%), H-1->L+5 (-22%)
38	37225.9702	268.629667	0.0053	Singlet-A	H-9->LUMO (86%)
39	37417.9315	267.251545	0.1436	Singlet-A	H-3->L+6 (44%), H-1->L+6 (-35%)
40	37699.421	265.256063	0.2483	Singlet-A	H-5->L+3 (-10%), H-3->L+6 (44%)
41	37989.7826	263.228672	0.1331	Singlet-A	H-4->L+3 (-13%), H-3->L+5 (28%), H-2->L+6 (16%)
42	38109.1534	262.40415	0.0001	Singlet-A	HOMO->L+7 (91%)
43	38148.6749	262.132303	0.3945	Singlet-A	H-7->LUMO (68%)
44	39146.3896	255.451399	0.0003	Singlet-A	HOMO->L+9 (28%), HOMO->L+10 (42%)
45	39236.7243	254.863273	0.0225	Singlet-A	H-4->L+5 (82%)
46	39520.6334	253.032382	0.0064	Singlet-A	H-4->L+6 (80%), H-2->L+6 (-10%)
47	39856.969	250.897152	0.0007	Singlet-A	H-5->L+5 (80%)
48	39903.7494	250.603017	0.0124	Singlet-A	H-5->L+6 (70%), HOMO->L+8 (18%)
49	40420.7544	247.397659	0.1675	Singlet-A	H-5->L+6 (-18%), HOMO->L+8 (37%), HOMO->L+13 (15%)
50	41014.3826	243.816909	0.001	Singlet-A	H-6->L+1 (21%), H-6->L+2 (62%)

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
51	41236.9931	242.500707	0.002	Singlet-A	H-10->LUMO (95%)
52	41332.9738	241.937589	0.0004	Singlet-A	H-8->L+2 (27%), H-6->L+3 (53%)
53	41501.5448	240.954886	0.0044	Singlet-A	H-4->L+10 (11%), H-2->L+9 (17%), H-2->L+10 (33%)
54	41658.0174	240.04983	0.0001	Singlet-A	H-6->L+1 (60%), H-6->L+2 (-19%)
55	41710.4438	239.748108	0.0015	Singlet-A	H-5->L+10 (13%), H-3->L+9 (15%), H-3->L+10 (22%), H-1->L+10 (10%)
56	41813.6835	239.15616	0.0039	Singlet-A	H-11->LUMO (90%)
57	42075.8155	237.666219	0.0406	Singlet-A	H-12->LUMO (43%), H-7->L+1 (27%)
58	42387.9542	235.91608	0.0191	Singlet-A	H-13->LUMO (45%), H-7->L+4 (-30%)
59	42794.4605	233.675104	0.0452	Singlet-A	H-8->L+2 (35%), H-6->L+3 (-32%), H-6->L+4 (-10%)
60	43035.6219	232.365644	0.0019	Singlet-A	H-8->L+1 (41%), H-6->L+4 (50%)
61	43087.2418	232.087263	0.0126	Singlet-A	H-8->L+3 (74%)
62	43390.5083	230.46515	0	Singlet-A	H-9->L+1 (12%), H-8->L+1 (36%), H-8->L+2 (-16%), H-6->L+4 (-29%)
63	43528.4301	229.734911	0.0024	Singlet-A	H-9->L+1 (11%), H-9->L+2 (35%), H-1->L+7 (32%)
64	43715.552	228.751544	0.0046	Singlet-A	H-9->L+1 (-12%), H-9->L+2 (-14%), H-7->L+2 (12%), H-1->L+7 (42%)
65	43726.8438	228.692472	0.0014	Singlet-A	H-7->L+1 (18%), H-7->L+2 (54%)
66	43799.4342	228.313451	0.0456	Singlet-A	H-2->L+7 (39%), HOMO->L+9 (21%), HOMO->L+10 (-13%)
67	44101.8942	226.74763	0.0134	Singlet-A	H-2->L+7 (37%), HOMO->L+9 (-15%), HOMO->L+10 (16%)
68	44318.8589	225.637579	0.0019	Singlet-A	H-9->L+3 (68%), H-7->L+3 (-10%)
69	44336.6032	225.547274	0.0071	Singlet-A	H-9->L+1 (51%), H-9->L+2 (-27%)
70	44465.6528	224.892684	0.0018	Singlet-A	H-7->L+3 (78%)
71	44710.847	223.659373	0.0616	Singlet-A	HOMO->L+8 (-19%), HOMO->L+12 (46%), HOMO->L+13 (18%)
72	44743.916	223.494072	0.0031	Singlet-A	H-8->L+4 (84%)
73	44897.969	222.727224	0.003	Singlet-A	H-12->LUMO (15%), H-3->L+7 (39%), H-1->L+7 (-17%)
74	45660.9747	219.005399	0.0132	Singlet-A	H-4->L+8 (10%), H-3->L+7 (11%), H-2->L+8 (35%)
75	45683.5584	218.897134	0.0003	Singlet-A	H-9->L+4 (62%), H-1->L+8 (13%)
76	45854.5491	218.080871	0.0074	Singlet-A	H-9->L+4 (-20%), H-1->L+8 (25%), HOMO->L+11 (23%)
77	45854.5491	218.080871	0.0318	Singlet-A	H-12->LUMO (-10%), H-7->L+1 (10%), H-3->L+7 (20%), H-2->L+8 (-17%)
78	46013.4414	217.3278	0.1192	Singlet-A	H-15->LUMO (25%), H-13->LUMO (25%), H-7->L+4 (24%)
79	46683.6928	214.207562	0.0008	Singlet-A	H-6->L+5 (85%)
80	46748.2176	213.911899	0.002	Singlet-A	H-5->L+8 (10%), H-4->L+7 (-17%), H-3->L+8 (25%), HOMO->L+11 (-18%)
81	46901.464	213.212961	0.0036	Singlet-A	H-14->LUMO (18%), H-6->L+6 (52%)
82	46959.5363	212.949292	0.0002	Singlet-A	H-4->L+7 (61%)
83	47005.5102	212.741016	0.0047	Singlet-A	H-14->LUMO (53%), H-6->L+6 (-24%)
84	47055.517	212.514932	0.0031	Singlet-A	H-1->L+9 (-20%), HOMO->L+13 (30%)
85	47416.8558	210.895468	0.0023	Singlet-A	H-10->L+1 (18%), H-10->L+2 (19%), H-8->L+5 (31%)
86	47594.299	210.109198	0.0085	Singlet-A	H-15->LUMO (-10%), H-11->L+2 (-15%), H-10->L+3 (19%), H-8->L+6 (16%)
87	47646.7254	209.878012	0.0024	Singlet-A	H-5->L+7 (82%)
88	47743.5126	209.45254	0.0046	Singlet-A	H-3->L+9 (-12%), H-3->L+10 (-11%), H-1->L+9 (21%), H-1->L+10 (43%)
89	47798.3587	209.212205	0.1836	Singlet-A	H-15->LUMO (47%), H-7->L+4 (-14%)
90	47894.3394	208.792942	0.001	Singlet-A	H-16->LUMO (85%)
91	48100.0122	207.900155	0.0018	Singlet-A	H-10->L+1 (61%), H-8->L+5 (-19%)
92	48135.5008	207.746878	0.0059	Singlet-A	H-17->LUMO (63%)
93	48179.8616	207.555598	0.0171	Singlet-A	H-10->L+2 (30%), H-9->L+5 (-15%), H-8->L+5 (-24%), H-6->L+6 (13%)
94	48296.8128	207.053	0.0001	Singlet-A	H-18->LUMO (82%)
95	48322.6227	206.94241	0	Singlet-A	H-2->L+9 (46%), H-2->L+10 (-18%)
96	48400.0525	206.611346	0.0088	Singlet-A	H-9->L+6 (14%), H-8->L+6 (55%)
97	48538.7808	206.020832	0.0019	Singlet-A	H-19->LUMO (95%)
98	48648.473	205.556298	0.0071	Singlet-A	H-11->L+1 (68%), H-11->L+2 (-11%)
99	48755.7454	205.104033	0.0138	Singlet-A	H-7->L+5 (85%)
100	48903.3459	204.484986	0.0643	Singlet-A	H-10->L+2 (-10%), H-9->L+5 (-18%), H-1->L+10 (12%), HOMO->L+12 (18%), HOMO->L+13 (-12%)

Table S12: Energy and composition of TD-DFT calculated transitions of **2a**

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	18560.5587	538.776884	0.0001	Singlet-A	HOMO->LUMO (99%)
2	23801.5856	420.140077	0.0088	Singlet-A	H-1->LUMO (98%)
3	24135.5014	414.327418	0.0005	Singlet-A	H-4->LUMO (22%), H-2->LUMO (76%)
4	26302.7282	380.188699	0.0435	Singlet-A	H-5->LUMO (10%), H-3->LUMO (87%)
5	26490.6566	377.491586	0.0003	Singlet-A	HOMO->L+1 (96%)
6	27099.6094	369.009008	0.0002	Singlet-A	H-4->LUMO (75%), H-2->LUMO (-22%)
7	27703.7229	360.962317	0.0006	Singlet-A	HOMO->L+2 (97%)
8	27844.8709	359.132569	0.0008	Singlet-A	HOMO->L+3 (89%)
9	28252.1837	353.954941	0.0017	Singlet-A	HOMO->L+4 (85%)
10	28307.8363	353.259072	0.0173	Singlet-A	H-5->LUMO (81%), H-3->LUMO (-11%)
11	31328.4035	319.199157	0.0023	Singlet-A	H-1->L+1 (95%)
12	31415.512	318.314086	0.0002	Singlet-A	H-6->LUMO (99%)
13	32113.1864	311.39856	0.004	Singlet-A	H-4->L+1 (12%), H-2->L+1 (72%)
14	32208.3605	310.478393	0	Singlet-A	H-7->LUMO (99%)
15	32440.6498	308.255231	0.0001	Singlet-A	H-8->LUMO (99%)
16	32568.0862	307.049052	0.0077	Singlet-A	H-1->L+2 (54%), HOMO->L+5 (25%)
17	32622.9323	306.532837	0.0268	Singlet-A	H-1->L+2 (-37%), HOMO->L+5 (49%)
18	32799.569	304.882055	0	Singlet-A	H-9->LUMO (100%)
19	32926.1989	303.709518	0.0139	Singlet-A	H-1->L+3 (69%)
20	33239.9507	300.842805	0.0088	Singlet-A	H-1->L+4 (55%), HOMO->L+6 (15%)
21	33431.1054	299.122625	0.0161	Singlet-A	H-2->L+2 (33%), H-2->L+3 (12%), H-1->L+4 (-11%)
22	33612.5814	297.507647	0.0012	Singlet-A	H-3->L+1 (39%), H-1->L+4 (12%), HOMO->L+6 (-20%)
23	33684.3653	296.873636	0.0556	Singlet-A	H-2->L+2 (31%), H-2->L+3 (-21%), HOMO->L+6 (-10%)
24	33757.7622	296.228166	0.0544	Singlet-A	H-3->L+1 (23%), H-2->L+3 (-13%), H-2->L+4 (16%), HOMO->L+6 (16%)
25	34312.6755	291.437489	0.0063	Singlet-A	H-2->L+4 (26%), HOMO->L+6 (-15%)
26	34665.1422	288.474224	0.0034	Singlet-A	H-11->LUMO (-16%), H-5->L+2 (13%), H-3->L+2 (56%)
27	34666.7554	288.4608	0.0071	Singlet-A	H-11->LUMO (69%), H-3->L+2 (10%)
28	34743.3786	287.824628	0.0005	Singlet-A	H-4->L+1 (61%), H-2->L+1 (-15%)
29	35342.6526	282.94424	0.0936	Singlet-A	H-3->L+3 (39%), H-3->L+4 (26%), H-2->L+3 (-11%)
30	35708.8309	280.042772	0.0129	Singlet-A	H-5->L+1 (49%), H-4->L+2 (-10%), H-3->L+1 (-10%), H-3->L+4 (-11%)
31	36021.7762	277.609853	0.0028	Singlet-A	H-5->L+1 (28%), H-4->L+2 (13%), H-3->L+3 (-12%), H-3->L+4 (18%)
32	36078.2354	277.175419	0.0013	Singlet-A	H-13->LUMO (-22%), H-12->LUMO (73%)
33	36348.433	275.115024	0.0134	Singlet-A	H-4->L+2 (52%)
34	36664.6045	272.742612	0.0088	Singlet-A	H-13->LUMO (-19%), H-12->LUMO (-11%), H-5->L+2 (22%), H-4->L+3 (11%), H-3->L+2 (-11%)
35	36680.7357	272.622667	0.0061	Singlet-A	H-13->LUMO (36%), H-12->LUMO (10%), H-4->L+3 (27%)
36	36977.5498	270.43436	0.0054	Singlet-A	H-13->LUMO (-12%), H-5->L+2 (-17%), H-4->L+4 (20%)
37	37185.6422	268.920997	0.0075	Singlet-A	H-5->L+3 (11%), H-4->L+4 (-17%), H-1->L+5 (37%)
38	37255.0064	268.4203	0.0052	Singlet-A	H-5->L+4 (-10%), H-4->L+4 (16%), H-1->L+5 (21%)
39	37676.8373	265.415059	0.001	Singlet-A	H-5->L+3 (18%), H-5->L+4 (30%), H-1->L+6 (-19%)
40	38279.3376	261.23754	0.1154	Singlet-A	H-10->LUMO (-17%), H-2->L+5 (27%), H-1->L+6 (-15%)
41	38365.6395	260.649897	0.0904	Singlet-A	H-10->LUMO (-16%), H-6->L+1 (21%), H-6->L+3 (10%)
42	38448.7152	260.086714	0.0065	Singlet-A	H-6->L+1 (37%), H-6->L+3 (15%)
43	38492.2694	259.792424	0.104	Singlet-A	H-10->LUMO (27%), H-5->L+2 (-10%), H-2->L+5 (32%)
44	38685.0373	258.497877	0.0067	Singlet-A	HOMO->L+7 (46%), HOMO->L+8 (12%)
45	38857.6411	257.349641	0.0036	Singlet-A	HOMO->L+7 (-17%), HOMO->L+8 (71%)
46	39232.6915	254.889471	0.2043	Singlet-A	H-1->L+6 (36%)
47	39360.128	254.064214	0.0154	Singlet-A	H-7->L+1 (69%), H-7->L+3 (17%)
48	39464.9808	253.389202	0.0039	Singlet-A	H-3->L+5 (60%), H-2->L+6 (-20%)
49	39654.5224	252.178047	0.0195	Singlet-A	H-8->L+1 (-25%), H-6->L+1 (-14%), H-6->L+3 (29%)
50	39702.916	251.870669	0.007	Singlet-A	H-8->L+1 (44%), H-8->L+4 (-10%), H-6->L+1 (-11%), H-6->L+3 (26%)

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
51	39845.6771	250.968254	0.0685	Singlet-A	H-2->L+6 (20%)
52	39918.2675	250.511874	0.0302	Singlet-A	H-3->L+6 (27%), HOMO->L+12 (28%)
53	40163.4618	248.982522	0.0003	Singlet-A	H-9->L+1 (86%), H-9->L+4 (-10%)
54	40324.7738	247.986512	0.0007	Singlet-A	H-6->L+2 (94%)
55	40404.6232	247.49643	0.003	Singlet-A	HOMO->L+7 (-12%), HOMO->L+11 (10%), HOMO->L+13 (10%), HOMO->L+14 (42%)
56	40553.0302	246.590697	0.0161	Singlet-A	H-3->L+6 (43%), HOMO->L+12 (-16%)
57	40618.3616	246.194076	0.0004	Singlet-A	H-7->L+1 (-19%), H-7->L+3 (74%)
58	40845.005	244.827979	0.0031	Singlet-A	H-8->L+1 (20%), H-8->L+2 (15%), H-8->L+4 (58%)
59	40939.3725	244.263637	0.0051	Singlet-A	HOMO->L+9 (86%)
60	41126.4944	243.152259	0.0001	Singlet-A	H-7->L+2 (94%)
61	41319.2622	242.017874	0.0034	Singlet-A	HOMO->L+10 (88%)
62	41370.8821	241.7159	0.0015	Singlet-A	H-9->L+2 (-13%), H-9->L+4 (-23%), H-8->L+2 (50%)
63	41410.4035	241.48521	0	Singlet-A	H-9->L+2 (21%), H-9->L+4 (25%), H-8->L+2 (31%), H-8->L+4 (-14%)
64	41546.7122	240.692933	0.0808	Singlet-A	H-5->L+5 (17%), H-4->L+5 (43%), H-2->L+5 (- 11%)
65	41710.4438	239.748108	0.0005	Singlet-A	H-14->LUMO (98%)
66	41779.0014	239.354691	0.0395	Singlet-A	H-5->L+5 (45%), H-4->L+5 (-11%)
67	41788.6802	239.299254	0.0004	Singlet-A	H-9->L+2 (61%), H-9->L+4 (-36%)
68	41837.0738	239.022453	0.0012	Singlet-A	HOMO->L+11 (75%)
69	42091.1402	237.579689	0.0056	Singlet-A	H-4->L+6 (33%), H-2->L+14 (11%)
70	42272.6162	236.559762	0.0001	Singlet-A	H-15->LUMO (96%)
71	42461.3512	235.508285	0.0015	Singlet-A	H-11->L+1 (-38%), H-6->L+4 (52%)
72	42464.5774	235.490392	0.0024	Singlet-A	H-11->L+1 (46%), H-6->L+4 (45%)
73	42566.204	234.92816	0.0182	Singlet-A	H-1->L+7 (40%)
74	42677.5093	234.315455	0.1205	Singlet-A	H-5->L+6 (12%), H-5->L+14 (14%), H-3->L+14 (10%)
75	42913.8314	233.025104	0.0755	Singlet-A	H-5->L+6 (21%), H-4->L+6 (-15%), H-1->L+7 (- 10%)
76	43159.8322	231.696916	0.0012	Singlet-A	H-8->L+3 (90%)
77	43204.193	231.459016	0.0315	Singlet-A	H-16->LUMO (10%), H-10->L+1 (39%), H-1- >L+8 (-25%)
78	43306.6261	230.911546	0	Singlet-A	H-7->L+4 (98%)
79	43382.4427	230.507998	0.0131	Singlet-A	H-17->LUMO (-17%), H-10->L+2 (40%)
80	43559.0794	229.573263	0.0582	Singlet-A	H-5->L+6 (18%), H-1->L+7 (35%)
81	43581.663	229.4543	0.0156	Singlet-A	H-12->L+1 (19%), H-11->L+2 (52%), H-9->L+3 (-13%)
82	43589.7286	229.411843	0.0073	Singlet-A	H-9->L+3 (82%)
83	43692.9683	228.869779	0.0106	Singlet-A	H-11->L+2 (-20%), H-10->L+1 (14%), H-1- >L+8 (50%)
84	44005.107	227.246351	0.0044	Singlet-A	H-13->L+1 (-12%), H-12->L+1 (39%), H-11- >L+3 (-22%)
85	44184.1634	226.325435	0.004	Singlet-A	H-12->L+1 (14%), H-11->L+3 (57%), H-11- >L+4 (-11%)
86	44492.2693	224.758147	0.0041	Singlet-A	H-11->L+4 (61%)
87	44575.345	224.339262	0.0621	Singlet-A	H-11->L+4 (11%), H-2->L+8 (-16%), HOMO- >L+13 (19%)
88	44665.6797	223.885544	0.0037	Singlet-A	H-9->L+7 (29%), H-8->L+10 (25%), H-1->L+10 (-21%)
89	44695.5224	223.736058	0.0109	Singlet-A	H-13->L+1 (28%), H-1->L+9 (11%)
90	44764.8866	223.389374	0.0162	Singlet-A	H-13->L+1 (40%)
91	44877.805	222.827298	0.0043	Singlet-A	H-2->L+8 (32%), H-1->L+12 (-14%), HOMO- >L+13 (17%)
92	44900.3886	222.715221	0.0018	Singlet-A	H-2->L+7 (70%)
93	44977.8184	222.331815	0.001	Singlet-A	H-6->L+5 (19%), H-1->L+9 (55%)
94	45231.0782	221.086925	0.0002	Singlet-A	H-13->L+2 (-17%), H-12->L+2 (75%)
95	45299.6358	220.752326	0.0008	Singlet-A	H-13->L+3 (-10%), H-12->L+3 (45%), H-10- >L+3 (24%)
96	45376.259	220.37956	0.0014	Singlet-A	H-6->L+5 (40%), H-6->L+11 (-10%), H-1- >L+11 (16%)
97	45497.243	219.793538	0.0024	Singlet-A	H-1->L+10 (66%)
98	45579.5122	219.396819	0.0047	Singlet-A	H-12->L+3 (-15%), H-10->L+3 (55%)
99	45639.1976	219.1099	0.0265	Singlet-A	H-12->L+3 (-12%), H-12->L+4 (-14%), H-10- >L+4 (-11%), HOMO->L+15 (17%)
100	45668.2338	218.970588	0.0075	Singlet-A	H-12->L+4 (-15%), H-3->L+8 (33%)

Table S13: Energy and composition of TD-DFT calculated transitions of **2b**

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	19780.884	505.53858	0.0001	Singlet-A	HOMO->LUMO (99%)
2	25121.1178	398.071459	0.0224	Singlet-A	H-1->LUMO (98%)
3	25228.3902	396.378838	0.0008	Singlet-A	H-4->LUMO (17%), H-2->LUMO (82%)
4	26707.6213	374.424959	0.0003	Singlet-A	HOMO->L+1 (96%)
5	27290.7642	366.424331	0.0664	Singlet-A	H-3->LUMO (86%)
6	28057.8027	356.407096	0.0016	Singlet-A	HOMO->L+3 (91%)
7	28127.1669	355.528164	0.0017	Singlet-A	HOMO->L+2 (71%), HOMO->L+4 (25%)
8	28286.8658	353.520962	0.0006	Singlet-A	HOMO->L+2 (-25%), HOMO->L+4 (72%)
9	28498.991	350.889615	0.0001	Singlet-A	H-4->LUMO (80%), H-2->LUMO (-17%)
10	29583.0077	338.03189	0.0161	Singlet-A	H-5->LUMO (88%), H-3->LUMO (-10%)
11	31646.1882	315.993824	0.011	Singlet-A	H-1->L+1 (92%)
12	32243.0426	310.144428	0.0061	Singlet-A	H-4->L+1 (10%), H-2->L+1 (76%)
13	32756.0147	305.287444	0.0194	Singlet-A	H-1->L+4 (13%), HOMO->L+5 (67%)
14	33025.4058	302.797188	0.0226	Singlet-A	H-1->L+2 (43%), H-1->L+4 (20%), HOMO->L+5 (-11%)
15	33227.8523	300.952343	0.0023	Singlet-A	H-1->L+3 (53%)
16	33230.272	300.930429	0.0046	Singlet-A	H-1->L+2 (40%), H-1->L+4 (-28%)
17	33503.6958	298.474534	0.0081	Singlet-A	H-2->L+2 (20%), H-2->L+4 (31%), HOMO->L+6 (21%), HOMO->L+7 (-15%)
18	33795.6706	295.895889	0.0013	Singlet-A	H-3->L+1 (55%), H-2->L+2 (11%), H-1->L+3 (-15%)
19	33871.4872	295.233567	0.1358	Singlet-A	H-2->L+3 (51%), H-1->L+4 (-26%)
20	34005.3762	294.071148	0.0638	Singlet-A	H-3->L+1 (-21%), H-2->L+2 (46%), HOMO->L+6 (-17%)
21	34458.6629	290.202787	0	Singlet-A	H-3->L+3 (19%), H-2->L+4 (24%), H-1->L+3 (-20%), HOMO->L+6 (-14%)
22	35054.7107	285.268365	0.0128	Singlet-A	H-4->L+1 (13%), H-3->L+2 (64%)
23	35103.1043	284.87509	0.002	Singlet-A	H-4->L+1 (54%), H-3->L+2 (-10%), H-2->L+1 (-11%)
24	35537.8402	281.390201	0.1024	Singlet-A	H-4->L+1 (-12%), H-3->L+4 (62%), H-2->L+3 (-12%)
25	35608.0109	280.835681	0.0076	Singlet-A	H-11->LUMO (74%), H-6->LUMO (14%)
26	35837.0739	279.040639	0	Singlet-A	HOMO->L+6 (21%), HOMO->L+7 (63%)
27	36051.6189	277.380054	0.0094	Singlet-A	H-5->L+1 (46%), H-3->L+3 (17%)
28	36358.1117	275.041787	0.0074	Singlet-A	H-5->L+1 (-32%), H-3->L+3 (32%), H-2->L+4 (-12%)
29	36375.0494	274.913716	0.0001	Singlet-A	H-7->LUMO (98%)
30	36407.3118	274.6701	0.0003	Singlet-A	H-11->LUMO (-12%), H-6->LUMO (84%)
31	36627.5027	273.018886	0	Singlet-A	HOMO->L+8 (98%)
32	36827.5296	271.535998	0.0115	Singlet-A	H-4->L+2 (65%), H-4->L+4 (13%)
33	36921.8971	270.841988	0	Singlet-A	H-8->LUMO (97%)
34	36950.1267	270.635066	0	Singlet-A	H-9->LUMO (99%)
35	37096.1141	269.570014	0.0117	Singlet-A	H-5->L+2 (12%), H-4->L+3 (50%)
36	37259.0392	268.391247	0.012	Singlet-A	H-4->L+2 (-13%), H-4->L+4 (50%), H-1->L+5 (17%)
37	37263.072	268.362201	0.0009	Singlet-A	H-13->LUMO (-16%), H-12->LUMO (79%)
38	37544.5614	266.350161	0.0008	Singlet-A	H-5->L+3 (-35%), H-1->L+5 (41%)
39	37561.4992	266.230055	0.0371	Singlet-A	H-10->LUMO (-11%), H-5->L+2 (39%), H-4->L+3 (-12%), H-3->L+2 (-13%)
40	37853.4739	264.176546	0.0064	Singlet-A	H-5->L+4 (56%), H-1->L+6 (10%)
41	38113.9928	262.370832	0.002	Singlet-A	H-13->LUMO (72%), H-12->LUMO (14%)
42	38417.2594	260.299672	0.1954	Singlet-A	H-10->LUMO (-27%), H-5->L+2 (-12%), H-2->L+5 (33%)
43	38576.1517	259.227517	0.1526	Singlet-A	H-10->LUMO (29%), H-5->L+2 (13%), H-2->L+5 (33%)
44	38610.8338	258.994666	0.0125	Singlet-A	H-5->L+3 (29%), H-2->L+6 (-18%), H-1->L+5 (22%)
45	39149.6158	255.430348	0.0001	Singlet-A	HOMO->L+9 (95%)
46	39164.9405	255.330402	0.0038	Singlet-A	HOMO->L+10 (97%)
47	39310.1213	254.387412	0.1853	Singlet-A	H-5->L+4 (-15%), H-1->L+6 (40%), HOMO->L+12 (11%)
48	39506.1154	253.125368	0.0051	Singlet-A	H-3->L+5 (71%)
49	39566.6074	252.738374	0.0023	Singlet-A	HOMO->L+11 (91%)
50	39844.064	250.978414	0.0658	Singlet-A	H-5->L+3 (13%), H-4->L+4 (-12%), H-2->L+6 (28%), H-2->L+7 (-17%)

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
51	40019.8941	249.875724	0.0322	Singlet-A	H-4->L+5 (-11%), H-3->L+6 (16%), HOMO->L+12 (36%)
52	40080.3861	249.498595	0.0296	Singlet-A	H-1->L+6 (10%), H-1->L+7 (67%)
53	40542.545	246.654471	0.0003	Singlet-A	H-2->L+6 (-12%), H-2->L+7 (-27%), H-1->L+8 (37%)
54	40613.5222	246.223412	0.0177	Singlet-A	H-3->L+6 (36%), H-3->L+7 (-16%), HOMO->L+12 (-13%)
55	40672.4011	245.866969	0	Singlet-A	H-1->L+8 (47%), HOMO->L+14 (-19%)
56	41370.8821	241.7159	0.002	Singlet-A	H-1->L+8 (11%), HOMO->L+13 (17%), HOMO->L+14 (42%)
57	41870.1427	238.833674	0.0147	Singlet-A	H-5->L+6 (13%), H-4->L+5 (-20%), H-3->L+7 (31%)
58	41950.7987	238.374484	0.1357	Singlet-A	H-5->L+7 (10%), H-4->L+5 (39%), H-2->L+5 (-12%)
59	42038.7138	237.875974	0.0024	Singlet-A	H-5->L+5 (70%)
60	42183.8946	237.057296	0.0005	Singlet-A	H-11->L+1 (21%), H-6->L+1 (44%)
61	42331.495	236.230731	0.0058	Singlet-A	H-7->L+1 (14%), H-2->L+8 (64%)
62	42386.3411	235.925058	0.0115	Singlet-A	H-7->L+1 (36%), H-6->L+4 (13%), H-2->L+8 (-27%)
63	42564.5909	234.937064	0.0046	Singlet-A	H-11->L+1 (33%), H-6->L+1 (-12%)
64	42565.3974	234.932612	0.0496	Singlet-A	H-16->LUMO (-28%), H-10->L+1 (38%)
65	42611.3714	234.67914	0.0037	Singlet-A	H-4->L+6 (36%), H-2->L+6 (-15%)
66	42937.2216	232.898162	0.0069	Singlet-A	H-17->LUMO (17%), H-11->L+1 (25%), H-10->L+2 (-21%), H-8->L+1 (12%)
67	43037.235	232.356934	0.001	Singlet-A	H-9->L+1 (57%), H-9->L+3 (11%), H-8->L+4 (-16%), H-7->L+1 (11%)
68	43045.3006	232.313397	0.003	Singlet-A	H-9->L+4 (-13%), H-8->L+1 (51%), H-8->L+3 (10%)
69	43052.5597	232.274227	0.0069	Singlet-A	H-14->LUMO (89%)
70	43166.2846	231.662282	0.0786	Singlet-A	H-5->L+6 (-16%), H-5->L+7 (10%), H-1->L+9 (49%)
71	43240.4882	231.264734	0.0003	Singlet-A	H-1->L+10 (88%)
72	43329.2098	230.791193	0.1332	Singlet-A	H-5->L+6 (19%), H-5->L+7 (-10%), H-1->L+9 (42%), HOMO->L+15 (10%)
73	43439.7085	230.204123	0.009	Singlet-A	H-4->L+7 (39%), H-2->L+7 (-13%)
74	43559.8859	229.569013	0.002	Singlet-A	H-15->LUMO (82%)
75	43592.1483	229.399109	0.0023	Singlet-A	H-7->L+4 (-13%), H-6->L+1 (23%), H-6->L+3 (-19%), H-3->L+8 (23%)
76	43606.6664	229.322735	0.0005	Singlet-A	H-7->L+1 (31%), H-7->L+3 (-24%), H-6->L+4 (-24%)
77	43630.8632	229.195557	0.0004	Singlet-A	H-3->L+8 (69%)
78	43808.3064	228.267213	0.0104	Singlet-A	H-12->L+1 (24%), H-11->L+2 (54%), H-6->L+2 (10%)
79	43941.3888	227.575875	0.0051	Singlet-A	H-5->L+7 (-19%), H-3->L+6 (20%), H-3->L+7 (22%)
80	44110.7664	226.702023	0	Singlet-A	H-12->L+1 (30%), H-11->L+2 (-16%), H-11->L+4 (-19%)
81	44176.9043	226.362624	0.0056	Singlet-A	H-11->L+3 (45%), H-8->L+1 (-11%), H-8->L+3 (16%)
82	44262.3997	225.925392	0.0011	Singlet-A	H-9->L+1 (27%), H-9->L+3 (-27%), H-8->L+4 (26%)
83	44300.308	225.732065	0.0013	Singlet-A	H-11->L+3 (30%), H-9->L+4 (20%), H-8->L+1 (18%), H-8->L+3 (-18%)
84	44347.895	225.489845	0.0011	Singlet-A	H-1->L+11 (73%)
85	44433.3904	225.055975	0.0024	Singlet-A	H-12->L+1 (14%), H-11->L+4 (41%), H-6->L+2 (-10%), H-4->L+8 (-13%)
86	44494.689	224.745924	0.0002	Singlet-A	H-6->L+2 (-12%), H-4->L+8 (47%)
87	44548.7285	224.473298	0.0377	Singlet-A	H-7->L+2 (51%), H-1->L+12 (10%), HOMO->L+13 (18%)
88	44616.4795	224.132431	0	Singlet-A	H-11->L+2 (-10%), H-11->L+4 (12%), H-6->L+2 (53%)
89	44634.2238	224.043327	0.0291	Singlet-A	H-7->L+2 (36%), H-1->L+12 (-12%), HOMO->L+13 (-22%)
90	44722.9454	223.598869	0.0069	Singlet-A	H-2->L+9 (25%)
91	44740.6898	223.510188	0.0009	Singlet-A	H-2->L+10 (49%)
92	44747.1422	223.477959	0.0009	Singlet-A	H-4->L+6 (11%), H-4->L+7 (14%), H-2->L+9 (27%)
93	45017.3398	222.136626	0.0184	Singlet-A	H-13->L+1 (61%), H-8->L+2 (-12%)
94	45116.5467	221.64817	0.0024	Singlet-A	H-8->L+2 (51%)
95	45117.3533	221.644207	0.0003	Singlet-A	H-9->L+2 (-15%), H-2->L+9 (23%), H-2->L+11 (15%)
96	45133.4845	221.564989	0.0109	Singlet-A	H-8->L+2 (-21%), H-2->L+10 (26%)
97	45142.3566	221.521443	0	Singlet-A	H-9->L+2 (75%)
98	45152.8419	221.470002	0.0097	Singlet-A	H-16->LUMO (10%), H-10->L+1 (13%), H-10->L+3 (49%)
99	45301.249	220.744466	0	Singlet-A	H-2->L+9 (-10%), H-2->L+11 (41%)
100	45417.3936	220.179962	0.0337	Singlet-A	H-12->L+3 (10%), H-5->L+6 (-15%), HOMO->L+12 (-13%), HOMO->L+15 (24%)

Table S14: Energy and composition of TD-DFT calculated transitions of **2b**

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	19780.884	505.53858	0.0001	Singlet-A	HOMO->LUMO (99%)
2	25121.1178	398.071459	0.0224	Singlet-A	H-1->LUMO (98%)
3	25228.3902	396.378838	0.0008	Singlet-A	H-4->LUMO (17%), H-2->LUMO (82%)
4	26707.6213	374.424959	0.0003	Singlet-A	HOMO->L+1 (96%)
5	27290.7642	366.424331	0.0664	Singlet-A	H-3->LUMO (86%)
6	28057.8027	356.407096	0.0016	Singlet-A	HOMO->L+3 (91%)
7	28127.1669	355.528164	0.0017	Singlet-A	HOMO->L+2 (71%), HOMO->L+4 (25%)
8	28286.8658	353.520962	0.0006	Singlet-A	HOMO->L+2 (-25%), HOMO->L+4 (72%)
9	28498.991	350.889615	0.0001	Singlet-A	H-4->LUMO (80%), H-2->LUMO (-17%)
10	29583.0077	338.03189	0.0161	Singlet-A	H-5->LUMO (88%), H-3->LUMO (-10%)
11	31646.1882	315.993824	0.011	Singlet-A	H-1->L+1 (92%)
12	32243.0426	310.144428	0.0061	Singlet-A	H-4->L+1 (10%), H-2->L+1 (76%)
13	32756.0147	305.287444	0.0194	Singlet-A	H-1->L+4 (13%), HOMO->L+5 (67%)
14	33025.4058	302.797188	0.0226	Singlet-A	H-1->L+2 (43%), H-1->L+4 (20%), HOMO->L+5 (-11%)
15	33227.8523	300.952343	0.0023	Singlet-A	H-1->L+3 (53%)
16	33230.272	300.930429	0.0046	Singlet-A	H-1->L+2 (40%), H-1->L+4 (-28%)
17	33503.6958	298.474534	0.0081	Singlet-A	H-2->L+2 (20%), H-2->L+4 (31%), HOMO->L+6 (21%), HOMO->L+7 (-15%)
18	33795.6706	295.895889	0.0013	Singlet-A	H-3->L+1 (55%), H-2->L+2 (11%), H-1->L+3 (-15%)
19	33871.4872	295.233567	0.1358	Singlet-A	H-2->L+3 (51%), H-1->L+4 (-26%)
20	34005.3762	294.071148	0.0638	Singlet-A	H-3->L+1 (-21%), H-2->L+2 (46%), HOMO->L+6 (-17%)
21	34458.6629	290.202787	0	Singlet-A	H-3->L+3 (19%), H-2->L+4 (24%), H-1->L+3 (-20%), HOMO->L+6 (-14%)
22	35054.7107	285.268365	0.0128	Singlet-A	H-4->L+1 (13%), H-3->L+2 (64%)
23	35103.1043	284.87509	0.002	Singlet-A	H-4->L+1 (54%), H-3->L+2 (-10%), H-2->L+1 (-11%)
24	35537.8402	281.390201	0.1024	Singlet-A	H-4->L+1 (-12%), H-3->L+4 (62%), H-2->L+3 (-12%)
25	35608.0109	280.835681	0.0076	Singlet-A	H-11->LUMO (74%), H-6->LUMO (14%)
26	35837.0739	279.040639	0	Singlet-A	HOMO->L+6 (21%), HOMO->L+7 (63%)
27	36051.6189	277.380054	0.0094	Singlet-A	H-5->L+1 (46%), H-3->L+3 (17%)
28	36358.1117	275.041787	0.0074	Singlet-A	H-5->L+1 (-32%), H-3->L+3 (32%), H-2->L+4 (-12%)
29	36375.0494	274.913716	0.0001	Singlet-A	H-7->LUMO (98%)
30	36407.3118	274.6701	0.0003	Singlet-A	H-11->LUMO (-12%), H-6->LUMO (84%)
31	36627.5027	273.018886	0	Singlet-A	HOMO->L+8 (98%)
32	36827.5296	271.535998	0.0115	Singlet-A	H-4->L+2 (65%), H-4->L+4 (13%)
33	36921.8971	270.841988	0	Singlet-A	H-8->LUMO (97%)
34	36950.1267	270.635066	0	Singlet-A	H-9->LUMO (99%)
35	37096.1141	269.570014	0.0117	Singlet-A	H-5->L+2 (12%), H-4->L+3 (50%)
36	37259.0392	268.391247	0.012	Singlet-A	H-4->L+2 (-13%), H-4->L+4 (50%), H-1->L+5 (17%)
37	37263.072	268.362201	0.0009	Singlet-A	H-13->LUMO (-16%), H-12->LUMO (79%)
38	37544.5614	266.350161	0.0008	Singlet-A	H-5->L+3 (-35%), H-1->L+5 (41%)
39	37561.4992	266.230055	0.0371	Singlet-A	H-10->LUMO (-11%), H-5->L+2 (39%), H-4->L+3 (-12%), H-3->L+2 (-13%)
40	37853.4739	264.176546	0.0064	Singlet-A	H-5->L+4 (56%), H-1->L+6 (10%)
41	38113.9928	262.370832	0.002	Singlet-A	H-13->LUMO (72%), H-12->LUMO (14%)
42	38417.2594	260.299672	0.1954	Singlet-A	H-10->LUMO (-27%), H-5->L+2 (-12%), H-2->L+5 (33%)
43	38576.1517	259.227517	0.1526	Singlet-A	H-10->LUMO (29%), H-5->L+2 (13%), H-2->L+5 (33%)
44	38610.8338	258.994666	0.0125	Singlet-A	H-5->L+3 (29%), H-2->L+6 (-18%), H-1->L+5 (22%)
45	39149.6158	255.430348	0.0001	Singlet-A	HOMO->L+9 (95%)
46	39164.9405	255.330402	0.0038	Singlet-A	HOMO->L+10 (97%)
47	39310.1213	254.387412	0.1853	Singlet-A	H-5->L+4 (-15%), H-1->L+6 (40%), HOMO->L+12 (11%)
48	39506.1154	253.125368	0.0051	Singlet-A	H-3->L+5 (71%)
49	39566.6074	252.738374	0.0023	Singlet-A	HOMO->L+11 (91%)
50	39844.064	250.978414	0.0658	Singlet-A	H-5->L+3 (13%), H-4->L+4 (-12%), H-2->L+6 (28%), H-2->L+7 (-17%)

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
51	40019.8941	249.875724	0.0322	Singlet-A	H-4->L+5 (-11%), H-3->L+6 (16%), HOMO->L+12 (36%)
52	40080.3861	249.498595	0.0296	Singlet-A	H-1->L+6 (10%), H-1->L+7 (67%)
53	40542.545	246.654471	0.0003	Singlet-A	H-2->L+6 (-12%), H-2->L+7 (-27%), H-1->L+8 (37%)
54	40613.5222	246.223412	0.0177	Singlet-A	H-3->L+6 (36%), H-3->L+7 (-16%), HOMO->L+12 (-13%)
55	40672.4011	245.866969	0	Singlet-A	H-1->L+8 (47%), HOMO->L+14 (-19%)
56	41370.8821	241.7159	0.002	Singlet-A	H-1->L+8 (11%), HOMO->L+13 (17%), HOMO->L+14 (42%)
57	41870.1427	238.833674	0.0147	Singlet-A	H-5->L+6 (13%), H-4->L+5 (-20%), H-3->L+7 (31%)
58	41950.7987	238.374484	0.1357	Singlet-A	H-5->L+7 (10%), H-4->L+5 (39%), H-2->L+5 (-12%)
59	42038.7138	237.875974	0.0024	Singlet-A	H-5->L+5 (70%)
60	42183.8946	237.057296	0.0005	Singlet-A	H-11->L+1 (21%), H-6->L+1 (44%)
61	42331.495	236.230731	0.0058	Singlet-A	H-7->L+1 (14%), H-2->L+8 (64%)
62	42386.3411	235.925058	0.0115	Singlet-A	H-7->L+1 (36%), H-6->L+4 (13%), H-2->L+8 (-27%)
63	42564.5909	234.937064	0.0046	Singlet-A	H-11->L+1 (33%), H-6->L+1 (-12%)
64	42565.3974	234.932612	0.0496	Singlet-A	H-16->LUMO (-28%), H-10->L+1 (38%)
65	42611.3714	234.67914	0.0037	Singlet-A	H-4->L+6 (36%), H-2->L+6 (-15%)
66	42937.2216	232.898162	0.0069	Singlet-A	H-17->LUMO (17%), H-11->L+1 (25%), H-10->L+2 (-21%), H-8->L+1 (12%)
67	43037.235	232.356934	0.001	Singlet-A	H-9->L+1 (57%), H-9->L+3 (11%), H-8->L+4 (-16%), H-7->L+1 (11%)
68	43045.3006	232.313397	0.003	Singlet-A	H-9->L+4 (-13%), H-8->L+1 (51%), H-8->L+3 (10%)
69	43052.5597	232.274227	0.0069	Singlet-A	H-14->LUMO (89%)
70	43166.2846	231.662282	0.0786	Singlet-A	H-5->L+6 (-16%), H-5->L+7 (10%), H-1->L+9 (49%)
71	43240.4882	231.264734	0.0003	Singlet-A	H-1->L+10 (88%)
72	43329.2098	230.791193	0.1332	Singlet-A	H-5->L+6 (19%), H-5->L+7 (-10%), H-1->L+9 (42%), HOMO->L+15 (10%)
73	43439.7085	230.204123	0.009	Singlet-A	H-4->L+7 (39%), H-2->L+7 (-13%)
74	43559.8859	229.569013	0.002	Singlet-A	H-15->LUMO (82%)
75	43592.1483	229.399109	0.0023	Singlet-A	H-7->L+4 (-13%), H-6->L+1 (23%), H-6->L+3 (-19%), H-3->L+8 (23%)
76	43606.6664	229.322735	0.0005	Singlet-A	H-7->L+1 (31%), H-7->L+3 (-24%), H-6->L+4 (-24%)
77	43630.8632	229.195557	0.0004	Singlet-A	H-3->L+8 (69%)
78	43808.3064	228.267213	0.0104	Singlet-A	H-12->L+1 (24%), H-11->L+2 (54%), H-6->L+2 (10%)
79	43941.3888	227.575875	0.0051	Singlet-A	H-5->L+7 (-19%), H-3->L+6 (20%), H-3->L+7 (22%)
80	44110.7664	226.702023	0	Singlet-A	H-12->L+1 (30%), H-11->L+2 (-16%), H-11->L+4 (-19%)
81	44176.9043	226.362624	0.0056	Singlet-A	H-11->L+3 (45%), H-8->L+1 (-11%), H-8->L+3 (16%)
82	44262.3997	225.925392	0.0011	Singlet-A	H-9->L+1 (27%), H-9->L+3 (-27%), H-8->L+4 (26%)
83	44300.308	225.732065	0.0013	Singlet-A	H-11->L+3 (30%), H-9->L+4 (20%), H-8->L+1 (18%), H-8->L+3 (-18%)
84	44347.895	225.489845	0.0011	Singlet-A	H-1->L+11 (73%)
85	44433.3904	225.055975	0.0024	Singlet-A	H-12->L+1 (14%), H-11->L+4 (41%), H-6->L+2 (-10%), H-4->L+8 (-13%)
86	44494.689	224.745924	0.0002	Singlet-A	H-6->L+2 (-12%), H-4->L+8 (47%)
87	44548.7285	224.473298	0.0377	Singlet-A	H-7->L+2 (51%), H-1->L+12 (10%), HOMO->L+13 (18%)
88	44616.4795	224.132431	0	Singlet-A	H-11->L+2 (-10%), H-11->L+4 (12%), H-6->L+2 (53%)
89	44634.2238	224.043327	0.0291	Singlet-A	H-7->L+2 (36%), H-1->L+12 (-12%), HOMO->L+13 (-22%)
90	44722.9454	223.598869	0.0069	Singlet-A	H-2->L+9 (25%)
91	44740.6898	223.510188	0.0009	Singlet-A	H-2->L+10 (49%)
92	44747.1422	223.477959	0.0009	Singlet-A	H-4->L+6 (11%), H-4->L+7 (14%), H-2->L+9 (27%)
93	45017.3398	222.136626	0.0184	Singlet-A	H-13->L+1 (61%), H-8->L+2 (-12%)
94	45116.5467	221.64817	0.0024	Singlet-A	H-8->L+2 (51%)
95	45117.3533	221.644207	0.0003	Singlet-A	H-9->L+2 (-15%), H-2->L+9 (23%), H-2->L+11 (15%)
96	45133.4845	221.564989	0.0109	Singlet-A	H-8->L+2 (-21%), H-2->L+10 (26%)
97	45142.3566	221.521443	0	Singlet-A	H-9->L+2 (75%)
98	45152.8419	221.470002	0.0097	Singlet-A	H-16->LUMO (10%), H-10->L+1 (13%), H-10->L+3 (49%)
99	45301.249	220.744466	0	Singlet-A	H-2->L+9 (-10%), H-2->L+11 (41%)
100	45417.3936	220.179962	0.0337	Singlet-A	H-12->L+3 (10%), H-5->L+6 (-15%), HOMO->L+12 (-13%), HOMO->L+15 (24%)

Table S15: Energy and composition of TD-DFT calculated transitions of **3a**

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	18005.6454	555.381368	0.0002	Singlet-A	HOMO->LUMO (98%)
2	22065.0619	453.205164	0.0095	Singlet-A	H-1->LUMO (99%)
3	22365.1022	447.125164	0.0002	Singlet-A	H-4->LUMO (23%), H-2->LUMO (76%)
4	24239.5477	412.548952	0.0004	Singlet-A	H-4->LUMO (75%), H-2->LUMO (-23%)
5	25680.0638	389.407132	0.0431	Singlet-A	H-5->LUMO (33%), H-3->LUMO (61%)
6	26265.6264	380.725738	0.0005	Singlet-A	HOMO->L+1 (98%)
7	26355.1546	379.432417	0.0232	Singlet-A	H-5->LUMO (61%), H-3->LUMO (-37%)
8	27176.2326	367.96859	0.0404	Singlet-A	HOMO->L+3 (95%)
9	27245.5968	367.031784	0.005	Singlet-A	HOMO->L+2 (90%)
10	28183.6261	354.815948	0.0084	Singlet-A	HOMO->L+4 (90%)
11	29808.8445	335.470904	0.0066	Singlet-A	H-1->L+1 (96%)
12	30441.9941	328.493593	0.0007	Singlet-A	H-2->L+1 (79%), H-1->L+2 (-12%)
13	30950.9334	323.092033	0.0036	Singlet-A	H-1->L+2 (81%)
14	31420.3514	318.26506	0.0277	Singlet-A	H-1->L+3 (78%)
15	31638.9291	316.066323	0.0156	Singlet-A	H-4->L+3 (10%), H-2->L+3 (46%), H-1->L+4 (-37%)
16	31739.7491	315.062352	0.0004	Singlet-A	H-2->L+2 (81%)
17	32322.892	309.378257	0.0823	Singlet-A	H-2->L+3 (31%), H-1->L+4 (52%)
18	32448.7154	308.17861	0.0083	Singlet-A	H-4->L+1 (81%), H-2->L+1 (-10%)
19	32845.5429	304.455312	0.0834	Singlet-A	H-4->L+4 (11%), H-2->L+4 (69%)
20	33239.1442	300.850105	0.0003	Singlet-A	H-5->L+1 (40%), H-4->L+2 (10%), H-3->L+1 (37%)
21	33581.1256	297.786326	0.007	Singlet-A	H-4->L+3 (45%), HOMO->L+5 (38%)
22	33771.4738	296.107895	0.0272	Singlet-A	H-5->L+3 (16%), H-4->L+2 (57%)
23	33868.261	295.261691	0.0065	Singlet-A	H-5->L+2 (44%), H-3->L+2 (16%), HOMO->L+5 (-19%)
24	33968.2744	294.392346	0.0068	Singlet-A	H-4->L+4 (-15%), H-3->L+1 (-18%), HOMO->L+6 (49%)
25	34125.5536	293.035539	0.0375	Singlet-A	H-5->L+2 (18%), H-5->L+4 (13%), H-4->L+3 (-17%), HOMO->L+5 (29%)
26	34148.9438	292.834825	0.0027	Singlet-A	H-5->L+1 (-35%), H-3->L+1 (40%), HOMO->L+6 (15%)
27	34326.387	291.321076	0.0001	Singlet-A	H-5->L+3 (-14%), H-4->L+2 (10%), H-4->L+4 (35%), H-2->L+4 (-14%)
28	34638.5258	288.695889	0.0142	Singlet-A	H-9->LUMO (72%), H-3->L+3 (11%)
29	34773.2213	287.577614	0.0009	Singlet-A	H-9->LUMO (-13%), H-5->L+3 (-10%), H-3->L+3 (64%)
30	34832.1002	287.091503	0.0084	Singlet-A	H-6->LUMO (68%), H-3->L+2 (-13%)
31	35076.4878	285.091257	0.0839	Singlet-A	H-6->LUMO (-15%), H-3->L+4 (60%)
32	35204.7309	284.052732	0.0297	Singlet-A	H-6->LUMO (10%), H-5->L+2 (-14%), H-5->L+4 (14%), H-3->L+2 (51%)
33	35441.8595	282.152238	0.0214	Singlet-A	H-5->L+3 (34%), H-4->L+4 (11%), H-1->L+5 (11%), HOMO->L+6 (21%)
34	35645.1126	280.543369	0.0293	Singlet-A	H-5->L+4 (41%), H-3->L+4 (-27%)
35	36450.0595	274.347975	0.0014	Singlet-A	H-11->LUMO (88%)
36	36676.7029	272.652644	0.0014	Singlet-A	H-8->LUMO (77%), H-7->LUMO (-14%)
37	37171.9307	269.020194	0.0011	Singlet-A	H-10->LUMO (95%)
38	37964.7792	263.402032	0.0096	Singlet-A	H-2->L+6 (35%), H-1->L+5 (56%)
39	38022.045	263.005317	0.2639	Singlet-A	H-8->LUMO (11%), H-7->LUMO (44%), H-1->L+6 (15%)
40	38104.3141	262.437476	0.0796	Singlet-A	H-7->LUMO (-15%), H-2->L+5 (42%), H-1->L+6 (27%)
41	38332.5706	260.874756	0.0017	Singlet-A	HOMO->L+7 (95%)
42	38893.1298	257.114819	0.4613	Singlet-A	H-2->L+5 (-24%), H-1->L+6 (37%), HOMO->L+8 (-14%)
43	39114.9338	255.656831	0.0896	Singlet-A	H-2->L+6 (45%), H-1->L+5 (-20%)
44	39521.44	253.027218	0.0023	Singlet-A	H-4->L+10 (10%), HOMO->L+9 (24%), HOMO->L+10 (42%)
45	40344.9378	247.862571	0.0587	Singlet-A	H-4->L+5 (58%), HOMO->L+8 (-22%)
46	40418.3347	247.412469	0.138	Singlet-A	H-4->L+5 (30%), H-2->L+5 (-13%), HOMO->L+8 (27%)
47	40515.9285	246.816508	0.0011	Singlet-A	H-4->L+6 (40%), H-3->L+5 (41%)
48	40716.7619	245.599098	0	Singlet-A	H-4->L+6 (-42%), H-3->L+5 (44%)
49	40990.9923	243.956036	0.0117	Singlet-A	H-5->L+6 (12%), H-3->L+6 (74%)
50	41102.2976	243.295402	0.0127	Singlet-A	H-12->LUMO (73%)

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
51	41231.3472	242.533914	0.0048	Singlet-A	H-13->LUMO (88%)
52	41437.02	241.330096	0.0163	Singlet-A	H-12->LUMO (-10%), H-5->L+5 (74%)
53	41549.9384	240.674244	0.0053	Singlet-A	H-5->L+6 (39%), H-5->L+10 (-10%), H-1->L+7 (15%)
54	41608.0107	240.338335	0.0053	Singlet-A	H-5->L+6 (39%), H-5->L+9 (11%), H-5->L+10 (14%)
55	41626.5616	240.231228	0.0114	Singlet-A	H-4->L+9 (13%), H-4->L+10 (29%), H-2->L+10 (15%)
56	41909.6642	238.60845	0.0021	Singlet-A	H-1->L+7 (70%)
57	42629.1157	234.581455	0.0014	Singlet-A	H-9->L+1 (18%), H-2->L+7 (58%)
58	42696.8667	234.209223	0.0141	Singlet-A	H-9->L+1 (69%), H-2->L+7 (-20%)
59	42954.9659	232.801954	0.0056	Singlet-A	H-6->L+1 (85%)
60	43659.8994	229.04313	0.0518	Singlet-A	H-16->LUMO (-14%), H-7->L+1 (53%)
61	43727.6504	228.688254	0.0161	Singlet-A	H-9->L+2 (68%), H-6->L+1 (-10%)
62	43826.8573	228.170593	0.0097	Singlet-A	H-7->L+2 (34%), H-4->L+7 (-22%), H-2->L+7 (14%)
63	43907.5133	227.751454	0.0004	Singlet-A	H-9->L+3 (77%)
64	44034.1432	227.096505	0.0139	Singlet-A	H-6->L+2 (80%)
65	44158.3534	226.457719	0.0129	Singlet-A	H-6->L+3 (67%)
66	44381.7706	225.317735	0.0025	Singlet-A	H-11->L+3 (22%), H-9->L+4 (59%)
67	44454.361	224.949809	0.0657	Singlet-A	HOMO->L+9 (32%), HOMO->L+10 (-18%)
68	44589.0565	224.270276	0.012	Singlet-A	H-8->L+1 (77%)
69	44685.8437	223.784518	0.0038	Singlet-A	H-11->L+1 (86%)
70	44767.3062	223.3773	0.0118	Singlet-A	H-6->L+4 (36%), H-1->L+8 (35%)
71	44779.4046	223.316949	0.0136	Singlet-A	H-4->L+8 (15%), H-2->L+8 (27%), HOMO->L+11 (-11%)
72	44847.1557	222.979581	0.0015	Singlet-A	H-14->LUMO (82%)
73	44968.9462	222.37568	0.0003	Singlet-A	H-10->L+1 (46%), H-6->L+4 (14%), H-4->L+7 (-10%)
74	45111.7074	221.671947	0.0202	Singlet-A	H-10->L+1 (32%), H-7->L+2 (11%), H-4->L+7 (32%)
75	45260.1144	220.945089	0.0171	Singlet-A	H-5->L+7 (46%), H-3->L+7 (27%)
76	45342.3835	220.544207	0.0095	Singlet-A	H-6->L+4 (-21%), H-1->L+8 (26%)
77	45470.6266	219.922195	0.0243	Singlet-A	H-4->L+8 (14%), HOMO->L+8 (-10%), HOMO->L+11 (22%)
78	45584.3515	219.373528	0.0001	Singlet-A	H-11->L+2 (73%), H-8->L+2 (11%)
79	45681.1387	218.908729	0.0402	Singlet-A	H-7->L+3 (76%)
80	45762.6013	218.519047	0.0017	Singlet-A	H-11->L+2 (-12%), H-8->L+2 (69%)
81	45901.3296	217.858613	0.0359	Singlet-A	H-11->L+3 (54%), H-9->L+4 (-16%)
82	46069.9006	217.061462	0.0142	Singlet-A	H-10->L+2 (-13%), H-8->L+3 (47%)
83	46130.3926	216.776824	0.0068	Singlet-A	H-5->L+7 (-27%), H-3->L+7 (50%)
84	46169.9141	216.591263	0.0001	Singlet-A	H-11->L+4 (43%), H-7->L+4 (-33%)
85	46222.3405	216.3456	0.0022	Singlet-A	H-10->L+2 (73%)
86	46474.7938	215.170401	0.0007	Singlet-A	H-11->L+4 (28%), H-7->L+4 (59%)
87	46558.676	214.78274	0.0176	Singlet-A	H-11->L+4 (-10%), H-10->L+3 (29%), H-8->L+4 (23%), H-2->L+9 (-16%)
88	46586.099	214.656307	0.0025	Singlet-A	H-8->L+3 (10%), H-1->L+9 (39%)
89	46782.8997	213.753317	0.011	Singlet-A	H-10->L+3 (14%), H-5->L+8 (12%), H-2->L+9 (22%), HOMO->L+12 (13%)
90	46936.9526	213.051752	0.0039	Singlet-A	H-1->L+10 (49%), HOMO->L+13 (11%)
91	47041.8054	212.576875	0.0024	Singlet-A	H-10->L+3 (-37%), H-8->L+4 (50%)
92	47415.2427	210.902643	0.001	Singlet-A	H-10->L+4 (81%)
93	47477.3478	210.626761	0.0116	Singlet-A	H-5->L+8 (36%), H-4->L+10 (19%), H-2->L+9 (-17%)
94	47579.781	210.173309	0.0092	Singlet-A	H-17->LUMO (54%), H-15->LUMO (21%)
95	47606.3974	210.055802	0.0199	Singlet-A	H-4->L+8 (31%), H-2->L+8 (-29%), H-1->L+10 (18%)
96	47738.6733	209.473773	0.0123	Singlet-A	H-17->LUMO (-13%), H-15->LUMO (71%)
97	47824.9752	209.09577	0.0001	Singlet-A	H-4->L+9 (-24%), H-2->L+10 (45%)
98	48784.7816	204.981957	0.0025	Singlet-A	H-16->LUMO (64%), H-7->L+1 (16%)
99	48807.3653	204.88711	0.0235	Singlet-A	H-5->L+8 (11%), H-4->L+9 (27%), H-4->L+10 (-14%), HOMO->L+12 (-23%)
100	49313.0784	202.785961	0.022	Singlet-A	H-12->L+1 (89%)

Table S16: Energy and composition of TD-DFT calculated transitions of **3b**

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	19968.8125	500.780906	0.0003	Singlet-A	HOMO->LUMO (98%)
2	24206.4787	413.112544	0.0198	Singlet-A	H-1->LUMO (98%)
3	24283.9085	411.795326	0.0005	Singlet-A	H-3->LUMO (27%), H-2->LUMO (72%)
4	26318.0528	379.96732	0.0009	Singlet-A	H-3->LUMO (70%), H-2->LUMO (-27%)
5	26796.3429	373.185253	0.029	Singlet-A	HOMO->L+1 (-34%), HOMO->L+2 (63%)
6	27159.2949	368.198072	0.0708	Singlet-A	H-5->LUMO (29%), H-4->LUMO (63%)
7	27295.6035	366.359366	0.0081	Singlet-A	HOMO->L+1 (64%), HOMO->L+2 (32%)
8	27681.9458	361.246283	0.0019	Singlet-A	HOMO->L+3 (87%)
9	28441.7253	351.596111	0.0102	Singlet-A	H-5->LUMO (68%), H-4->LUMO (-29%)
10	28671.5949	348.777249	0.0143	Singlet-A	HOMO->L+4 (83%)
11	30819.4642	324.470275	0.0297	Singlet-A	H-1->L+1 (85%)
12	31237.2622	320.130488	0.0128	Singlet-A	H-2->L+1 (38%), H-2->L+2 (-27%), H-1->L+3 (15%)
13	31418.7382	318.2814	0.0038	Singlet-A	H-1->L+1 (11%), H-1->L+2 (68%)
14	31482.4565	317.637221	0.0034	Singlet-A	H-2->L+1 (43%), H-2->L+2 (13%), H-1->L+3 (-16%), H-1->L+4 (10%)
15	32120.4454	311.328186	0.0744	Singlet-A	H-2->L+2 (27%), H-1->L+3 (56%)
16	32414.8398	308.500676	0.0104	Singlet-A	H-1->L+4 (78%)
17	32673.7456	306.056126	0.0616	Singlet-A	H-2->L+3 (42%), H-2->L+4 (-18%), H-1->L+2 (14%)
18	32981.045	303.204462	0.0119	Singlet-A	H-3->L+4 (10%), H-2->L+3 (24%), H-2->L+4 (58%)
19	33243.177	300.813608	0.0116	Singlet-A	H-3->L+1 (42%), H-3->L+2 (-12%), HOMO->L+5 (26%)
20	33444.817	298.999992	0.0015	Singlet-A	H-5->L+1 (-13%), H-5->L+2 (12%), H-4->L+1 (-21%), H-4->L+2 (16%), HOMO->L+6 (28%)
21	33474.6597	298.733433	0.0019	Singlet-A	H-3->L+1 (-30%), H-3->L+2 (-10%), HOMO->L+5 (44%)
22	33725.4998	296.511543	0.0145	Singlet-A	H-5->L+3 (-10%), H-4->L+3 (-13%), H-3->L+2 (31%), H-2->L+2 (-16%), HOMO->L+5 (14%)
23	33837.6117	295.529132	0.0398	Singlet-A	H-4->L+1 (14%), H-3->L+3 (20%), HOMO->L+6 (36%)
24	34081.9994	293.410017	0	Singlet-A	H-4->L+1 (27%), H-3->L+3 (-22%), H-2->L+3 (13%)
25	34636.1061	288.716058	0.145	Singlet-A	H-5->L+3 (11%), H-4->L+3 (46%), H-3->L+2 (13%)
26	34680.4669	288.346752	0.0037	Singlet-A	H-5->L+1 (12%), H-5->L+2 (-18%), H-4->L+2 (46%), H-3->L+4 (-10%)
27	34801.4509	287.344342	0.0001	Singlet-A	H-5->L+1 (10%), H-5->L+2 (-14%), H-4->L+1 (-10%), H-3->L+4 (36%), HOMO->L+6 (14%)
28	35003.0909	285.689056	0.0242	Singlet-A	H-5->L+4 (23%), H-4->L+4 (53%)
29	35288.6131	283.377529	0.0407	Singlet-A	H-3->L+3 (28%), H-3->L+4 (26%)
30	35411.2102	282.396448	0.0124	Singlet-A	H-5->L+3 (47%), H-5->L+4 (-17%), H-4->L+3 (-22%)
31	35435.407	282.203616	0.0189	Singlet-A	H-5->L+1 (43%), H-5->L+2 (26%), H-4->L+1 (-16%)
32	36321.0099	275.322741	0.0148	Singlet-A	H-8->LUMO (95%)
33	36662.1848	272.760613	0.0019	Singlet-A	H-7->LUMO (15%), H-5->L+4 (34%), H-4->L+4 (-29%)
34	37088.855	269.622775	0.0003	Singlet-A	H-7->LUMO (82%)
35	37782.4966	264.672822	0.0076	Singlet-A	H-2->L+6 (38%), H-1->L+5 (51%)
36	37842.9886	264.249742	0.023	Singlet-A	H-2->L+5 (49%), H-1->L+6 (36%)
37	38154.3208	262.093514	0.3323	Singlet-A	H-6->LUMO (64%)
38	38283.3704	261.210021	0.0361	Singlet-A	H-11->LUMO (88%)
39	38679.3914	258.535609	0.4447	Singlet-A	H-2->L+5 (-20%), H-1->L+6 (39%), HOMO->L+8 (11%)
40	38932.6512	256.853815	0.1085	Singlet-A	H-2->L+6 (38%), H-1->L+5 (-25%)
41	38989.917	256.476566	0.0115	Singlet-A	H-9->LUMO (94%)
42	39389.9707	253.87173	0.0001	Singlet-A	H-10->LUMO (-16%), HOMO->L+7 (-23%), HOMO->L+9 (10%), HOMO->L+10 (30%)
43	39477.8858	253.306372	0.0006	Singlet-A	H-10->LUMO (82%)
44	40000.5366	249.996646	0.0018	Singlet-A	HOMO->L+7 (68%), HOMO->L+10 (10%)
45	40013.4416	249.916018	0.0024	Singlet-A	H-3->L+5 (78%)
46	40169.9142	248.942528	0.0081	Singlet-A	H-4->L+5 (34%), H-3->L+6 (39%)
47	40415.915	247.427282	0.1788	Singlet-A	H-4->L+6 (11%), HOMO->L+8 (40%)
48	40447.3709	247.234858	0.0018	Singlet-A	H-4->L+5 (45%), H-3->L+6 (-41%)
49	40565.1286	246.517152	0.0127	Singlet-A	H-5->L+6 (16%), H-4->L+6 (64%)
50	41061.163	243.539132	0.0029	Singlet-A	H-5->L+5 (82%)

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
51	41328.941	241.961196	0.0059	Singlet-A	H-5->L+6 (72%), H-4->L+6 (-14%)
52	41463.6365	241.17518	0.0113	Singlet-A	H-5->L+10 (24%), H-4->L+10 (16%), H-1->L+10 (15%)
53	41641.0797	240.147472	0.0033	Singlet-A	H-3->L+10 (29%), H-2->L+10 (20%), HOMO->L+10 (13%)
54	41854.0115	238.925724	0.0447	Singlet-A	H-12->LUMO (63%), H-6->L+1 (24%)
55	41953.2184	238.360736	0.0318	Singlet-A	H-13->LUMO (60%), H-6->L+4 (-15%)
56	43354.2131	230.65809	0.012	Singlet-A	H-8->L+1 (87%)
57	43471.9709	230.033279	0.0047	Singlet-A	H-1->L+7 (83%)
58	43530.8498	229.722141	0.0104	Singlet-A	H-8->L+2 (83%)
59	43789.7555	228.363915	0.0043	Singlet-A	H-8->L+3 (50%), H-7->L+1 (29%)
60	43943.8085	227.563344	0.0058	Singlet-A	H-7->L+1 (31%), H-7->L+2 (-29%)
61	44015.5923	227.192217	0.0054	Singlet-A	H-13->LUMO (-10%), H-3->L+7 (14%), H-2->L+7 (51%)
62	44089.7958	226.80985	0.0044	Singlet-A	H-7->L+1 (13%), H-7->L+2 (29%), H-6->L+2 (-23%)
63	44163.9994	226.428769	0.0176	Singlet-A	H-6->L+1 (-20%), H-6->L+2 (26%)
64	44230.1373	226.090187	0.0932	Singlet-A	HOMO->L+9 (36%), HOMO->L+10 (-14%)
65	44367.2525	225.391464	0.0362	Singlet-A	H-14->LUMO (25%), H-12->LUMO (-11%), H-6->L+2 (43%)
66	44588.2499	224.274333	0.0011	Singlet-A	H-7->L+3 (47%), H-7->L+4 (-10%), H-1->L+8 (-20%)
67	44657.6141	223.92598	0.0147	Singlet-A	H-3->L+8 (16%), H-2->L+8 (25%)
68	44743.1094	223.498101	0.0133	Singlet-A	H-15->LUMO (16%), H-6->L+3 (32%), H-2->L+7 (29%)
69	44809.2474	223.168221	0.0239	Singlet-A	H-8->L+3 (14%), H-8->L+4 (55%)
70	44931.8445	222.559303	0.0038	Singlet-A	H-6->L+3 (-36%), H-6->L+4 (43%)
71	45125.4189	221.604591	0.0139	Singlet-A	H-7->L+3 (16%), H-1->L+8 (40%)
72	45223.8192	221.122412	0.0056	Singlet-A	H-11->L+1 (-15%), H-11->L+2 (27%), H-8->L+3 (-14%)
73	45446.4298	220.039287	0.0546	Singlet-A	H-11->L+1 (32%), HOMO->L+12 (19%)
74	45573.8662	219.423999	0.0242	Singlet-A	H-14->LUMO (-12%), H-11->L+1 (35%), H-11->L+2 (23%), H-8->L+4 (11%)
75	45593.2237	219.330839	0.0009	Singlet-A	H-7->L+3 (10%), H-7->L+4 (82%)
76	45764.2144	218.511344	0.003	Singlet-A	H-11->L+3 (67%), H-11->L+4 (-11%)
77	45811.8014	218.284365	0.0079	Singlet-A	H-9->L+1 (76%)
78	45949.7232	217.629167	0.0034	Singlet-A	H-14->LUMO (17%), H-11->L+2 (14%), H-5->L+7 (12%), H-4->L+7 (16%)
79	46044.0907	217.183136	0.0003	Singlet-A	H-10->L+1 (-13%), H-3->L+7 (58%)
80	46172.3338	216.579912	0.0216	Singlet-A	H-9->L+2 (53%)
81	46309.449	215.938652	0.0111	Singlet-A	H-10->L+1 (68%)
82	46510.2824	215.00622	0.0044	Singlet-A	H-10->L+2 (21%), H-9->L+3 (33%), H-2->L+9 (-14%)
83	46655.4632	214.337171	0.0167	Singlet-A	H-9->L+2 (12%), H-1->L+9 (35%), HOMO->L+13 (12%)
84	46699.0174	214.137268	0.0165	Singlet-A	H-5->L+8 (11%), H-4->L+8 (18%), HOMO->L+11 (18%)
85	46832.0998	213.528756	0.0049	Singlet-A	H-11->L+3 (14%), H-11->L+4 (70%)
86	46832.9064	213.525078	0.0185	Singlet-A	H-14->LUMO (-12%), H-6->L+1 (14%), H-5->L+7 (12%), H-4->L+7 (22%)
87	46970.0216	212.901754	0.0054	Singlet-A	H-16->LUMO (83%)
88	47109.5565	212.271156	0.0003	Singlet-A	H-10->L+2 (52%), H-9->L+3 (-40%)
89	47187.7928	211.919215	0.0009	Singlet-A	H-3->L+8 (-11%), H-1->L+10 (39%)
90	47317.649	211.337634	0.0643	Singlet-A	H-9->L+4 (23%), H-2->L+9 (23%)
91	47387.8197	211.024691	0.0012	Singlet-A	H-10->L+3 (78%)
92	47451.5379	210.741326	0	Singlet-A	H-9->L+4 (50%), H-2->L+9 (-14%)
93	47560.4235	210.258851	0.1716	Singlet-A	H-15->LUMO (31%), H-6->L+4 (-12%)
94	47663.6632	209.803429	0.0154	Singlet-A	H-3->L+8 (28%), H-2->L+8 (-21%), H-1->L+10 (25%)
95	47863.6901	208.926641	0.0009	Singlet-A	H-10->L+4 (52%), H-5->L+7 (-20%), H-4->L+7 (17%)
96	47893.5328	208.796458	0.0002	Singlet-A	H-18->LUMO (38%), H-17->LUMO (-18%), H-3->L+9 (12%), H-2->L+10 (-14%)
97	47937.8936	208.603242	0.0021	Singlet-A	H-10->L+4 (34%), H-5->L+7 (37%), H-4->L+7 (-18%)
98	47940.3133	208.592713	0.0007	Singlet-A	H-18->LUMO (41%), H-3->L+9 (-16%), H-2->L+10 (22%)
99	48054.0382	208.099056	0.0075	Singlet-A	H-17->LUMO (49%), H-13->L+1 (10%)
100	48158.0845	207.649455	0.0012	Singlet-A	H-19->LUMO (97%)

Table S17: Energy and composition of TD-DFT calculated transitions of **4a**

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	20548.7291	486.648101	0.0001	Singlet-A	HOMO->LUMO (97%)
2	23906.4384	418.297357	0.0137	Singlet-A	H-1->LUMO (99%)
3	24660.572	405.505598	0.0003	Singlet-A	H-5->LUMO (12%), H-2->LUMO (80%)
4	26641.4834	375.354475	0.0003	Singlet-A	H-5->LUMO (55%), H-3->LUMO (20%), H-2->LUMO (-18%)
5	27945.6909	357.836922	0.0655	Singlet-A	H-7->LUMO (57%), H-4->LUMO (37%)
6	28670.7883	348.787061	0.0001	Singlet-A	HOMO->L+1 (96%)
7	28733.7	348.023401	0.0103	Singlet-A	H-7->LUMO (-31%), H-6->LUMO (-13%), H-4->LUMO (53%)
8	29481.3811	339.197135	0	Singlet-A	H-5->LUMO (-24%), H-3->LUMO (74%)
9	29750.7722	336.12573	0.0004	Singlet-A	HOMO->L+2 (94%)
10	29970.1565	333.665258	0.0003	Singlet-A	H-6->LUMO (80%)
11	30071.783	332.537648	0.0008	Singlet-A	HOMO->L+3 (89%)
12	30697.6736	325.757584	0.0023	Singlet-A	HOMO->L+4 (90%)
13	31585.6962	316.599006	0.0064	Singlet-A	H-1->L+1 (96%)
14	32494.6893	307.742595	0.0032	Singlet-A	H-8->LUMO (-28%), H-2->L+1 (41%), H-1->L+2 (-24%)
15	32520.4992	307.498355	0.0016	Singlet-A	H-8->LUMO (68%), H-2->L+1 (16%), H-1->L+2 (-11%)
16	32867.32	304.253587	0.0008	Singlet-A	H-2->L+1 (29%), H-1->L+2 (59%)
17	32911.6808	303.843491	0.0001	Singlet-A	H-9->LUMO (98%)
18	33306.0886	300.245403	0.0174	Singlet-A	H-1->L+3 (82%)
19	33873.9069	295.212478	0.0165	Singlet-A	H-2->L+2 (77%)
20	33998.9237	294.126958	0.0107	Singlet-A	H-1->L+4 (80%)
21	34262.6688	291.862845	0.0228	Singlet-A	H-2->L+3 (64%)
22	34601.424	289.005447	0.0011	Singlet-A	H-10->LUMO (10%), H-5->L+1 (51%), H-3->L+1 (19%), H-2->L+1 (-10%)
23	34992.6056	285.774661	0.0307	Singlet-A	H-2->L+4 (69%)
24	35353.1379	282.860323	0.0473	Singlet-A	HOMO->L+5 (75%)
25	35467.6694	281.946916	0.013	Singlet-A	H-7->L+1 (47%), H-4->L+1 (26%)
26	35966.9301	278.033182	0.0153	Singlet-A	H-10->LUMO (-18%), H-7->L+2 (48%), H-4->L+2 (11%)
27	36102.4322	276.989649	0.0213	Singlet-A	H-12->LUMO (15%), H-5->L+2 (40%), H-3->L+2 (16%)
28	36212.1243	276.150604	0.0063	Singlet-A	H-7->L+3 (10%), H-5->L+3 (27%), H-3->L+3 (16%)
29	36392.7938	274.779674	0.0092	Singlet-A	H-4->L+1 (14%), HOMO->L+6 (29%)
30	36412.9578	274.627512	0.0004	Singlet-A	H-7->L+1 (-17%), H-4->L+1 (39%)
31	36533.1352	273.724112	0.0036	Singlet-A	H-5->L+1 (-10%), H-3->L+1 (30%), H-3->L+3 (-20%), HOMO->L+6 (-19%)
32	36607.3387	273.16927	0.0336	Singlet-A	H-12->LUMO (59%), HOMO->L+6 (14%)
33	36812.205	271.649036	0.0015	Singlet-A	H-7->L+4 (35%), H-5->L+4 (-19%)
34	37096.9206	269.564153	0.0027	Singlet-A	H-11->LUMO (80%)
35	37133.2158	269.300673	0.0052	Singlet-A	H-6->L+1 (49%), H-6->L+3 (-20%), H-4->L+3 (-11%)
36	37523.5909	266.499015	0.0175	Singlet-A	H-4->L+2 (-26%), H-4->L+3 (37%)
37	37594.5682	265.995874	0.0037	Singlet-A	H-3->L+1 (23%), H-3->L+2 (-13%), H-3->L+3 (31%)
38	37763.9458	264.802838	0.0111	Singlet-A	H-4->L+2 (36%), H-4->L+3 (30%)
39	37813.1459	264.458292	0.0269	Singlet-A	H-7->L+3 (34%), H-5->L+3 (-12%)
40	38153.5142	262.099054	0.0326	Singlet-A	H-5->L+4 (16%), H-4->L+4 (37%)
41	38175.2914	261.94954	0.0009	Singlet-A	H-6->L+1 (15%), H-6->L+2 (-20%), H-6->L+3 (41%)
42	38240.6227	261.502018	0.017	Singlet-A	H-13->LUMO (57%)
43	38322.0853	260.946134	0.0047	Singlet-A	H-13->LUMO (31%), H-7->L+4 (12%), H-4->L+4 (-23%)
44	38584.2173	259.173328	0.0789	Singlet-A	H-10->LUMO (-13%), H-5->L+2 (-13%), H-3->L+2 (40%)
45	38639.0634	258.805445	0.1907	Singlet-A	H-10->LUMO (33%), H-7->L+2 (19%), H-3->L+2 (16%)
46	39112.5141	255.672647	0.0065	Singlet-A	H-6->L+2 (56%), H-6->L+3 (14%)
47	39224.6259	254.941883	0.0028	Singlet-A	H-2->L+5 (42%), H-1->L+5 (12%), H-1->L+6 (-10%)
48	39316.5738	254.345662	0.0151	Singlet-A	H-2->L+5 (-19%), H-1->L+5 (20%), HOMO->L+7 (11%)
49	39698.8832	251.896255	0.0029	Singlet-A	H-2->L+6 (13%), HOMO->L+7 (38%), HOMO->L+14 (-15%)
50	39930.3659	250.435972	0.119	Singlet-A	H-1->L+6 (32%), HOMO->L+11 (27%)

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
51	40048.1237	249.699588	0.0086	Singlet-A	H-8->L+1 (71%)
52	40408.656	247.47173	0.0004	Singlet-A	H-9->L+1 (74%), H-9->L+4 (-12%)
53	40513.5088	246.83125	0.0025	Singlet-A	H-5->L+4 (-21%), H-3->L+4 (73%)
54	40610.296	246.242972	0.0557	Singlet-A	H-2->L+6 (22%), H-1->L+5 (12%)
55	40713.5357	245.61856	0.0006	Singlet-A	H-14->LUMO (97%)
56	40897.4314	244.514134	0.0095	Singlet-A	HOMO->L+8 (90%)
57	40949.0512	244.205902	0.0007	Singlet-A	H-6->L+4 (74%), H-4->L+4 (10%)
58	41031.3203	243.716262	0.0956	Singlet-A	H-8->L+4 (19%), H-5->L+5 (11%)
59	41270.0621	242.306396	0.0543	Singlet-A	H-8->L+2 (26%), H-8->L+4 (18%), H-5->L+5 (-10%)
60	41320.0688	242.01315	0.0015	Singlet-A	H-15->LUMO (91%)
61	41484.607	241.053266	0.0182	Singlet-A	H-8->L+2 (-13%), H-4->L+5 (18%)
62	41524.935	240.819161	0.0018	Singlet-A	H-9->L+4 (25%), H-8->L+2 (35%), H-4->L+5 (10%)
63	41645.919	240.119566	0.0005	Singlet-A	H-9->L+2 (28%), H-9->L+4 (14%), H-8->L+2 (-12%), H-8->L+4 (30%)
64	41721.7357	239.683221	0.0553	Singlet-A	H-1->L+7 (15%)
65	41910.4707	238.603858	0.2171	Singlet-A	
66	41938.7003	238.44325	0.0215	Singlet-A	H-5->L+5 (-14%), H-4->L+5 (17%), H-1->L+7 (10%)
67	41971.7693	238.255384	0.0042	Singlet-A	H-9->L+2 (59%), H-9->L+4 (-30%)
68	42263.744	236.609421	0.0071	Singlet-A	H-7->L+5 (-11%), HOMO->L+7 (16%), HOMO->L+14 (18%)
69	42625.8894	234.59921	0.0033	Singlet-A	H-7->L+5 (23%), H-4->L+6 (34%)
70	42692.8339	234.231347	0.0287	Singlet-A	H-7->L+5 (35%), H-4->L+6 (-16%)
71	43007.3923	232.518166	0.017	Singlet-A	H-8->L+3 (42%), H-5->L+6 (-18%)
72	43013.8448	232.483286	0.0069	Singlet-A	H-8->L+3 (49%), H-5->L+6 (18%)
73	43150.1534	231.748886	0.0018	Singlet-A	H-7->L+6 (-18%), H-1->L+7 (41%)
74	43344.5344	230.709596	0.038	Singlet-A	H-16->LUMO (14%), H-10->L+1 (44%), H-1->L+8 (24%)
75	43401.8002	230.40519	0.0003	Singlet-A	H-17->LUMO (12%), H-10->L+2 (27%), H-9->L+3 (45%)
76	43405.833	230.383783	0.0025	Singlet-A	H-17->LUMO (-11%), H-10->L+2 (-23%), H-9->L+3 (49%)
77	43652.6403	229.081218	0.0123	Singlet-A	H-7->L+6 (11%), H-3->L+5 (39%)
78	43835.7294	228.124412	0.041	Singlet-A	H-7->L+6 (20%), H-5->L+5 (15%), H-3->L+5 (-15%), HOMO->L+9 (25%)
79	43878.4771	227.902167	0.0202	Singlet-A	H-10->L+1 (-15%), H-1->L+8 (64%)
80	43945.4216	227.554991	0.0175	Singlet-A	H-6->L+5 (13%), HOMO->L+9 (50%)
81	43994.6218	227.300511	0.045	Singlet-A	H-7->L+6 (11%), H-6->L+5 (43%), HOMO->L+9 (-12%)
82	44169.6453	226.399826	0.007	Singlet-A	H-2->L+7 (12%), HOMO->L+10 (58%)
83	44377.7378	225.33821	0.007	Singlet-A	H-2->L+7 (23%), H-1->L+11 (25%), HOMO->L+13 (21%)
84	44568.8925	224.371741	0.0012	Singlet-A	H-12->L+1 (76%)
85	44824.572	223.091924	0.0033	Singlet-A	H-9->L+7 (18%), H-9->L+9 (18%), H-8->L+7 (25%), H-8->L+9 (-12%)
86	44839.8966	223.015679	0.0028	Singlet-A	H-2->L+7 (20%)
87	44868.9328	222.871358	0.0011	Singlet-A	H-6->L+5 (11%), H-6->L+10 (12%), H-3->L+12 (10%), HOMO->L+12 (12%)
88	44965.72	222.391635	0.002	Singlet-A	H-12->L+2 (-19%), H-11->L+1 (58%)
89	45023.7923	222.104791	0.0072	Singlet-A	H-2->L+8 (69%)
90	45107.6746	221.691765	0.002	Singlet-A	H-5->L+6 (-22%), H-3->L+6 (61%)
91	45302.8621	220.736606	0.0209	Singlet-A	H-11->L+1 (12%), H-2->L+11 (-11%), H-1->L+13 (16%), HOMO->L+15 (11%)
92	45458.5282	219.980725	0.0031	Singlet-A	H-6->L+6 (56%), HOMO->L+12 (-12%)
93	45597.2565	219.31144	0.0433	Singlet-A	H-1->L+10 (12%)
94	45694.0437	218.846904	0.0078	Singlet-A	H-10->L+3 (81%)
95	45723.0798	218.707927	0.0038	Singlet-A	H-12->L+2 (46%), HOMO->L+12 (14%)
96	45772.28	218.47284	0.0084	Singlet-A	H-1->L+10 (42%), HOMO->L+12 (23%)
97	45931.9789	217.713241	0.0167	Singlet-A	H-1->L+9 (68%)
98	46006.1824	217.362091	0.03	Singlet-A	H-12->L+3 (15%), H-1->L+9 (-14%)
99	46174.7534	216.568563	0.054	Singlet-A	H-12->L+3 (10%)
100	46239.2782	216.266351	0.016	Singlet-A	H-12->L+3 (-20%), H-11->L+2 (40%)

Table S18: Energy and composition of TD-DFT calculated transitions of **4b**

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	22515.1224	444.145931	0.0001	Singlet-A	HOMO->LUMO (97%)
2	26011.56	384.444455	0.0247	Singlet-A	H-1->LUMO (98%)
3	26589.8635	376.083164	0.001	Singlet-A	H-3->LUMO (-22%), H-2->LUMO (76%)
4	28630.4603	349.278352	0.0007	Singlet-A	H-3->LUMO (71%), H-2->LUMO (22%)
5	29223.2819	342.192914	0.0011	Singlet-A	HOMO->L+1 (80%)
6	29395.0792	340.192994	0.0902	Singlet-A	H-5->LUMO (25%), H-4->LUMO (61%)
7	30124.2094	331.958919	0.0007	Singlet-A	HOMO->L+1 (-10%), HOMO->L+2 (68%), HOMO->L+3 (-15%)
8	30529.1026	327.556304	0.0021	Singlet-A	HOMO->L+3 (-22%), HOMO->L+4 (64%)
9	30804.1395	324.631694	0.0041	Singlet-A	H-5->LUMO (53%), H-4->LUMO (-24%)
10	31043.6878	322.126677	0.0001	Singlet-A	HOMO->L+2 (15%), HOMO->L+3 (46%), HOMO->L+4 (19%)
11	32068.8256	311.829318	0	Singlet-A	H-6->LUMO (88%), H-5->LUMO (10%)
12	32416.453	308.485324	0.015	Singlet-A	H-1->L+1 (87%)
13	32605.9946	306.692071	0.0002	Singlet-A	H-7->LUMO (97%)
14	33155.2619	301.61125	0.003	Singlet-A	H-2->L+1 (47%), H-1->L+2 (13%)
15	33304.4755	300.259945	0.0331	Singlet-A	H-2->L+1 (-24%), H-1->L+2 (55%)
16	33949.7235	294.553209	0.0006	Singlet-A	H-2->L+2 (11%), H-1->L+3 (-28%), H-1->L+4 (38%)
17	34142.4914	292.890167	0.0142	Singlet-A	H-2->L+2 (23%), H-1->L+3 (49%)
18	34337.6789	291.225276	0.0076	Singlet-A	H-2->L+2 (-24%), H-1->L+2 (15%), H-1->L+4 (27%)
19	34731.2802	287.924889	0.0276	Singlet-A	H-2->L+3 (-22%), H-2->L+4 (35%)
20	34877.2675	286.719709	0.0004	Singlet-A	H-8->LUMO (96%)
21	35017.609	285.570611	0.0455	Singlet-A	H-3->L+1 (-18%), HOMO->L+5 (57%)
22	35328.9411	283.054054	0.0165	Singlet-A	H-3->L+1 (26%), H-2->L+3 (20%), HOMO- >L+5 (13%)
23	35345.0723	282.92487	0.0228	Singlet-A	H-3->L+1 (22%), H-2->L+3 (-22%), H-2->L+4 (- 17%)
24	35418.4693	282.338571	0.0002	Singlet-A	H-9->LUMO (98%)
25	35728.1883	279.891046	0.025	Singlet-A	H-5->L+1 (15%), H-4->L+1 (43%)
26	36068.5566	277.249797	0.0078	Singlet-A	H-3->L+2 (23%), HOMO->L+6 (38%)
27	36251.6458	275.849545	0.0243	Singlet-A	H-5->L+2 (11%), H-4->L+2 (16%), HOMO- >L+6 (13%)
28	36516.1974	273.851077	0.0164	Singlet-A	H-4->L+4 (-11%), H-3->L+2 (21%), HOMO- >L+6 (-16%)
29	36921.8971	270.841988	0.0212	Singlet-A	H-10->LUMO (-16%), H-5->L+3 (15%), H-4- >L+3 (19%)
30	37012.2318	270.180951	0.0081	Singlet-A	H-5->L+1 (33%), H-4->L+1 (-21%)
31	37131.6027	269.312372	0.0053	Singlet-A	H-6->L+1 (33%), H-6->L+2 (21%), H-6->L+3 (- 10%)
32	37189.675	268.891836	0.0154	Singlet-A	H-5->L+1 (-16%), H-3->L+3 (26%)
33	37509.0728	266.602165	0.0588	Singlet-A	H-4->L+2 (-16%), H-3->L+3 (19%)
34	37881.7035	263.979681	0.0007	Singlet-A	H-5->L+2 (32%), H-4->L+2 (-13%), H-4->L+4 (10%)
35	37930.9037	263.637273	0.0069	Singlet-A	H-12->LUMO (33%), H-3->L+4 (14%), H-1- >L+5 (11%)
36	37969.6186	263.368461	0.002	Singlet-A	H-7->L+1 (39%), H-7->L+2 (28%), H-7->L+3 (- 14%)
37	38158.3536	262.065814	0.0309	Singlet-A	H-12->LUMO (51%), H-1->L+5 (-14%)
38	38454.3611	260.048528	0.0012	Singlet-A	H-5->L+3 (-10%), H-5->L+4 (23%), H-4->L+3 (11%), H-4->L+4 (-20%)
39	38703.5882	258.373977	0.2749	Singlet-A	H-10->LUMO (36%), H-4->L+3 (26%)
40	39045.5696	256.111003	0.0276	Singlet-A	H-6->L+1 (36%), H-6->L+2 (-30%)
41	39056.0549	256.042246	0.0033	Singlet-A	H-2->L+5 (50%), H-1->L+6 (-13%)
42	39080.2517	255.883715	0.0448	Singlet-A	H-11->LUMO (34%), H-6->L+2 (10%), H-5- >L+3 (-19%)
43	39187.5242	255.183256	0.0222	Singlet-A	H-2->L+6 (-14%), H-1->L+5 (18%), HOMO- >L+7 (-17%)
44	39333.5115	254.236136	0.0116	Singlet-A	H-11->LUMO (43%), H-5->L+3 (22%)
45	39466.5939	253.378845	0.0092	Singlet-A	H-5->L+4 (11%), H-2->L+6 (-13%), HOMO- >L+7 (38%), HOMO->L+14 (-13%)
46	39581.932	252.640523	0.0037	Singlet-A	H-7->L+1 (-44%), H-7->L+2 (47%)
47	39815.0278	251.161447	0.1501	Singlet-A	H-1->L+6 (37%), HOMO->L+11 (-23%)
48	39958.5955	250.259046	0.0053	Singlet-A	H-13->LUMO (92%)
49	40363.4886	247.748654	0.0728	Singlet-A	H-2->L+6 (28%), H-1->L+5 (11%)
50	40426.4003	247.363107	0.0033	Singlet-A	H-6->L+2 (11%), H-6->L+3 (69%)

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
51	40680.4667	245.818222	0.0473	Singlet-A	H-8->L+1 (12%), H-8->L+4 (12%), H-3->L+5 (19%), HOMO->L+11 (-16%)
52	40935.3397	244.287701	0.0227	Singlet-A	H-8->L+1 (27%), H-8->L+4 (17%), H-3->L+5 (-14%)
53	40971.6349	244.071295	0.0019	Singlet-A	H-7->L+2 (12%), H-7->L+3 (77%)
54	41028.0941	243.735426	0	Singlet-A	H-6->L+4 (77%), H-5->L+4 (10%)
55	41141.819	243.061688	0.0081	Singlet-A	H-4->L+5 (30%), H-3->L+14 (-15%), HOMO->L+7 (-13%)
56	41425.7282	241.395877	0.0012	Singlet-A	H-9->L+1 (13%), H-3->L+5 (11%)
57	41469.2824	241.142345	0.0013	Singlet-A	H-9->L+1 (33%), H-9->L+4 (20%)
58	41511.2235	240.898705	0.0005	Singlet-A	H-7->L+4 (89%)
59	41559.6171	240.618194	0.0194	Singlet-A	H-4->L+5 (-12%), H-3->L+6 (-12%), H-1->L+7 (16%)
60	41710.4438	239.748108	0.2087	Singlet-A	H-4->L+6 (10%), H-3->L+5 (15%), H-2->L+5 (12%), HOMO->L+15 (10%)
61	41895.9526	238.686541	0.0055	Singlet-A	H-5->L+5 (21%), HOMO->L+7 (13%), HOMO->L+10 (13%), HOMO->L+14 (18%)
62	42028.2285	237.93532	0.0018	Singlet-A	H-8->L+1 (43%), H-8->L+4 (-38%)
63	42200.8323	236.962151	0.0006	Singlet-A	H-5->L+5 (30%)
64	42400.8592	235.844277	0.0091	Singlet-A	HOMO->L+10 (69%)
65	42517.0038	235.200016	0.0568	Singlet-A	H-4->L+6 (45%)
66	42570.2368	234.905905	0.0005	Singlet-A	H-9->L+1 (45%), H-9->L+4 (-40%)
67	42669.4437	234.359746	0.0633	Singlet-A	H-16->LUMO (35%), H-10->L+1 (41%)
68	42694.447	234.222497	0.0174	Singlet-A	H-3->L+6 (40%), H-2->L+6 (11%)
69	42817.0442	233.551853	0.0326	Singlet-A	H-5->L+6 (18%), H-1->L+7 (35%)
70	42886.4083	233.174108	0.004	Singlet-A	H-17->LUMO (30%), H-10->L+2 (-13%), H-10->L+3 (-19%)
71	43033.2022	232.378709	0.0052	Singlet-A	H-14->LUMO (86%)
72	43157.4125	231.709906	0.0076	Singlet-A	H-8->L+2 (44%), H-8->L+3 (18%), H-8->L+4 (20%)
73	43289.6883	231.001894	0.0443	Singlet-A	H-5->L+6 (-11%), HOMO->L+8 (53%)
74	43422.7707	230.293918	0.0705	Singlet-A	H-5->L+6 (14%), HOMO->L+8 (38%)
75	43446.9675	230.165661	0.0106	Singlet-A	H-8->L+2 (-22%), H-8->L+3 (66%)
76	43610.6992	229.301529	0.0015	Singlet-A	H-15->LUMO (88%)
77	43641.3485	229.140491	0.0004	Singlet-A	H-9->L+2 (50%), H-9->L+3 (23%), H-9->L+4 (24%)
78	43732.4898	228.662947	0.0039	Singlet-A	HOMO->L+9 (54%)
79	43970.425	227.425594	0.0014	Singlet-A	H-9->L+2 (-25%), H-9->L+3 (71%)
80	44041.4022	227.059074	0.0107	Singlet-A	H-6->L+5 (46%)
81	44221.2651	226.135548	0.0022	Singlet-A	H-10->L+1 (14%), H-10->L+2 (41%), H-10->L+3 (-26%)
82	44272.885	225.871885	0.0057	Singlet-A	H-6->L+5 (23%), H-2->L+7 (24%), H-1->L+11 (11%), HOMO->L+13 (-12%)
83	44317.2458	225.645792	0.0051	Singlet-A	H-7->L+5 (33%), HOMO->L+12 (10%)
84	44597.9286	224.22566	0.0047	Singlet-A	H-2->L+7 (16%), H-1->L+11 (-16%), HOMO->L+12 (10%), HOMO->L+13 (18%)
85	44708.4274	223.671477	0.0103	Singlet-A	H-7->L+5 (-26%), HOMO->L+12 (45%)
86	44871.3525	222.85934	0.0026	Singlet-A	H-9->L+7 (35%), H-9->L+8 (11%), H-8->L+7 (16%), H-8->L+8 (-25%)
87	44900.3886	222.715221	0.0049	Singlet-A	H-12->L+1 (11%), H-10->L+2 (-17%), H-10->L+4 (60%)
88	44941.5232	222.511372	0.0071	Singlet-A	H-12->L+1 (76%)
89	45050.4088	221.973568	0.0047	Singlet-A	H-2->L+11 (-13%), H-1->L+10 (30%)
90	45217.3667	221.153966	0.0068	Singlet-A	H-7->L+5 (15%), H-7->L+9 (-13%), H-6->L+6 (17%), H-6->L+12 (10%), HOMO->L+12 (14%)
91	45353.6754	220.489297	0.0044	Singlet-A	H-1->L+9 (23%), H-1->L+10 (-20%)
92	45402.069	220.25428	0.008	Singlet-A	H-6->L+6 (60%)
93	45546.4432	219.556112	0.0247	Singlet-A	H-1->L+9 (31%), H-1->L+10 (24%)
94	45577.0925	219.408467	0.0062	Singlet-A	H-1->L+8 (78%)
95	45679.5256	218.916459	0.0536	Singlet-A	H-12->L+2 (25%), H-11->L+1 (-12%), H-1->L+9 (-10%)
96	45715.0142	218.746514	0.0326	Singlet-A	H-12->L+3 (-13%), H-11->L+1 (51%)
97	45814.2211	218.272837	0.0188	Singlet-A	H-7->L+6 (59%)
98	45910.2018	217.816512	0.0317	Singlet-A	H-12->L+2 (19%), H-7->L+6 (18%)
99	46056.9957	217.122282	0.0339	Singlet-A	H-12->L+2 (18%)
100	46229.5995	216.311629	0.0165	Singlet-A	H-2->L+10 (40%)