Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.
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Supporting Information

Highly Efficient Single Emissive Layer Orange and Two-Element White Organic Light-Emitting Diodes by Solution Processe

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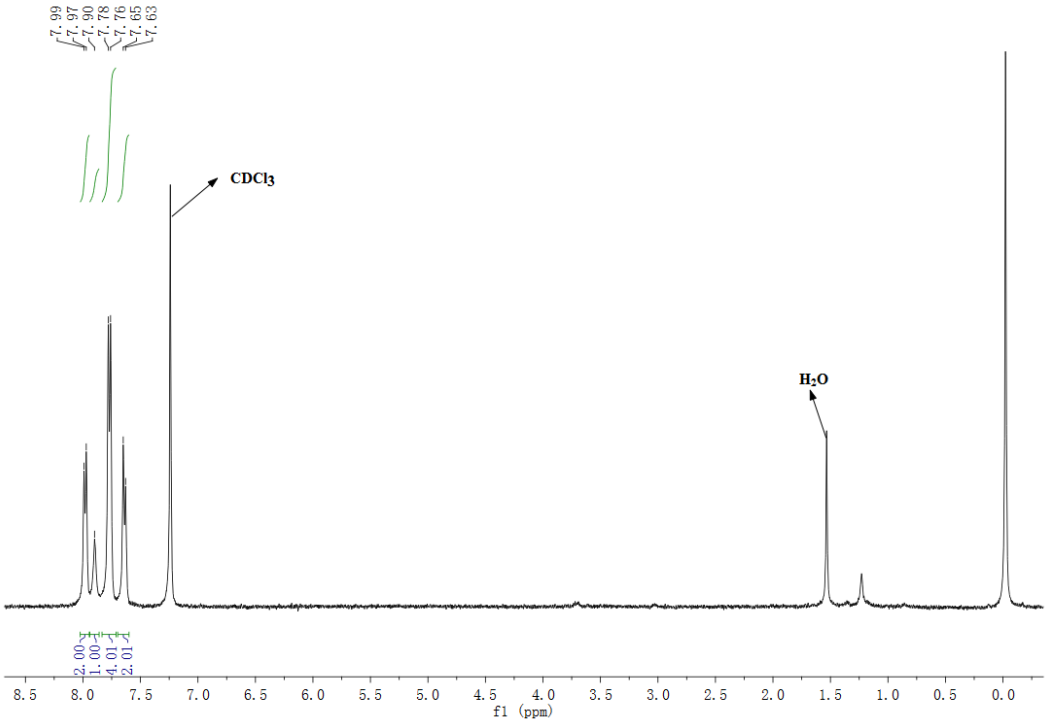
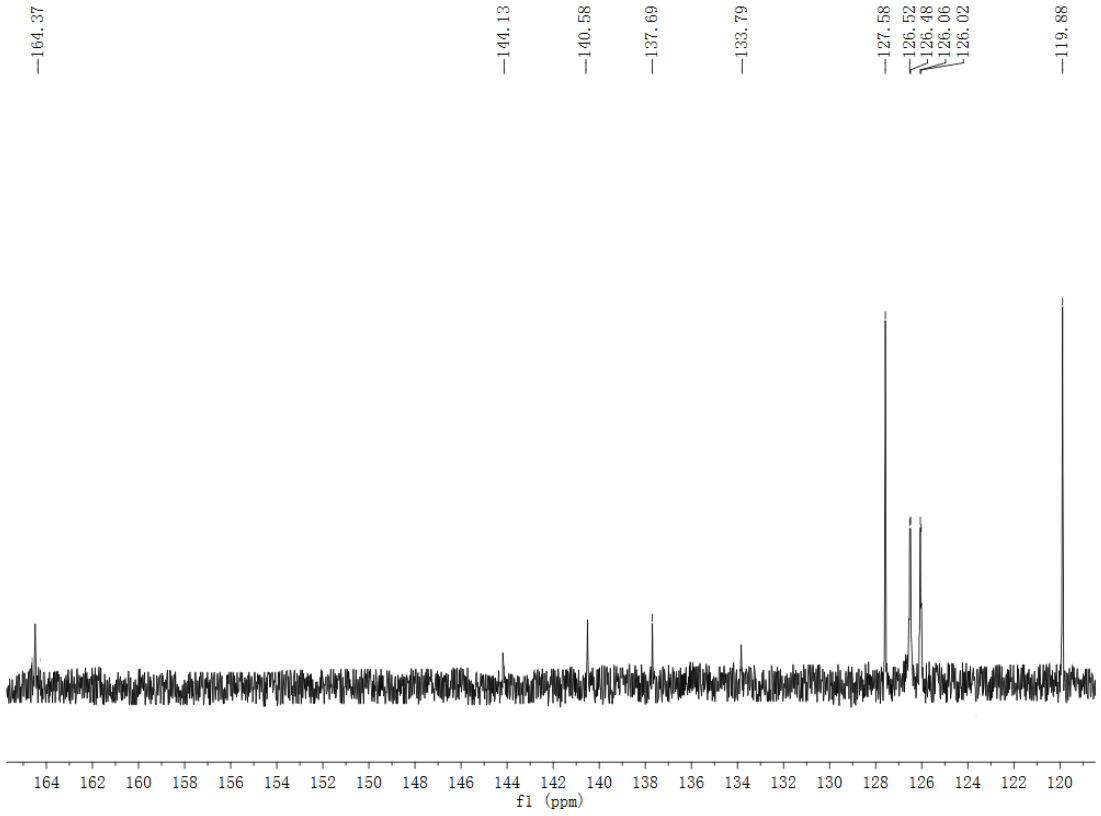
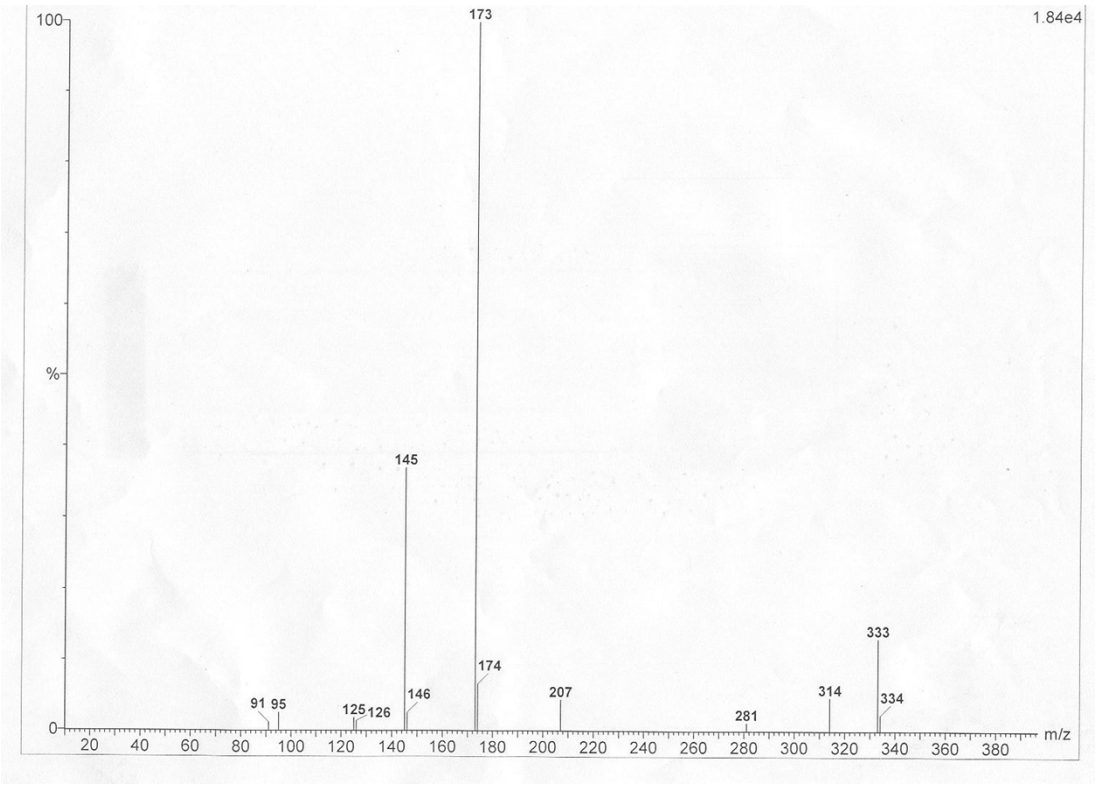
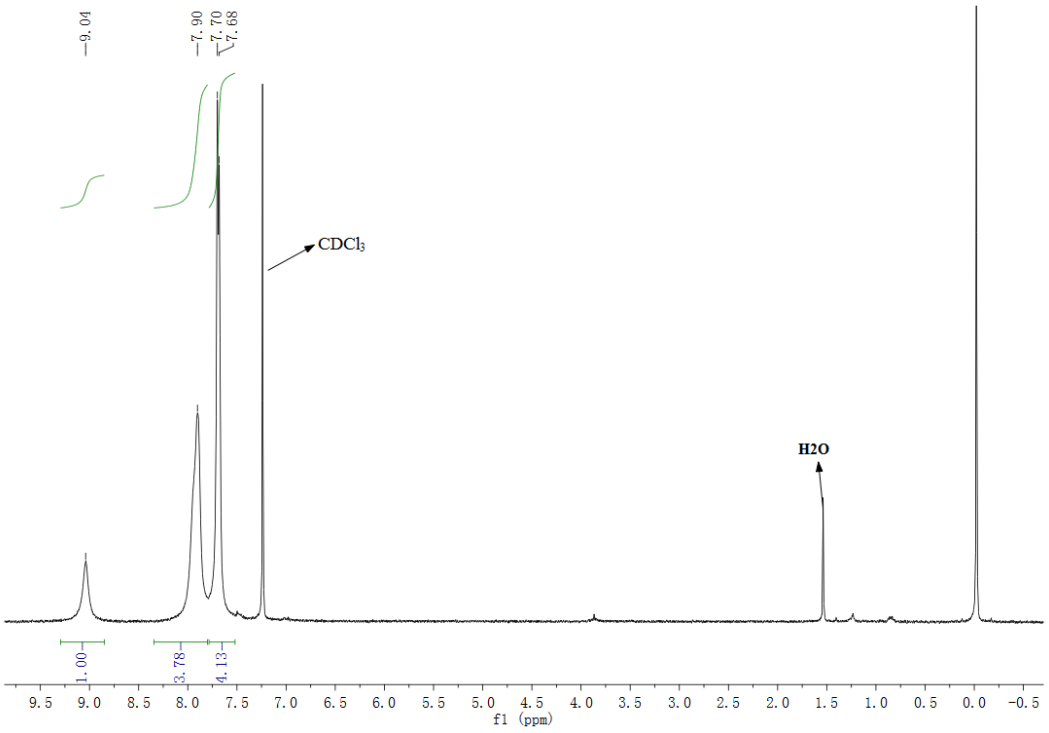
^{1}HNMR, ^{13}CNMR and MS(EI) of **1**:







^{1}HNMR, ^{13}CNMR and MS(EI) of **2**: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7.68
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H2O
1.00
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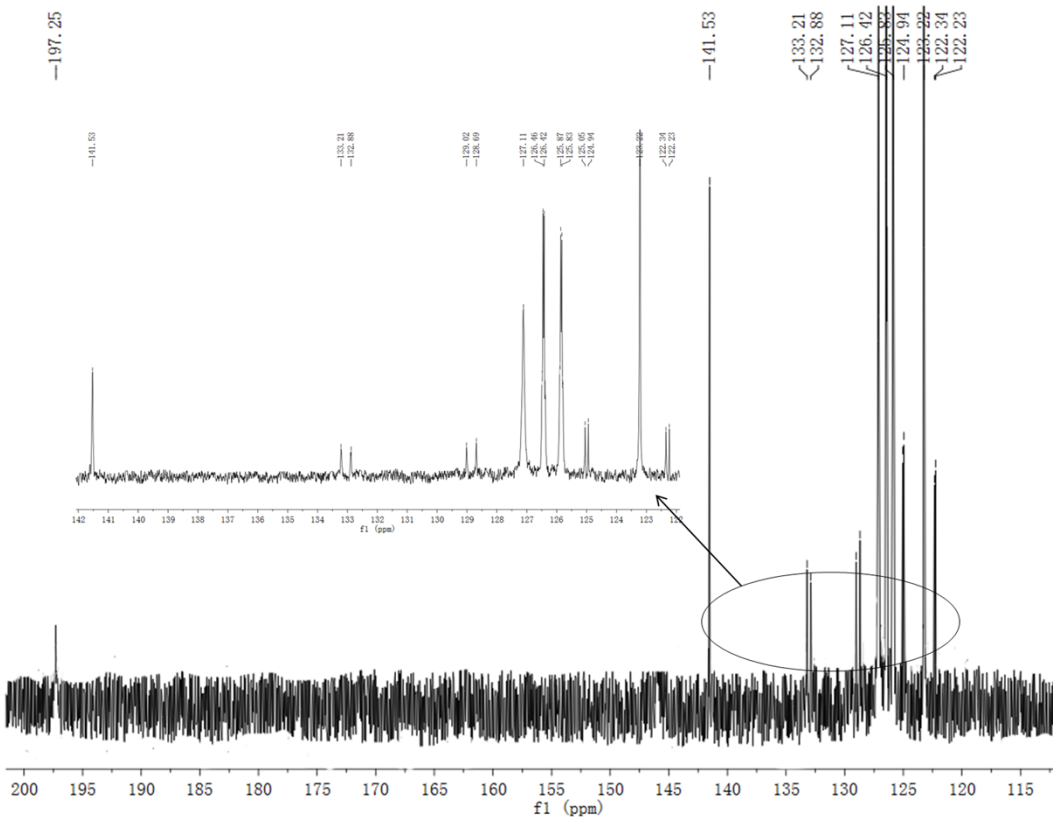
f1 (ppm)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132.88
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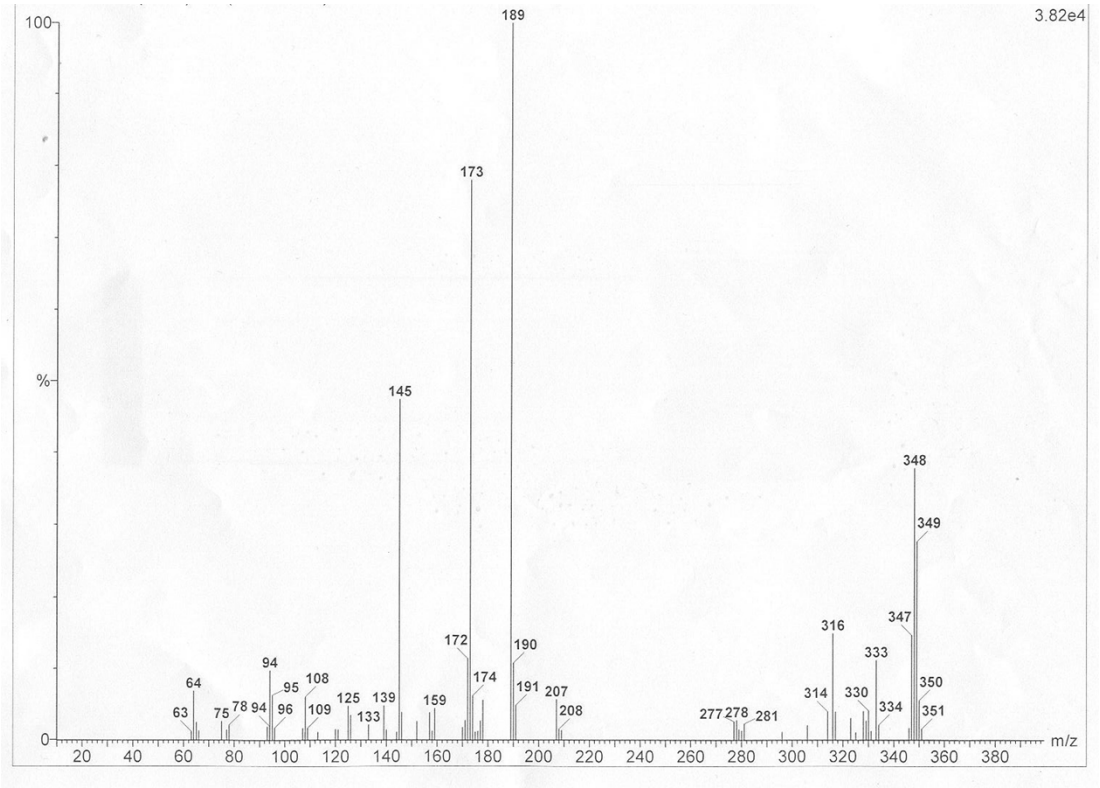
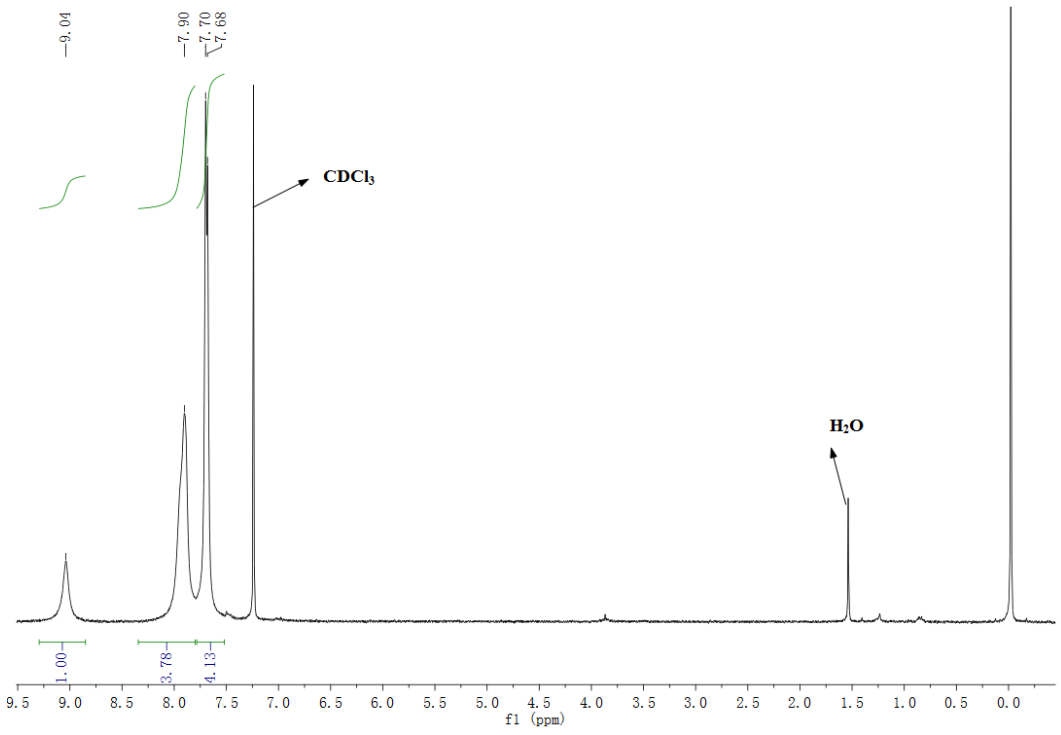
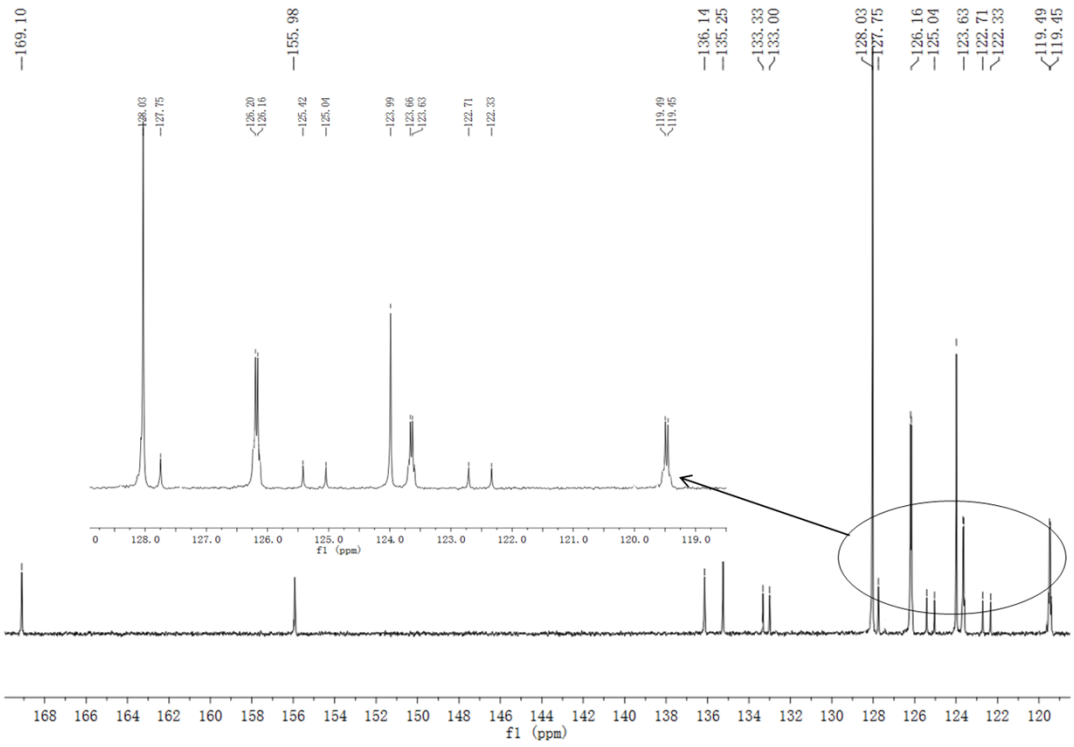
122.23
f1 (ppm)



^{1}HNMR, ^{13}CNMR and MS(EI) of **3**:

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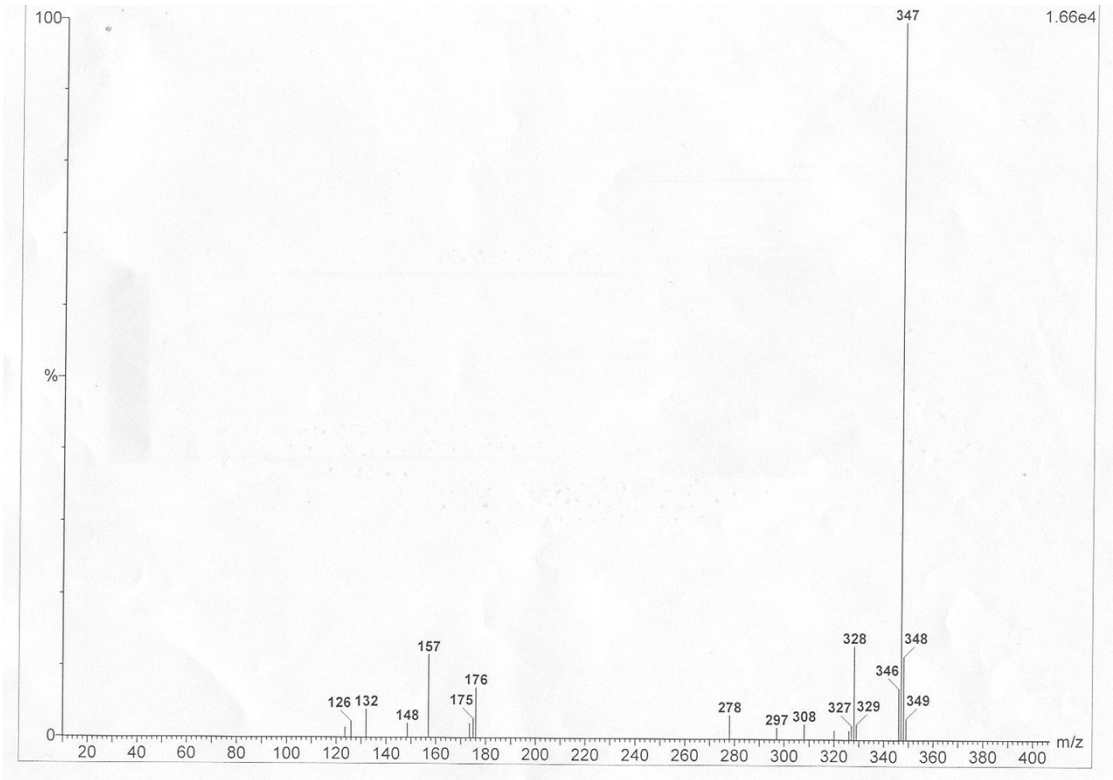
f1 (ppm)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%
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1.66e4
328
348
346
349
157
176
175
126
132
148
278
297
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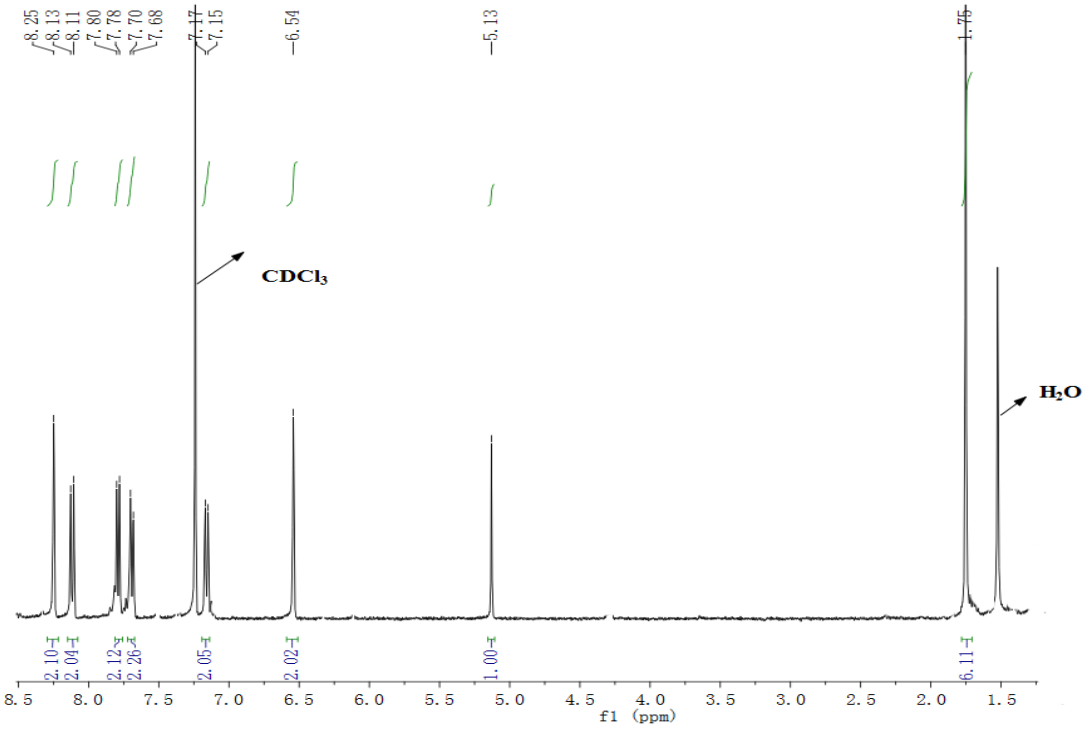
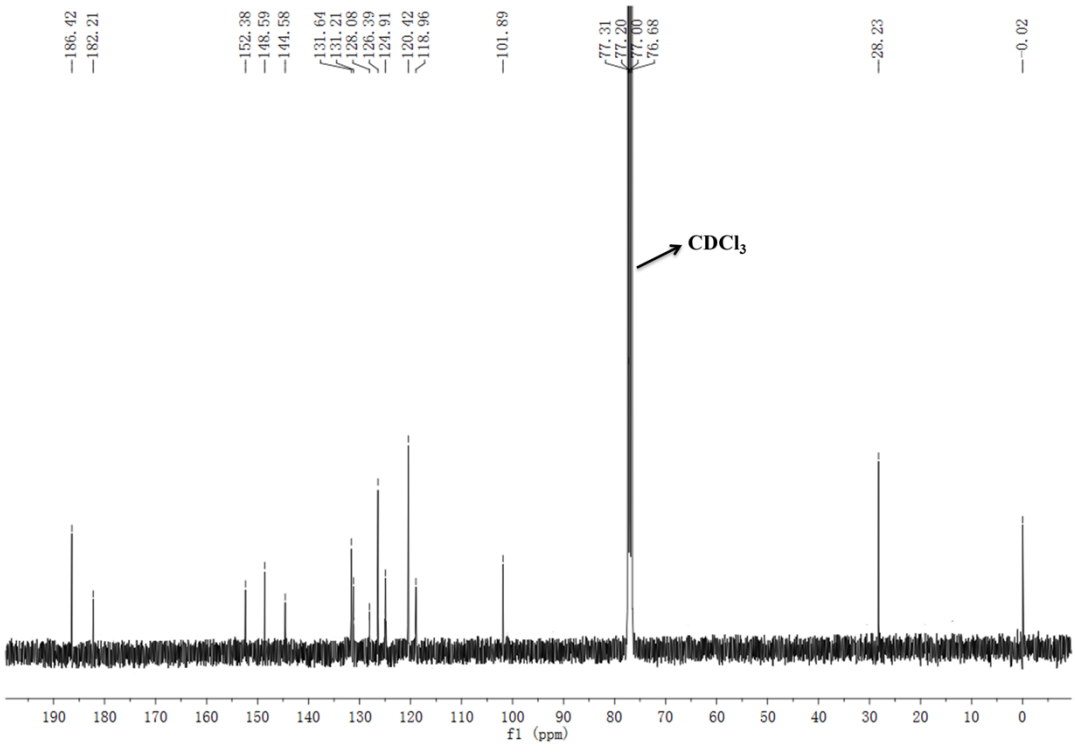
327
329
m/z

^{1}HNMR, ^{13}CNMR and MALDI-TOF mass spectra of $(CF_3BT\text{-}CF_3P)_2Ir(acac)$:





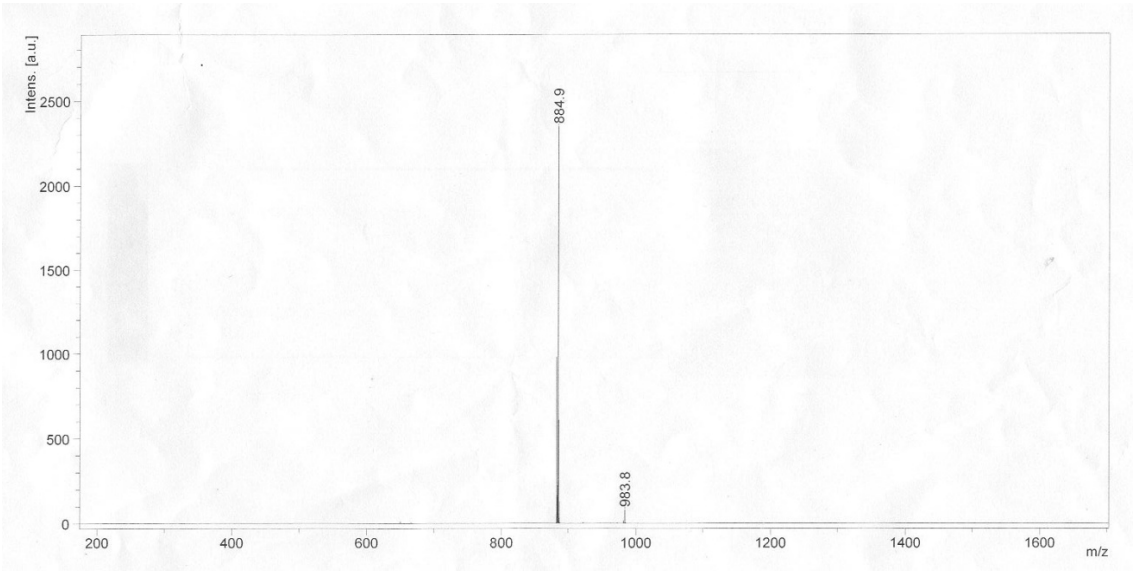


Fig. S1 The NMR spectra and mass spectra (MS) of all compounds.

Table S1. The photoluminescent quantum yields of $(CF_3BT\text{-}CF_3P)_2Ir(acac)$ under different doping concentrations in solid states.

Doping concentration [a]	20:1	10:1	5:1	0:1
Φ_P (%)	67	62	42	1.8

[a] The w/w concentration of PVK: iridium complex.

Table S2. Frontier molecular orbital (FMO) energies (*E*, eV) and compositions (%) of $(CF_3BT\text{-}CF_3P)_2Ir(acac)$ in the lowest-triplet excited state in the gas phase under vacuum.

FMO[a]	*E* (eV)	MO composition (%)[b]				Assignment
		Ir	PBT-1	PBT-2	acac	
L	–2.73	4	94	1	1	π*(PBT-1)
H	–5.70	40	33	21	6	d(Ir)+π(PBT-1+ PBT-2)
H−1	–5.95	30	8	7	55	d(Ir)+π(acac)
H−2	–6.35	12	52	13	23	d(Ir)+π(PBT-1+ PBT-2+acac)

[a] H=HOMO, L=LUMO, H−1=HOMO−1, H−2=HOMO−2. [b] PBT=2-phenyl benzothiazole.

Table S3. Calculated orbital transition analyses based on the geometry optimization of the lowest-lying triplet state.

State	Configuration [a]	Assignment[b]	MLCT[c] (%)
S_0-T_1	H→L(22%)	d(Ir)+π(PBT-1+ PBT-2) →π*(PBT-1)/MLCT/LLCT/IL	23.5
	H−1→L(55%)	d(Ir)+π(acac) →π*(PBT-1)/MLCT/LLCT	
	H−2→L(16%)	d(Ir)+π(PBT-1+PBT-2+acac)→π*(PBT-1)/MLCT/LLCT/IL	

[a] H=HOMO, L=LUMO, H−1=HOMO−1, H−2=HOMO−2. [b] PBT=2-phenyl benzothiazole. MLCT, LLCT and IL denote metal-to-ligand charge transfer, ligand-to-ligand charge transfer and intraligand, respectively. [c] $MLCT(\%) = \sum_{m,n}[C_I(m \to n)]^2(\%(M)_m - \%(M)_n)$,[1] where $\%(M)_{m,n}$ is the molecular orbital (MO) composition contributed from the metal to the orbital involved in the transition model of MO(m)→MO(n), C_I(m→n) is the corresponding coefficients of the I-th eigenvector of the configuration interaction (CI) matrix, so $[C_I(m \to n)]^2$ is the contribution of this electron transition model to the $S_0 \to T_1$ transition.

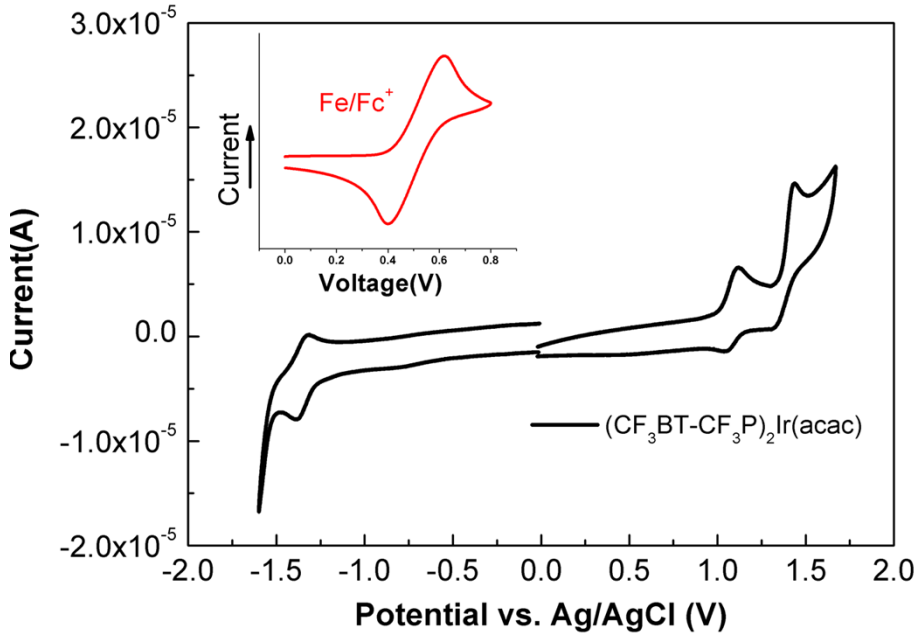


Fig. S2 Cyclic voltammogram of $(CF_3BT\text{-}CF_3P)_2Ir(acac)$ in CH_2Cl_2 with 0.1 M Bu_4NPF_6 as the electrolyte at a potential scan rate of 30 mV s^{-1}. The inset shows the redox curve of ferrocene. The first oxidation peak was used to calculate the HOMO level of $(CF3BT\text{-}CF3P)_2Ir(acac)$.

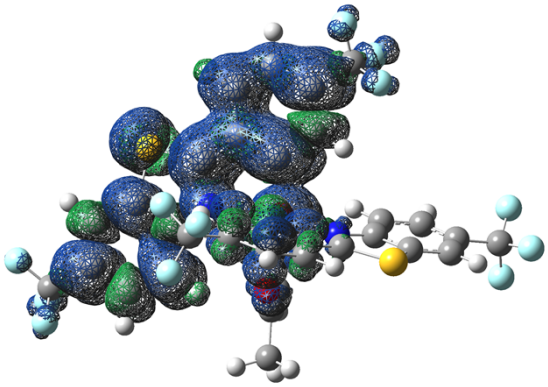


Fig. S3 The spin density of the triplet electronic configuration of $(CF_3BT\text{-}CF_3P)_2Ir(acac)$ (the blue balloons indicate regions where the spin density is positive and the green balloons the regions where the spin density is negative).

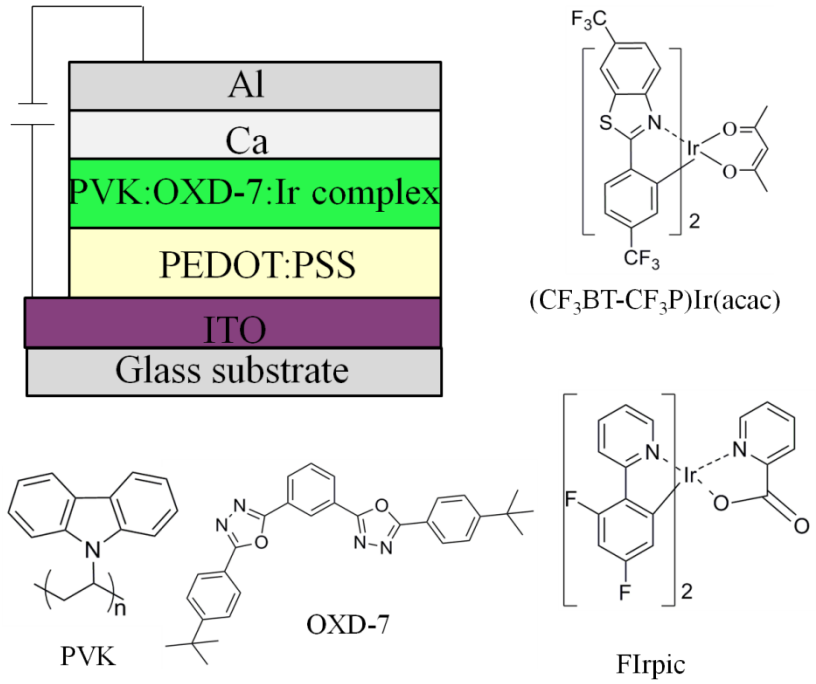


Fig. S4 The device configuration of monochromatic orange OLEDs and two−element WOLEDs together with the molecular structures of compounds used in these devices.

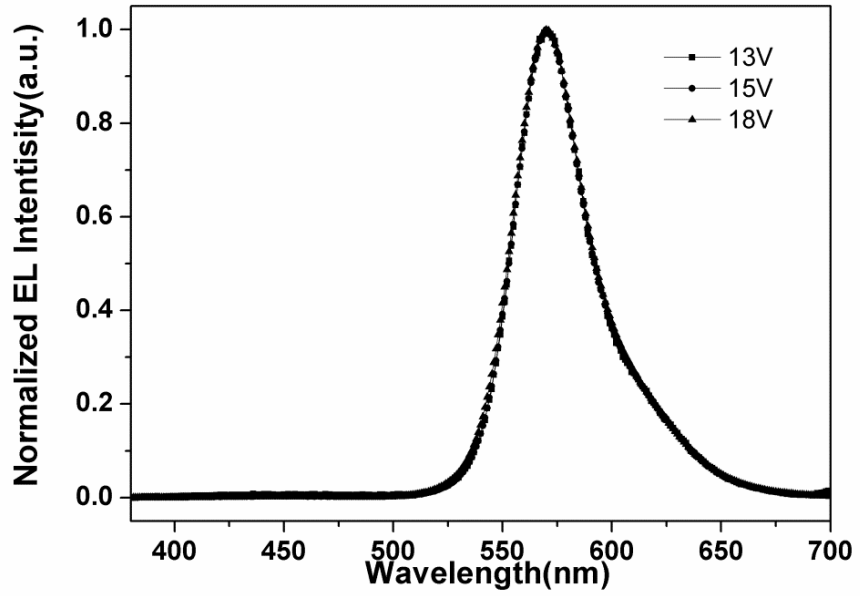


Fig. S5 The EL spectra of device A under various driving voltages.

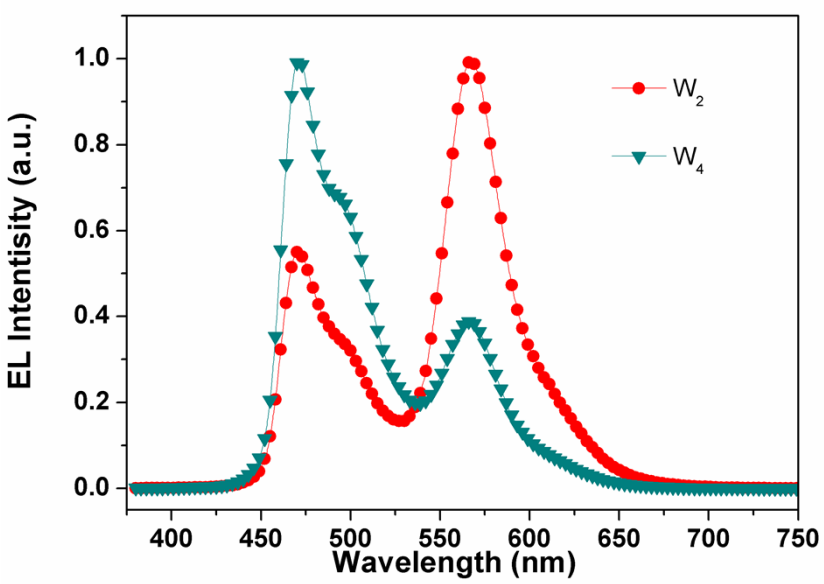


Fig. S6 The EL spectrum of W_2 and W_4 at 12 V.

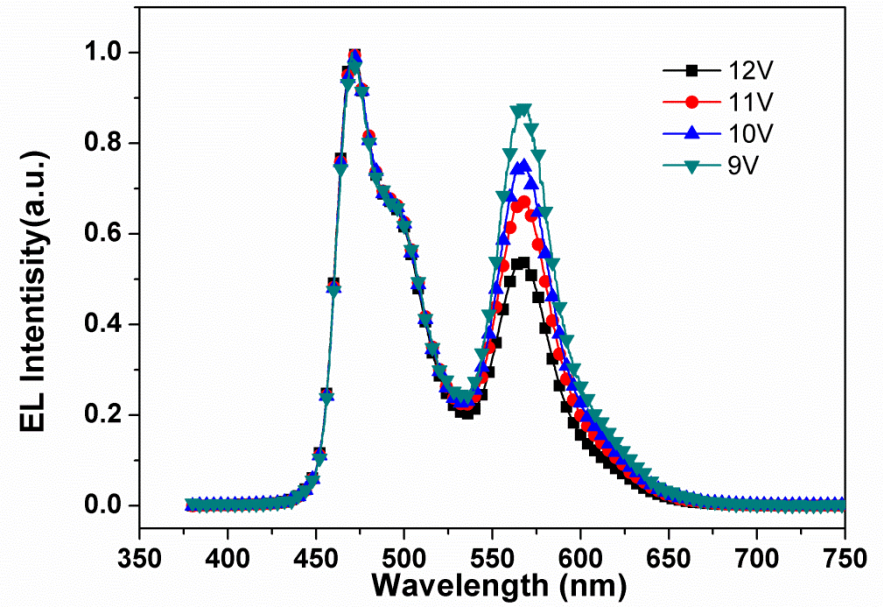


Fig. S7 The EL spectra of device W_3 under various driving voltages.

References

1 S. I. Gorelsky and A. B. P. Lever, *Can. J. Anal. Sci. Spectr.*, 2003, **48**, 93.