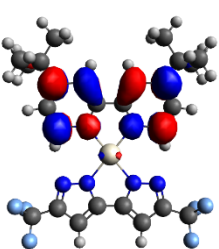
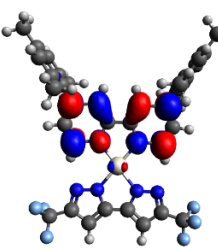
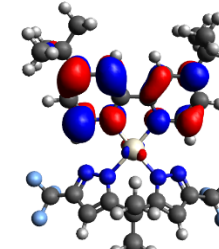
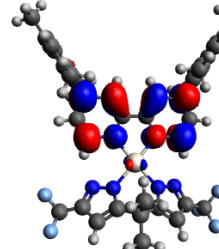
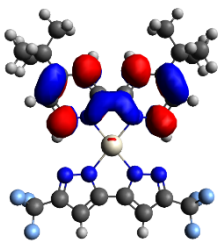
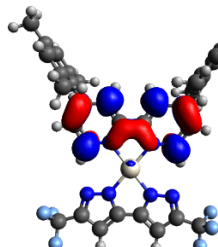
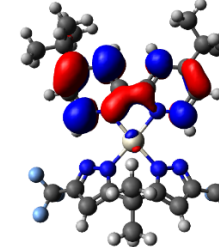
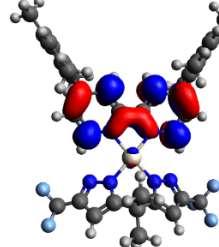
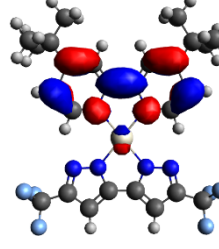
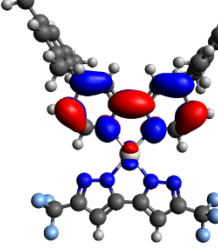
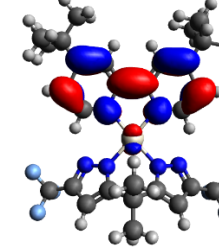
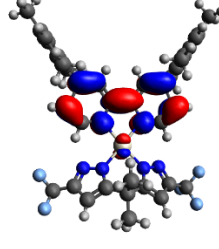
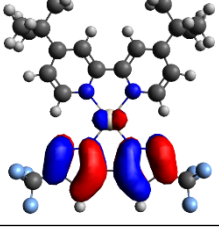
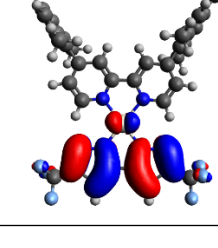
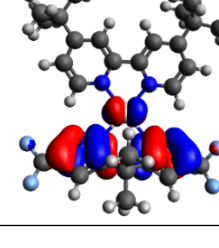
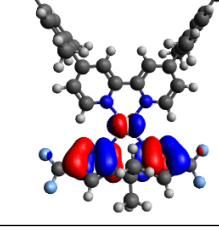


Efficient Pt(II) Emitters Assembled from Neutral Bipyridine and Dianionic Bipyrazolate:
Designs, Photophysical Characterizations and Fabrication of Non-doped OLEDs

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Robertson,^{c,*} Gene-Hsiang Lee,^d Xiao Wei Sun,^{b,*} and Yun Chi^{a,*}

Supplementary Information

Table S1 Molecular orbital distributions and energy (isodensity=0.030 a.u.).

	1	2	3	4
LUMO+ 2				
LUMO+ 1				
LUMO				
HOMO				

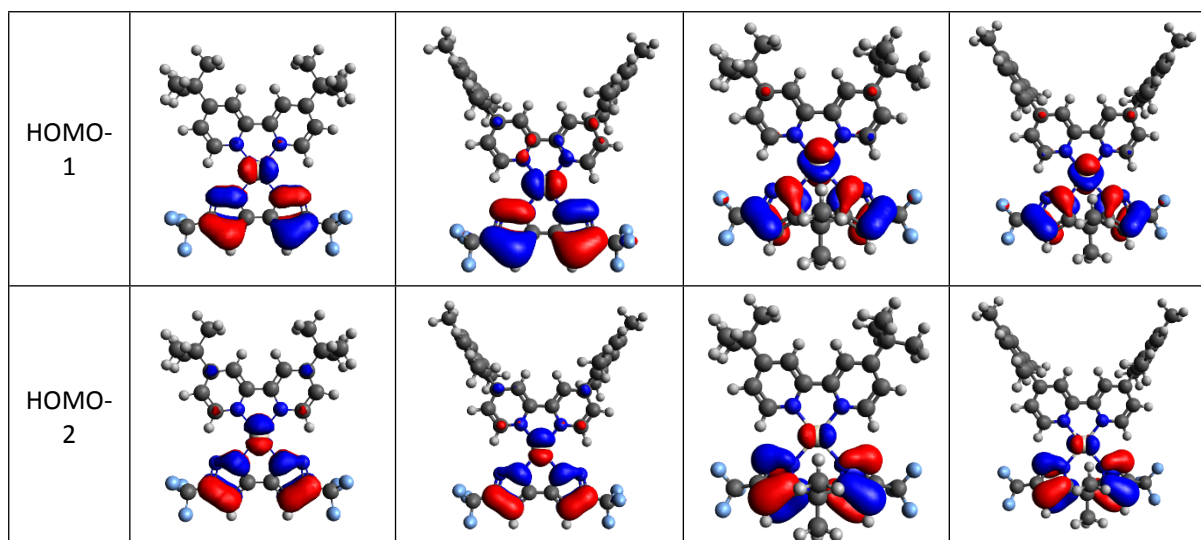


Table S2 Molecular orbital distributions and energy (isodensity=0.030 a.u.).

	1		2		3		4	
	vacuum	In DCM	vacuum	In DCM	vacuum	In DCM	vacuum	In DCM
LUMO+2	-2.08eV	-1.21 eV	-1.74eV	-1.39 eV	-1.49eV	-1.17 eV	-1.77eV	-1.34 eV
LUMO+1	-2.24 eV	-1.40 eV	-1.88 eV	-1.57 eV	-1.75 eV	-1.38 eV	-1.82 eV	-1.53 eV
LUMO	-2.80 eV	-2.51eV	-2.84 eV	-2.58eV	-2.76 eV	-2.39eV	-2.76 eV	-2.52eV
HOMO	-5.10 eV	-5.70 eV	-5.18 eV	-5.73 eV	-5.64 eV	-6.19 eV	-5.47 eV	-6.19 eV
HOMO-1	-5.91 eV	-6.30 eV	-5.86 eV	-6.33 eV	-5.82 eV	-6.24 eV	-5.70 eV	-6.26 eV
HOMO-2	-6.01 eV	-6.32 eV	-5.99 eV	-6.36 eV	-5.95 eV	-6.36 eV	-5.86 eV	-6.34 eV

Table S3. Contributions from component parts of **1** to selected molecular orbitals

	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1
Pt	44.79	37.02	8.12	4.27	1.93
bipyridine	8.56	4.86	0.74	93.72	95.06
bispyrazole	46.6	58.08	91.12	2	3

Table S4. Contributions from component parts of **2** to selected molecular orbitals

	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1
Pt	43.29	36.23	7.82	4.36	1.87
bipyridine	10.28	4.92	0.72	93.64	95.82
bispyrazole	46.44	58.77	91.47	1.97	2.3

Table S5. Contributions from component parts of **3** to selected molecular orbitals

	HOMO-3	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1
Pt	24.86	13.02	41.97	29.69	4.15	2.25
bipyridine	1.32	3.28	7.15	3.7	94.54	96.4
bispyrazole	73.82	83.64	50.87	66.61	1.29	1.32

Table S6. Contributions from component parts of **4** to selected molecular orbitals

	HOMO-3	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1
Pt	22.56	13.63	40.79	28.02	4.28	2.28
bipyridine	2.23	4.46	8.05	3.68	94.37	96.47
bispyrazole	75.21	81.9	51.17	68.25	1.31	1.23

Table S7 The wavelengths, oscillator strengths and major contributions of the singlet optical transitions in lowest 70 states for **1** in DCM.

No.	Wavelength (nm)	Osc. Strength	Major contri
1	479.48	0.0008	HOMO->LUMO (97%)
2	392.51	0.0084	H-1->LUMO (95%)
3	382.22	0.1989	H-2->LUMO (98%)
4	371.21	0.0041	H-3->LUMO (99%)
5	332.28	0.0001	HOMO->L+1 (98%)
6	315.99	0.0035	H-1->L+3 (12%), HOMO->L+2 (23%), HOMO->L+3 (62%)
7	315.78	0.0095	HOMO->L+2 (75%), HOMO->L+3 (19%)
8	300.65	0.1568	H-4->LUMO (72%), H-1->L+1 (13%)
9	289.32	0.0062	H-5->LUMO (11%), H-3->L+3 (68%), H-1->L+1 (13%)
10	286.55	0.0481	H-2->L+1 (95%)
11	285.44	0.0883	H-4->LUMO (11%), H-3->L+3 (12%), H-2->L+2 (11%), H-2->L+3 (12%), H-1->L+1 (51%)
12	285.26	0.0145	H-2->L+3 (81%)
13	280.37	0.0104	H-5->LUMO (78%)
14	278.14	0.0001	H-1->L+3 (73%), HOMO->L+3 (18%)
15	274.18	0.0825	H-1->L+2 (89%)
16	272.10	0.256	H-2->L+2 (69%)
17	271.48	0.0019	H-3->L+1 (99%)
18	269.51	0	H-7->LUMO (95%)
19	265.61	0.0592	H-6->LUMO (91%)

20	264.83	0	H-8->LUMO (82%), H-3->L+2 (17%)
21	263.21	0.0002	H-8->LUMO (17%), H-3->L+2 (82%)
22	262.41	0.1718	HOMO->L+4 (76%)
23	254.93	0.0437	H-9->LUMO (83%)
24	253.55	0.0014	H-10->LUMO (92%)
25	240.81	0.0034	HOMO->L+5 (93%)
26	239.33	0.0564	H-11->LUMO (34%), H-4->L+1 (58%)
27	234.45	0.1678	H-1->L+4 (82%)
28	234.27	0.0938	H-2->L+4 (74%)
29	231.67	0.0468	H-13->LUMO (15%), H-4->L+2 (51%)
30	229.42	0.0026	H-10->L+3 (88%)
31	227.53	0.0323	H-3->L+4 (96%)
32	225.86	0.0473	H-12->LUMO (70%)
33	225.71	0.1415	H-11->LUMO (54%), H-5->L+1 (13%), H-4->L+1 (22%)
34	221.39	0	H-14->LUMO (93%)
35	221.06	0.0268	H-5->L+1 (10%), HOMO->L+6 (85%)
36	219.84	0.0539	H-5->L+1 (71%), HOMO->L+6 (11%)
37	218.58	0.0013	H-5->L+3 (28%), H-4->L+3 (63%)
38	217.73	0.0002	H-7->L+1 (89%)
39	216.63	0.245	H-13->LUMO (61%), H-4->L+2 (20%)
40	215.64	0.0372	H-2->L+5 (88%)
41	215.63	0.0094	H-13->LUMO (11%), H-6->L+1 (19%), H-5->L+2 (52%), H-1->L+5 (13%)
42	215.20	0	H-8->L+1 (78%), H-7->L+2 (17%)
43	214.45	0.0425	H-6->L+1 (20%), H-1->L+5 (66%)
44	214.38	0.0049	H-17->LUMO (12%), H-15->LUMO (83%)
45	213.24	0.0001	H-5->L+3 (56%), H-4->L+3 (36%)
46	211.28	0.024	H-6->L+1 (51%), H-5->L+2 (25%)
47	210.35	0.1987	HOMO->L+8 (75%)
48	209.78	0	H-16->LUMO (98%)
49	209.54	0.1327	H-9->L+1 (12%), HOMO->L+7 (59%)
50	208.19	0	H-8->L+1 (12%), H-7->L+2 (60%), H-3->L+5 (20%)
51	207.52	0.0691	H-6->L+2 (94%)
52	207.41	0.0001	H-7->L+2 (13%), H-3->L+5 (75%)
53	206.78	0.0001	H-17->LUMO (82%), H-15->LUMO (13%)
54	206.66	0.0003	H-9->L+3 (12%), H-6->L+3 (75%)
55	206.06	0	H-10->L+1 (12%), H-8->L+2 (81%)
56	204.04	0.0004	HOMO->L+9 (98%)
57	203.53	0.0157	H-9->L+1 (58%), H-2->L+6 (12%)
58	202.54	0.0002	H-10->L+1 (85%), H-8->L+2 (10%)
59	200.41	0.0969	H-9->L+2 (91%)
60	199.79	0.0056	H-1->L+6 (91%)
61	198.14	0.0001	H-10->L+2 (92%)
62	197.63	0.0126	H-2->L+6 (76%)
63	197.22	0.0931	H-9->L+3 (42%), H-7->L+3 (25%), H-6->L+3 (10%)

64	196.91	0.1259	H-9->L+3 (30%), H-7->L+3 (29%), H-4->L+4 (16%)
65	196.34	0.0025	H-18->LUMO (51%), H-7->L+3 (11%), H-4->L+4 (19%)
66	195.77	0.1456	H-8->L+3 (74%), H-1->L+7 (16%)
67	195.36	0.0033	HOMO->L+10 (92%)
68	194.14	0.0033	H-18->LUMO (32%), H-7->L+3 (10%), H-4->L+4 (48%)
69	194.05	0.0021	H-19->LUMO (77%), H-12->L+1 (10%)
70	193.94	0.0123	H-7->L+4 (70%), H-3->L+6 (14%)

Table S8 The wavelengths, oscillator strengths and major contributions of the singlet optical transitions in lowest 70 states for **2** in DCM.

No.	Wavelength (nm)	Osc. Strength	Major contribs
1	489.16	0.001	HOMO->LUMO (98%)
2	397.99	0.0107	H-1->LUMO (95%)
3	387.39	0.2161	H-2->LUMO (98%)
4	376.19	0.0036	H-7->LUMO (99%)
5	366.73	0.0039	H-3->LUMO (98%)
6	364.89	0	H-4->LUMO (98%)
7	354.27	0.0012	H-5->LUMO (99%)
8	354.15	0	H-6->LUMO (99%)
9	345.48	0	HOMO->L+1 (98%)
10	328.56	0.0146	HOMO->L+2 (99%)
11	317.85	0.0001	H-1->L+3 (14%), HOMO->L+3 (82%)
12	303.08	0.0845	H-8->LUMO (52%), H-1->L+1 (35%)
13	295.73	0.0516	H-2->L+1 (94%)
14	294.24	0.0749	H-8->LUMO (14%), H-7->L+3 (12%), H-2->L+2 (19%), H-1->L+1 (49%)
15	289.65	0.0756	H-7->L+3 (69%)
16	288.77	0.0339	H-4->L+2 (24%), H-3->L+1 (68%)
17	288.04	0.0123	H-4->L+1 (64%), H-3->L+2 (26%)
18	286.09	0.0002	H-2->L+3 (91%)
19	282.36	0.102	H-1->L+2 (85%)
20	282.28	0.0227	H-9->LUMO (63%), H-2->L+2 (16%)
21	280.22	0.0012	H-7->L+1 (67%), H-1->L+3 (23%)
22	279.18	0.0538	H-7->L+1 (23%), H-1->L+3 (38%)
23	279.01	0.0139	H-6->L+2 (17%), H-5->L+1 (56%)
24	278.94	0.0001	H-6->L+1 (73%), H-5->L+2 (22%)

25	278.43	0.3151	H-9->LUMO (19%), H-2->L+2 (36%)
26	271.84	0	H-7->L+2 (97%)
27	271.73	0.0001	H-11->LUMO (95%)
28	267.85	0.041	H-10->LUMO (94%)
29	266.82	0	H-12->LUMO (97%)
30	265.10	0.002	H-4->L+1 (29%), H-3->L+2 (69%)
31	264.72	0.0004	H-4->L+2 (70%), H-3->L+1 (26%)
32	263.33	0.1257	HOMO->L+4 (68%), HOMO->L+6 (12%)
33	260.61	0.0001	H-6->L+1 (15%), H-5->L+2 (73%)
34	260.54	0.0007	H-6->L+2 (74%), H-5->L+1 (15%)
35	256.34	0.0486	H-13->LUMO (85%)
36	254.95	0.0001	H-14->LUMO (95%)
37	246.90	0.0031	HOMO->L+5 (79%), HOMO->L+7 (12%)
38	243.49	0	HOMO->L+4 (17%), HOMO->L+6 (83%)
39	240.86	0.1712	H-15->LUMO (14%), H-8->L+1 (77%)
40	239.79	0	HOMO->L+5 (20%), HOMO->L+7 (57%), HOMO->L+9 (16%)
41	237.24	0.0025	H-6->L+6 (11%), H-5->L+5 (23%), H-5->L+6 (11%), H-4->L+8 (14%), H-3->L+7 (10%)
42	237.22	0.0065	H-6->L+5 (24%), H-6->L+6 (10%), H-5->L+6 (10%), H-3->L+8 (15%)
43	235.17	0.217	H-8->L+2 (40%), H-2->L+4 (30%)
44	234.67	0.1571	H-1->L+4 (69%), H-1->L+6 (13%)
45	233.34	0.0042	H-8->L+2 (25%), H-2->L+4 (38%)
46	231.62	0.0001	HOMO->L+8 (100%)
47	230.88	0.0084	HOMO->L+7 (23%), HOMO->L+9 (74%)
48	230.08	0.0034	H-14->L+3 (68%), H-3->L+3 (23%)
49	227.73	0.0109	H-14->L+3 (13%), H-7->L+4 (27%), H-3->L+3 (49%)
50	227.58	0.0013	H-4->L+3 (98%)
51	227.40	0.0214	H-7->L+4 (52%), H-7->L+6 (11%), H-3->L+3 (27%)
52	225.67	0.0917	H-15->LUMO (14%), H-9->L+1 (81%)
53	224.74	0	H-5->L+3 (96%)
54	224.61	0	H-6->L+3 (97%)
55	223.99	0.0048	H-16->LUMO (55%)
56	222.55	0.0015	H-11->L+1 (88%)
57	221.93	0.0001	H-18->LUMO (59%), H-12->L+1 (13%), H-11->L+2 (13%)
58	221.60	0.0132	H-15->LUMO (42%), H-2->L+5 (18%), H-2->L+7 (10%)
59	220.71	0.0713	HOMO->L+10 (93%)
60	219.91	0.0543	H-10->L+1 (24%), H-9->L+2 (50%)
61	219.71	0.006	H-18->LUMO (14%), H-12->L+1 (58%)
62	219.47	0.0642	H-15->LUMO (19%), H-2->L+5 (51%)
63	218.99	0.0425	H-10->L+1 (13%), H-1->L+5 (65%)
64	218.01	0.0026	H-9->L+3 (46%), H-8->L+3 (37%)
65	216.87	0.0643	H-2->L+4 (14%), H-2->L+6 (62%)
66	216.84	0.0006	H-1->L+4 (15%), H-1->L+6 (78%)
67	216.09	0.0923	H-10->L+1 (33%), H-9->L+2 (16%), H-2->L+6 (18%)

68	215.02	0.1912	H-17->LUMO (55%)
69	214.14	0.0471	H-2->L+5 (25%), H-2->L+7 (43%), H-2->L+9 (14%)
70	213.72	0.1102	H-13->L+1 (13%), H-1->L+5 (13%), H-1->L+7 (39%), H-1->L+9 (12%)

Table S9 The wavelengths, oscillator strengths and major contributions of the singlet optical transitions in lowest 70 states for **3** in DCM.

N o.	Wavelength (nm)	Osc. Strength	Major contribs
1	398.83	0.008	HOMO->LUMO (91%)
2	384.31	0.1068	H-3->LUMO (10%), H-1->LUMO (85%)
3	381.78	0.0195	H-4->LUMO (34%), H-3->LUMO (52%), H-1->LUMO (14%)
4	366.20	0.0006	H-2->LUMO (92%)
5	349.94	0.0007	H-4->LUMO (62%), H-3->LUMO (38%)
6	302.70	0.0686	H-5->LUMO (43%), HOMO->L+1 (35%)
7	295.83	0.0145	H-4->L+3 (17%), H-3->L+3 (11%), H-1->L+1 (19%), HOMO->L+1 (32%)
8	294.53	0.0001	H-6->LUMO (11%), H-1->L+1 (18%), HOMO->L+3 (44%)
9	293.38	0.0362	H-5->LUMO (14%), H-4->L+3 (29%), H-3->L+3 (16%), H-1->L+1 (16%)
10	291.05	0.0198	H-1->L+1 (27%), H-1->L+3 (42%)
11	289.65	0.1035	H-5->LUMO (19%), H-1->L+1 (10%), H-1->L+3 (42%), HOMO->L+1 (15%)
12	286.02	0.0024	H-4->L+1 (18%), H-3->L+1 (63%)
13	284.78	0.0098	H-7->LUMO (17%), H-6->LUMO (35%), HOMO->L+2 (15%), HOMO->L+3 (17%)
14	284.11	0.0225	H-7->LUMO (59%), H-6->LUMO (20%)
15	281.54	0.0068	H-2->L+1 (53%), H-1->L+2 (18%)
16	279.58	0.1099	H-6->LUMO (18%), H-2->L+1 (16%), HOMO->L+2 (47%)
17	275.18	0.2869	H-5->LUMO (10%), H-2->L+1 (10%), H-1->L+2 (52%)
18	274.06	0.0108	H-8->LUMO (18%), H-4->L+2 (16%), H-3->L+2 (37%)
19	273.29	0.0467	H-8->LUMO (51%), H-4->L+2 (12%), H-3->L+2 (21%)
20	270.62	0.0704	H-4->L+1 (44%), H-3->L+1 (12%), H-2->L+2 (19%)
21	266.38	0.017	H-4->L+1 (17%), H-3->L+1 (11%), H-2->L+2 (62%)
22	263.23	0.005	H-9->LUMO (95%)
23	258.63	0.0002	H-4->L+2 (61%), H-3->L+2 (28%)
24	256.83	0.0001	H-2->L+3 (78%), HOMO->L+3 (17%)
25	249.24	0.0022	H-4->L+3 (35%), H-3->L+3 (61%)
26	241.91	0.0091	H-10->L+3 (17%), H-8->L+3 (15%), H-7->L+3 (11%), H-6-

			>L+3 (38%)
27	241.62	0.0695	H-11->LUMO (17%), H-10->LUMO (11%), H-5->L+1 (48%)
28	240.21	0.0273	H-10->LUMO (55%), H-5->L+1 (14%), H-5->L+2 (16%)
29	234.74	0.0882	H-13->LUMO (10%), H-10->LUMO (22%), H-6->L+1 (10%), H-5->L+2 (34%)
30	229.89	0.0007	H-11->LUMO (10%), H-7->L+1 (37%), H-6->L+1 (24%), H-5->L+2 (12%)
31	227.97	0.0681	H-11->LUMO (13%), H-7->L+1 (25%), H-6->L+1 (44%)
32	225.38	0.0223	H-12->LUMO (13%), H-11->LUMO (13%), H-8->L+1 (22%), H-7->L+1 (16%)
33	224.03	0.0578	H-11->LUMO (14%), H-8->L+1 (44%), H-7->L+2 (10%)
34	223.23	0.0346	H-14->LUMO (17%), H-12->LUMO (12%), H-6->L+2 (42%)
35	221.80	0.023	H-14->LUMO (10%), H-11->LUMO (12%), H-7->L+2 (14%)
36	221.29	0.0436	H-14->LUMO (18%), H-7->L+2 (11%), H-6->L+2 (10%)
37	220.59	0.0389	H-14->LUMO (30%), H-6->L+2 (21%)
38	218.82	0.0655	HOMO->L+5 (79%)
39	218.50	0.0638	H-9->L+1 (23%), H-8->L+2 (21%), H-7->L+2 (16%), HOMO->L+4 (11%)
40	217.56	0.2261	H-13->LUMO (21%), H-9->L+1 (15%), H-8->L+2 (14%), H-1->L+5 (14%)
41	216.91	0.0479	H-13->LUMO (34%), HOMO->L+4 (24%)
42	215.20	0.0202	H-1->L+4 (83%)
43	214.83	0.0017	H-1->L+5 (44%), HOMO->L+4 (14%)
44	214.26	0.0097	H-7->L+3 (13%), H-5->L+3 (55%), H-1->L+5 (12%)
45	213.02	0.0154	H-9->L+1 (34%), H-8->L+2 (22%)
46	212.10	0.0237	H-12->LUMO (13%), H-8->L+2 (16%), H-7->L+2 (11%), HOMO->L+4 (15%)
47	211.56	0.0015	H-4->L+4 (23%), H-3->L+4 (67%)
48	211.39	0.0058	H-17->LUMO (21%), H-15->LUMO (45%), H-4->L+5 (10%), H-3->L+5 (13%)
49	210.67	0.0539	H-15->LUMO (19%), H-4->L+5 (29%), H-3->L+5 (39%)
50	209.05	0.0019	H-8->L+3 (22%), H-2->L+5 (51%)
51	208.47	0.0046	H-2->L+4 (88%)
52	207.50	0.0024	H-9->L+2 (80%)
53	206.89	0.0012	H-16->LUMO (67%), H-15->LUMO (10%)
54	205.44	0.0004	H-17->LUMO (55%), H-16->LUMO (18%), H-15->LUMO (19%)
55	205.15	0.0366	H-8->L+3 (11%), H-2->L+5 (22%), HOMO->L+7 (54%)
56	203.43	0.0058	H-4->L+5 (14%), H-1->L+7 (48%), HOMO->L+6 (28%)
57	203.07	0.08	H-8->L+3 (17%), H-4->L+4 (27%), H-3->L+4 (10%), HOMO->L+7 (14%)
58	202.83	0.0595	H-8->L+3 (12%), H-4->L+4 (38%), H-3->L+4 (13%)
59	202.58	0.036	H-4->L+5 (38%), H-3->L+5 (26%), H-1->L+7 (14%)
60	200.94	0.0197	H-4->L+7 (10%), H-3->L+7 (55%), H-2->L+6 (11%)
61	200.62	0.1093	H-1->L+6 (73%)

62	199.72	0.0114	H-10->L+3 (43%), H-4->L+6 (12%), H-3->L+6 (10%)
63	199.21	0.0297	H-9->L+3 (29%), H-3->L+7 (21%), H-2->L+6 (16%), HOMO->L+6 (11%)
64	198.82	0.0003	H-8->L+3 (10%), H-3->L+6 (19%), H-2->L+7 (28%), HOMO->L+7 (10%)
65	198.00	0.072	H-10->L+1 (62%), H-9->L+3 (11%)
66	197.91	0.0196	H-4->L+6 (12%), H-3->L+6 (19%), H-2->L+7 (48%)
67	196.06	0.1559	H-10->L+1 (14%), H-9->L+3 (33%), HOMO->L+6 (22%)
68	195.84	0.0006	H-22->LUMO (10%), H-18->LUMO (81%)
69	195.33	0.1895	H-20->LUMO (19%), H-11->L+1 (49%)
70	194.43	0.0558	H-2->L+6 (51%), HOMO->L+6 (11%)

Table S10 The wavelengths, oscillator strengths and major contributions of the singlet optical transitions in lowest 70 states for **4** in DCM.

No.	Wavelength (nm)	Osc. Strength	Major contribs
1	410.42	0.0097	HOMO->LUMO (90%)
2	394.66	0.1065	H-3->LUMO (17%), H-1->LUMO (74%)
3	392.58	0.0337	H-8->LUMO (29%), H-3->LUMO (44%), H-1->LUMO (24%)
4	377.64	0.0011	H-2->LUMO (91%)
5	364.08	0.0046	H-8->LUMO (12%), H-4->LUMO (64%), H-3->LUMO (19%)
6	360.04	0.005	H-5->LUMO (88%)
7	357.53	0.0023	H-8->LUMO (51%), H-4->LUMO (23%), H-3->LUMO (19%)
8	349.15	0.0015	H-6->LUMO (97%)
9	348.93	0.0008	H-7->LUMO (96%)
10	306.62	0.0432	H-9->LUMO (34%), HOMO->L+1 (48%)
11	299.18	0.0624	H-9->LUMO (17%), H-8->L+3 (12%), H-1->L+2 (16%), HOMO->L+1 (35%)
12	298.44	0.0069	H-1->L+1 (83%)
13	296.60	0.0009	H-10->LUMO (11%), HOMO->L+2 (27%), HOMO->L+3 (36%)
14	294.97	0.069	H-9->LUMO (21%), H-8->L+3 (38%), H-3->L+3 (19%)
15	291.45	0.0368	H-1->L+3 (79%)
16	291.02	0.0015	H-8->L+1 (19%), H-3->L+1 (70%)
17	289.27	0.0138	H-10->LUMO (13%), HOMO->L+2 (27%), HOMO->L+3 (30%)
18	288.66	0.0003	H-11->LUMO (52%), H-2->L+1 (19%)
19	288.01	0.006	H-11->LUMO (10%), H-2->L+1 (37%), H-1->L+2 (23%)
20	286.20	0.1156	H-10->LUMO (45%), HOMO->L+2 (23%)
21	286.14	0.1084	H-11->LUMO (14%), H-5->L+1 (10%), H-5->L+2 (19%), H-4->L+1 (45%)
22	284.14	0.0065	H-5->L+1 (42%), H-4->L+2 (22%), HOMO->L+2 (12%)
23	281.35	0.1058	H-8->L+2 (19%), H-3->L+2 (48%), H-1->L+2 (11%)
24	280.25	0.2739	H-9->LUMO (10%), H-8->L+2 (10%), H-3->L+2 (10%), H-2-

			>L+1 (20%), H-1->L+2 (29%)
25	278.96	0.0119	H-12->LUMO (54%), H-8->L+1 (12%), H-2->L+2 (18%)
26	276.46	0.0913	H-12->LUMO (32%), H-8->L+1 (26%), H-2->L+2 (28%)
27	276.17	0.0051	H-6->L+1 (72%), H-6->L+2 (22%)
28	275.91	0.0015	H-7->L+1 (69%), H-7->L+2 (24%)
29	272.52	0.0073	H-8->L+1 (35%), H-3->L+1 (18%), H-2->L+2 (40%)
30	268.34	0.0048	H-13->LUMO (84%)
31	266.12	0.0012	H-13->LUMO (14%), H-8->L+2 (43%), H-4->L+2 (10%), H-3->L+2 (24%)
32	262.82	0.0013	H-5->L+2 (26%), H-4->L+1 (21%), H-4->L+2 (38%)
33	262.14	0.0011	H-8->L+2 (12%), H-5->L+1 (18%), H-5->L+2 (43%), H-4->L+2 (17%)
34	258.98	0	H-2->L+3 (78%), HOMO->L+3 (19%)
35	258.30	0.0003	H-7->L+1 (26%), H-7->L+2 (62%), H-6->L+2 (10%)
36	258.19	0.0009	H-7->L+2 (10%), H-6->L+1 (25%), H-6->L+2 (65%)
37	251.26	0.0024	H-8->L+3 (33%), H-3->L+3 (64%)
38	243.32	0.0085	H-14->LUMO (75%), H-9->L+2 (15%)
39	242.23	0.1103	H-10->L+3 (14%), H-9->L+1 (53%)
40	242.07	0.0508	H-14->L+3 (13%), H-12->L+3 (18%), H-10->L+3 (32%), H-9->L+1 (24%)
41	237.30	0.1302	H-14->LUMO (18%), H-10->L+1 (13%), H-9->L+2 (42%)
42	236.97	0.0051	H-7->L+4 (39%), H-7->L+5 (11%), H-4->L+7 (13%)
43	236.78	0.0044	H-6->L+4 (11%), H-6->L+5 (41%), H-5->L+6 (12%), H-5->L+7 (14%)
44	231.39	0.0014	H-10->L+1 (71%), H-9->L+2 (16%)
45	229.39	0.0125	H-15->LUMO (10%), H-11->L+1 (81%)
46	227.08	0.0348	H-12->L+1 (57%), H-11->L+2 (10%)
47	226.88	0.0825	H-18->LUMO (11%), H-10->L+2 (59%)
48	226.45	0.0002	H-4->L+3 (79%)
49	225.55	0.0035	H-5->L+3 (84%)
50	225.38	0.0038	H-16->LUMO (20%), H-11->L+2 (20%), HOMO->L+4 (26%)
51	223.60	0.0948	H-11->L+2 (30%), HOMO->L+4 (31%)
52	223.43	0.0075	H-18->LUMO (29%), H-15->LUMO (18%), H-10->L+2 (13%)
53	222.67	0.0002	H-6->L+3 (93%)
54	222.47	0.0005	H-7->L+3 (93%)
55	222.38	0.0005	H-18->LUMO (19%), H-1->L+4 (39%)
56	221.94	0.0027	HOMO->L+4 (10%), HOMO->L+5 (62%)
57	221.51	0.1946	H-13->L+1 (25%), H-12->L+2 (43%)
58	221.42	0.0183	H-11->L+3 (33%), H-9->L+3 (18%)
59	220.45	0.0775	H-18->LUMO (19%), H-15->LUMO (28%), H-1->L+4 (11%), HOMO->L+9 (10%)
60	219.63	0.0033	H-1->L+4 (16%), H-1->L+5 (78%)
61	219.37	0.0979	H-11->L+2 (13%), HOMO->L+4 (10%), HOMO->L+6 (11%)
62	218.16	0.0305	HOMO->L+9 (62%)
63	217.77	0.0011	H-3->L+4 (46%), H-3->L+5 (10%)

64	217.19	0.0747	H-17->LUMO (29%), HOMO->L+6 (32%), HOMO->L+8 (12%)
65	216.99	0.0207	H-2->L+4 (60%)
66	216.16	0.0074	H-13->L+1 (23%), H-12->L+2 (17%), H-1->L+6 (22%), H-1->L+8 (12%)
67	215.40	0.014	H-13->L+1 (19%), H-12->L+2 (15%), H-1->L+6 (23%), H-1->L+8 (10%)
68	215.25	0.003	H-2->L+5 (62%)
69	214.54	0.0172	H-3->L+5 (36%), H-1->L+9 (13%)
70	214.43	0.0038	H-3->L+5 (25%), H-1->L+9 (31%)

Table S11 The estimated emission energy, determined by subtracting the total energy of the S0 state from that of the minimized T1 state, both at the minimized T1 state geometry.

	Singlet energy / a.u.	Triplet energy/ a.u.	Energy difference / a.u.	Energy difference / eV	Emission / nm
1	-2053.14922605	-2053.21799387	0.068767	1.87	663
2	-2436.70601081	-2436.63936765	0.066643	1.81	685
3	-2171.15264034	-2171.06642693	0.086214	2.35	530
4	-2554.64168544	-2554.55633685	0.085349	2.32	534

Table S12: Dimer calculations

Dimer calculations were carried out for complex **1** by fixing the Pt-Pt distance at 3.484 Å or 3.44 Å. A greater interaction is found between the two monomers when the distance is shorter.

	Singlet energy / a.u.
1	-2053.2180
1 dimer with Pt-Pt distance 3.484	-4106.4499
E(dimer)-E(monomer)*2	-0.0139 a.u. = -0.38 eV
	Singlet energy / a.u.
1	-2053.2180
1 dimer with Pt-Pt distance 3.44	-4106.4538
E(dimer)-E(monomer)*2	-0.0178 a.u. = -0.48 eV