Supporting Information:

Synthesis and Characterization of Luminescent Cyclometalated Platinum(II) Complexes with Tunable Emissive Colors and Their Application Studies in Organic Memories and OLEDs

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Table S1a Crystal and structure determination data of **4**

empirical formula	$C_{40}H_{37}N_5Pt$
formula weight	782.84
temp, K	299
wavelength, Å	0.71073
crystal system	Monoclinic
space group	*C*2/*c*
a, Å	14.3245(12)
b, Å	13.9107(11)
c, Å	16.7445(14)
β, deg	104.782(1)
volume, Å^3	3226.1(5)
Z, Å^3	4
density (calcd), g cm^{-3}	1.612
crystal size	0.50 mm × 0.18 mm × 0.16 mm
index ranges	$-17 \le h \le 17$
	$-16 \le k \le 16$
	$-11 \le l \le 19$
reflections collected/unique	8718/2822
GoF on F^2	1.05
final *R* indices [$I > 2\sigma(I)$]	$R_1 = 0.016$
	$wR_2 = 0.040$
largest diff peak and hole, e Å^{-3}	0.46 and −0.52

Table S1b Selected bond lengths [Å] and angles [°] for **4** with estimated standard deviations in parentheses

Pt1—C8	1.944(3)	Pt1—N3	2.103(3)
Pt1—N1^{i}	2.011(2)	Pt1—N1	2.011(2)
C8—Pt1—N1^{i}	80.03(6)	C8—Pt1—N3	180.000(1)
C8—Pt1—N1	80.03(6)	N1^{i}—Pt1—N3	99.97(6)
N1^{i}—Pt1—N1	160.05(12)	N1—Pt1—N3	99.97(6)

The representation i refers to the symmetrical component of the complex

Table S1c Computed bond lengths [Å] and angles [°] of complex **4** optimized at the PBE0 level

Pt1—C8	1.938	Pt1—N3	2.114
Pt1—N1^{i}	2.027	Pt1—N1	2.027
C8—Pt1—N1^{i}	79.81	C8—Pt1—N3	180.00
C8—Pt1—N1	79.81	N1^{i}—Pt1—N3	100.19
N1^{i}—Pt1—N1	159.62	N1—Pt1—N3	100.19

The representation i refers to the symmetrical component of the complex

Table S2 Selected singlet excited states (S_n) of **4**–**6** computed by TDDFT/CPCM (CH_2Cl_2) at the optimized ground-state geometries

Complex	S_n	Excitation[a]	Coefficient[b]	Vertical excitation energy (nm)	f[c]
4	1	H→L	0.71	496	0.000
	2	H→L+1	0.70	444	0.000
	3	H-1→L	0.70	376	0.012
	4	H-3→L	0.62	358	0.279
	5	H-2→L	0.66	351	0.143
	6	H-2→L+1	0.47	346	0.134
		H-1→L+1	-0.42		
	7	H→L+2	0.69	337	0.050
	8	H-1→L+1	0.55	337	0.008
		H-2→L+1	0.42		
	9	H-4→L	0.70	326	0.000
	10	H-3→L+1	0.65	318	0.022
5	1	H→L	0.71	529	0.000
	2	H→L+1	0.70	469	0.000
	3	H-1→L	0.70	383	0.010
	4	H-3→L	0.61	358	0.255
	5	H-2→L	0.66	352	0.155
	6	H→L+2	0.70	350	0.038
	7	H-1→L+1	0.54	349	0.127
		H-2→L+1	0.32		
		H-3→L	0.31		
	8	H-2→L+1	0.54	340	0.030
		H-1→L+1	-0.42		
	9	H-5→L	0.70	326	0.000
	10	H→L+3	0.70	324	0.001
6	1	H→L	0.70	463	0.004
	2	H→L+2	0.70	416	0.000
	3	H→L+1	0.70	411	1.225
	4	H→L+3	0.66	369	0.414
	5	H-1→L	0.67	361	0.027

6	H-3→L	0.62	355	0.286
7	H-2→L	0.63	346	0.149
8	H-2→L+2	0.55	344	0.138
	H-3→L	0.31		
9	H→L+4	0.60	343	0.110
10	H-1→L+2	0.63	325	0.000

[a]The orbitals involved in the excitations (H = HOMO and L = LUMO).

[b]The coefficients in the configuration interaction (CI) expansion that are less than or equal to 0.3 are not listed.

[c]Oscillator strengths.

Table S3 Cartesian coordinates of the optimized structure of **4** at the S_0 state

1	C	0.000000	0.000000	-1.759353
2	C	0.269715	-1.190910	-3.849826
3	C	0.000000	0.000000	-4.526627
4	C	-0.269715	1.190910	-3.849826
5	H	0.459943	-2.086489	-4.431072
6	H	-0.459943	2.086489	-4.431072
7	C	-0.536408	2.260118	-1.487205
8	C	-0.708746	3.088139	0.538416
9	C	-0.981451	4.121458	-0.378133
10	C	-0.743958	3.322048	1.915434
11	C	-1.291584	5.414690	0.040316
12	C	-1.054257	4.608173	2.331610
13	H	-0.534421	2.519540	2.614029
14	C	-1.323213	5.637193	1.410439
15	H	-1.494786	6.214891	-0.663692
16	H	-1.090124	4.828589	3.394078
17	H	-1.559525	6.630632	1.778795
18	C	0.536408	-2.260118	-1.487205
19	C	0.981451	-4.121458	-0.378133
20	C	0.708746	-3.088139	0.538416
21	C	1.291584	-5.414690	0.040316
22	C	0.743958	-3.322048	1.915434
23	C	1.323213	-5.637193	1.410439
24	H	1.494786	-6.214891	-0.663692
25	C	1.054257	-4.608173	2.331610
26	H	0.534421	-2.519540	2.614029
27	H	1.559525	-6.630632	1.778795
28	H	1.090124	-4.828589	3.394078
29	C	-0.281628	1.192811	-2.449474
30	C	0.281628	-1.192811	-2.449474
31	N	-0.437566	1.946585	-0.179735
32	N	0.437566	-1.946585	-0.179735
33	Pt	0.000000	0.000000	0.178842
34	H	0.000000	0.000000	-5.611811
35	N	-0.876105	3.563925	-1.641876
36	N	0.876105	-3.563925	-1.641876
37	C	1.069032	-4.292687	-2.887309
38	H	1.580084	-3.634079	-3.594024
39	H	1.763965	-5.109184	-2.672717
40	C	-1.069032	4.292687	-2.887309
41	H	-1.580084	3.634079	-3.594024
42	H	-1.763965	5.109184	-2.672717
43	C	-1.075493	-0.225982	3.114200
44	C	1.075493	0.225982	3.114200
45	C	-0.703866	-0.147904	4.490998
46	C	-2.404254	-0.504980	2.755054
47	C	0.703866	0.147904	4.490998
48	C	-1.664050	-0.349239	5.489067
49	C	-3.336464	-0.700095	3.764803
50	H	-2.686477	-0.564565	1.706287
51	C	-2.975355	-0.624242	5.123180
52	H	-1.387329	-0.291254	6.539523
53	H	-4.368691	-0.916711	3.500891
54	H	-3.730206	-0.782618	5.888316
55	C	2.404254	0.504980	2.755054
56	H	2.686477	0.564565	1.706287
57	C	3.336464	0.700095	3.764803
58	C	1.664050	0.349239	5.489067
59	C	2.975355	0.624242	5.123180
60	H	1.387329	0.291254	6.539523
61	H	3.730206	0.782618	5.888316
62	H	4.368691	0.916711	3.500891
63	N	0.000000	0.000000	2.293011
64	C	0.232562	4.836345	-3.465265
65	H	0.714120	5.475857	-2.715022
66	H	0.922477	4.004370	-3.656927
67	C	0.000000	5.625012	-4.750126
68	H	-0.492769	4.980108	-5.489784
69	H	-0.698337	6.447805	-4.548532
70	C	1.291863	6.180783	-5.335616
71	H	1.101146	6.742335	-6.254976
72	H	1.787235	6.854956	-4.628611
73	H	1.995118	5.375901	-5.575195
74	C	-0.232562	-4.836345	-3.465265
75	H	-0.714120	-5.475857	-2.715022
76	H	-0.922477	-4.004370	-3.656927
77	C	0.000000	-5.625012	-4.750126
78	H	0.698337	-6.447805	-4.548532
79	H	0.492769	-4.980108	-5.489784
80	C	-1.291863	-6.180783	-5.335616
81	H	-1.101146	-6.742335	-6.254976
82	H	-1.787235	-6.854956	-4.628611
83	H	-1.995118	-5.375901	-5.575195

Table S4 Cartesian coordinates of the optimized structure of **4** at the T_1 state

1	C	0.000000	0.000000	-1.752814	55	C	2.405212	0.467442	2.730074
2	C	0.269954	-1.198175	-3.863119	56	H	2.666107	0.517995	1.676960
3	C	0.000000	0.000000	-4.522683	57	C	3.353361	0.651938	3.734510
4	C	-0.269954	1.198175	-3.863119	58	C	1.668553	0.324752	5.474333
5	H	0.450502	-2.095073	-4.443858	59	C	2.992114	0.582051	5.083298
6	H	-0.450502	2.095073	-4.443858	60	H	1.408320	0.274499	6.527346
7	C	-0.530703	2.245078	-1.484203	61	H	3.750603	0.729794	5.845922
8	C	-0.690580	3.104051	0.550930	62	H	4.385741	0.852561	3.466614
9	C	-0.958752	4.134719	-0.378344	63	N	0.000000	0.000000	2.296198
10	C	-0.720307	3.372489	1.921162	64	C	0.235733	4.822311	-3.472700
11	C	-1.251357	5.432460	0.021892	65	H	0.723035	5.466666	-2.729811
12	C	-1.016929	4.674103	2.323605	66	H	0.919920	3.985013	-3.661560
13	H	-0.516588	2.592561	2.645859	67	C	0.000000	5.600786	-4.762815
14	C	-1.277919	5.687752	1.395158	68	H	-0.497345	4.949704	-5.494222
15	H	-1.447023	6.221615	-0.697268	69	H	-0.696723	6.426501	-4.566289
16	H	-1.043716	4.905252	3.384603	70	C	1.289177	6.149759	-5.360771
17	H	-1.502230	6.691047	1.744086	71	H	1.095652	6.703386	-6.284564
18	C	0.530703	-2.245078	-1.484203	72	H	1.789590	6.829434	-4.662416
19	C	0.958752	-4.134719	-0.378344	73	H	1.990150	5.341543	-5.596118
20	C	0.690580	-3.104051	0.550930	74	C	-0.235733	-4.822311	-3.472700
21	C	1.251357	-5.432460	0.021892	75	H	-0.723035	-5.466666	-2.729811
22	C	0.720307	-3.372489	1.921162	76	H	-0.919920	-3.985013	-3.661560
23	C	1.277919	-5.687752	1.395158	77	C	0.000000	-5.600786	-4.762815
24	H	1.447023	-6.221615	-0.697268	78	H	0.696723	-6.426501	-4.566289
25	C	1.016929	-4.674103	2.323605	79	H	0.497345	-4.949704	-5.494222
26	H	0.516588	-2.592561	2.645859	80	C	-1.289177	-6.149759	-5.360771
27	H	1.502230	-6.691047	1.744086	81	H	-1.095652	-6.703386	-6.284564
28	H	1.043716	-4.905252	3.384603	82	H	-1.789590	-6.829434	-4.662416
29	C	-0.283651	1.201617	-2.428232	83	H	-1.990150	-5.341543	-5.596118
30	C	0.283651	-1.201617	-2.428232					
31	N	-0.432130	1.956028	-0.152841					
32	N	0.432130	-1.956028	-0.152841					
33	Pt	0.000000	0.000000	0.204441					
34	H	0.000000	0.000000	-5.610585					
35	N	-0.867360	3.562072	-1.637701					
36	N	0.867360	-3.562072	-1.637701					
37	C	1.062659	-4.281259	-2.883066					
38	H	1.569610	-3.617245	-3.587761					
39	H	1.758036	-5.100813	-2.676662					
40	C	-1.062659	4.281259	-2.883066					
41	H	-1.569610	3.617245	-3.587761					
42	H	-1.758036	5.100813	-2.676662					
43	C	-1.088169	-0.211405	3.119865					
44	C	1.088169	0.211405	3.119865					
45	C	-0.715977	-0.139245	4.489226					
46	C	-2.405212	-0.467442	2.730074					
47	C	0.715977	0.139245	4.489226					
48	C	-1.668553	-0.324752	5.474333					
49	C	-3.353361	-0.651938	3.734510					
50	H	-2.666107	-0.517995	1.676960					
51	C	-2.992114	-0.582051	5.083298					
52	H	-1.408320	-0.274499	6.527346					
53	H	-4.385741	-0.852561	3.466614					
54	H	-3.750603	-0.729794	5.845922					

Table S5 Cartesian coordinates of the optimized structure of **5** at the S_0 state

1	C	-2.701405	0.000001	0.000000	55	C	2.851900	1.139013	-3.207247
2	C	-4.792192	-1.178032	-0.320965	56	C	4.548251	0.570319	-1.597711
3	C	-5.469087	0.000003	0.000000	57	C	4.219724	1.025881	-2.877039
4	C	-4.792190	1.178037	0.320964	58	H	5.592230	0.469540	-1.306688
5	H	-5.373335	-2.064364	-0.550702	59	H	2.569290	1.489354	-4.194828
6	H	-5.373332	2.064371	0.550701	60	N	1.350227	-0.000001	0.000000
7	C	-2.429942	2.233781	0.637963	61	C	-4.399729	4.829491	-0.045359
8	C	-0.404481	3.049106	0.863979	62	H	-3.646368	5.485315	-0.499305
9	C	-1.321480	4.071057	1.175361	63	H	-4.583850	4.020051	-0.763557
10	C	0.972648	3.277021	0.924423	64	C	-5.688063	5.608235	0.200721
11	C	-0.903106	5.347946	1.547245	65	H	-6.430890	4.946812	0.666069
12	C	1.388619	4.546575	1.296930	66	H	-5.494353	6.408889	0.926459
13	H	1.671058	2.482579	0.685509	67	C	-6.262995	6.203460	-1.078289
14	C	0.467127	5.565100	1.602282	68	H	-7.185071	6.757314	-0.878401
15	H	-1.607136	6.140156	1.779481	69	H	-5.552814	6.893918	-1.545913
16	H	2.451183	4.762078	1.353952	70	H	-6.494748	5.420647	-1.808564
17	H	0.835307	6.545964	1.886569	71	C	-4.399734	-4.829485	0.045362
18	C	-2.429945	-2.233778	-0.637964	72	H	-3.646374	-5.485310	0.499309
19	C	-1.321486	-4.071056	-1.175362	73	H	-4.583853	-4.020045	0.763560
20	C	-0.404486	-3.049107	-0.863982	74	C	-5.688070	-5.608228	-0.200715
21	C	-0.903115	-5.347947	-1.547246	75	H	-5.494362	-6.408884	-0.926452
22	C	0.972643	-3.277024	-0.924428	76	H	-6.430896	-4.946806	-0.666063
23	C	0.467119	-5.565101	-1.602284	77	C	-6.263001	-6.203452	1.078296
24	H	-1.607145	-6.140156	-1.779481	78	H	-7.185078	-6.757304	0.878410
25	C	1.388613	-4.546578	-1.296934	79	H	-5.552819	-6.893910	1.545920
26	H	1.671054	-2.482582	-0.685513	80	H	-6.494752	-5.420637	1.808570
27	H	0.835297	-6.545966	-1.886572	81	C	3.549643	0.240608	-0.679029
28	H	2.451176	-4.762083	-1.353957	82	C	5.336659	1.382576	-3.865630
29	C	-3.391836	1.179454	0.332839	83	C	4.792129	1.865095	-5.213327
30	C	-3.391838	-1.179450	-0.332840	84	H	4.180965	2.767602	-5.105722
31	N	-1.122279	1.923008	0.533822	85	H	5.626132	2.107050	-5.880706
32	N	-1.122281	-1.923008	-0.533825	86	H	4.185563	1.097469	-5.705683
33	Pt	-0.762938	0.000000	-0.000001	87	C	6.213412	0.145625	-4.122511
34	H	-6.554271	0.000004	0.000000	88	H	7.022879	0.386996	-4.821583
35	N	-2.585289	3.521430	1.034546	89	H	6.668860	-0.225188	-3.199024
36	N	-2.585294	-3.521428	-1.034546	90	H	5.621467	-0.668096	-4.555160
37	C	-3.831628	-4.244555	-1.242690	91	C	6.209160	2.503645	-3.276877
38	H	-4.542322	-3.570634	-1.727735	92	H	7.019387	2.763164	-3.968536
39	H	-3.621486	-5.038284	-1.964740	93	H	5.614530	3.405506	-3.095812
40	C	-3.831622	4.244557	1.242693	94	H	6.663438	2.205155	-2.327021
41	H	-4.542316	3.570637	1.727737	95	C	5.336658	-1.382579	3.865630
42	H	-3.621478	5.038286	1.964742	96	C	6.209157	-2.503649	3.276879
43	C	2.173948	-0.365038	1.035710	97	H	6.663437	-2.205161	2.327023
44	C	2.173948	0.365035	-1.035710	98	H	7.019384	-2.763169	3.968538
45	C	3.549644	-0.240611	0.679029	99	H	5.614527	-3.405510	3.095814
46	C	1.834013	-0.818536	2.316553	100	C	4.792127	-1.865097	5.213328
47	C	4.548251	-0.570323	1.597711	101	H	5.626129	-2.107053	5.880707
48	C	2.851898	-1.139016	3.207247	102	H	4.185562	-1.097470	5.705684
49	H	0.790033	-0.917389	2.605893	103	H	4.180961	-2.767603	5.105724
50	C	4.219723	-1.025884	2.877039	104	C	6.213412	-0.145629	4.122512
51	H	5.592230	-0.469544	1.306689	105	H	5.621468	0.668093	4.555159
52	H	2.569288	-1.489356	4.194829	106	H	7.022878	-0.387000	4.821584
53	C	1.834014	0.818533	-2.316553	107	H	6.668861	0.225183	3.199024
54	H	0.790033	0.917388	-2.605894					

Table S6 Cartesian coordinates of the optimized structure of **5** at the T_1 state

1	C	-2.687656	0.000001	0.000000	55	C	2.831498	1.087214	-3.231843
2	C	-4.798242	-1.189882	-0.304738	56	C	4.546467	0.545700	-1.605436
3	C	-5.457804	0.000003	0.000002	57	C	4.192793	0.984894	-2.903165
4	C	-4.798240	1.189887	0.304742	58	H	5.592906	0.457249	-1.327802
5	H	-5.379085	-2.081276	-0.510687	59	H	2.543366	1.420267	-4.221940
6	H	-5.379082	2.081281	0.510692	60	N	1.368584	-0.000001	0.000000
7	C	-2.419347	2.226076	0.606380	61	C	-4.409685	4.834031	-0.050147
8	C	-0.385040	3.075189	0.816864	62	H	-3.667775	5.501304	-0.507162
9	C	-1.315133	4.094554	1.123093	63	H	-4.595715	4.027799	-0.771422
10	C	0.985416	3.338484	0.875041	64	C	-5.701950	5.598083	0.218709
11	C	-0.915762	5.376940	1.477988	65	H	-6.432385	4.923411	0.685092
12	C	1.386918	4.624389	1.234765	66	H	-5.508291	6.391864	0.952370
13	H	1.710403	2.565720	0.646739	67	C	-6.299732	6.203450	-1.045037
14	C	0.457647	5.627724	1.530440	68	H	-7.225152	6.745475	-0.827850
15	H	-1.635567	6.157789	1.702500	69	H	-5.602485	6.906795	-1.513254
16	H	2.448031	4.851264	1.284879	70	H	-6.532201	5.427221	-1.782181
17	H	0.806003	6.619055	1.803618	71	C	-4.409690	-4.834027	0.050148
18	C	-2.419351	-2.226073	-0.606381	72	H	-3.667780	-5.501300	0.507163
19	C	-1.315139	-4.094552	-1.123096	73	H	-4.595719	-4.027795	0.771424
20	C	-0.385045	-3.075189	-0.816868	74	C	-5.701957	-5.598077	-0.218705
21	C	-0.915770	-5.376939	-1.477992	75	H	-5.508299	-6.391858	-0.952367
22	C	0.985411	-3.338485	-0.875048	76	H	-6.432392	-4.923404	-0.685087
23	C	0.457639	-5.627724	-1.530447	77	C	-6.299737	-6.203444	1.045041
24	H	-1.635576	-6.157787	-1.702503	78	H	-7.225158	-6.745468	0.827855
25	C	1.386911	-4.624390	-1.234772	79	H	-5.602490	-6.906791	1.513256
26	H	1.710399	-2.565722	-0.646746	80	H	-6.532204	-5.427216	1.782186
27	H	0.805994	-6.619055	-1.803625	81	C	3.562463	0.232249	-0.691945
28	H	2.448023	-4.851266	-1.284888	82	C	5.302416	1.333050	-3.894507
29	C	-3.363325	1.192586	0.320065	83	C	4.754869	1.792031	-5.248406
30	C	-3.363326	-1.192583	-0.320064	84	H	4.141187	2.694120	-5.155708
31	N	-1.087555	1.941178	0.500173	85	H	5.590035	2.027740	-5.915249
32	N	-1.087558	-1.941177	-0.500176	86	H	4.155714	1.013300	-5.731640
33	Pt	-0.732541	0.000000	-0.000002	87	C	6.182990	0.092210	-4.124293
34	H	-6.545741	0.000003	0.000003	88	H	6.986793	0.332212	-4.828665
35	N	-2.574218	3.527994	0.997771	89	H	6.646579	-0.259378	-3.197700
36	N	-2.574223	-3.527992	-0.997772	90	H	5.596608	-0.731577	-4.543972
37	C	-3.820334	-4.236721	-1.223430	91	C	6.161823	2.468375	-3.310800
38	H	-4.524929	-3.550178	-1.699678	92	H	6.965700	2.723232	-4.009860
39	H	-3.615543	-5.024977	-1.954589	93	H	5.560025	3.367056	-3.140998
40	C	-3.820328	4.236725	1.223431	94	H	6.624438	2.185874	-2.360414
41	H	-4.524922	3.550183	1.699680	95	C	5.302410	-1.333055	3.894513
42	H	-3.615534	5.024981	1.954589	96	C	6.161815	-2.468382	3.310808
43	C	2.192001	-0.348685	1.049046	97	H	6.624432	-2.185882	2.360422
44	C	2.192003	0.348681	-1.049045	98	H	6.965692	-2.723239	4.009869
45	C	3.562462	-0.232253	0.691948	99	H	5.560017	-3.367062	3.141005
46	C	1.821261	-0.775326	2.324134	100	C	4.754860	-1.792035	5.248411
47	C	4.546464	-0.545705	1.605440	101	H	5.590025	-2.027744	5.915255
48	C	2.831493	-1.087217	3.231845	102	H	4.155705	-1.013302	5.731644
49	H	0.772361	-0.860842	2.593130	103	H	4.141177	-2.694123	5.155713
50	C	4.192788	-0.984898	2.903169	104	C	6.182984	-0.092216	4.124299
51	H	5.592904	-0.457255	1.327808	105	H	5.596603	0.731572	4.543977
52	H	2.543359	-1.420270	4.221941	106	H	6.986787	-0.332218	4.828672
53	C	1.821265	0.775324	-2.324133	107	H	6.646575	0.259371	3.197706
54	H	0.772365	0.860840	-2.593131					

Table S7 Cartesian coordinates of the optimized structure of **6** at the S_0 state

1	C	0.000000	0.000000	4.640224	55	C	-0.000276	-3.407519	-0.874001
2	C	1.220595	0.001721	6.730369	56	C	-0.000320	-1.691337	-2.611692
3	C	0.000000	0.000000	7.407338	57	C	-0.000429	-3.046548	-2.248096
4	C	-1.220595	-0.001721	6.730369	58	H	-0.000425	-1.417654	-3.663106
5	H	2.135975	0.013169	7.311462	59	H	-0.000360	-4.462185	-0.615544
6	H	-2.135975	-0.013169	7.311462	60	N	0.000000	0.000000	0.579722
7	C	-2.323333	0.017109	4.369396	61	C	-4.625111	-1.357953	6.340811
8	C	-3.171974	0.005003	2.345132	62	H	-5.123600	-1.977392	5.584863
9	C	-4.238551	0.025050	3.264092	63	H	-3.648034	-1.820895	6.530219
10	C	-3.413386	-0.006313	0.968956	64	C	-5.448722	-1.339795	7.624632
11	C	-5.569658	0.028588	2.849572	65	H	-4.949397	-0.706341	8.369717
12	C	-4.737374	-0.000587	0.556276	66	H	-6.420162	-0.869056	7.424863
13	H	-2.589528	-0.019770	0.264629	67	C	-5.662937	-2.734227	8.199437
14	C	-5.798034	0.016057	1.480322	68	H	-6.255841	-2.697509	9.118133
15	H	-6.393083	0.035848	3.556045	69	H	-6.189853	-3.377902	7.486844
16	H	-4.962552	-0.010261	-0.505699	70	H	-4.707537	-3.214392	8.437041
17	H	-6.820217	0.017075	1.115025	71	C	4.625111	1.357953	6.340811
18	C	2.323333	-0.017109	4.369396	72	H	5.123600	1.977392	5.584863
19	C	4.238551	-0.025050	3.264092	73	H	3.648034	1.820895	6.530219
20	C	3.171974	-0.005003	2.345132	74	C	5.448722	1.339795	7.624632
21	C	5.569658	-0.028588	2.849572	75	H	6.420162	0.869056	7.424863
22	C	3.413386	0.006313	0.968956	76	H	4.949397	0.706341	8.369717
23	C	5.798034	-0.016057	1.480322	77	C	5.662937	2.734227	8.199437
24	H	6.393083	-0.035848	3.556045	78	H	6.255841	2.697509	9.118133
25	C	4.737374	0.000587	0.556276	79	H	6.189853	3.377902	7.486844
26	H	2.589528	0.019770	0.264629	80	H	4.707537	3.214392	8.437041
27	H	6.820217	-0.017075	1.115025	81	C	-0.000381	-4.056458	-3.245051
28	H	4.962552	0.010261	-0.505699	82	C	-0.000060	-0.720384	-1.616303
29	C	-1.225232	0.007751	5.330019	83	C	0.000000	-4.924466	-4.100098
30	C	1.225232	-0.007751	5.330019	84	C	0.000381	4.056458	-3.245051
31	N	-1.996876	0.001118	3.061380	85	C	0.000000	4.924466	-4.100098
32	N	1.996876	-0.001118	3.061380	86	C	0.002166	-5.934887	-5.097127
33	Pt	0.000000	0.000000	2.702986	87	C	0.003187	-7.295798	-4.738489
34	H	0.000000	0.000000	8.492463	88	C	-0.000458	-5.593893	-6.462571
35	N	-3.669454	0.044019	4.526837	89	C	0.005094	-8.280695	-5.714364
36	N	3.669454	-0.044019	4.526837	90	H	-0.000036	-7.569275	-3.688518
37	C	4.421330	-0.042477	5.773895	91	C	0.001420	-6.582408	-7.434770
38	H	3.908918	-0.695549	6.484682	92	H	-0.006515	-4.547564	-6.749592
39	H	5.384397	-0.515564	5.564051	93	C	0.003822	-7.927397	-7.064051
40	C	-4.421330	0.042477	5.773895	94	H	-0.000048	-9.327320	-5.427777
41	H	-3.908918	0.695549	6.484682	95	H	-0.006612	-6.309330	-8.484981
42	H	-5.384397	0.515564	5.564051	96	C	-0.002166	5.934887	-5.097127
43	C	-0.000096	1.096881	-0.238011	97	C	-0.003187	7.295798	-4.738489
44	C	0.000096	-1.096881	-0.238011	98	C	0.000458	5.593893	-6.462571
45	C	0.000060	0.720384	-1.616303	99	C	-0.005094	8.280695	-5.714364
46	C	0.000043	2.454166	0.125573	100	H	0.000036	7.569275	-3.688518
47	C	0.000320	1.691337	-2.611692	101	C	-0.001420	6.582408	-7.434770
48	C	0.000276	3.407519	-0.874001	102	H	0.006515	4.547564	-6.749592
49	H	0.000029	2.740233	1.174145	103	C	-0.003822	7.927397	-7.064051
50	C	0.000429	3.046548	-2.248096	104	H	0.000048	9.327320	-5.427777
51	H	0.000425	1.417654	-3.663106	105	H	0.006612	6.309330	-8.484981
52	H	0.000360	4.462185	-0.615544	106	C	0.063573	-8.991898	-8.114993
53	C	-0.000043	-2.454166	0.125573	107	C	-0.063573	8.991898	-8.114993
54	H	-0.000029	-2.740233	1.174145	108	F	1.334117	-9.311406	-8.432763

109	F	-0.532628	-8.607148	-9.256414
110	F	-0.529726	-10.129394	-7.714339
111	F	0.529726	10.129394	-7.714339
112	F	-1.334117	9.311406	-8.432763
113	F	0.532628	8.607148	-9.256414

Table S8 Cartesian coordinates of the optimized structure of **6** at the T_1 state

1	C	-4.625978	0.000065	-0.000020	55	C	0.858439	3.410857	-0.144266
2	C	-6.736148	0.003672	-1.228175	56	C	2.611642	1.689201	-0.073025
3	C	-7.395751	0.000061	-0.000049	57	C	2.227024	3.053404	-0.130096
4	C	-6.736174	-0.003548	1.228091	58	H	3.665478	1.430561	-0.063383
5	H	-7.317085	-0.011783	-2.142736	59	H	0.594583	4.461940	-0.188308
6	H	-7.317129	0.011904	2.142640	60	N	-0.564127	0.000041	0.000019
7	C	-4.357537	-0.024756	2.307121	61	C	-6.340391	1.327069	4.623807
8	C	-2.323263	0.006013	3.181202	62	H	-5.594612	1.949472	5.134628
9	C	-3.253255	-0.019486	4.245393	63	H	-6.524315	1.792482	3.646890
10	C	-0.953059	0.032499	3.450879	64	C	-7.632510	1.292483	5.433219
11	C	-2.853834	-0.013078	5.575945	65	H	-8.366771	0.658383	4.918440
12	C	-0.551441	0.035379	4.786065	66	H	-7.441166	0.812462	6.402122
13	H	-0.227711	0.052200	2.645829	67	C	-8.222265	2.679378	5.656164
14	C	-1.480665	0.013180	5.831775	68	H	-9.147726	2.629896	6.237898
15	H	-3.573399	-0.022644	6.388568	69	H	-7.521095	3.323645	6.197783
16	H	0.509494	0.057303	5.018024	70	H	-8.452385	3.167841	4.703053
17	H	-1.132480	0.019726	6.860064	71	C	-6.340283	-1.326947	-4.623889
18	C	-4.357490	0.024889	-2.307156	72	H	-5.594482	-1.949344	-5.134685
19	C	-3.253169	0.019622	-4.245406	73	H	-6.524234	-1.792361	-3.646977
20	C	-2.323198	-0.005877	-3.181197	74	C	-7.632376	-1.292373	-5.433344
21	C	-2.853722	0.013216	-5.575950	75	H	-7.441002	-0.812356	-6.402243
22	C	-0.952989	-0.032363	-3.450847	76	H	-8.366657	-0.658274	-4.918593
23	C	-1.480548	-0.013043	-5.831753	77	C	-8.222114	-2.679272	-5.656301
24	H	-3.573271	0.022781	-6.388587	78	H	-9.147556	-2.629799	-6.238067
25	C	-0.551345	-0.035242	-4.786025	79	H	-7.520922	-3.323539	-6.197892
26	H	-0.227656	-0.052065	-2.645783	80	H	-8.452264	-3.167732	-4.703195
27	H	-1.132343	-0.019588	-6.860035	81	C	3.220158	4.057472	-0.171988
28	H	0.509595	-0.057166	-5.017964	82	C	1.627136	0.728499	-0.031081
29	C	-5.301382	-0.013987	1.234669	83	C	4.079916	4.920177	-0.206763
30	C	-5.301357	0.014117	-1.234724	84	C	3.220035	-4.057504	0.172052
31	N	-3.025909	0.000706	2.003796	85	C	4.079763	-4.920238	0.206833
32	N	-3.025868	-0.000572	-2.003804	86	C	5.078030	5.927524	-0.248368
33	Pt	-2.671426	0.000070	0.000000	87	C	4.715201	7.285924	-0.287858
34	H	-8.483645	0.000059	-0.000060	88	C	6.440653	5.578793	-0.246388
35	N	-4.512301	-0.055120	3.666070	89	C	5.692625	8.268269	-0.327180
36	N	-4.512227	0.055256	-3.666108	90	H	3.665278	7.558633	-0.284587
37	C	-5.758614	0.066686	-4.409591	91	C	7.413498	6.565676	-0.286097
38	H	-6.466595	0.713566	-3.885330	92	H	6.724169	4.532320	-0.211168
39	H	-5.556126	0.547481	-5.371610	93	C	7.040646	7.909304	-0.326291
40	C	-5.758704	-0.066559	4.409526	94	H	5.409411	9.315229	-0.351100
41	H	-6.466668	-0.713448	3.885252	95	H	8.463634	6.293529	-0.278337
42	H	-5.556233	-0.547349	5.371551	96	C	5.077819	-5.927644	0.248420
43	C	0.253076	-1.102638	0.046528	97	C	4.714907	-7.286025	0.287929
44	C	0.253110	1.102694	-0.046486	98	C	6.440459	-5.578997	0.246406
45	C	1.627114	-0.728483	0.031126	99	C	5.692271	-8.268424	0.327237
46	C	-0.134858	-2.446800	0.103288	100	H	3.664967	-7.558669	0.284684
47	C	2.611591	-1.689215	0.073075	101	C	7.413251	-6.565940	0.286104
48	C	0.858335	-3.410818	0.144317	102	H	6.724038	-4.532542	0.211172
49	H	-1.187582	-2.713605	0.114504	103	C	7.040320	-7.909539	0.326317
50	C	2.226931	-3.053407	0.130150	104	H	5.408992	-9.315368	0.351164
51	H	3.665434	-1.430608	0.063436	105	H	8.463402	-6.293858	0.278328
52	H	0.594447	-4.461893	0.188362	106	C	8.094443	8.972001	-0.424642
53	C	-0.134784	2.446869	-0.103243	107	C	8.093995	-8.972358	0.424657
54	H	-1.187500	2.713706	-0.114461	108	F	8.398665	9.248889	-1.706571

109	F	9.237375	8.601056	0.174548
110	F	7.697659	10.124600	0.138257
111	F	7.697429	-10.124602	-0.139135
112	F	8.397439	-9.250029	1.706601
113	F	9.237298	-8.601171	-0.173662

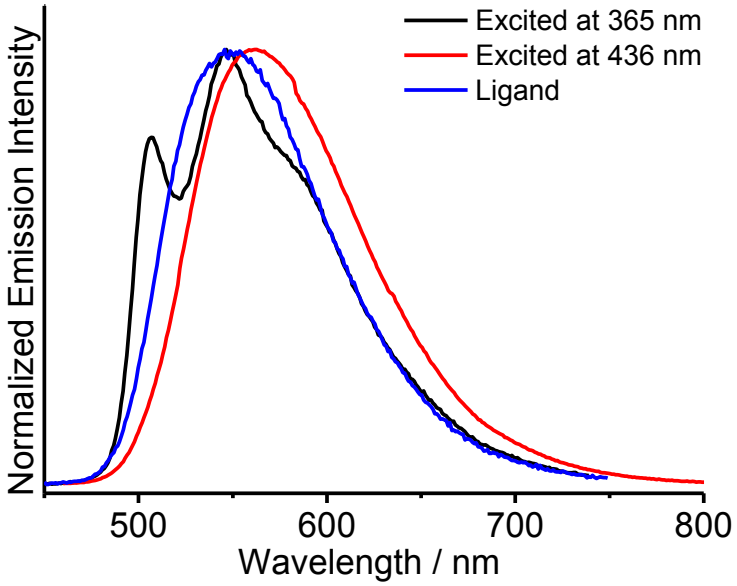

Figure S1 Normalized emission spectra of complex **1** with different excitation wavelengths and its corresponding free alkynyl ligand in degassed CH_2Cl_2 at 298 K

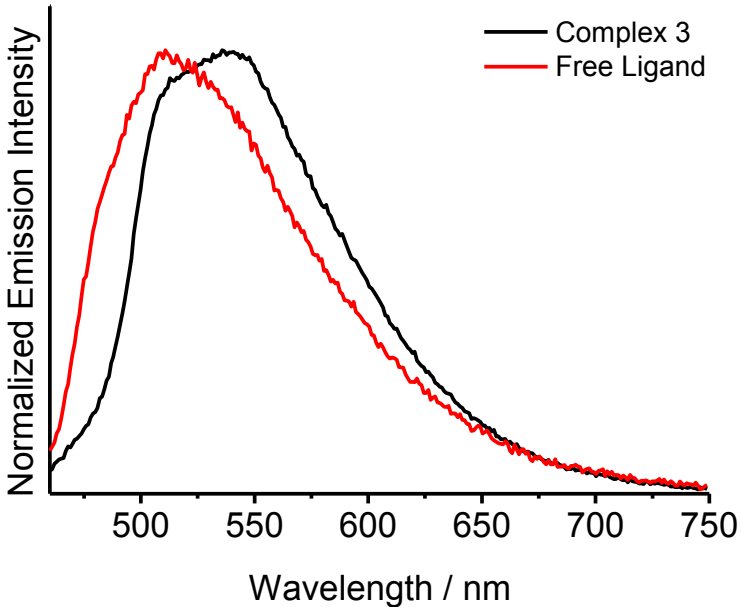

Figure S2 Normalized emission spectra of complex **3** and its corresponding free alkynyl ligand upon excitation at 436 nm in degassed CH_2Cl_2 at 298 K

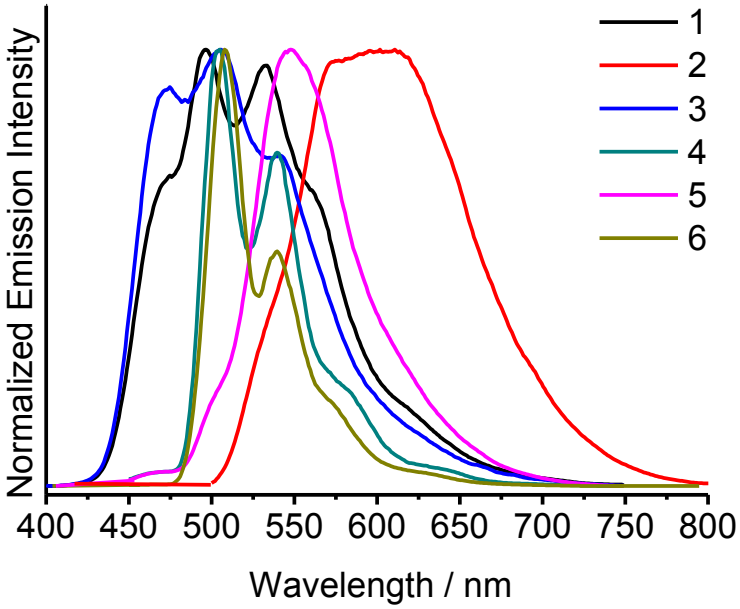

Figure S3 Normalized emission spectra of complexes **1**–**6** upon excitation at 400 nm in butyronitrile glass at 77 K

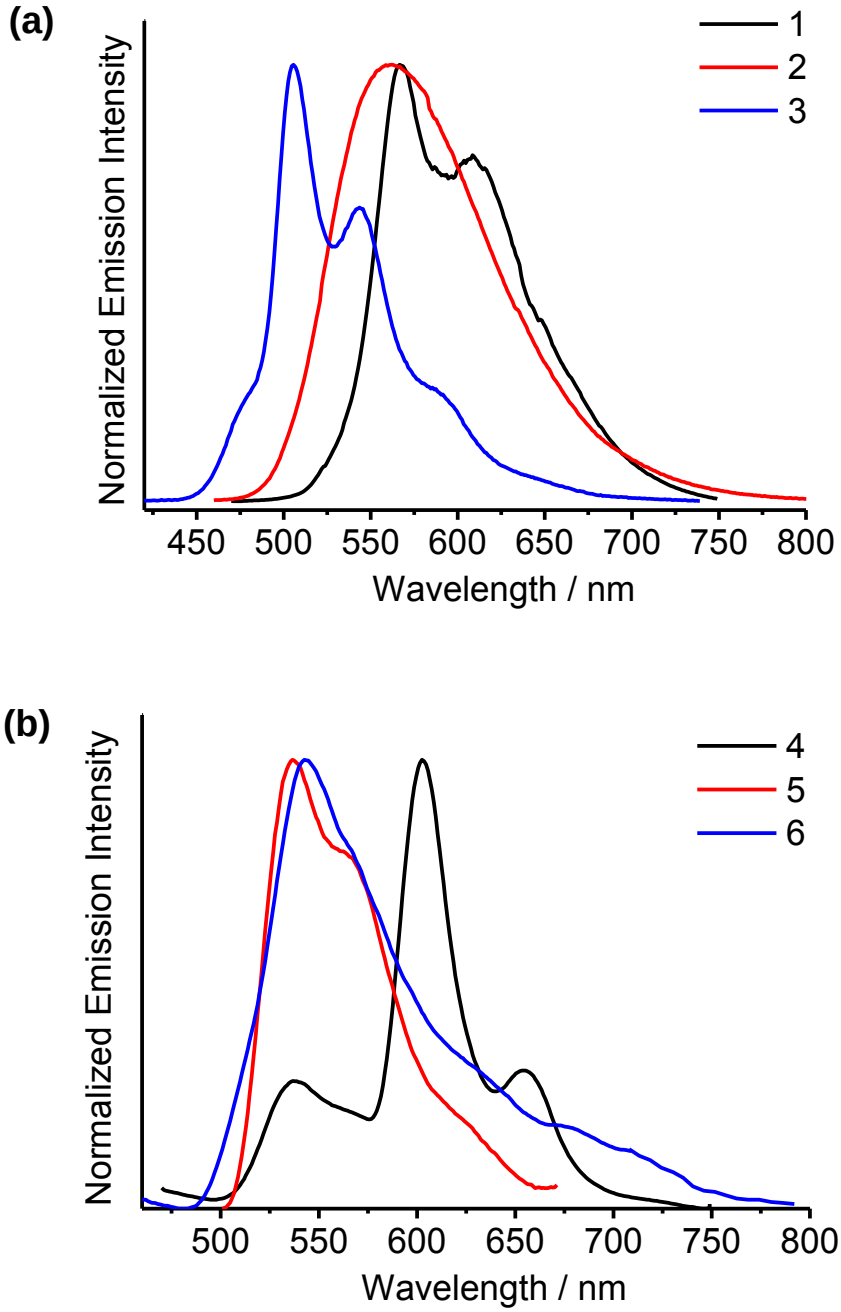

Figure S4 Normalized emission spectra of (a) **1**–**3** and **4**–**6** upon excitation at 400 nm in solid state at 77 K

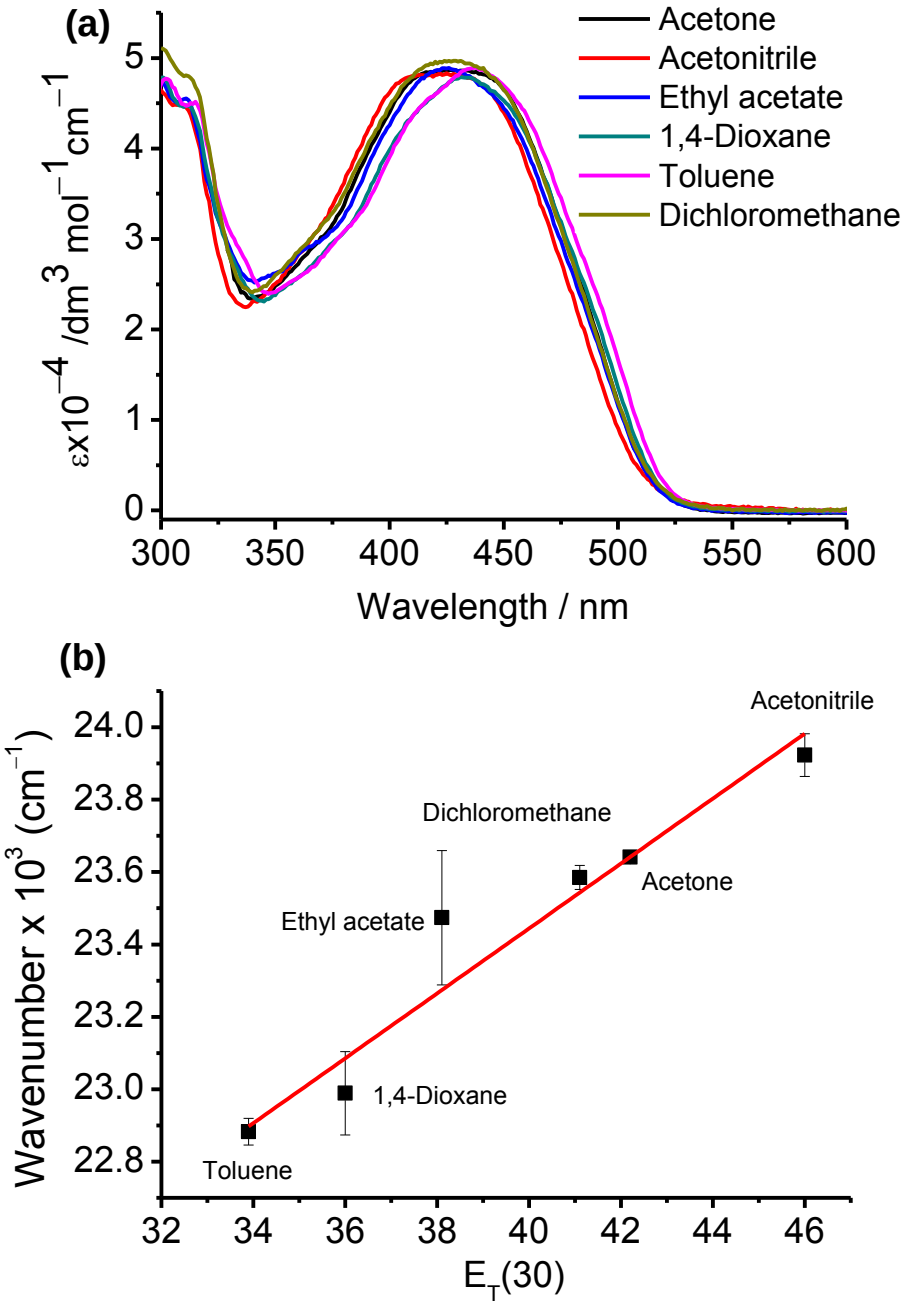

Figure S5 (a) Electronic absorption spectra of **1** in acetone (——) , acetonitrile (——), ethyl acetate (——), 1,4-dioxane (——), toluene (——) and dichloromethane (——) at 298 K at a concentration of 5 × 10^{-5} M. (b) Plot of absorption maximum as a function of empirical parameters of solvent polarity $E_T(30)$.

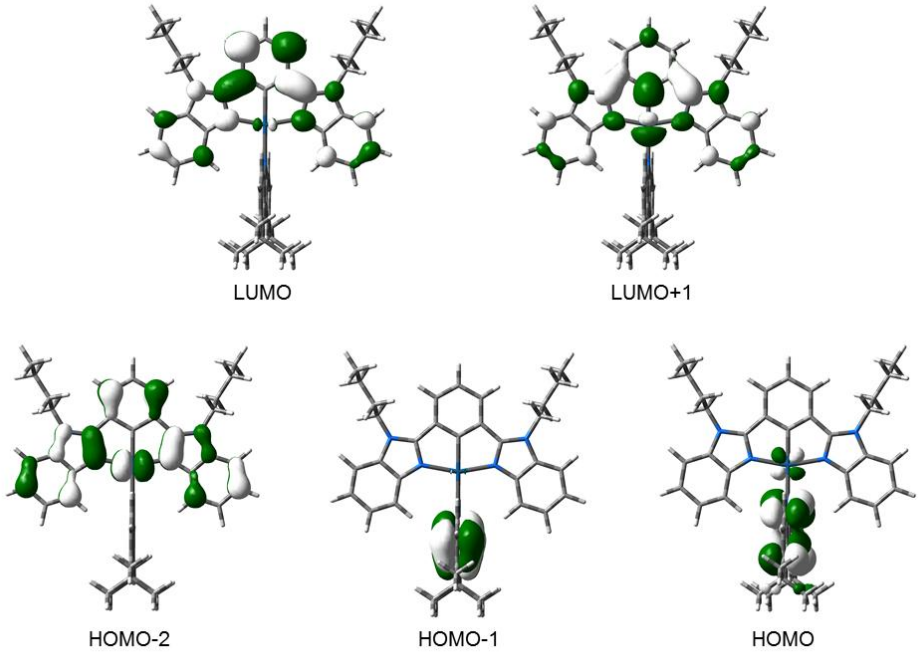

Figure S6 Spatial plots (isovalue = 0.03) of selected molecular orbitals of complex **5**

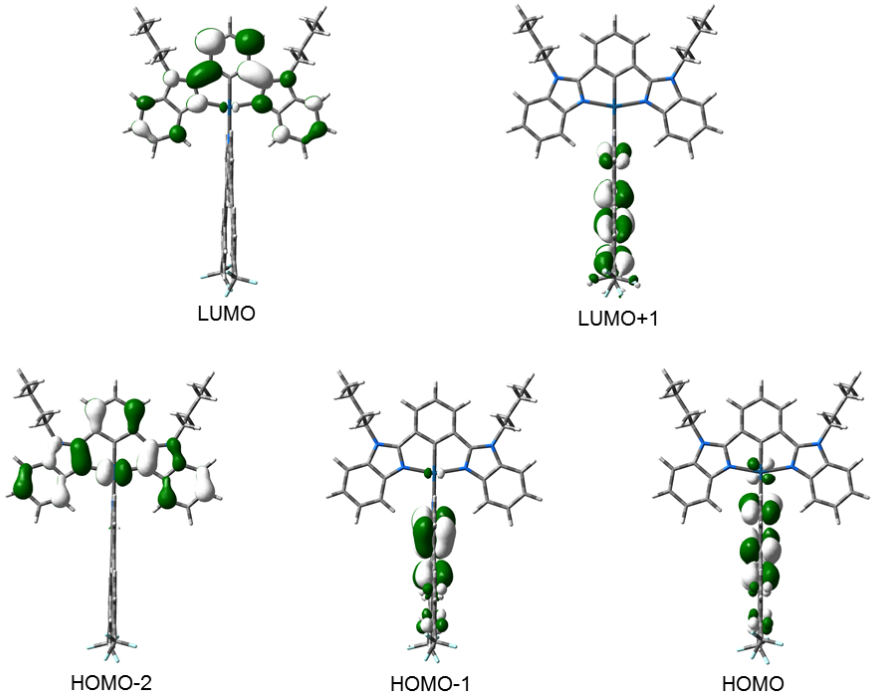

Figure S7 Spatial plots (isovalue = 0.03) of selected molecular orbitals of complex **6**