Electronic Supplementary Information

for

Platinum(II) cyclometallates featuring broad emission bands and their applications in color-tunable OLEDs and high color-rendering WOLEDs

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Table S1 Computed electronic density of the frontier orbitals for **1** (up) and **2** (bottom).

	% of electronic density	
	HOMO	LUMO
Phenylpyridine	56.09	89.25
Pt	23.87	5.18
acac	7.79	2.30
Phenoxy group	11.85	3.24
F-group	0.40	0.03

	% of electronic density	
	HOMO	LUMO
Phenylpyridine	57.35	88.51
Pt	19.56	5.48
acac	5.30	2.62
Phenoxy group	16.11	2.43
F-group	1.67	0.97

Table S2 Calculated position of the 0-0 peaks, oscillator strength (f) and major contributions for the 10 first transitions for **1** (top) and **2** (below).

No.	(nm)	f	Major contributions
1	375.2	0.0959	HOMO−>LUMO (90%)
2	341.4	0.0085	H-2−>LUMO (97%)
3	340.1	0.1476	H-1−>LUMO (89%)
4	326.1	0.062	HOMO−>L+1 (78%)
5	316.5	0.0688	H-3−>LUMO (54%), HOMO−>L+2 (31%)
6	311.3	0.0003	H-2−>L+1 (96%)
7	305.5	0.0397	H-1−>L+1 (75%), HOMO−>L+1 (12%)
8	304.3	0.2177	H-3−>LUMO (23%), HOMO−>L+2 (61%)
9	287.6	0.1606	H-1−>L+2 (67%)
10	287.2	0.0106	H-6−>LUMO (10%), HOMO−>L+4 (36%), HOMO−>L+5 (21%)

No.	(nm)	f	Major contributions
1	387.1	0.076	HOMO−>LUMO (91%)
2	348.8	0.0153	H-2−>LUMO (91%)
3	346.6	0.1489	H-1−>LUMO (87%)
4	328.9	0.0417	H-3−>LUMO (21%), HOMO−>L+1 (59%)
5	321.5	0.0492	H-3−>LUMO (31%), HOMO−>L+1 (21%), HOMO−>L+2 (36%)
6	311.1	0.2381	H-3−>LUMO (31%), H-1−>L+2 (10%), HOMO−>L+2 (48%)
7	309.3	0.0005	H-2−>L+1 (86%)
8	306.0	0.0162	H-1−>L+1 (76%), HOMO−>L+1 (11%)
9	293.9	0.1925	H-1−>L+2 (75%)
10	290.3	0.0001	H-7−>LUMO (17%), H-1−>L+4 (11%), HOMO−>L+4 (52%)

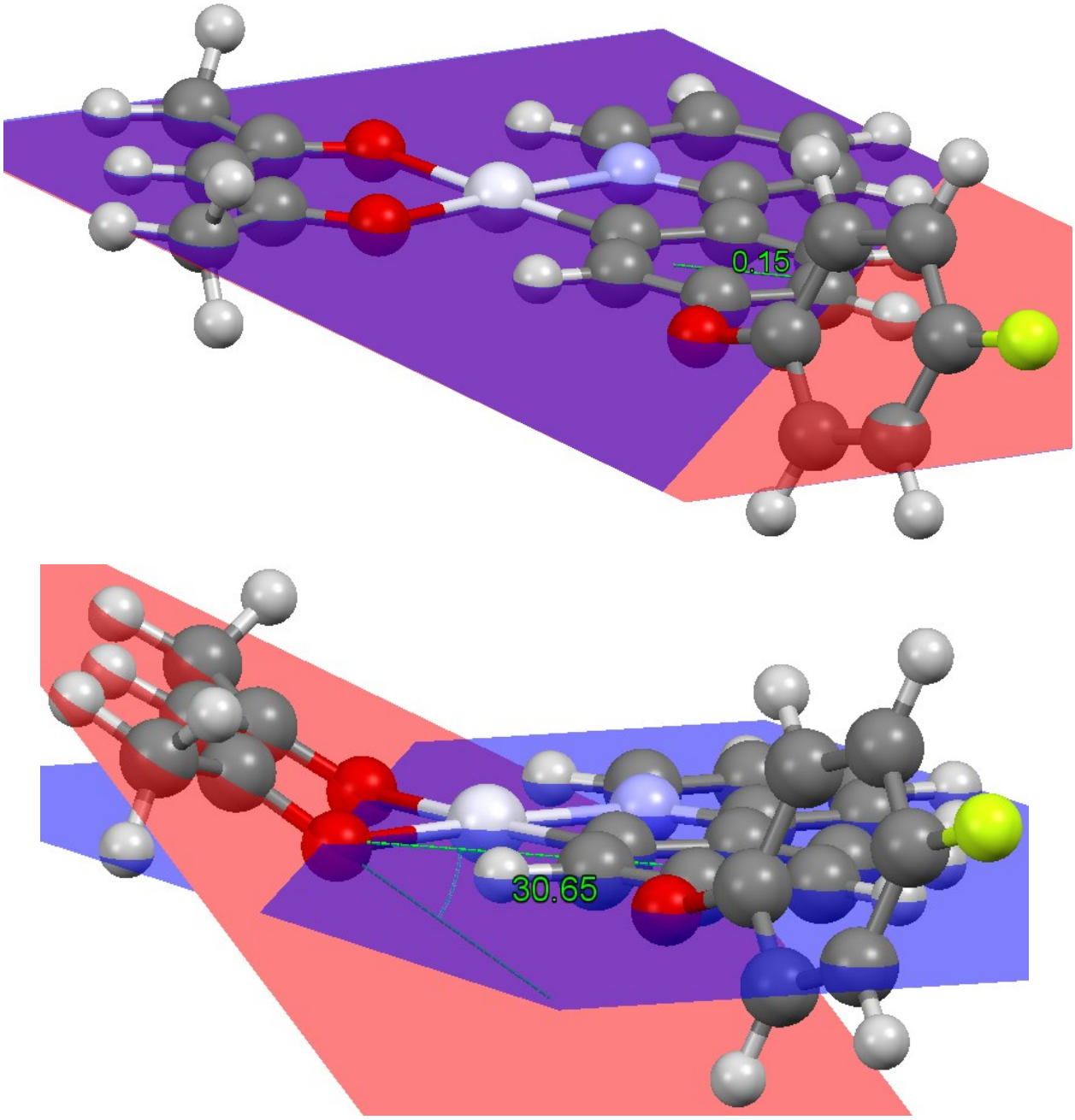


Fig. S1 The angles of acac ligand bending from singlet (top) to triplet (below) states in **1**.

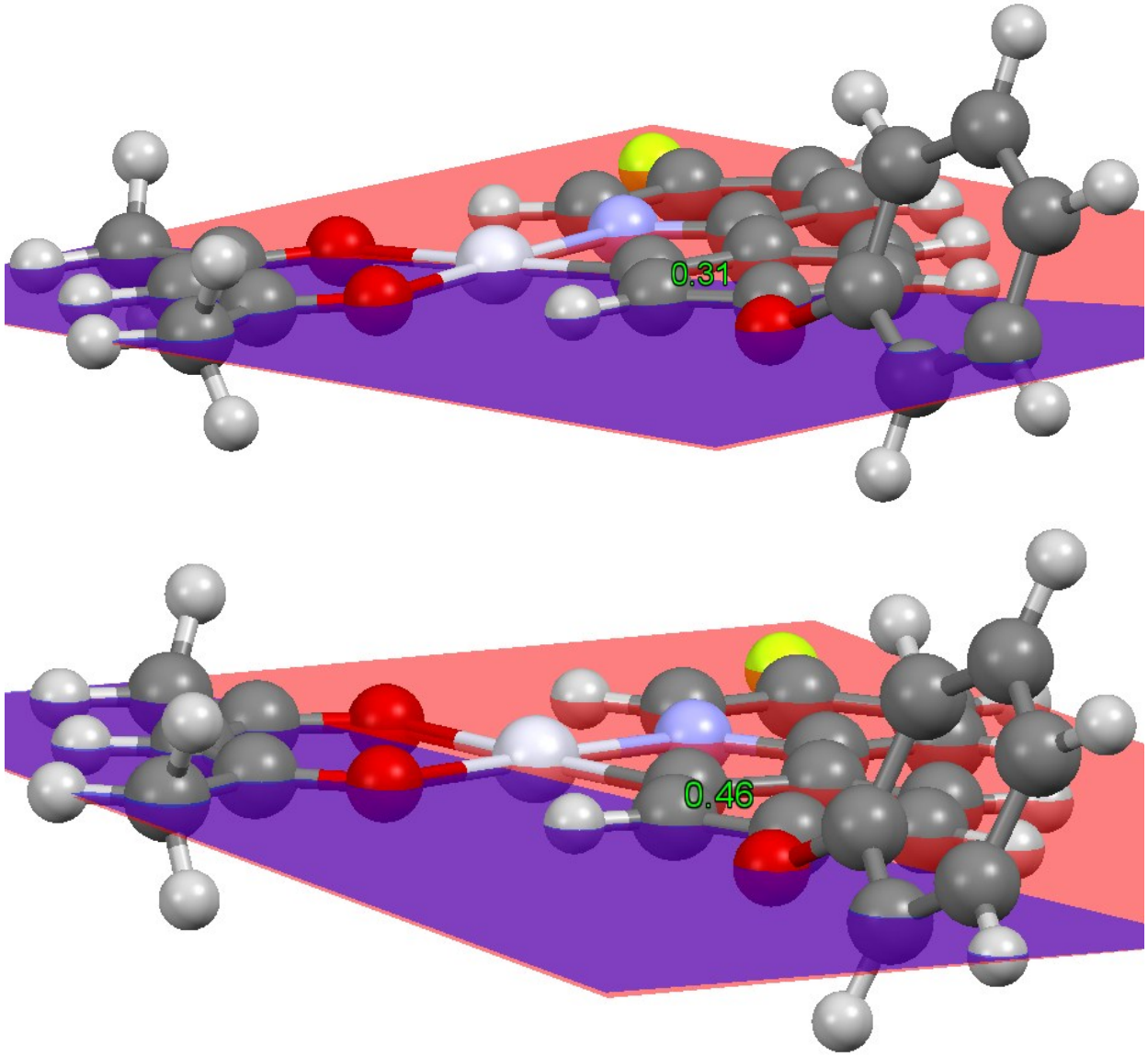


Fig. S2 The angles of acac ligand bending from singlet (top) to triplet (below) states in **2**.

Table S3 Conformational changes between singlet and triplet states of **1**

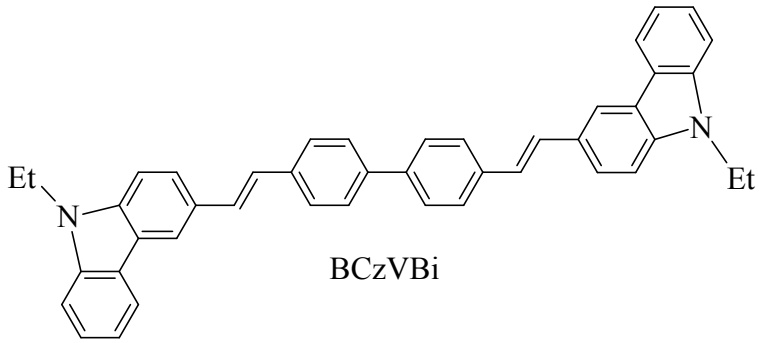
Tag	Atom	NA	NB	NC	Singlet conformation			Triplet conformation			Conformational change		
					Bond	Angle	Dihedral	Bond	Angle	Dihedral	Bond	Angle	Dihedral
1	C												
2	C	1			1.40			1.40			0.00		
3	C	2	1		1.42	118.51		1.42	118.66		0.00	0.15	
4	C	3	2	1	1.40	120.36	0.40	1.40	120.26	0.50	0.00	-0.10	0.10
5	C	4	3	2	1.39	120.69	-0.21	1.39	120.66	-0.28	0.00	-0.03	-0.07
6	C	1	2	3	1.40	120.43	-0.20	1.40	120.41	-0.20	0.00	-0.02	0.01
7	H	1	2	3	1.09	120.77	179.90	1.09	120.74	-179.83	0.00	-0.03	-359.73
8	H	4	3	2	1.09	120.74	179.34	1.09	120.82	179.36	0.00	0.08	0.02
9	H	5	4	3	1.08	120.46	179.38	1.08	120.39	179.35	0.00	-0.08	-0.03
10	C	3	2	1	1.46	115.09	-179.87	1.46	115.37	-179.36	0.00	0.27	0.51
11	C	10	3	2	1.40	126.80	179.96	1.40	126.72	-179.62	0.00	-0.08	-359.58
12	C	11	10	3	1.39	120.08	179.76	1.39	120.00	179.90	0.00	-0.09	0.13
13	H	11	10	3	1.08	119.57	-0.20	1.08	119.71	-0.06	0.00	0.13	0.14
14	C	10	3	2	2.36	143.25	-0.33	2.36	143.27	0.27	0.00	0.02	0.59
15	C	14	10	3	1.39	91.99	-179.70	1.39	91.98	-179.91	0.00	0.00	-0.22
16	H	12	11	10	1.09	120.04	-179.95	1.09	119.97	-179.93	0.00	-0.08	0.02
17	H	14	10	3	1.08	145.34	0.25	1.08	145.20	0.00	0.00	-0.14	-0.24
18	H	15	14	10	1.08	119.77	179.97	1.08	119.82	179.99	0.00	0.05	0.02
19	N	14	10	3	1.35	29.91	0.34	1.35	29.79	0.15	0.00	-0.12	-0.20
20	Pt	2	1	6	1.99	127.18	179.74	2.00	127.02	-179.26	0.01	-0.16	-358.99
21	O	20	2	1	2.05	94.10	-0.26	2.03	95.85	-2.78	-0.02	1.75	-2.52
22	O	20	2	1	2.14	175.16	-176.92	2.11	175.28	169.60	-0.03	0.12	346.52
23	C	22	20	2	2.39	95.33	176.94	2.40	92.98	-147.38	0.00	-2.36	-324.32
24	C	22	20	2	1.28	123.77	177.11	1.32	120.51	-134.48	0.04	-3.25	-311.59
25	C	21	20	2	1.29	124.87	179.94	1.33	120.81	139.77	0.04	-4.06	-40.17
26	H	23	22	20	1.08	142.01	179.79	1.09	143.26	165.69	0.00	1.25	-14.10
27	C	24	22	20	1.51	114.96	179.61	1.50	116.24	156.31	-0.01	1.28	-23.29
28	H	27	24	22	1.09	112.59	179.60	1.09	111.83	179.25	0.00	-0.76	-0.35
29	H	27	24	22	1.10	109.45	-59.02	1.10	110.85	-60.05	0.00	1.40	-1.02
30	H	27	24	22	1.10	109.48	58.11	1.10	111.04	58.39	0.00	1.56	0.29
31	C	25	21	20	1.51	113.43	-179.80	1.50	115.25	-155.05	-0.01	1.82	24.75
32	H	31	25	21	1.10	109.54	58.96	1.10	110.93	61.22	0.00	1.39	2.25
33	H	31	25	21	1.09	112.36	-179.68	1.09	111.56	-178.25	0.00	-0.80	1.44
34	H	31	25	21	1.10	109.56	-58.28	1.10	111.33	-57.43	0.00	1.77	0.85
35	O	6	1	2	1.38	115.70	-177.75	1.38	115.84	-177.80	0.00	0.14	-0.04
36	C	35	6	1	1.39	120.60	-161.64	1.39	120.59	-159.23	0.00	-0.01	2.41
37	C	36	35	6	1.40	117.84	-123.27	1.40	117.74	-126.01	0.00	-0.10	-2.73
38	C	36	35	6	1.40	121.24	61.26	1.40	121.32	58.51	0.00	0.08	-2.75
39	C	37	36	35	1.40	119.81	-175.52	1.40	119.78	-175.56	0.00	-0.03	-0.05
40	H	37	36	35	1.09	119.35	4.11	1.09	119.36	4.05	0.00	0.02	-0.06
41	C	38	36	35	1.39	119.63	175.84	1.39	119.62	175.90	0.00	-0.01	0.06

42	H	38	36	35	1.09	119.95	-3.92	1.09	120.00	-3.88	0.00	0.05	0.04
43	C	39	37	36	1.39	118.76	-0.41	1.39	118.78	-0.43	0.00	0.02	-0.02
44	H	39	37	36	1.08	121.33	179.84	1.08	121.31	179.84	0.00	-0.02	0.00
45	H	41	38	36	1.08	121.26	-179.95	1.08	121.25	-179.96	0.00	-0.02	-0.02
46	F	43	39	37	1.35	118.99	-179.75	1.35	119.00	-179.71	0.00	0.01	0.04

Table S4 Conformational changes between singlet and triplet states of **2**

Tag	Atom	NA	NB	NC	Singlet conformation			Triplet conformation			Conformational change		
					Bond	Angle	Dihedral	Bond	Angle	Dihedral	Bond	Angle	Dihedral
1	C												
2	C	1			1.40			1.39			-0.01		
3	C	2	1		1.42	118.52		1.48	118.82		0.05	0.29	
4	C	3	2	1	1.40	120.38	0.45	1.44	118.92	0.84	0.04	-1.46	0.39
5	C	4	3	2	1.39	120.62	-0.23	1.37	120.36	-0.99	-0.02	-0.27	-0.77
6	C	1	2	3	1.40	120.42	-0.22	1.40	120.71	0.49	0.00	0.29	0.70
7	H	1	2	3	1.09	120.79	179.85	1.09	120.50	179.88	0.00	-0.29	0.03
8	H	4	3	2	1.09	120.80	179.32	1.09	120.29	178.09	0.00	-0.51	-1.23
9	H	5	4	3	1.08	120.53	179.34	1.08	120.39	178.67	0.00	-0.14	-0.67
10	C	3	2	1	1.46	115.06	-179.64	1.40	115.67	-179.57	-0.06	0.61	0.07
11	C	10	3	2	1.40	126.86	179.84	1.43	127.46	179.64	0.02	0.60	-0.19
12	C	11	10	3	1.39	120.57	-179.99	1.37	121.61	-179.65	-0.02	1.03	0.34
13	H	11	10	3	1.08	119.68	-0.04	1.08	118.58	0.24	0.00	-1.10	0.27
14	C	10	3	2	2.36	143.08	-0.06	2.40	142.95	0.22	0.04	-0.14	0.28
15	C	14	10	3	1.38	90.70	179.97	1.38	89.64	179.55	-0.01	-1.06	-0.42
16	H	14	10	3	1.08	146.90	0.11	1.08	148.66	-0.33	0.00	1.76	-0.44
17	N	14	10	3	1.35	29.71	-0.06	1.35	31.41	-0.58	0.00	1.71	-0.52
18	Pt	2	1	6	1.99	127.21	-179.89	1.97	127.69	-178.94	-0.02	0.48	0.95
19	O	18	2	1	2.04	94.22	-0.52	2.06	93.84	-0.72	0.01	-0.38	-0.21
20	O	18	2	1	2.14	175.04	178.40	2.14	175.51	178.36	0.00	0.48	-0.05
21	C	20	18	2	2.39	95.39	-179.07	2.40	95.46	-179.38	0.00	0.08	-0.31
22	C	20	18	2	1.28	123.86	-179.09	1.28	123.80	-179.44	0.00	-0.07	-0.35
23	C	19	18	2	1.29	124.86	-179.86	1.29	124.72	-179.60	0.00	-0.14	0.26
24	H	21	20	18	1.08	142.09	-179.91	1.08	141.94	-179.79	0.00	-0.15	0.12
25	C	22	20	18	1.51	114.98	179.99	1.51	114.83	-179.94	0.00	-0.16	-359.93
26	H	25	22	20	1.09	112.58	179.01	1.09	112.61	179.02	0.00	0.03	0.01
27	H	25	22	20	1.10	109.45	-59.60	1.10	109.42	-59.56	0.00	-0.03	0.04
28	H	25	22	20	1.10	109.47	57.52	1.10	109.44	57.50	0.00	-0.03	-0.02
29	C	23	19	18	1.51	113.36	179.85	1.51	113.50	179.66	0.00	0.13	-0.19
30	H	29	23	19	1.10	109.54	59.24	1.10	109.52	59.11	0.00	-0.02	-0.13
31	H	29	23	19	1.09	112.36	-179.39	1.09	112.40	-179.49	0.00	0.04	-0.10
32	H	29	23	19	1.10	109.53	-57.98	1.10	109.50	-58.07	0.00	-0.03	-0.10
33	O	6	1	2	1.38	115.99	-176.97	1.37	117.08	-176.81	-0.01	1.08	0.15
34	C	33	6	1	1.39	120.98	-153.98	1.39	121.15	-149.75	0.00	0.17	4.22
35	C	34	33	6	1.40	117.18	-133.32	1.40	116.71	-141.83	0.00	-0.47	-8.51
36	C	34	33	6	1.40	121.82	51.19	1.40	122.10	42.13	0.00	0.28	-9.07
37	C	35	34	33	1.40	119.42	-175.64	1.40	119.25	-176.58	0.00	-0.17	-0.94
38	H	35	34	33	1.09	119.15	4.07	1.09	119.22	3.45	0.00	0.07	-0.62
39	C	36	34	33	1.40	119.16	175.84	1.40	119.01	176.67	0.00	-0.15	0.83
40	H	36	34	33	1.09	119.98	-3.86	1.09	120.11	-2.49	0.00	0.14	1.37
41	C	37	35	34	1.40	120.36	-0.34	1.40	120.57	-0.49	0.00	0.21	-0.15

42	H	37	35	34	1.09	119.46	179.91	1.09	119.43	-179.88	0.00	-0.02	-359.79
43	H	39	36	34	1.09	119.32	-179.94	1.09	119.28	-179.89	0.00	-0.05	0.06
44	H	41	37	35	1.09	120.21	-179.81	1.09	120.14	-179.81	0.00	-0.07	0.00
45	H	12	11	10	1.08	121.76	-179.99	1.08	122.94	179.93	0.00	1.18	359.92
46	F	15	14	10	1.34	118.92	-179.99	1.35	118.83	179.96	0.00	-0.09	359.95



BCzVBi

Fig. S3 The molecular structure of the blue emitter BCzVBi.

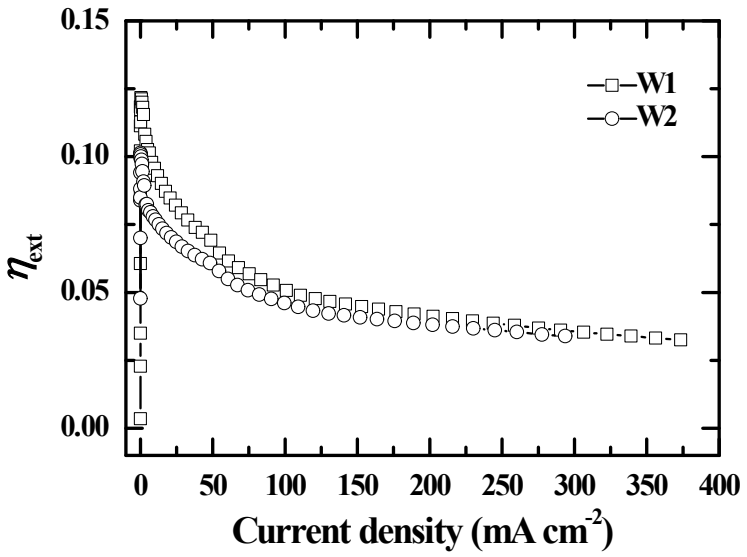


Fig. S4 The $\eta_{ext} - J$ curves of WOLEDs **W1** and **W2**.

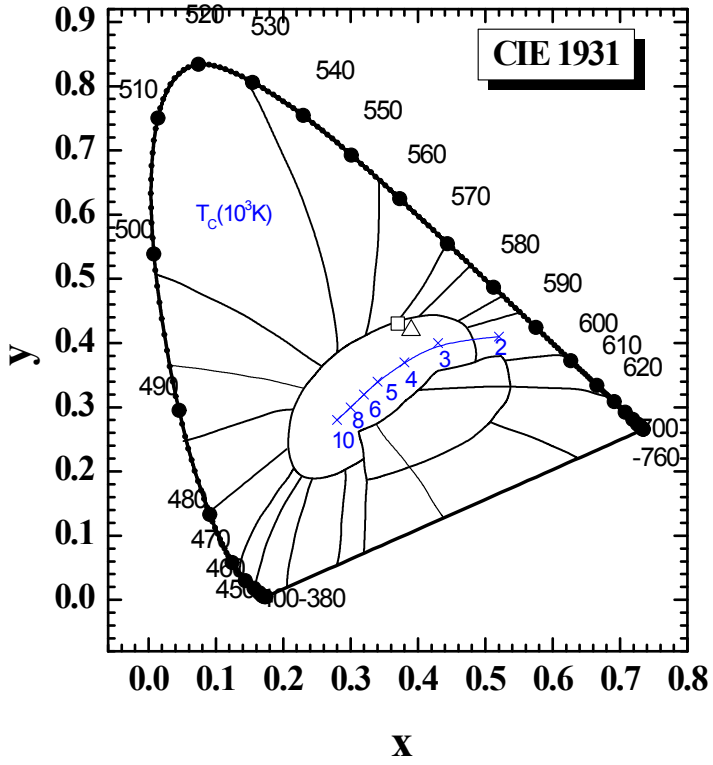


Fig. S5 The CIE 1931 chromaticity diagram of **W1** (□) and **W2** (Δ).

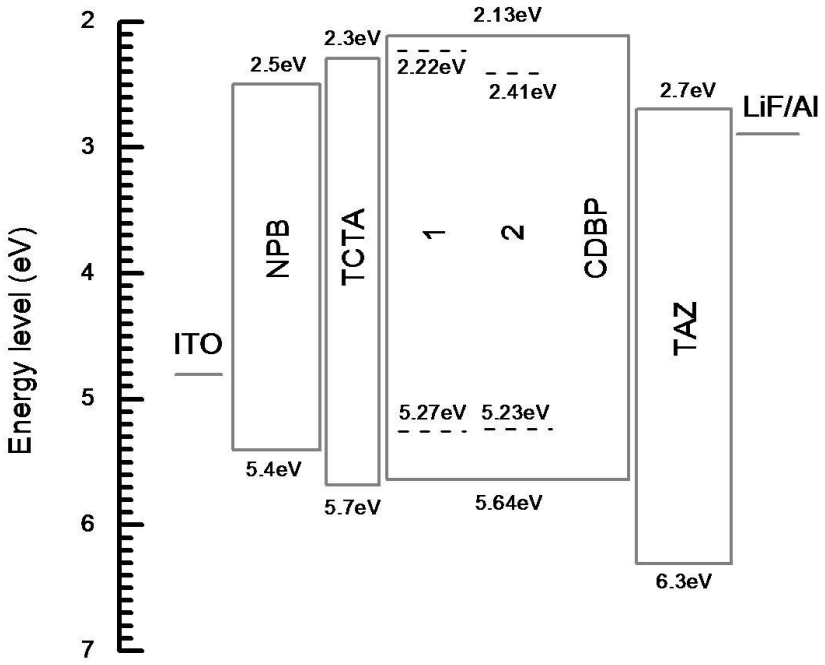


Fig. S6 The energy diagram of devices.

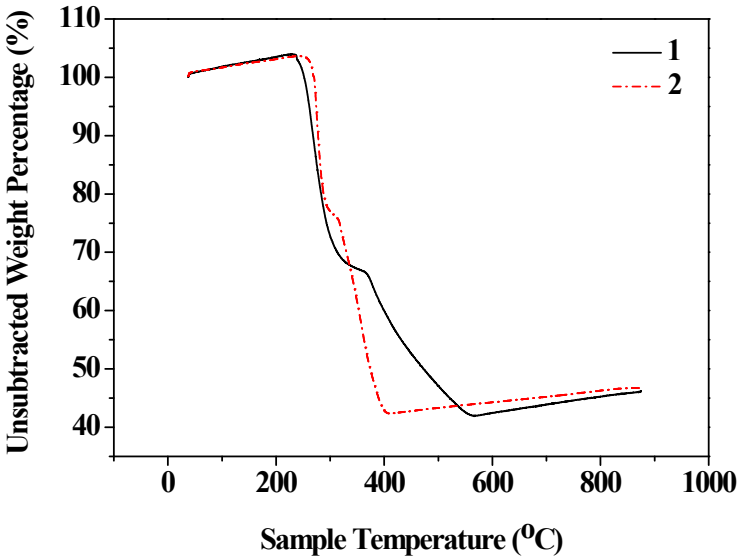


Fig. S7 The TGA curves of **1** and **2**.