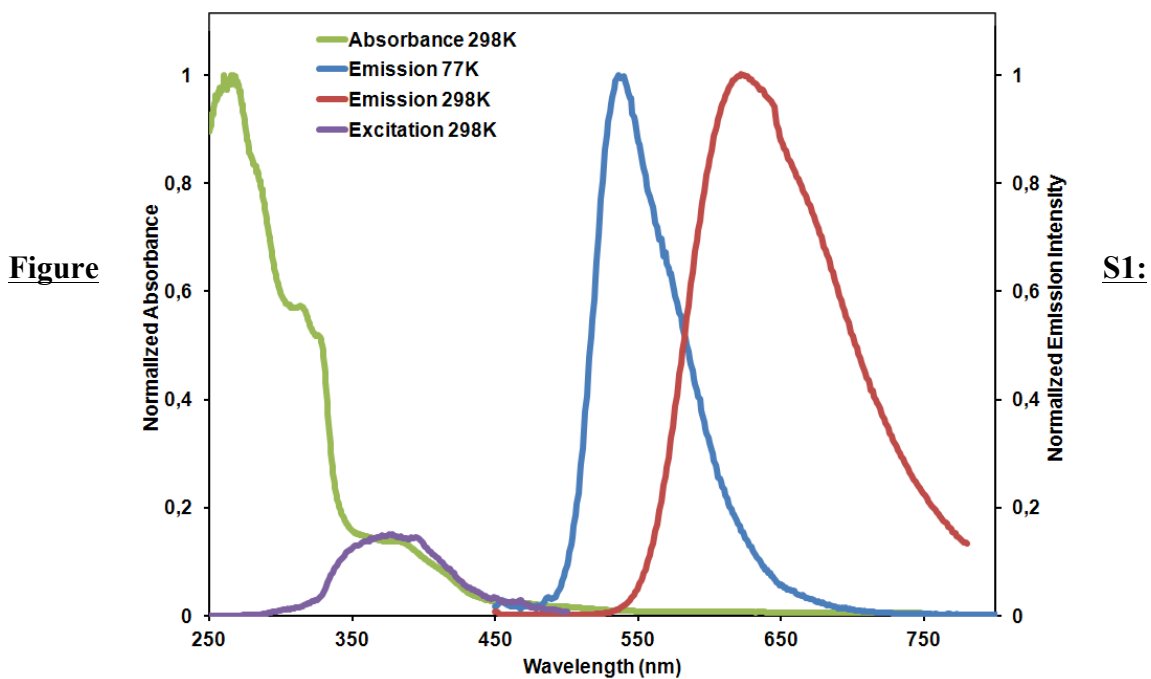


SUPPORTING INFORMATION

Intimate Electronic Coupling in Cationic Homodimeric Iridium(III) Complexes

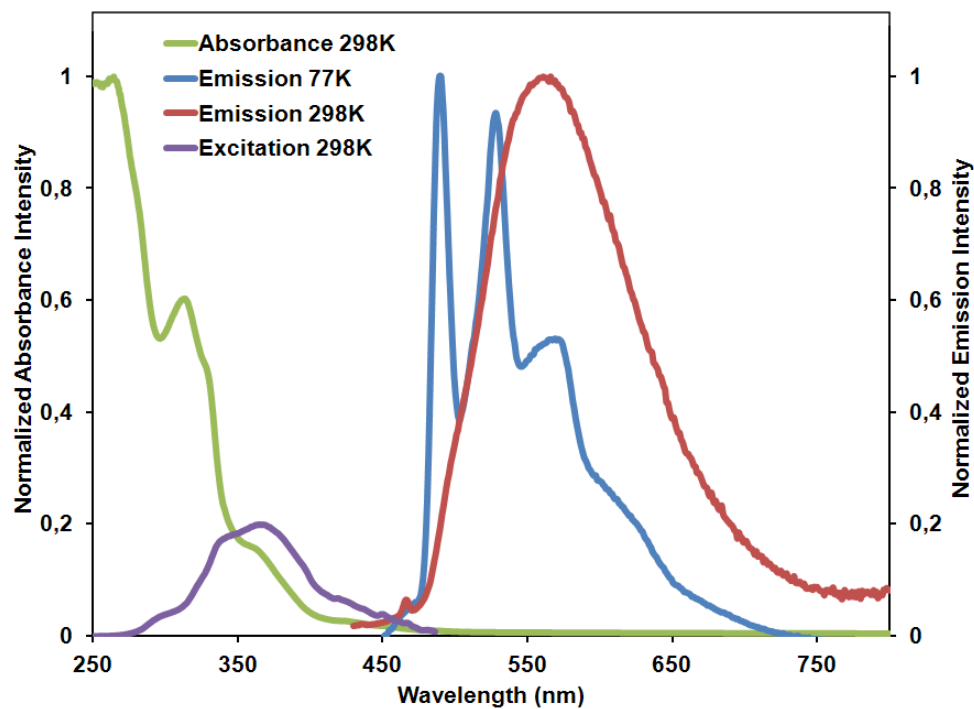
Ahmed M. Soliman, Daniel Fortin, Pierre D. Harvey and Eli Zysman-Colman**

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Energy and composition of TD-DFT calculated transitions	S9-S20
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Absorption (green), emission at 298 K (red) and 77 K (blue) and excitation spectra (purple) at 298 K for **10**:

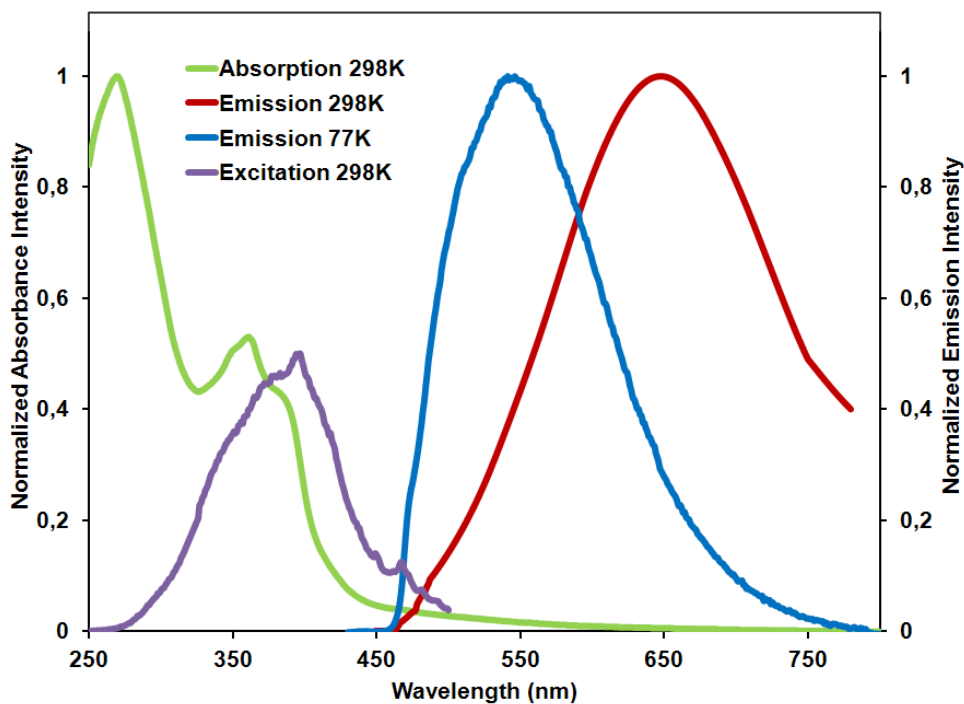
Figure S2: Absorption (green), emission at 298 K (red) and 77 K (blue) and excitation spectra (purple) at 298 K for **11**:



Figure

S3:

Absorption (green), emission at 298 K (red) and 77 K (blue) and excitation spectra (purple)
at
for



12:

Figure S4: Absorption (green), emission at 298 K (red) and 77 K (blue) and excitation spectra (purple) at 298 K for **13**:

Figure S5: Calculated (**10**-TMS) and experimental (**10**) absorption spectra:

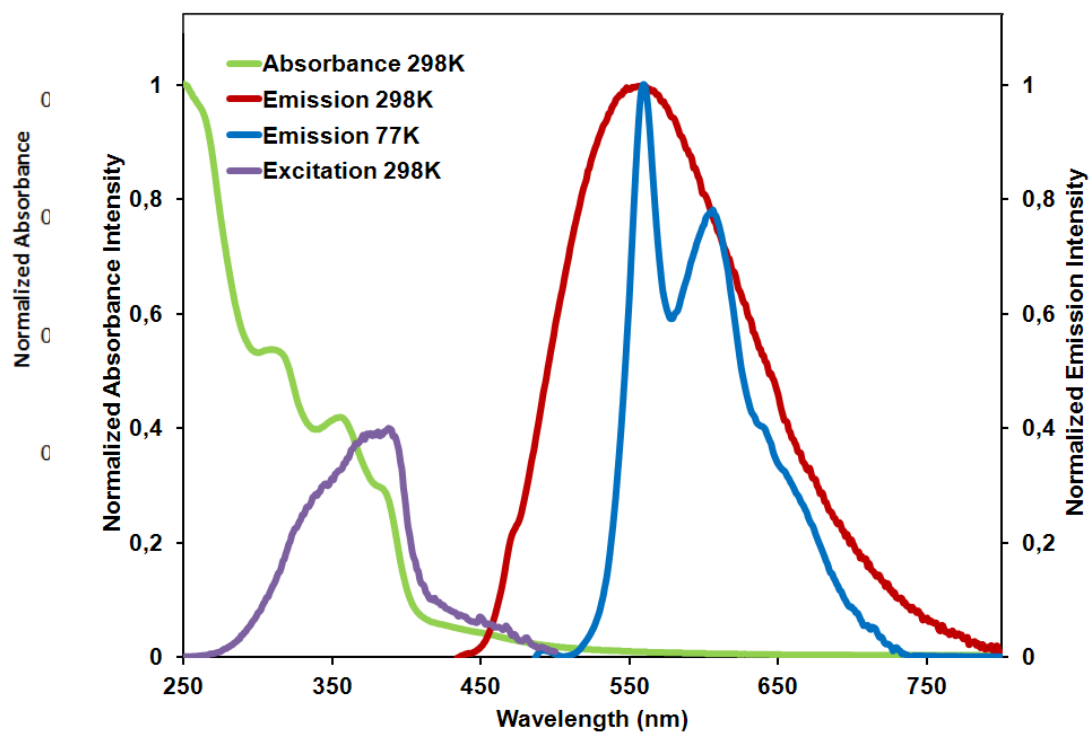


Figure S6: Calculated and experimental absorption spectra for **11**:

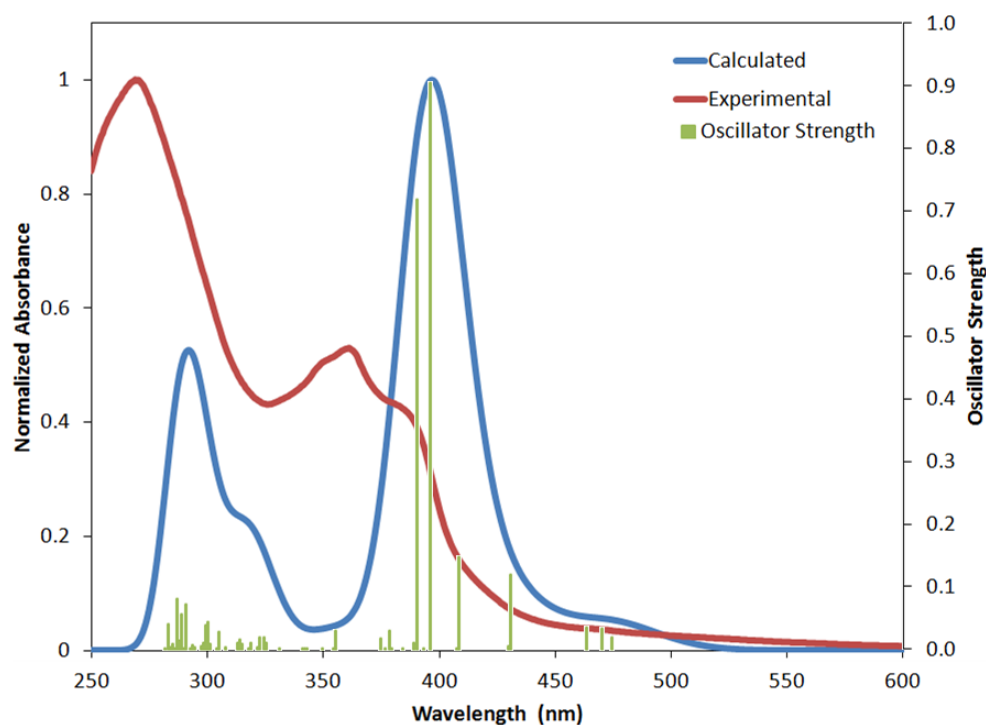


Figure S7: Calculated (**12**-TMS) and experimental (**12**) absorption spectra:

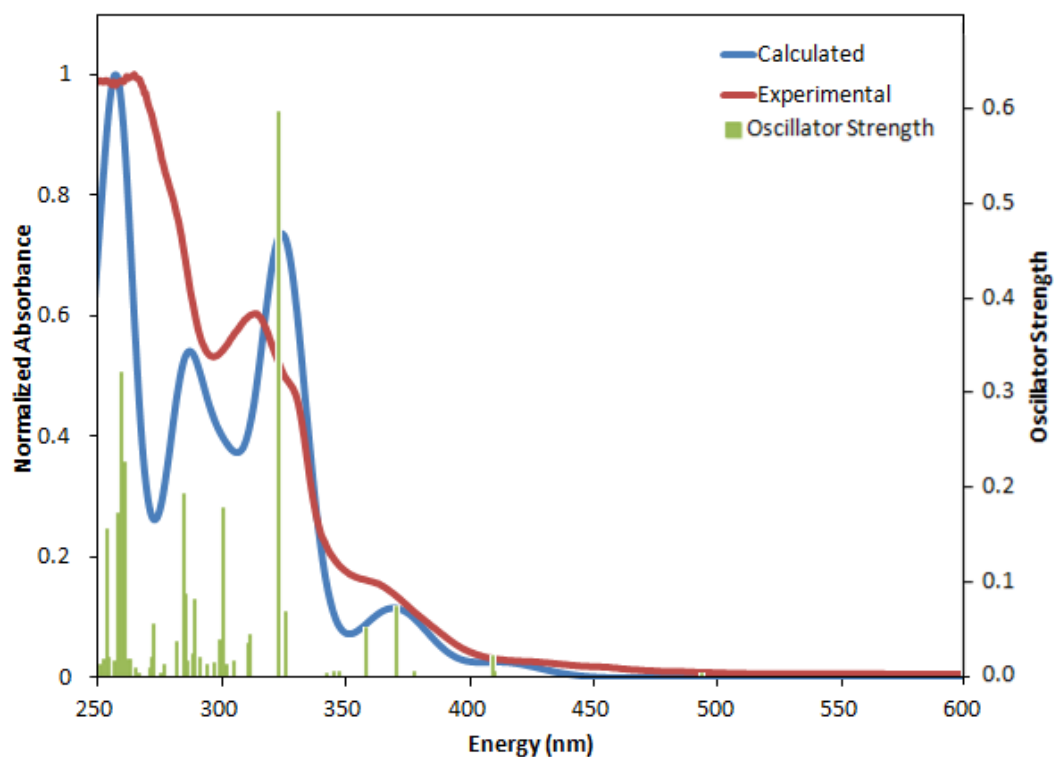


Figure S8: Calculated and experimental absorption spectra for **13**:

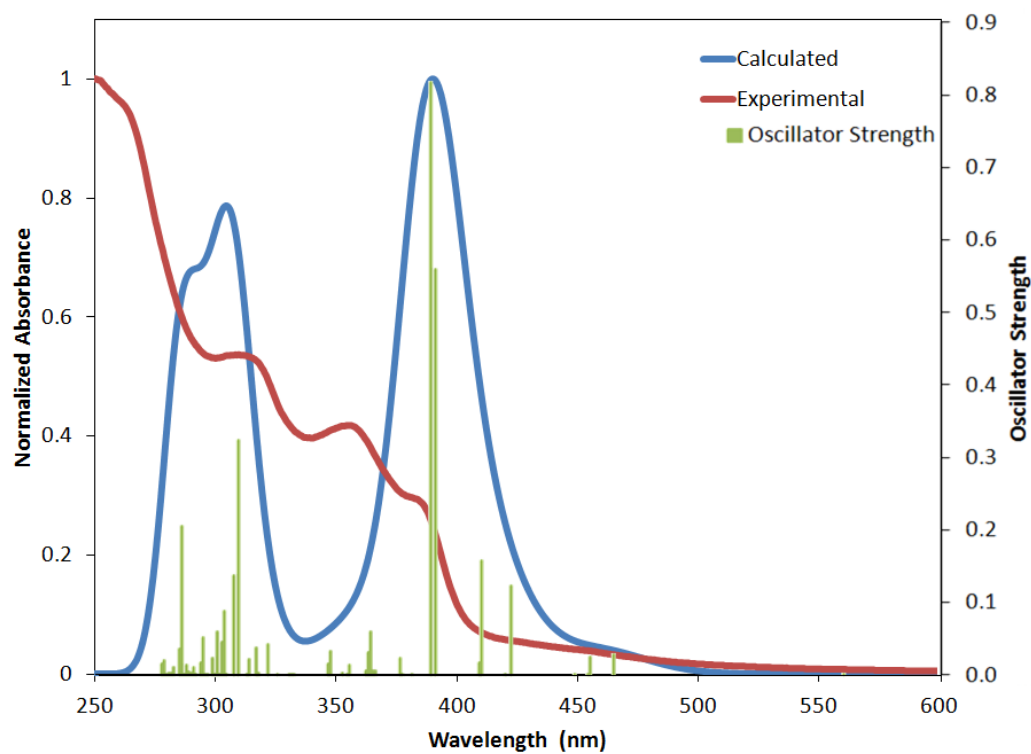


Figure S9: Cyclic voltammograms for **10**, **11**, **12** and **13** with scan rate of 200 mV/sec:

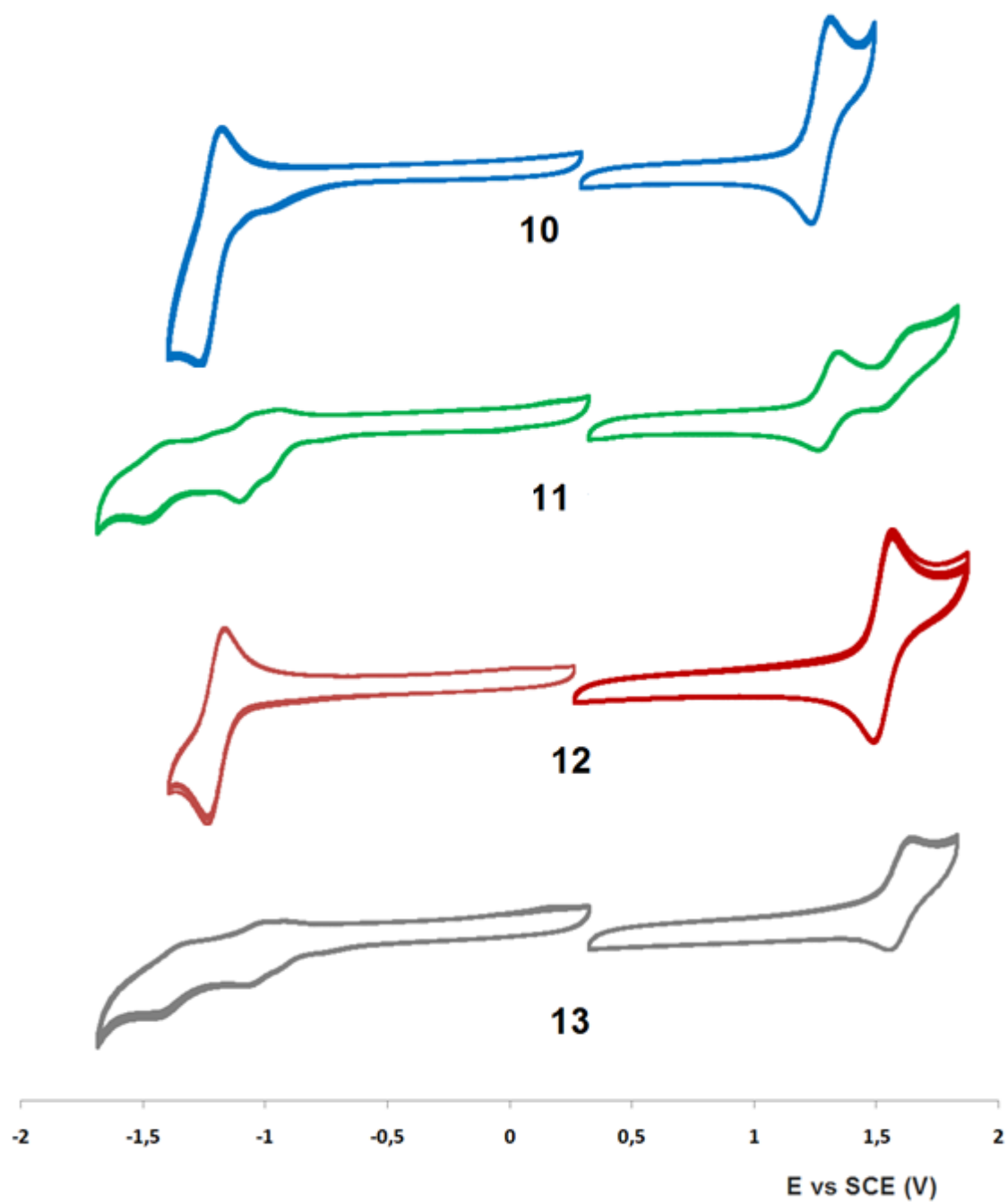


Table S1: Visualization of MOs of **10**:

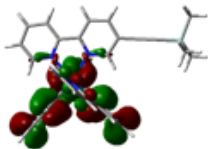
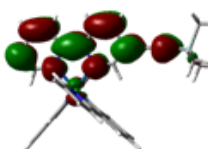
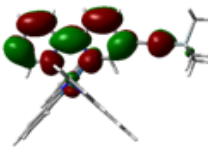
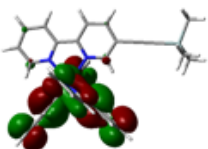
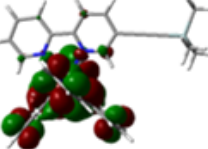
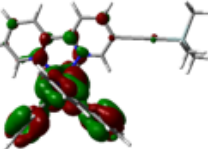
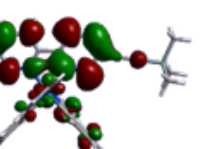
Orbital Energy (eV)	Image	Orbital Energy (eV)	Image	Orbital Energy (eV)	Image
HOMO -5.97		LUMO -3.04		HSOMO -3.90	
HOMO -1 -6.59		LUMO+1 -2.05			
HOMO -2 -6.67		LUMO+2 -1.98			

Table S2: Visualization of MOs of **11**:

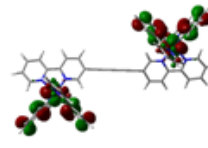
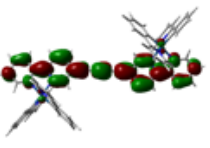
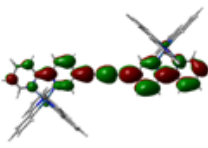
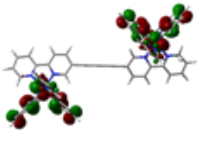
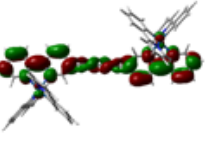
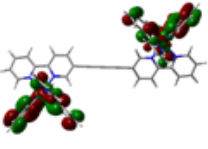
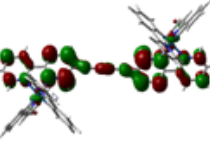
Orbital Energy (eV)	Image	Orbital Energy (eV)	Image	Orbital Energy (eV)	Image
HOMO -6.13		LUMO -3.68		HSOMO -4.27	
HOMO -1 -6.14		LUMO+1 -3.13			
HOMO -2 -6.74		LUMO+2 -2.35			

Table S3: Visualization of MOs of **12**:

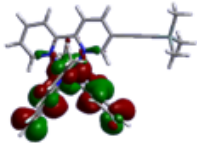
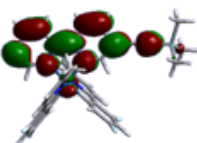
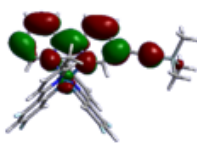
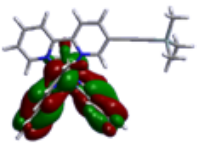
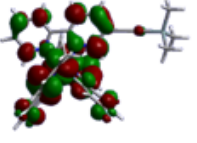
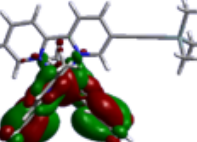
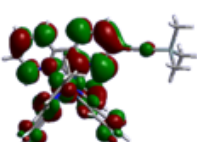
Orbital Energy (eV)	Image	Orbital Energy (eV)	Image	Orbital Energy (eV)	Image
HOMO -6.28		LUMO -3.13		HSOMO -4.25	
HOMO -1 -6.65		LUMO+1 -2.09			
HOMO -2 -6.80		LUMO+2 -2.05			

Table S4: Visualization of MOs of **13**:

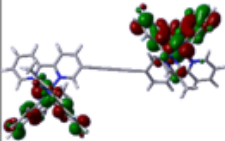
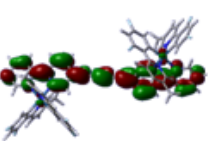
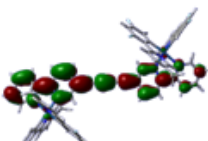
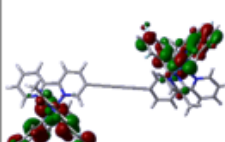
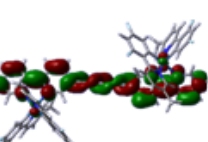
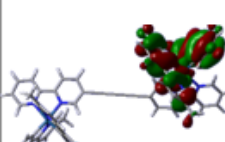
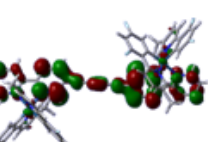
Orbital Energy (eV)	Image	Orbital Energy (eV)	Image	Orbital Energy (eV)	Image
HOMO -6.44		LUMO -3.73		HSOMO -4.40	
HOMO -1 -6.45		LUMO+1 -3.28			
HOMO -2 -6.81		LUMO+2 -2.43			

Table S5: Energy and composition of TD-DFT calculated transitions of **10**:

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	18155.6656	550.7922552	0.0002	Singlet-A	HOMO->LUMO (98%)
2	23140.2064	432.1482629	0.0012	Singlet-A	H-2->LUMO (94%)
3	24080.65536	415.27109	0.0451	Singlet-A	H-1->LUMO (92%)
4	25446.968	392.9741256	0.0489	Singlet-A	HOMO->L+1 (96%)
5	25633.28336	390.1177957	0.0468	Singlet-A	H-3->LUMO (87%)
6	26384.99728	379.0032606	0.0033	Singlet-A	HOMO->L+2 (-12%), HOMO->L+3 (83%)
7	26810.0544	372.9943942	0.002	Singlet-A	HOMO->L+2 (82%), HOMO->L+3 (12%)
8	27318.1872	366.0565003	0.0028	Singlet-A	H-4->LUMO (91%)
9	28289.28544	353.4907243	0.0085	Singlet-A	H-5->LUMO (96%)
10	28725.6344	348.1211193	0.0064	Singlet-A	HOMO->L+4 (98%)
11	30646.86032	326.2976989	0.1022	Singlet-A	H-2->L+1 (73%)
12	30847.69376	324.1733427	0.4761	Singlet-A	H-6->LUMO (77%), H-2->L+2 (13%) H-3->L+1 (16%), H-2->L+3 (14%), H-1->L+1 (61%)
13	30988.0352	322.7051969	0.013	Singlet-A	HOMO->L+5 (93%)
14	31387.2824	318.6003768	0.0214	Singlet-A	H-2->L+3 (-23%), HOMO->L+6 (59%)
15	31646.99472	315.9857702	0.0083	Singlet-A	H-2->L+1 (-13%), H-2->L+2 (-11%), H-1->L+3 (47%)
16	31741.36224	315.04634	0.0131	Singlet-A	H-2->L+3 (32%), H-1->L+1 (-18%), HOMO- >L+6 (22%)
17	31969.61872	312.7969741	0.0405	Singlet-A	H-2->L+2 (61%), H-1->L+3 (16%)
18	32133.3504	311.2031542	0.2533	Singlet-A	H-1->L+2 (68%)
19	32482.59088	307.8572161	0.008	Singlet-A	H-7->LUMO (94%)
20	32914.90704	303.8137093	0.0012	Singlet-A	H-3->L+1 (58%), H-2->L+3 (-10%)
21	33127.83888	301.8609224	0.0092	Singlet-A	H-3->L+3 (68%), H-1->L+3 (-14%)
22	33502.08272	298.4889054	0.1298	Singlet-A	H-3->L+2 (31%), H-2->L+4 (49%)
23	33936.81856	294.6652168	0.0134	Singlet-A	H-3->L+4 (13%), H-1->L+4 (71%)
24	34156.20288	292.7725905	0.0587	Singlet-A	H-3->L+2 (40%), H-2->L+4 (-30%)
25	34328.00016	291.3073862	0.0501	Singlet-A	H-8->LUMO (83%)
26	34745.79824	287.8045838	0.0239	Singlet-A	H-4->L+1 (67%)
27	34883.72	286.6666743	0.1616	Singlet-A	H-5->L+1 (36%), H-4->L+3 (-25%), H-1->L+5 (14%)
28	35287.80656	283.3840064	0.0396	Singlet-A	H-5->L+1 (43%), H-4->L+3 (40%)
29	35527.35488	281.4732488	0.0008	Singlet-A	H-4->L+2 (48%), H-3->L+4 (-16%)
30	35705.60464	280.0680762	0.0458	Singlet-A	H-4->L+2 (14%), HOMO->L+7 (64%)
31	35815.2968	279.2103066	0.004	Singlet-A	H-3->L+4 (49%), H-1->L+4 (-14%), HOMO- >L+7 (-21%)
32	35893.53312	278.6017182	0.0123	Singlet-A	H-5->L+3 (50%), H-2->L+5 (-12%)
33	35941.92672	278.2265981	0.0099	Singlet-A	H-9->LUMO (91%)
34	36066.13696	277.2683975	0.0056	Singlet-A	H-5->L+2 (73%)
35	36697.67344	272.4968387	0.0045	Singlet-A	H-2->L+5 (57%), H-1->L+6 (23%)
36	36784.78192	271.8515505	0.0064	Singlet-A	

37	36891.24784	271.0670033	0.0035	Singlet-A	H-2->L+6 (57%), H-1->L+5 (28%)
38	37096.92064	269.5641532	0.0001	Singlet-A	H-10->LUMO (92%) H-11->LUMO (-16%), H-6->L+2 (48%), H-4->L+4 (12%)
39	37766.36544	264.7858719	0.0154	Singlet-A	H-4->L+4 (74%)
40	37867.18544	264.0808891	0.0014	Singlet-A	H-6->L+1 (19%), H-5->L+3 (-11%), H-1->L+6 (32%)
41	37931.71024	263.6316669	0.3458	Singlet-A	H-4->L+3 (10%), H-2->L+6 (-18%), H-1->L+5 (39%)
42	38111.57312	262.3874897	0.1284	Singlet-A	H-6->L+1 (64%)
43	38322.08528	260.946134	0.126	Singlet-A	H-3->L+5 (65%)
44	38519.69248	259.6074723	0.0734	Singlet-A	H-5->L+4 (80%)
45	38725.36528	258.2286811	0.0181	Singlet-A	H-3->L+6 (76%), H-1->L+6 (-13%)
46	38822.95904	257.5795418	0.0073	Singlet-A	H-6->L+3 (86%)
47	39102.0288	255.7412059	0.0102	Singlet-A	H-11->LUMO (-23%), HOMO->L+11 (32%)
48	39573.05984	252.6971642	0.0855	Singlet-A	H-11->LUMO (38%), H-6->L+2 (10%), HOMO->L+11 (20%)
49	39616.61408	25242%	0.0955	Singlet-A	H-6->L+4 (67%)
50	39998.11696	250.0117696	0.0221	Singlet-A	H-4->L+5 (19%), HOMO->L+8 (50%), HOMO->L+14 (12%)
51	40122.3272	249.237786	0.0664	Singlet-A	H-12->LUMO (95%)
52	40438.49872	24729%	0.0079	Singlet-A	H-4->L+5 (72%), HOMO->L+8 (-10%)
53	40561.9024	246.5367601	0.1197	Singlet-A	H-4->L+6 (91%)
54	40803.06384	245.0796352	0.0035	Singlet-A	H-13->LUMO (88%)
55	40965.98896	244.1049332	0.0015	Singlet-A	H-5->L+5 (-18%), H-1->L+7 (58%)
56	41116.81568	243.2094955	0.0103	Singlet-A	H-5->L+5 (65%), H-1->L+7 (12%)
57	41149.07808	243.0188103	0.011	Singlet-A	H-8->L+1 (-10%), H-7->L+1 (-12%), H-2->L+7 (38%)
58	41193.43888	242.7571058	0.0156	Singlet-A	H-8->L+1 (21%), H-7->L+1 (32%), H-2->L+7 (15%)
59	41269.25552	242.3111315	0.0023	Singlet-A	H-7->L+2 (67%)
60	41427.34128	241.3864779	0.0015	Singlet-A	H-5->L+6 (79%)
61	41467.66928	241.1517255	0.0312	Singlet-A	H-9->L+1 (-19%), H-8->L+3 (17%), H-7->L+3 (23%)
62	41659.63056	240.0405348	0.0004	Singlet-A	H-2->L+11 (38%)
63	41798.35888	239.2438428	0.0329	Singlet-A	H-3->L+11 (21%), H-1->L+11 (12%)
64	41846.75248	238.9671697	0.0124	Singlet-A	H-15->LUMO (-34%), H-3->L+7 (39%)
65	42712.99792	234.1207709	0.0014	Singlet-A	H-15->LUMO (56%), H-3->L+7 (21%)
66	42771.8768	233.7984851	0.0016	Singlet-A	H-14->LUMO (52%), H-3->L+7 (20%)
67	42773.48992	233.7896678	0.0206	Singlet-A	H-9->L+1 (24%), H-8->L+1 (-15%), H-7->L+3 (25%)
68	43027.55632	232.4092013	0.0093	Singlet-A	H-8->L+2 (67%), H-7->L+4 (-12%)
69	43307.43264	23091%	0.0037	Singlet-A	H-9->L+3 (-19%), H-8->L+3 (18%), HOMO->L+9 (20%)
70	43380.02304	230.520855	0.0935	Singlet-A	H-6->L+5 (82%)
71	43495.36112	229.9095752	0.0107	Singlet-A	H-9->L+3 (22%), H-8->L+3 (-15%), HOMO->L+9 (18%), HOMO->L+11 (10%)
72	43600.21392	229.3566728	0.0329	Singlet-A	H-16->LUMO (55%)
73	43916.38544	227.705443	0.0179	Singlet-A	H-6->L+6 (84%)
74	43995.42832	227.2963438	0.0051	Singlet-A	H-17->LUMO (76%)
75	44185.77648	226.3171726	0.0166	Singlet-A	H-10->L+1 (60%)
76	44212.39296	226.1809264	0.0227	Singlet-A	

77	44369.67216	225.3791726	0.0047	Singlet-A	H-8->L+2 (10%), H-8->L+4 (28%), H-7->L+4 (38%)
78	44432.58384	225.0600603	0.0613	Singlet-A	H-10->L+1 (-10%), HOMO->L+8 (10%), HOMO->L+10 (23%), HOMO->L+13 (17%), HOMO->L+14 (-19%)
79	44576.15152	224.335203	0.0073	Singlet-A	H-4->L+7 (88%)
80	44673.74528	223.8451228	0.0045	Singlet-A	H-9->L+2 (79%)
81	44918.13296	22263%	0.0008	Singlet-A	H-10->L+3 (61%)
82	45135.0976	221.5570705	0.0096	Singlet-A	H-2->L+8 (52%)
83	45211.7208	221.1815835	0.001	Singlet-A	H-10->L+1 (11%), H-9->L+1 (28%), H-8->L+1 (20%), H-7->L+1 (-24%)
84	45377.0656	220.3756428	0.0024	Singlet-A	H-5->L+7 (12%), HOMO->L+10 (40%), HOMO->L+13 (-13%)
85	45405.2952	22024%	0.0044	Singlet-A	H-5->L+7 (71%)
86	45707.7552	218.781254	0.0043	Singlet-A	H-10->L+2 (47%)
87	45773.89312	21847%	0.0026	Singlet-A	H-10->L+2 (-11%), H-1->L+8 (33%), HOMO->L+12 (-12%)
88	45981.17904	217.4802867	0.001	Singlet-A	H-10->L+2 (-11%), H-9->L+4 (-28%), H-8->L+4 (30%)
89	46031.99232	217.240217	0.0012	Singlet-A	H-10->L+3 (-14%), H-9->L+3 (-24%), H-8->L+3 (-18%), H-7->L+3 (24%)
90	46315.90144	21591%	0.0007	Singlet-A	H-18->LUMO (36%), H-11->L+2 (33%), H-6->L+7 (-19%)
91	46496.57088	215.0696236	0.0014	Singlet-A	H-19->LUMO (-25%), H-3->L+8 (19%), HOMO->L+12 (32%)
92	46583.67936	214.6674573	0.0016	Singlet-A	H-19->LUMO (58%), H-6->L+7 (13%)
93	46689.33872	214.1816585	0.0017	Singlet-A	H-20->LUMO (-22%), H-19->LUMO (-12%), H-6->L+7 (30%)
94	47035.35296	21261%	0.0028	Singlet-A	H-1->L+9 (-19%), HOMO->L+13 (17%), HOMO->L+14 (26%)
95	47045.83824	212.5586529	0.0095	Singlet-A	H-11->L+1 (61%)
96	47131.3336	212.1730755	0.0016	Singlet-A	H-2->L+9 (46%), H-2->L+10 (-11%)
97	47166.01568	212.0170605	0.0333	Singlet-A	H-20->LUMO (24%), H-11->L+1 (-18%), H-11->L+2 (18%), H-11->L+4 (13%)
98	47195.8584	211.8829986	0.0006	Singlet-A	H-10->L+4 (-22%), H-9->L+4 (25%), H-7->L+5 (-16%)
99	47260.3832	21159%	0.0018	Singlet-A	H-9->L+4 (11%), H-8->L+5 (19%), H-7->L+5 (38%)
100	47489.44624	210.5731019	0.0085	Singlet-A	H-12->L+1 (30%), H-8->L+6 (16%), H-7->L+6 (26%)

Table 6: Energy and composition of TD-DFT calculated transitions of **11**:

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	15770.66768	634.0885626	0.0001	Singlet-A	H-1->L+1 (-10%), HOMO->LUMO (90%)
2	15782.76608	633.6024971	0	Singlet-A	H-1->LUMO (89%), HOMO->L+1 (-10%)
3	20820.53984	480.2949432	0.0182	Singlet-A	H-4->LUMO (-25%), HOMO->L+1 (53%)
4	20847.96288	479.6631718	0.0002	Singlet-A	H-5->LUMO (-13%), H-1->L+1 (67%)
5	20989.91744	476.4192155	0.0335	Singlet-A	H-4->LUMO (53%), HOMO->L+1 (31%)
6	21060.89472	474.813636	0	Singlet-A	H-5->LUMO (66%), H-1->L+1 (17%)
7	21327.86608	468.8701609	0.0351	Singlet-A	H-2->LUMO (83%)
8	21333.512	468.7460743	0.002	Singlet-A	H-3->LUMO (87%)
9	23004.70432	434.6936983	0.1189	Singlet-A	H-7->LUMO (84%)
10	23040.99952	434.0089496	0.0047	Singlet-A	H-6->LUMO (88%)
11	24243.58048	412.4803268	0.1474	Singlet-A	H-8->LUMO (89%)
12	24317.784	411.2216804	0.0006	Singlet-A	H-9->LUMO (84%)
13	25079.9832	398.72435	0.9056	Singlet-A	H-12->LUMO (49%), H-10->LUMO (34%)
14	25276.78384	395.6199516	0.0008	Singlet-A	H-11->LUMO (88%)
15	25444.54832	393.011496	0.7191	Singlet-A	H-12->LUMO (-33%), H-10->LUMO (57%)
16	25532.46336	391.6582532	0.011	Singlet-A	H-1->L+4 (47%), HOMO->L+3 (37%), HOMO->L+5 (12%)
17	25538.91584	391.5592996	0.0892	Singlet-A	H-1->L+3 (37%), H-1->L+5 (12%), HOMO->L+4 (47%)
18	25822.0184	387.2663959	0.0018	Singlet-A	H-1->L+5 (-25%), HOMO->L+2 (60%)
19	25826.0512	387.2059233	0.0001	Singlet-A	H-1->L+2 (60%), HOMO->L+5 (-25%)
20	26196.26224	381.7338485	0.0004	Singlet-A	H-2->L+1 (82%)
21	26221.2656	381.3698451	0.0302	Singlet-A	H-3->L+1 (87%)
22	26351.12176	379.4904859	0.0003	Singlet-A	H-4->L+1 (74%)
23	26495.496	377.4226382	0.0181	Singlet-A	H-5->L+1 (69%)
24	26515.66	377.1356248	0.0018	Singlet-A	H-1->L+6 (46%), HOMO->L+7 (-46%)
25	26522.91904	377.0324068	0.0199	Singlet-A	H-1->L+7 (-43%), HOMO->L+6 (44%)
26	27994.89104	357.2080343	0.0288	Singlet-A	H-6->L+1 (74%)
27	27998.11728	357.166873	0.0027	Singlet-A	H-7->L+1 (71%)
28	28068.288	356.2739559	0.0003	Singlet-A	H-13->LUMO (75%)
29	28450.59744	351.4864678	0.001	Singlet-A	H-7->L+1 (-14%), H-1->L+9 (-40%), HOMO->L+8 (41%)
30	28457.04992	351.4067701	0.03	Singlet-A	H-6->L+1 (-14%), H-1->L+8 (-40%), HOMO->L+9 (40%)
31	29087.77984	343.7869805	0.0004	Singlet-A	H-8->L+1 (85%)
32	29170.04896	342.8173883	0.001	Singlet-A	H-9->L+1 (79%)
33	29228.12128	342.1362565	0.0009	Singlet-A	H-1->L+3 (-21%), H-1->L+5 (40%), HOMO->L+2 (28%)
34	29228.12128	342.1362565	0.0013	Singlet-A	H-1->L+2 (27%), HOMO->L+3 (-19%), HOMO->L+5 (36%)
35	30084.688	332.3950044	0.0009	Singlet-A	H-10->L+1 (89%)
36	30087.10768	332.3682724	0.0135	Singlet-A	H-11->L+1 (89%)

37	30187.12112	331.2670977	0	Singlet-A	H-1->L+3 (-16%), H-1->L+4 (-24%), HOMO->L+3 (16%), HOMO->L+4 (25%)
38	30187.12112	331.2670977	0	Singlet-A	H-1->L+3 (-16%), H-1->L+4 (25%), HOMO->L+3 (-16%), HOMO->L+4 (24%)
39	30629.116	326.4867324	0.0096	Singlet-A	H-12->L+1 (74%)
40	30760.58528	325.0913436	0.0191	Singlet-A	H-5->L+3 (21%), H-5->L+5 (14%), H-4->L+4 (35%)
41	30777.52304	324.9124365	0.0315	Singlet-A	H-5->L+4 (30%), H-4->L+3 (16%), H-4->L+5 (16%)
42	30976.74336	322.8228314	0.0192	Singlet-A	H-5->L+3 (15%), H-5->L+5 (-12%), H-4->L+2 (54%)
43	31030.78288	322.2606416	0.004	Singlet-A	H-1->L+6 (24%), H-1->L+7 (-19%), HOMO->L+6 (-21%), HOMO->L+7 (22%)
44	31030.78288	322.2606416	0.0037	Singlet-A	H-1->L+6 (18%), H-1->L+7 (27%), HOMO->L+6 (25%), HOMO->L+7 (18%)
45	31037.23536	322.1936453	0.0076	Singlet-A	H-5->L+2 (38%), H-4->L+3 (15%), H-4->L+5 (-10%)
46	31081.59616	321.7337986	0.0314	Singlet-A	H-3->L+3 (28%), H-2->L+2 (22%), H-2->L+4 (16%)
47	31083.20928	321.7171017	0.0079	Singlet-A	H-3->L+2 (20%), H-3->L+4 (18%), H-2->L+3 (28%)
48	31324.37072	319.2402519	0.0108	Singlet-A	H-1->L+11 (31%), HOMO->L+10 (19%), HOMO->L+12 (-26%)
49	31328.40352	319.1991572	0.0421	Singlet-A	H-1->L+10 (19%), H-1->L+12 (-27%), HOMO->L+11 (32%)
50	31392.92832	31854%	0.0433	Singlet-A	H-3->L+5 (-20%), H-2->L+2 (33%)
51	31446.16128	318.0038387	0.0001	Singlet-A	H-3->L+2 (34%), H-2->L+5 (-18%)
52	31778.464	314.6785194	0.0088	Singlet-A	H-1->L+13 (19%), H-1->L+15 (-13%), HOMO->L+14 (31%)
53	31785.72304	31461%	0.0001	Singlet-A	H-5->L+7 (-10%), H-4->L+6 (10%), H-1->L+14 (34%), HOMO->L+13 (20%), HOMO->L+15 (-14%)
54	31892.18896	313.5564013	0.0155	Singlet-A	H-15->LUMO (74%)
55	31932.51696	313.1604068	0.0108	Singlet-A	H-3->L+7 (33%), H-2->L+6 (-33%)
56	31935.7432	313.1287704	0.1223	Singlet-A	H-3->L+6 (34%), H-2->L+7 (-34%)
57	32109.1536	311.4376705	0	Singlet-A	H-1->L+9 (45%), HOMO->L+8 (43%)
58	32109.96016	311.4298476	0.0022	Singlet-A	H-1->L+8 (45%), HOMO->L+9 (48%)
59	32142.22256	311.1172534	0	Singlet-A	H-14->LUMO (32%)
60	32180.93744	310.7429676	0.0289	Singlet-A	H-5->L+6 (-14%), H-4->L+7 (15%), H-2->L+4 (13%)
61	32205.9408	310.5017196	0	Singlet-A	H-14->LUMO (24%)
62	32425.32512	308.400917	0.0031	Singlet-A	H-1->L+15 (13%), HOMO->L+10 (52%), HOMO->L+12 (18%)
63	32435.00384	308.308889	0.0036	Singlet-A	H-1->L+10 (53%), H-1->L+12 (18%), HOMO->L+15 (13%)
64	32835.0576	304.5525341	0.0284	Singlet-A	H-7->L+2 (42%), H-6->L+3 (-22%)
65	32866.51344	304.2610534	0.0005	Singlet-A	H-7->L+3 (-21%), H-6->L+2 (39%)
66	33198.81616	301.21556	0.0081	Singlet-A	H-16->LUMO (16%), H-6->L+4 (14%)
67	33234.3048	300.8939125	0.0195	Singlet-A	H-17->LUMO (20%), H-13->L+1 (12%), H-7->L+4 (-11%)
68	33376.25936	299.6141626	0.0437	Singlet-A	H-17->LUMO (47%)
69	33494.01712	298.5607837	0.0392	Singlet-A	H-16->LUMO (23%)
70	33569.0272	29789%	0.0108	Singlet-A	H-7->L+7 (28%), H-6->L+6 (29%), H-1->L+11 (-11%)
71	33577.89936	297.8149375	0.1409	Singlet-A	H-7->L+6 (25%), H-6->L+7 (25%), HOMO->L+11 (13%)
72	33663.39472	297.0585731	0.0041	Singlet-A	H-18->LUMO (47%)
73	33677.10624	296.9376267	0.014	Singlet-A	H-1->L+11 (40%), H-1->L+15 (12%), HOMO->L+10 (-14%)
74	33683.55872	296.8807448	0.0433	Singlet-A	H-1->L+10 (-13%), HOMO->L+11 (37%), HOMO->L+15 (11%)
75	33720.66048	296.5540964	0.0015	Singlet-A	H-3->L+9 (25%), H-2->L+8 (-24%)
76	33961.82192	294.4482785	0.0037	Singlet-A	H-5->L+8 (-18%), H-4->L+9 (18%)

77	33972.3072	294.3573994	0.0946	Singlet-A	H-5->L+9 (-18%), H-4->L+8 (18%)
78	34077.16	293.4516844	0.0065	Singlet-A	H-9->L+2 (10%), H-3->L+8 (-12%), H-2->L+9 (13%)
79	34119.10112	293.090957	0.0976	Singlet-A	H-13->L+1 (23%), H-8->L+2 (22%)
80	34195.72432	292.4342209	0.001	Singlet-A	H-3->L+3 (-21%), H-3->L+5 (40%), H-2->L+2 (22%)
81	34198.95056	292.4066334	0	Singlet-A	H-3->L+2 (21%), H-2->L+3 (-20%), H-2->L+5 (38%)
82	34495.76464	28989%	0.0712	Singlet-A	H-19->LUMO (65%), H-8->L+2 (11%)
83	34553.83696	289.4034608	0.0005	Singlet-A	H-20->LUMO (58%), H-18->LUMO (-20%)
84	34598.19776	289.0323961	0.2364	Singlet-A	H-19->LUMO (-14%), H-13->L+1 (-21%), H-8->L+2 (27%)
85	34661.916	288.5010742	0.0024	Singlet-A	H-5->L+2 (20%), H-4->L+3 (-13%), H-4->L+5 (23%)
86	34748.21792	28778%	0.0563	Singlet-A	H-5->L+3 (-20%), H-5->L+5 (27%), H-4->L+2 (27%)
87	34812.74272	287.2511391	0.0131	Singlet-A	H-9->L+2 (33%), H-8->L+3 (13%)
88	34940.98576	28620%	0.0812	Singlet-A	H-9->L+3 (17%), H-9->L+5 (12%), H-8->L+4 (31%), H-5->L+5 (-14%)
89	34957.11696	286.0647808	0.0484	Singlet-A	H-9->L+2 (-10%), H-9->L+4 (26%), H-8->L+3 (10%), H-8->L+5 (17%), H-4->L+5 (-10%)
90	35066.00256	285.1765034	0.0004	Singlet-A	H-3->L+3 (-22%), H-3->L+5 (-13%), H-2->L+4 (41%)
91	35066.80912	28517%	0.0003	Singlet-A	H-3->L+4 (41%), H-2->L+3 (-22%), H-2->L+5 (-13%)
92	35228.92768	283.8576323	0.0076	Singlet-A	H-11->L+4 (17%), H-10->L+3 (17%), H-9->L+7 (11%), H-8->L+6 (-11%)
93	35230.5408	283.8446352	0.0737	Singlet-A	H-11->L+3 (16%), H-10->L+4 (17%), H-9->L+6 (-11%), H-8->L+7 (11%)
94	35310.39024	283.2027608	0.0037	Singlet-A	H-12->L+5 (-14%), H-12->L+10 (25%)
95	35424.1152	28229%	0.0395	Singlet-A	H-7->L+8 (24%), H-6->L+9 (25%)
96	35480.5744	281.8443661	0.011	Singlet-A	H-11->L+3 (-17%), H-10->L+2 (-15%), H-10->L+4 (-10%), H-9->L+6 (-20%), H-8->L+7 (21%)
97	35491.05968	281.7610996	0.0069	Singlet-A	H-11->L+2 (13%), H-11->L+4 (10%), H-10->L+3 (15%), H-9->L+7 (-21%), H-8->L+6 (22%)
98	35553.1648	281.2689125	0.0001	Singlet-A	H-1->L+12 (42%), HOMO->L+13 (-34%)
99	35555.58448	281.2497712	0.0006	Singlet-A	H-1->L+13 (-37%), HOMO->L+12 (44%)
100	35580.58784	28105%	0.0012	Singlet-A	H-11->L+2 (36%), H-10->L+5 (-22%)

Table S7: Energy and composition of TD-DFT calculated transitions of **12**:

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	19962.36	500.9427743	0.0001	Singlet-A	HOMO->LUMO (98%)
2	24112.91776	414.7154691	0.0035	Singlet-A	H-3->LUMO (28%), H-2->LUMO (65%)
3	24163.73104	413.8433747	0.0202	Singlet-A	H-1->LUMO (92%)
4	26262.40016	380.772509	0.0038	Singlet-A	H-3->LUMO (67%), H-2->LUMO (-30%)
5	26705.2016	374.4588844	0.0724	Singlet-A	H-4->LUMO (93%)
6	27666.62112	361.4463782	0.0503	Singlet-A	HOMO->L+1 (75%), HOMO->L+2 (21%)
7	28543.35184	350.3442783	0.0041	Singlet-A	HOMO->L+2 (17%), HOMO->L+3 (74%)
8	28720.79504	348.1797766	0.0035	Singlet-A	HOMO->L+1 (-17%), HOMO->L+2 (57%), HOMO->L+3 (-21%)
9	28970.02208	345.1844107	0.0028	Singlet-A	H-5->LUMO (95%)
10	30517.81072	327.6775025	0.067	Singlet-A	HOMO->L+4 (88%)
11	30779.94272	324.8868944	0.5964	Singlet-A	H-6->LUMO (82%)
12	31975.26464	312.7417431	0.0427	Singlet-A	H-4->L+1 (-10%), H-1->L+1 (76%)
13	32033.33696	312.1747826	0.0333	Singlet-A	H-3->L+1 (14%), H-2->L+1 (40%), H-2->L+2 (13%), H-1->L+3 (-16%)
14	32641.4832	306.3586277	0.0147	Singlet-A	H-2->L+1 (10%), H-1->L+2 (55%)
15	32667.29312	306.1165785	0.0038	Singlet-A	H-2->L+1 (22%), H-1->L+2 (-16%), H-1->L+3 (34%)
16	33027.82544	302.7750046	0.0107	Singlet-A	H-7->LUMO (89%)
17	33094.76992	302.1625479	0.1765	Singlet-A	H-3->L+2 (18%), H-2->L+2 (43%), H-1->L+3 (23%)
18	33357.70848	299.780784	0.0375	Singlet-A	H-3->L+3 (23%), H-2->L+3 (41%), H-1->L+2 (15%)
19	33601.2896	297.6076252	0.0136	Singlet-A	HOMO->L+5 (84%)
20	33844.87072	295.4657467	0.0118	Singlet-A	H-4->L+1 (-27%), HOMO->L+6 (52%)
21	34252.99008	291.9453156	0.0187	Singlet-A	H-3->L+1 (28%), H-1->L+4 (48%)
22	34459.46944	290.1959944	0.0797	Singlet-A	H-4->L+3 (-16%), H-3->L+1 (-16%), H-1->L+4 (26%)
23	34552.22384	289.416972	0.0229	Singlet-A	H-4->L+1 (42%), HOMO->L+6 (20%)
24	34794.9984	287.3976278	0.0154	Singlet-A	H-4->L+2 (14%), H-3->L+4 (16%), H-2->L+4 (59%)
25	34920.82176	286.3621042	0.0868	Singlet-A	H-4->L+3 (11%), H-3->L+1 (-14%), H-3->L+2 (26%), H-2->L+2 (-10%), H-1->L+4 (15%)
26	34999.05808	285.7219751	0.0395	Singlet-A	H-3->L+3 (50%), H-2->L+3 (-24%)
27	35123.26832	284.7115453	0.192	Singlet-A	H-4->L+3 (39%), H-3->L+2 (-21%)
28	35496.7056	281.7162841	0.0362	Singlet-A	H-4->L+2 (58%), H-2->L+4 (-11%)
29	36163.73072	276.5201433	0.012	Singlet-A	H-5->L+1 (65%), H-5->L+2 (19%)
30	36261.32448	275.7759167	0.0016	Singlet-A	H-9->LUMO (80%)
31	36663.79792	272.7486122	0.0542	Singlet-A	H-4->L+4 (69%)
32	36789.62128	271.8157908	0.0181	Singlet-A	H-8->LUMO (11%), H-5->L+3 (13%), H-3->L+4 (46%), H-2->L+4 (-10%)
33	36822.69024	271.5716841	0.0108	Singlet-A	H-8->LUMO (73%)
34	36850.91984	271.3636469	0.0069	Singlet-A	H-5->L+3 (72%), H-3->L+4 (-14%)
35	37481.64976	266.7972211	0.0009	Singlet-A	H-5->L+1 (-19%), H-5->L+2 (52%), HOMO- >L+7 (14%)
36	37722.00464	265.0972581	0.0076	Singlet-A	H-10->LUMO (-10%), H-6->L+1 (-20%), H-6- >L+2 (24%), HOMO->L+7 (-17%)

37	37798.62784	264.5598682	0.0011	Singlet-A	HOMO->L+7 (62%)
38	37977.68416	263.3125274	0.0166	Singlet-A	H-2->L+6 (-27%), H-1->L+5 (43%)
39	38009.94656	263.0890308	0.0062	Singlet-A	H-3->L+5 (10%), H-2->L+5 (41%), H-1->L+6 (-29%)
40	38222.07184	261.6289363	0.0174	Singlet-A	H-13->LUMO (77%)
41	38355.15424	260.721152	0.2261	Singlet-A	H-6->L+1 (28%), H-6->L+2 (14%), H-2->L+5 (-13%), H-1->L+6 (-16%)
42	38662.4536	258.6488717	0.3216	Singlet-A	H-6->L+1 (20%), H-6->L+2 (11%), H-1->L+6 (17%)
43	38828.60496	257.5420881	0.1712	Singlet-A	H-6->L+1 (11%), H-2->L+6 (29%), H-1->L+5 (15%)
44	39018.95312	256.2857073	0.0144	Singlet-A	H-12->LUMO (-20%), H-11->LUMO (63%), H-10->LUMO (10%)
45	39066.54016	255.9735251	0.0252	Singlet-A	H-12->LUMO (50%), H-11->LUMO (29%), H-10->LUMO (-10%)
46	39352.86896	254.1110792	0.0188	Singlet-A	H-6->L+3 (51%), H-5->L+4 (-20%)
47	39402.87568	253.7885834	0.0132	Singlet-A	H-6->L+3 (28%), H-5->L+4 (57%)
48	39602.096	252.5118873	0.1548	Singlet-A	H-12->LUMO (20%), H-10->LUMO (34%), H-6->L+2 (11%), H-5->L+4 (15%)
49	39726.30624	25172%	0.0171	Singlet-A	H-4->L+5 (-16%), HOMO->L+10 (-15%), HOMO->L+11 (23%)
50	39952.14304	250.2994643	0.0114	Singlet-A	H-6->L+4 (52%), H-3->L+5 (-16%)
51	39995.69728	250.0268949	0.0023	Singlet-A	H-6->L+4 (19%), H-3->L+5 (46%)
52	40239.2784	24851%	0.0138	Singlet-A	H-4->L+5 (22%), H-3->L+6 (43%), H-2->L+6 (-14%)
53	40398.97728	247.5310187	0.2242	Singlet-A	HOMO->L+8 (47%), HOMO->L+14 (10%)
54	40548.19088	246.6201274	0.0207	Singlet-A	H-4->L+5 (-16%), H-4->L+6 (50%), H-3->L+5 (-10%)
55	40623.20096	246.1647473	0.0037	Singlet-A	H-4->L+5 (32%), H-4->L+6 (27%), H-3->L+6 (-22%)
56	41324.1016	241.9895318	0.0121	Singlet-A	H-1->L+7 (69%)
57	41585.42704	240.4688544	0.0019	Singlet-A	H-7->L+1 (-25%), H-7->L+2 (44%)
58	41626.5616	240.2312277	0.0053	Singlet-A	H-4->L+10 (-13%), H-4->L+11 (22%), H-1->L+7 (24%)
59	41727.3816	239.6507908	0.0029	Singlet-A	H-2->L+7 (22%), H-2->L+11 (10%)
60	41758.03088	239.4748936	0.011	Singlet-A	H-5->L+5 (82%)
61	42063.71712	237.7345771	0.0147	Singlet-A	H-14->LUMO (11%), H-5->L+6 (58%)
62	42078.2352	237.6525525	0.0207	Singlet-A	H-14->LUMO (-19%), H-5->L+6 (31%), H-2->L+7 (15%)
63	42361.33776	236.0643107	0.0078	Singlet-A	H-16->LUMO (-35%), H-15->LUMO (48%)
64	42428.28224	235.6918421	0.0115	Singlet-A	H-16->LUMO (-16%), H-15->LUMO (-19%), H-14->LUMO (28%), H-2->L+7 (25%)
65	42774.29648	233.7852594	0.1144	Singlet-A	H-17->LUMO (12%), H-16->LUMO (27%), H-15->LUMO (18%), H-14->LUMO (15%), H-2->L+7 (10%)
66	42974.32336	232.6970902	0.0028	Singlet-A	H-17->LUMO (75%)
67	43508.26608	229.8413819	0.0006	Singlet-A	H-9->L+1 (22%), H-9->L+2 (10%), H-7->L+1 (33%), H-7->L+2 (18%)
68	43667.96496	229.000825	0.0427	Singlet-A	H-3->L+7 (28%), HOMO->L+9 (31%)
69	43765.55872	22849%	0.0056	Singlet-A	H-6->L+5 (39%), H-4->L+7 (45%)
70	43892.18864	227.830972	0.0123	Singlet-A	H-6->L+5 (45%), H-4->L+7 (-30%)
71	44004.30048	227.2505162	0.0075	Singlet-A	H-3->L+7 (32%), HOMO->L+9 (-11%)
72	44032.53008	227.1048241	0.0038	Singlet-A	H-9->L+3 (25%), H-7->L+3 (26%)
73	44192.22896	226.2841281	0.0006	Singlet-A	H-6->L+6 (87%)
74	44280.95056	225.8307438	0.01	Singlet-A	H-3->L+8 (14%), H-2->L+8 (29%)
75	44586.6368	224.2824469	0.0387	Singlet-A	H-8->L+1 (30%), H-1->L+9 (-14%)
76	44712.46016	223.6513036	0.0262	Singlet-A	H-9->L+1 (-11%), H-9->L+2 (18%), H-1->L+8 (31%)

77	44883.45088	222.799268	0.0016	Singlet-A	H-9->L+2 (-14%), H-8->L+1 (-13%), H-7->L+3 (14%)
78	44924.58544	222.595265	0.0079	Singlet-A	H-9->L+1 (-18%), H-9->L+2 (22%), H-1->L+8 (-16%)
79	44972.97904	222.3557392	0.0883	Singlet-A	H-9->L+1 (11%), HOMO->L+13 (13%), HOMO->L+14 (-12%)
80	45358.51472	220.4657728	0.0039	Singlet-A	H-8->L+1 (-27%), H-8->L+2 (44%)
81	45450.46256	22002%	0.0013	Singlet-A	H-8->L+3 (41%), H-4->L+8 (20%)
82	45645.65008	219.0789261	0.0006	Singlet-A	H-9->L+4 (13%), H-7->L+4 (43%)
83	45933.592	217.7055955	0.0105	Singlet-A	H-13->L+3 (-10%), H-9->L+3 (26%), H-7->L+3 (-15%)
84	45982.79216	217.4726573	0.0009	Singlet-A	H-18->LUMO (89%)
85	46056.18912	21713%	0.0013	Singlet-A	H-19->LUMO (30%), H-10->L+1 (-13%), H-10->L+2 (12%)
86	46194.91744	216.4740312	0.0234	Singlet-A	H-13->L+1 (17%), H-13->L+2 (11%), H-1->L+9 (-13%)
87	46269.92752	21612%	0.0015	Singlet-A	H-5->L+7 (85%)
88	46297.35056	215.9950813	0.0223	Singlet-A	H-1->L+9 (16%)
89	46382.84592	215.5969476	0.0143	Singlet-A	H-3->L+9 (16%), H-2->L+9 (44%)
90	46541.73824	21486%	0.0047	Singlet-A	H-20->LUMO (-28%), H-6->L+7 (30%)
91	46628.04016	214.4632278	0.025	Singlet-A	H-13->L+2 (19%), H-9->L+4 (14%), H-4->L+8 (10%)
92	46661.91568	214.3075323	0.0171	Singlet-A	H-13->L+2 (16%), H-8->L+3 (10%), H-4->L+8 (-16%)
93	46903.07712	213.2056277	0.0248	Singlet-A	H-20->LUMO (18%), H-13->L+3 (17%), H-6->L+7 (10%)
94	46949.8576	21299%	0.011	Singlet-A	H-12->L+1 (15%), H-11->L+1 (13%), H-1->L+9 (13%)
95	46974.0544	212.8834764	0.0017	Singlet-A	H-11->L+1 (14%), H-10->L+1 (13%)
96	47114.39584	212.2493523	0.0057	Singlet-A	H-13->L+3 (18%), H-12->L+1 (17%), H-10->L+2 (-15%)
97	47164.40256	212.0243119	0.0014	Singlet-A	H-13->L+2 (21%), H-9->L+4 (-17%), H-8->L+4 (31%)
98	47245.86512	211.658734	0.0148	Singlet-A	H-3->L+8 (-17%), HOMO->L+10 (27%), HOMO->L+11 (17%)
99	47376.52784	21107%	0.0034	Singlet-A	H-9->L+4 (18%), H-8->L+4 (48%)
100	47448.31168	210.7556549	0.0056	Singlet-A	H-10->L+1 (34%), H-10->L+2 (18%)

Table S8: Energy and composition of TD-DFT calculated transitions of **13**:

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	17845.14	560.3766628	0.0001	Singlet-A	H-1->L+1 (-11%), HOMO->LUMO (85%)
2	17857.2384	559.9970038	0	Singlet-A	H-1->LUMO (85%), HOMO->L+1 (-11%)
3	21543.2176	464.1832147	0.0284	Singlet-A	H-3->LUMO (23%), H-2->LUMO (67%)
4	21562.57504	463.766502	0.0043	Singlet-A	H-3->LUMO (68%), H-2->LUMO (-23%)
5	22016.66832	454.2013285	0.0256	Singlet-A	H-6->LUMO (12%), H-4->LUMO (69%)
6	22067.4816	453.1554702	0.0006	Singlet-A	H-7->LUMO (13%), H-5->LUMO (69%)
7	22318.32176	448.0623636	0.0007	Singlet-A	H-1->LUMO (12%), HOMO->L+1 (80%)
8	22328.00048	447.868138	0	Singlet-A	H-1->L+1 (81%), HOMO->LUMO (12%)
9	23735.44768	421.310781	0.1235	Singlet-A	H-6->LUMO (69%), H-4->LUMO (-16%)
10	23844.33328	419.3868574	0.0001	Singlet-A	H-7->LUMO (67%), H-5->LUMO (-18%)
11	24476.67632	408.5522017	0.1574	Singlet-A	H-12->LUMO (-10%), H-9->L+1 (10%), H-8->LUMO (73%)
12	24524.26336	407.7594443	0.0168	Singlet-A	H-9->LUMO (84%)
13	25613.92592	390.4126229	0.559	Singlet-A	H-12->LUMO (27%), H-8->LUMO (10%), H-3->L+1 (-25%), H-2->L+1 (24%)
14	25665.54576	389.6274053	0.0018	Singlet-A	H-3->L+1 (41%), H-2->L+1 (48%)
15	25746.20176	388.4068063	0.8172	Singlet-A	H-12->LUMO (44%), H-3->L+1 (24%), H-2->L+1 (-18%)
16	26284.17728	380.4570291	0.0007	Singlet-A	H-11->LUMO (-24%), H-10->LUMO (65%)
17	26315.63312	380.0022578	0.0482	Singlet-A	H-11->LUMO (65%), H-10->LUMO (24%)
18	26571.31264	376.345728	0.0002	Singlet-A	H-4->L+1 (75%)
19	26660.8408	375.0819442	0.0229	Singlet-A	H-5->L+1 (76%)
20	27433.52528	364.5174981	0.0061	Singlet-A	H-6->L+1 (10%), H-1->L+3 (-27%), HOMO->L+2 (44%)
21	27467.4008	364.067939	0.0067	Singlet-A	H-1->L+2 (46%), HOMO->L+3 (-29%)
22	27552.89616	362.9382531	0.0596	Singlet-A	H-1->L+4 (49%), HOMO->L+4 (25%)
23	27595.64384	362.3760351	0.0315	Singlet-A	H-1->L+5 (-29%), HOMO->L+5 (44%)
24	27703.72288	360.962317	0.0061	Singlet-A	H-13->LUMO (35%), H-6->L+1 (-20%), HOMO->L+2 (12%)
25	28286.86576	353.5209622	0.0136	Singlet-A	H-7->L+1 (73%)
26	28347.35776	352.7665642	0.0003	Singlet-A	H-13->LUMO (32%), H-6->L+1 (41%)
27	28482.05328	351.0982829	0.0036	Singlet-A	H-1->L+6 (54%), HOMO->L+6 (33%)
28	28499.7976	350.8796848	0.0041	Singlet-A	H-1->L+7 (-31%), HOMO->L+7 (57%)
29	28943.4056	345.5018438	0.0325	Singlet-A	H-9->L+1 (56%), H-8->L+1 (27%)
30	28949.05152	345.4344607	0.0154	Singlet-A	H-9->L+1 (-27%), H-8->L+1 (56%)
31	30183.08832	331.3113587	0.0014	Singlet-A	H-11->L+1 (12%), H-1->L+9 (32%), HOMO->L+8 (33%)
32	30205.672	331.0636492	0.0226	Singlet-A	H-10->L+1 (13%), H-1->L+8 (36%), HOMO->L+9 (36%)
33	30306.492	329.9623064	0.0012	Singlet-A	H-10->L+1 (69%)
34	30315.36416	329.8657389	0.0003	Singlet-A	H-11->L+1 (69%), HOMO->L+8 (-10%)
35	30391.1808	329.0428255	0.0019	Singlet-A	H-12->L+1 (71%)
36	30891.248	323.7162837	0.0011	Singlet-A	H-1->L+2 (26%), HOMO->L+3 (58%)

37	30903.3464	323.5895515	0.0002	Singlet-A	H-1->L+3 (58%), HOMO->L+2 (25%)
38	31267.91152	319.8166911	0.0424	Singlet-A	H-3->L+2 (33%), H-3->L+3 (-17%), H-2->L+2 (26%), H-2->L+3 (12%)
39	31282.4296	319.6682652	0.0074	Singlet-A	H-3->L+2 (-26%), H-3->L+3 (11%), H-2->L+2 (33%), H-2->L+3 (18%)
40	31617.152	316.284022	0.0032	Singlet-A	H-6->L+2 (13%), H-5->L+3 (17%), H-4->L+2 (43%)
41	31689.7424	315.5595231	0.002	Singlet-A	H-7->L+2 (10%), H-5->L+2 (35%), H-4->L+3 (17%)
42	31743.78192	315.0223255	0.0384	Singlet-A	H-4->L+4 (-18%), H-3->L+4 (30%)
43	31776.85088	314.6944937	0.0256	Singlet-A	H-5->L+5 (-18%), H-2->L+5 (32%), H-2->L+7 (-10%)
44	32026.07792	312.2455402	0.0213	Singlet-A	H-4->L+4 (19%), H-3->L+4 (34%)
45	32074.47152	311.7744276	0.0255	Singlet-A	H-5->L+5 (19%), H-2->L+5 (33%), H-2->L+7 (10%)
46	32150.28816	311.0392028	0.0001	Singlet-A	H-1->L+4 (-35%), HOMO->L+4 (60%)
47	32197.8752	310.5795006	0.0001	Singlet-A	H-1->L+5 (60%), HOMO->L+5 (35%)
48	32474.52528	307.9336777	0.3239	Singlet-A	H-13->L+1 (70%)
49	32666.48656	30612%	0.1381	Singlet-A	H-4->L+4 (-14%), H-3->L+6 (56%)
50	32690.68336	305.8975516	0.3616	Singlet-A	H-5->L+5 (-13%), H-2->L+7 (53%)
51	32966.52688	303.33799	0.0001	Singlet-A	H-1->L+6 (-35%), HOMO->L+6 (60%)
52	32983.46464	30318%	0.0001	Singlet-A	H-1->L+7 (60%), HOMO->L+7 (35%)
53	33162.52096	301.5452297	0.088	Singlet-A	H-4->L+6 (38%)
54	33189.944	301.2960793	0.0449	Singlet-A	H-5->L+7 (35%), H-4->L+7 (11%)
55	33362.54784	299.7372997	0.0011	Singlet-A	H-14->LUMO (-16%), H-7->L+2 (20%), H-6->L+3 (21%), H-5->L+2 (-17%)
56	33468.2072	298.791027	0.0602	Singlet-A	H-7->L+3 (18%), H-6->L+2 (39%)
57	33575.47968	297.8364001	0.0017	Singlet-A	
58	33654.52256	297.136885	0.0242	Singlet-A	H-8->L+2 (-12%), H-1->L+11 (12%), HOMO->L+10 (18%)
59	33697.27024	296.7599431	0.0138	Singlet-A	H-1->L+10 (18%), HOMO->L+11 (17%)
60	33716.62768	296.5895669	0.0209	Singlet-A	H-1->L+11 (12%), HOMO->L+10 (11%)
61	33875.52	295.1984206	0.0005	Singlet-A	H-1->L+9 (39%), HOMO->L+8 (-36%)
62	33877.13312	295.1843642	0.0013	Singlet-A	H-1->L+8 (-39%), HOMO->L+9 (42%)
63	33898.10368	295.0017527	0.0019	Singlet-A	H-2->L+2 (-15%), H-2->L+3 (42%)
64	33903.7496	294.9526267	0.0018	Singlet-A	H-3->L+2 (14%), H-3->L+3 (42%)
65	33962.62848	294.4412858	0.0006	Singlet-A	H-9->L+2 (11%)
66	34084.41904	293.3891872	0.0527	Singlet-A	H-17->LUMO (11%), H-3->L+9 (-10%), H-2->L+8 (-11%)
67	34127.97328	293.0147629	0.0381	Singlet-A	H-18->LUMO (-19%), H-16->LUMO (22%)
68	34143.29792	292.8832482	0.127	Singlet-A	H-17->LUMO (33%)
69	34189.27184	29249%	0.0167	Singlet-A	H-7->L+4 (-15%), H-6->L+4 (16%), H-4->L+4 (-11%)
70	34207.82272	292.3307947	0.0186	Singlet-A	H-7->L+5 (14%), H-6->L+5 (13%), H-5->L+5 (-11%)
71	34249.76384	291.9728161	0.0136	Singlet-A	
72	34257.82944	291.9040746	0.0109	Singlet-A	
73	34423.9808	290.4951655	0.002	Singlet-A	H-16->LUMO (26%), H-14->LUMO (25%)
74	34429.62672	290.4475288	0.0127	Singlet-A	H-17->LUMO (-10%), H-15->LUMO (40%)
75	34539.31888	289.5251072	0.0118	Singlet-A	H-1->L+10 (14%), H-1->L+12 (-10%)
76	34548.9976	289.4439982	0.0112	Singlet-A	H-15->LUMO (18%), H-1->L+13 (15%), HOMO->L+10 (-12%)

77	34571.58128	289.2549207	0.071	Singlet-A	H-5->L+9 (14%), H-4->L+8 (-11%)
78	34575.61408	289.2211828	0.0254	Singlet-A	H-5->L+8 (-12%), H-4->L+9 (14%)
79	34767.57536	287.6243136	0.0021	Singlet-A	H-4->L+6 (13%)
80	34786.9328	287.464263	0.0047	Singlet-A	H-7->L+7 (-10%), H-6->L+7 (-10%), H-5->L+7 (17%)
81	34927.27424	28631%	0.0145	Singlet-A	H-18->LUMO (26%)
82	34982.12032	285.8603169	0.0211	Singlet-A	H-5->L+3 (39%), H-4->L+2 (-25%), H-4->L+3 (-14%)
83	34989.37936	285.8010111	0.0086	Singlet-A	H-5->L+2 (-21%), H-5->L+3 (13%), H-4->L+3 (35%)
84	35085.36	285.0191647	0.0012	Singlet-A	H-2->L+4 (93%)
85	35132.14048	28464%	0.0091	Singlet-A	H-3->L+5 (90%)
86	35153.11104	284.4698436	0.2053	Singlet-A	H-9->L+7 (13%), H-8->L+7 (22%)
87	35156.33728	28444%	0.2447	Singlet-A	H-9->L+6 (22%), H-8->L+6 (-11%)
88	35357.17072	282.8280599	0.0365	Singlet-A	H-8->L+5 (-11%), H-1->L+14 (-10%), HOMO->L+14 (23%)
89	35384.59376	282.6088684	0.043	Singlet-A	H-1->L+15 (20%), HOMO->L+15 (13%)
90	35548.32544	28131%	0.0113	Singlet-A	H-12->L+3 (26%), H-12->L+10 (-12%), H-6->L+3 (-15%)
91	35767.70976	279.5817811	0.003	Singlet-A	H-12->L+2 (12%), H-1->L+11 (40%), HOMO->L+10 (-20%)
92	35796.74592	279.3550012	0.0032	Singlet-A	H-1->L+10 (-29%), HOMO->L+11 (55%)
93	35872.56256	278.7645846	0.0069	Singlet-A	H-24->LUMO (-13%), H-12->L+2 (25%), H-1->L+11 (-16%)
94	35896.75936	27858%	0.0039	Singlet-A	H-10->L+2 (14%), H-10->L+4 (52%)
95	35903.21184	278.5266133	0.0002	Singlet-A	H-2->L+6 (86%)
96	35924.1824	278.3640248	0.0004	Singlet-A	H-3->L+7 (86%)
97	35931.44144	278.3077884	0.0037	Singlet-A	H-11->L+2 (-18%), H-11->L+3 (-10%), H-11->L+5 (52%)
98	36134.69456	276.742342	0.0204	Singlet-A	H-24->LUMO (31%), H-23->LUMO (18%), H-19->LUMO (-15%)
99	36185.50784	27635%	0.0148	Singlet-A	H-10->L+2 (34%), H-10->L+3 (-15%), H-10->L+4 (-21%)
100	36208.89808	276.1752091	0.0122	Singlet-A	H-11->L+2 (29%), H-11->L+3 (13%), H-11->L+5 (24%)

Figure S10: ^1H NMR data for $[\text{Ir}(\text{ppy})_2(5\text{-ethynyl-2,2'-bipyridine})]\text{PF}_6$ (10).⁵

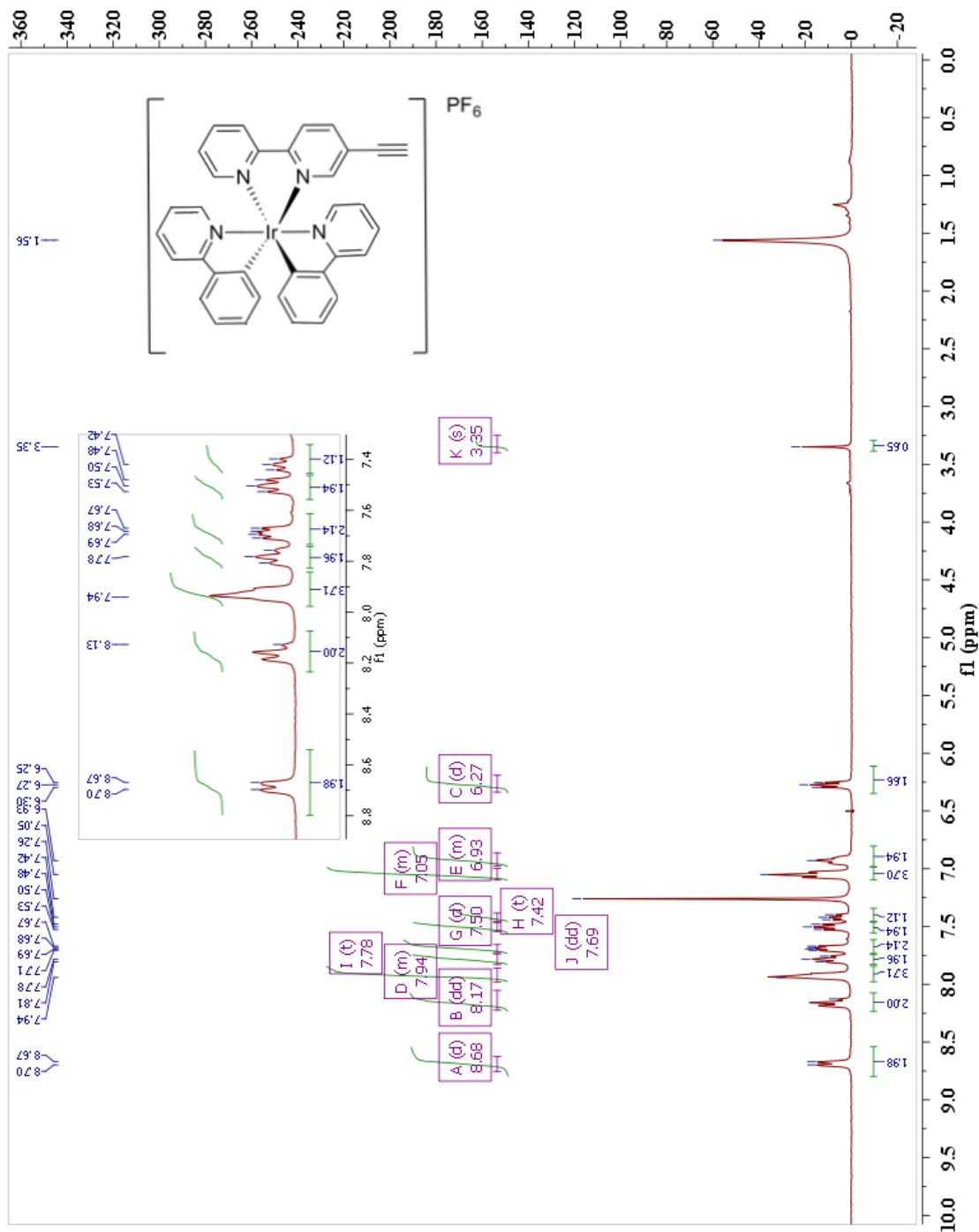


Figure S11: ^{13}C NMR data for $[\text{Ir}(\text{ppy})_2(5\text{-ethynyl-2,2'-bipyridine})]\text{PF}_6$ (10):⁵

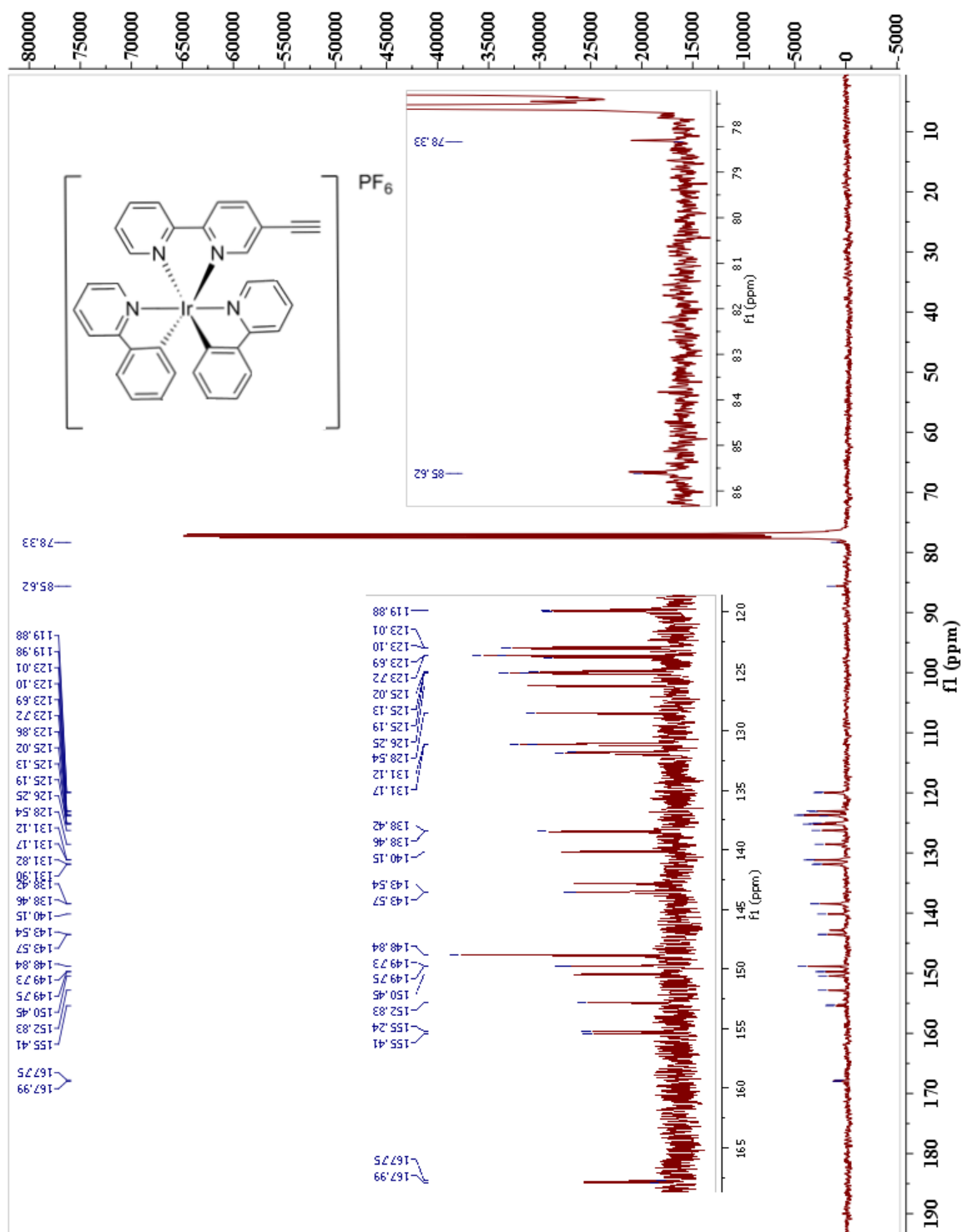


Figure S13: ^{13}C NMR data for **Bis[Ir(ppy)₂(5-ethynyl-2,2'-bipyridine)]-bis Hexafluorophosphate (11):**

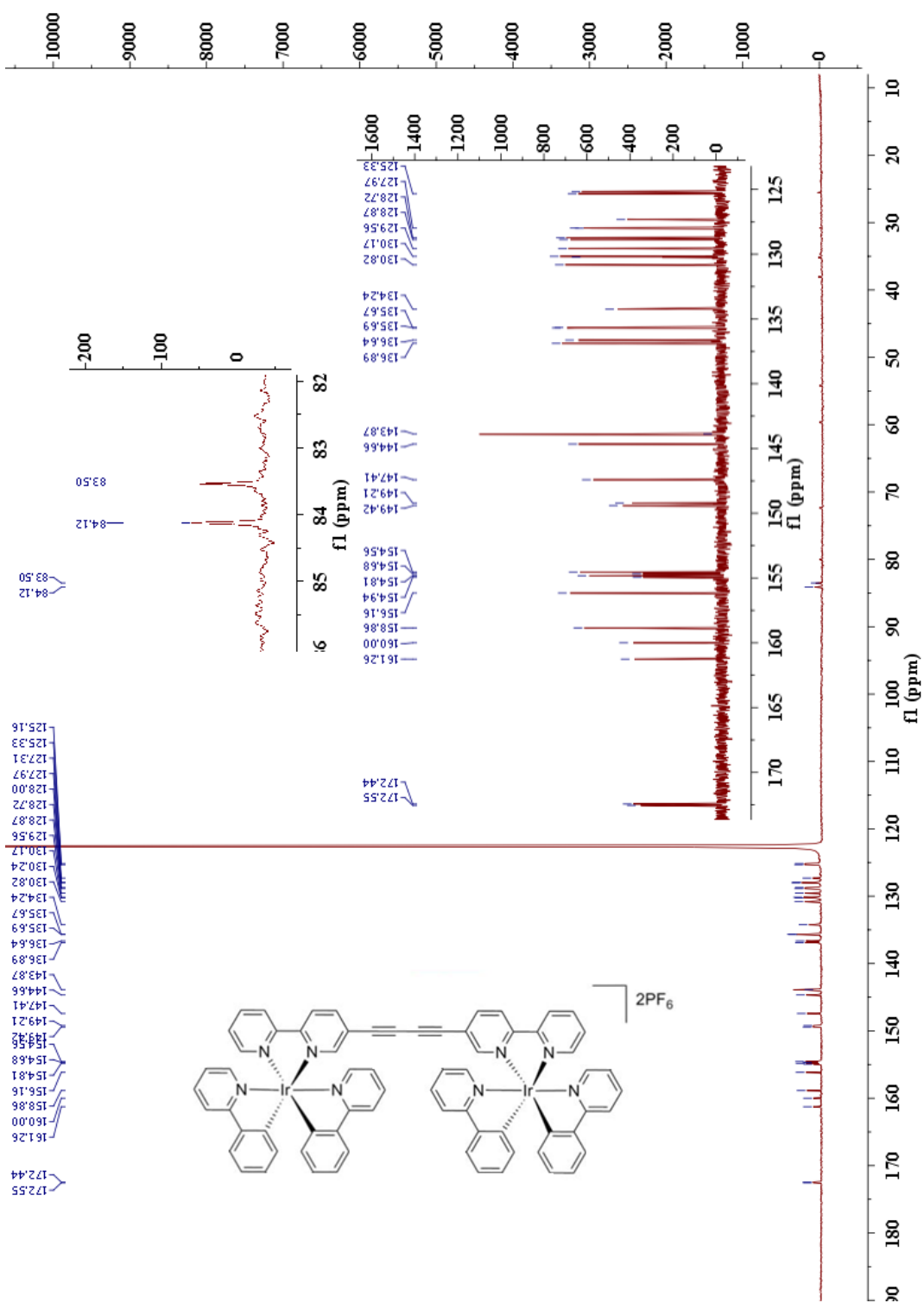


Figure S14: ^1H NMR data for $[\text{Ir}(\text{diF-Meppy})_2(5\text{-ethynyl-2,2'-bipyridine})]\text{PF}_6$ Hexafluorophosphate (12):

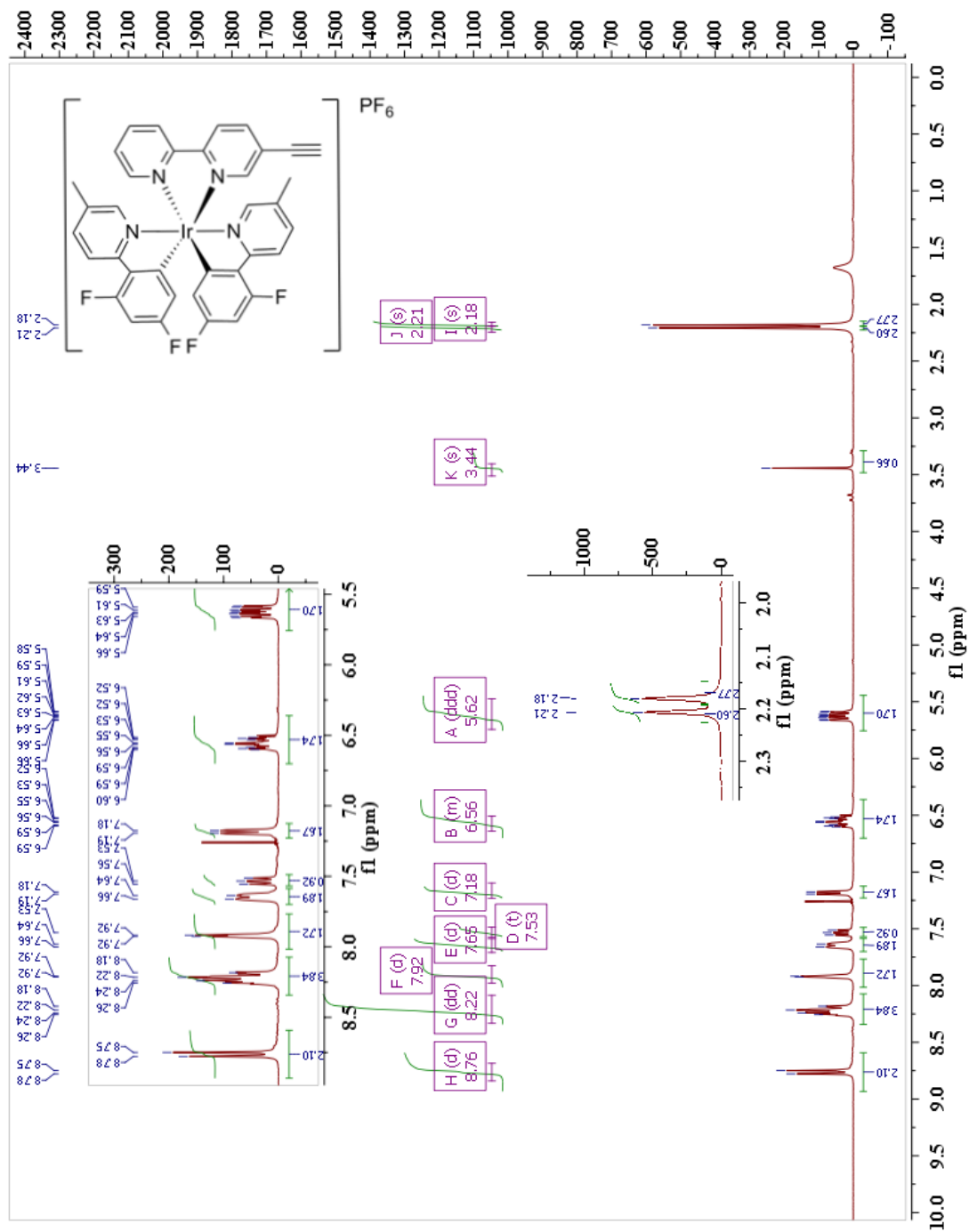


Figure S15: ^{13}C NMR data for $[\text{Ir}(\text{diF-Meppy})_2(5\text{-ethynyl-2,2'-bipyridine})]\text{PF}_6$ (12):

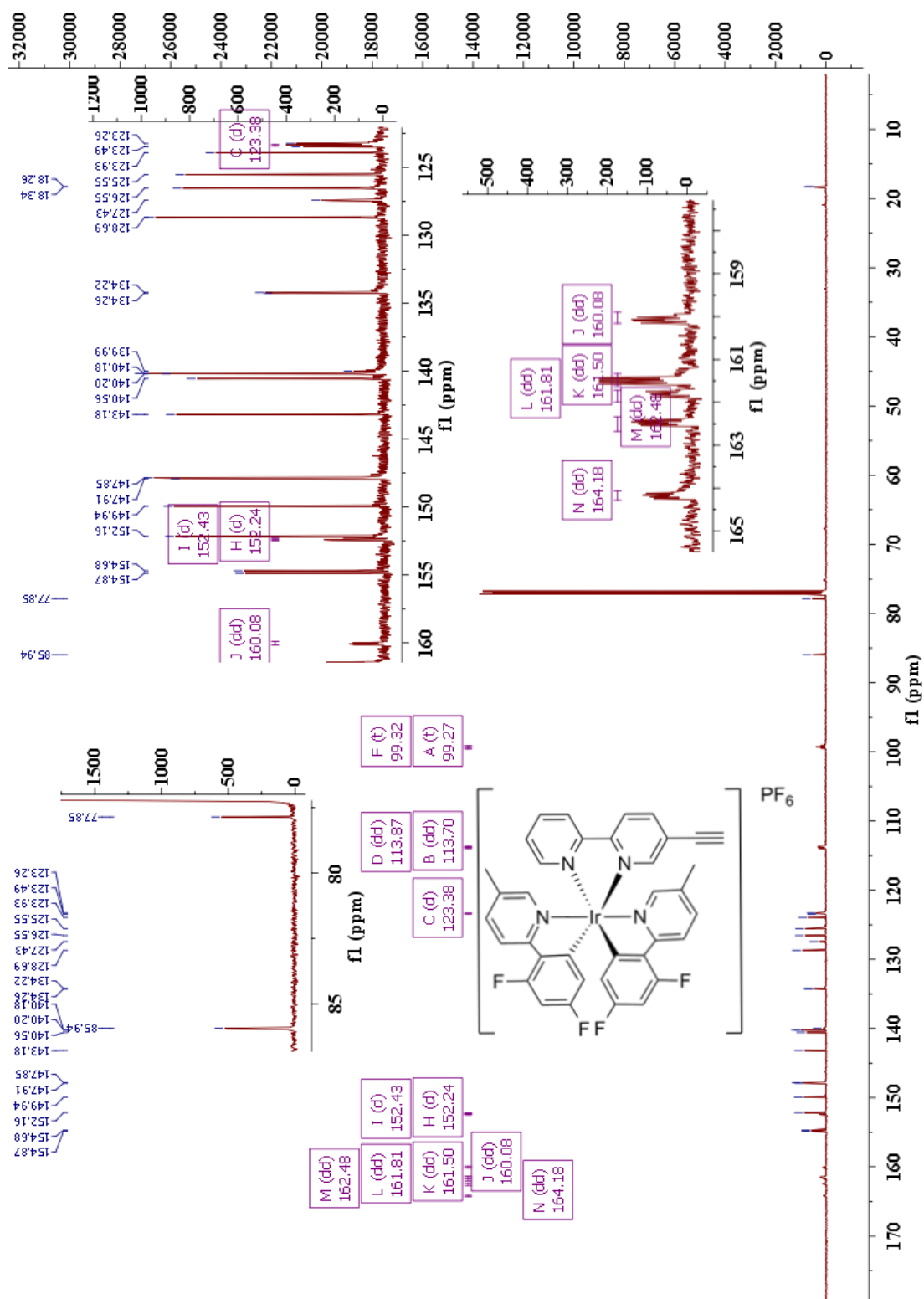


Figure S16: ^1H NMR data for **Bis[$\text{Ir}(\text{diF-Meppy})_2(5\text{-ethynyl-2,2'-bipyridine})$]-bis Hexafluorophosphate (13):**

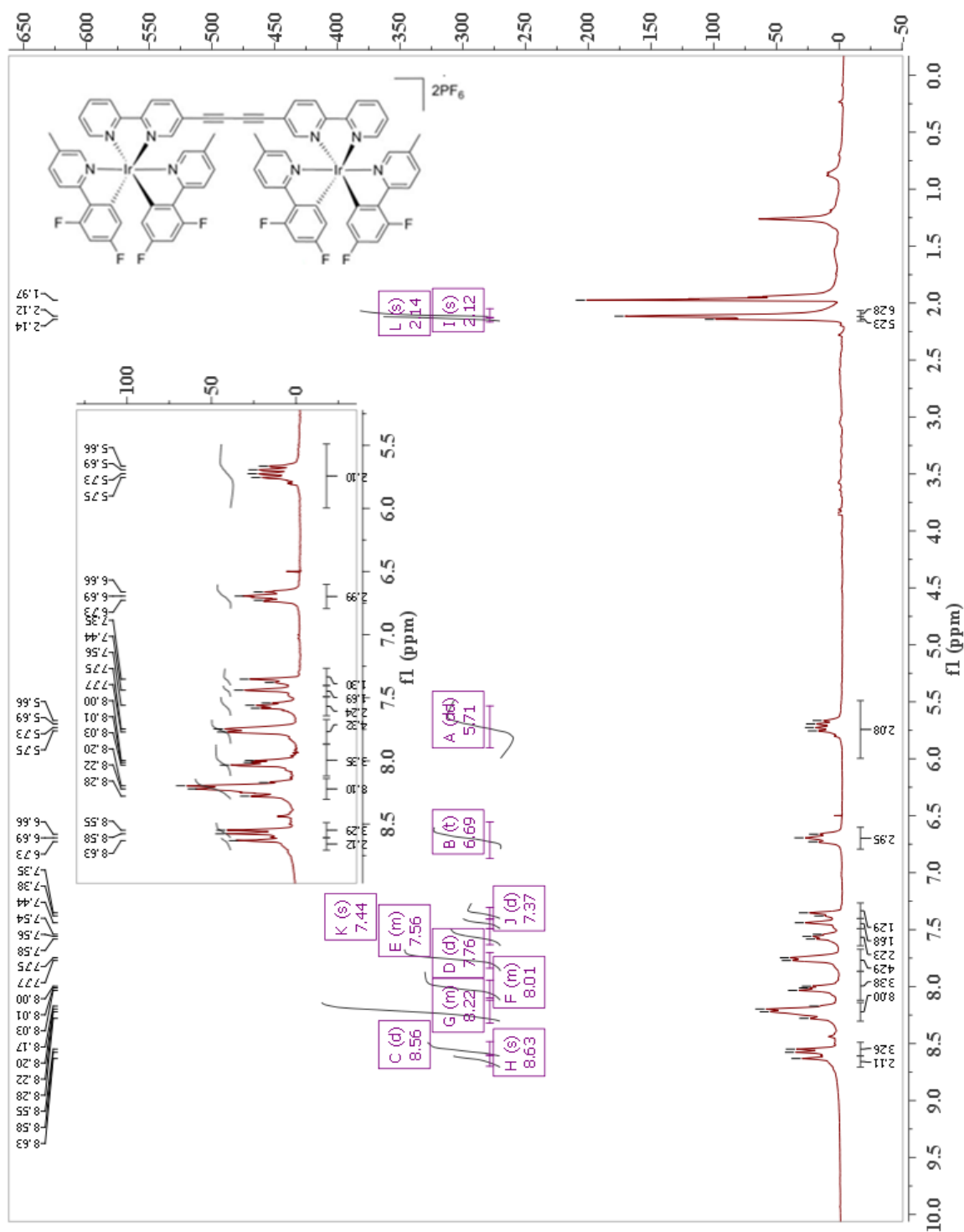
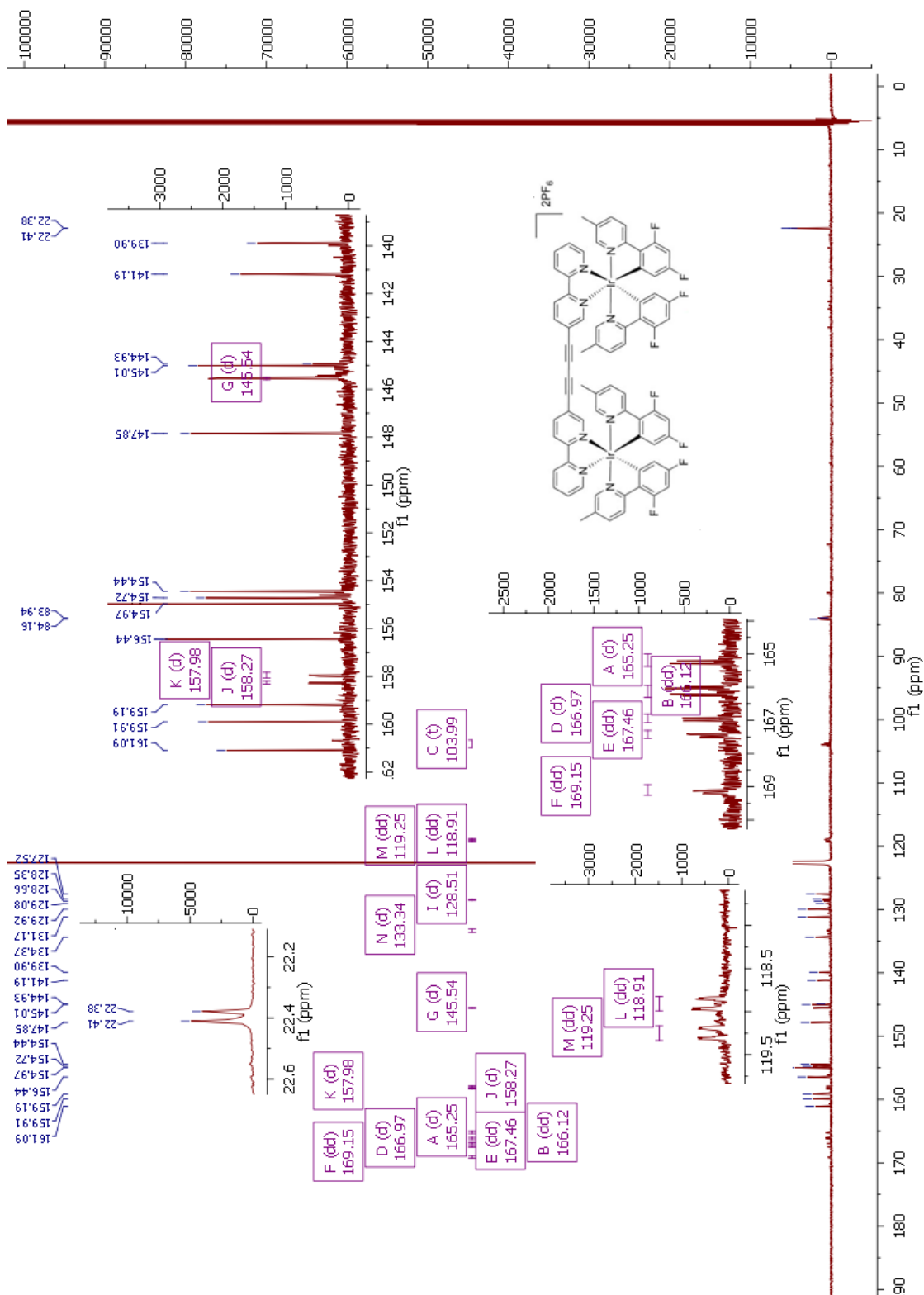


Figure S17: ^{13}C NMR data for **Bis[Ir(diF-Meppy) $_2$ (5-ethynyl-2,2'-bipyridine)]-bis Hexafluorophosphate (13):**



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