

Supporting Information

Syntheses, photoluminescence and electroluminescence of four heteroleptic iridium complexes with 2-(5-phenyl-1,3,4-oxadiazol-2-yl)-phenol derivatives as ancillary ligands

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Table S1 Selected bond lengths (Å) and angles (°) for **Ir1** and **Ir3**.

Fig. S1 TGA thermograms of **Ir1** - **Ir4**.

²⁰ **Fig. S2** Relative emission spectra of complexes **Ir1** - **Ir4** in degassed dichloromethane at 77 K.

Fig. S3 Cyclic voltammograms of complexes **Ir1**-**Ir4** in the negative range.

Fig. S1 The ¹³C-NMR spectra of **Ir1** in acetone-*d*₆.

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Fig. S2 The ¹³C-NMR spectra of **Ir2** in acetone-*d*₆.

Fig. S3 The ¹³C-NMR spectra of **Ir3** in acetone-*d*₆.

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Fig. S4 The ¹³C-NMR spectra of **Ir4** in acetone-*d*₆.

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Table S1 Selected bond lengths (Å) and angles (°) for **Ir1** and **Ir3**.

Ir1					
Ir(1)-C(39)	1.967(8)	Ir(1)-C(51)	1.977(7)	Ir(1)-N(5)	2.051(6)
Ir(1)-N(8)	2.054(6)	Ir(1)-N(6)	2.130(6)	Ir(1)-O(3)	2.150(5)
C(39)-Ir(1)-C(51)	88.2(3)	C(39)-Ir(1)-N(5)	94.5(3)	C(51)-Ir(1)-N(5)	80.8(3)
C(39)-Ir(1)-N(8)	80.5(3)	C(51)-Ir(1)-N(8)	94.9(2)	N(5)-Ir(1)-N(8)	173.5(2)
C(39)-Ir(1)-N(6)	175.3(2)	C(51)-Ir(1)-N(6)	96.2(2)	N(5)-Ir(1)-N(6)	88.0(2)
N(8)-Ir(1)-N(6)	97.3(2)	C(39)-Ir(1)-O(3)	92.2(2)	C(51)-Ir(1)-O(3)	174.5(2)
N(5)-Ir(1)-O(3)	93.8(2)	N(8)-Ir(1)-O(3)	90.5(2)	N(6)-Ir(1)-O(3)	83.7(2)

Ir3					
C(1)-Ir(1)	1.990(12)	C(13)-Ir(1)	2.006(11)	Ir(1)-N(3)	2.042(10)
Ir(1)-N(4)	2.055(10)	Ir(1)-N(1)	2.097(9)	Ir(1)-O(1)	2.145(8)
C(1)-Ir(1)-C(13)	90.4(5)	C(1)-Ir(1)-N(3)	80.5(5)	C(13)-Ir(1)-N(3)	91.6(5)
C(1)-Ir(1)-N(4)	95.9(5)	C(13)-Ir(1)-N(4)	81.0(5)	N(3)-Ir(1)-N(4)	171.8(4)
C(1)-Ir(1)-N(1)	92.2(4)	C(13)-Ir(1)-N(1)	176.5(5)	N(3)-Ir(1)-N(1)	91.1(4)
N(4)-Ir(1)-N(1)	96.4(4)	C(1)-Ir(1)-O(1)	174.3(4)	C(13)-Ir(1)-O(1)	91.8(4)
N(3)-Ir(1)-O(1)	94.2(4)	N(4)-Ir(1)-O(1)	89.6(4)	N(1)-Ir(1)-O(1)	85.8(4)

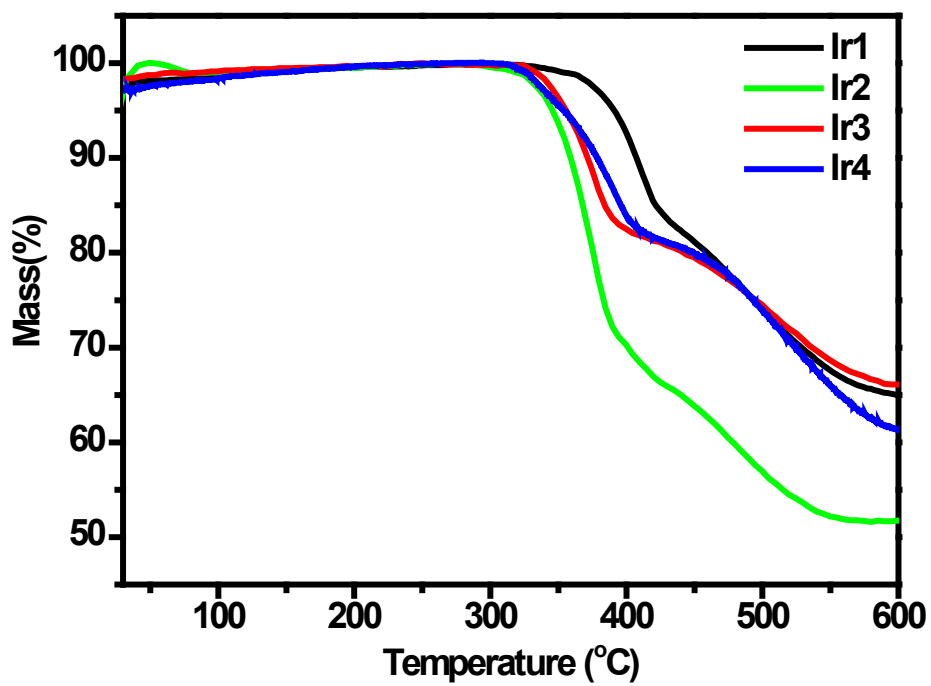
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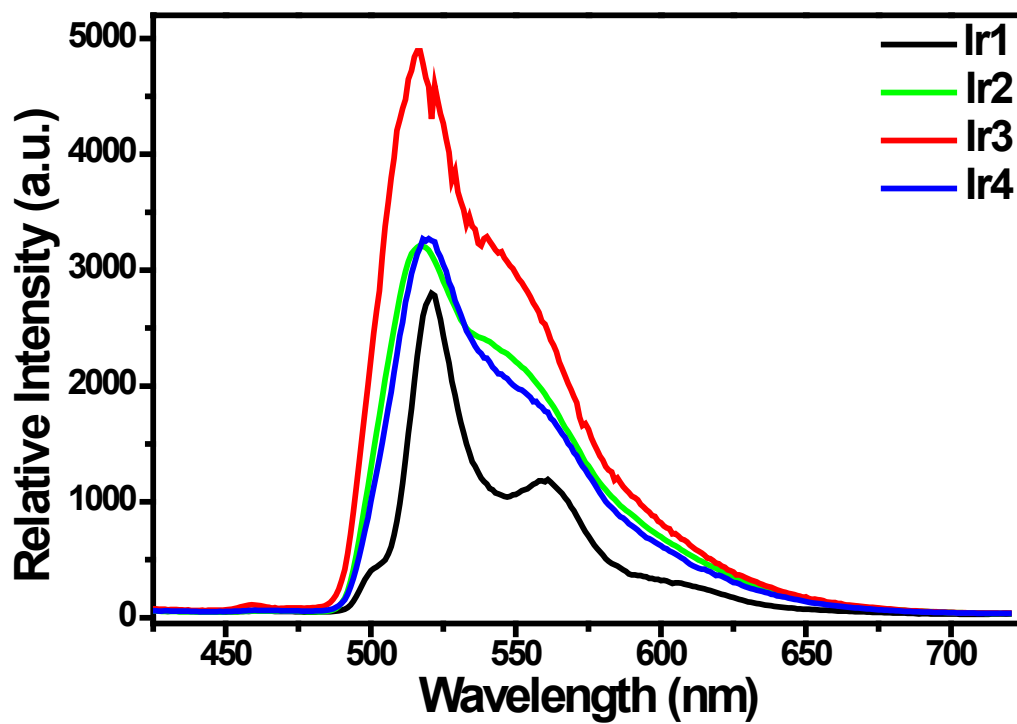
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Fig. S1 TGA thermograms of Ir1 - Ir4.

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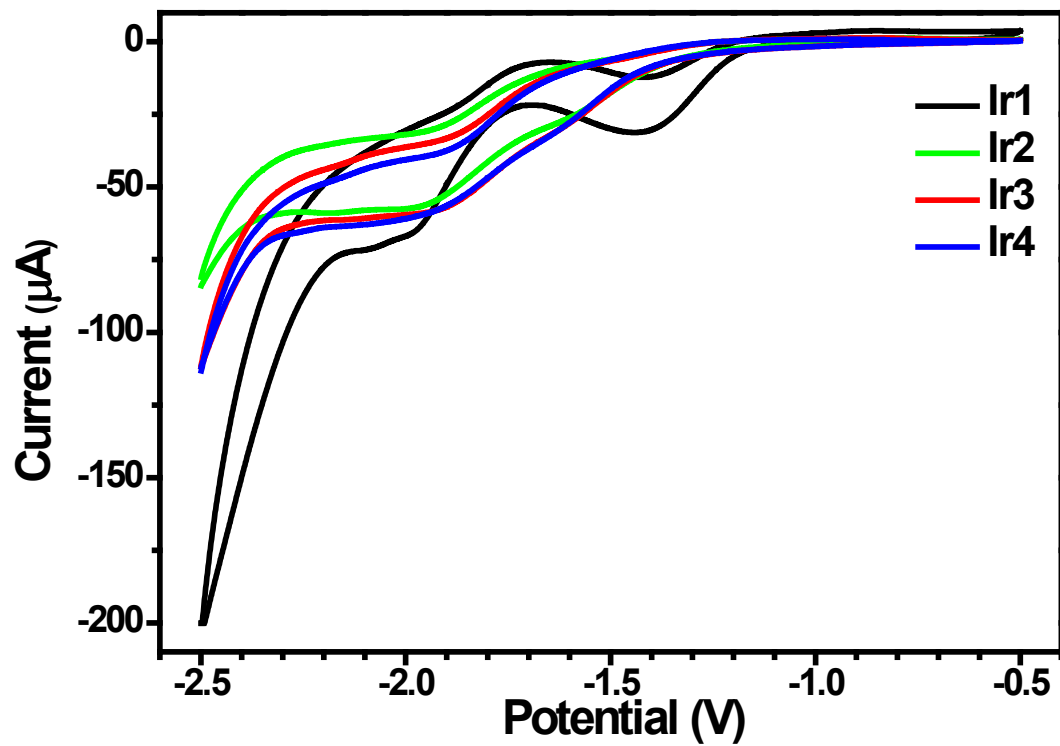


10 **Fig. S2** Relative emission spectra of complexes Ir1 - Ir4 in degassed dichloromethane at 77 K.

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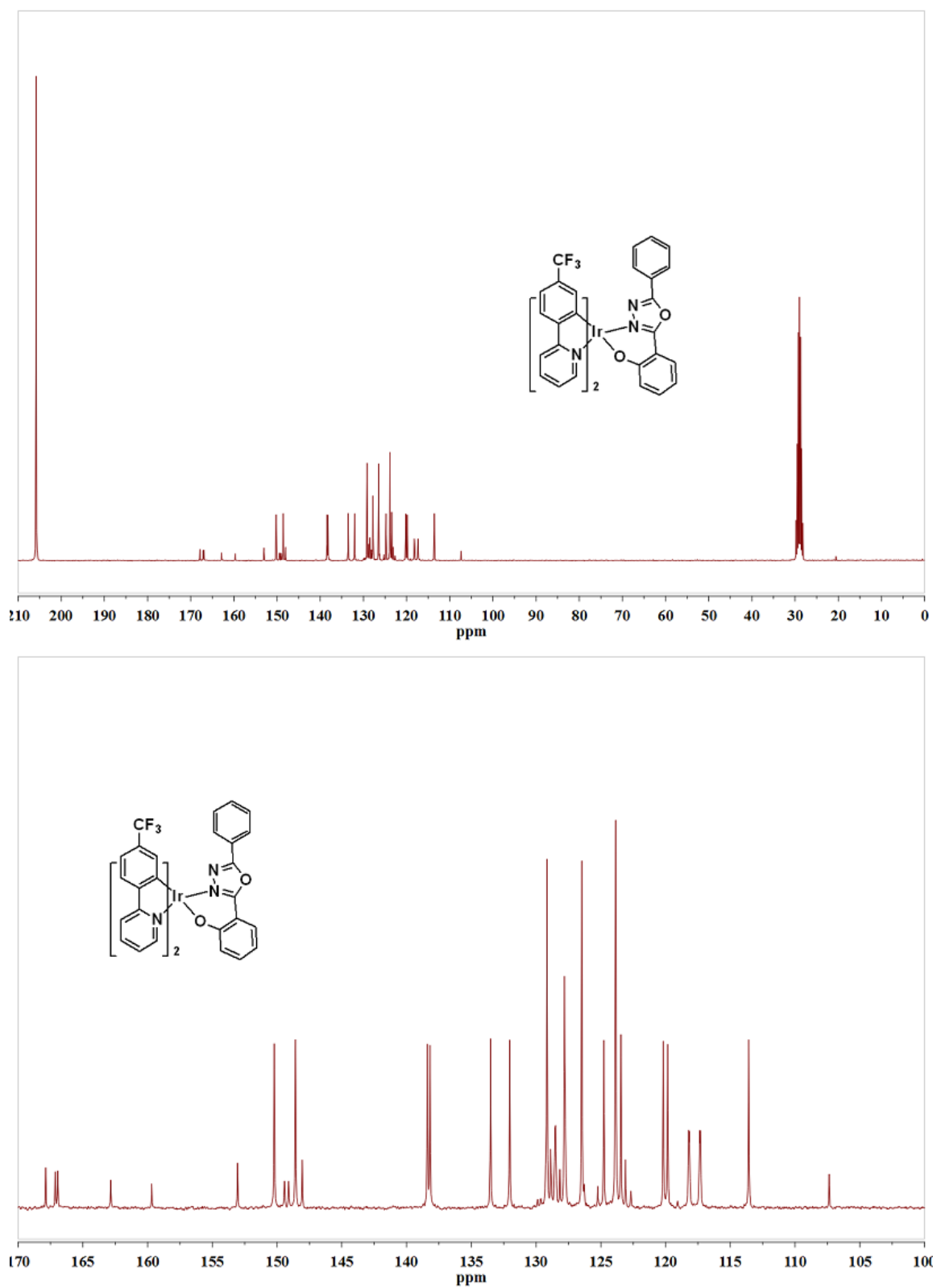
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10 **Fig. S3** Cyclic voltammograms of complexes **Ir1-Ir4** in the negative range.

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Fig. S4 The ^{13}C -NMR spectra of **Ir1** in $\text{acetone-}d_6$.

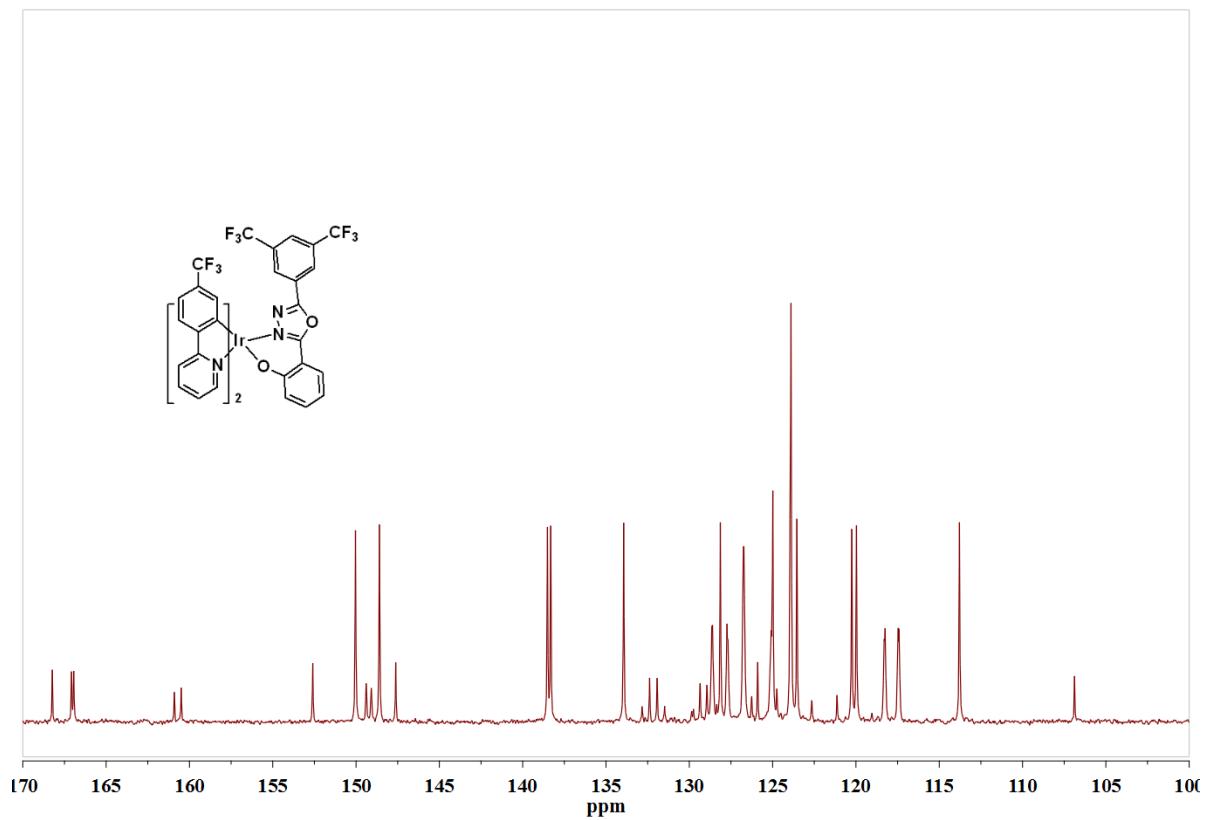
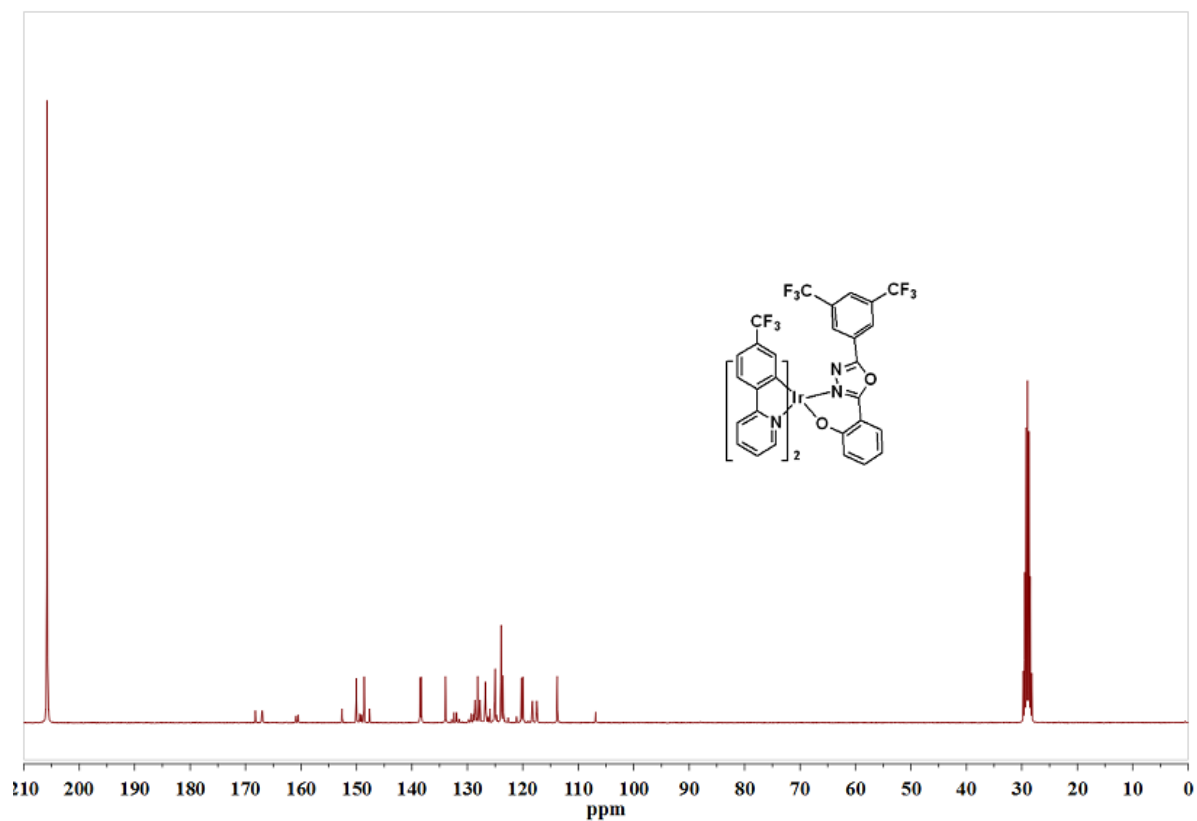
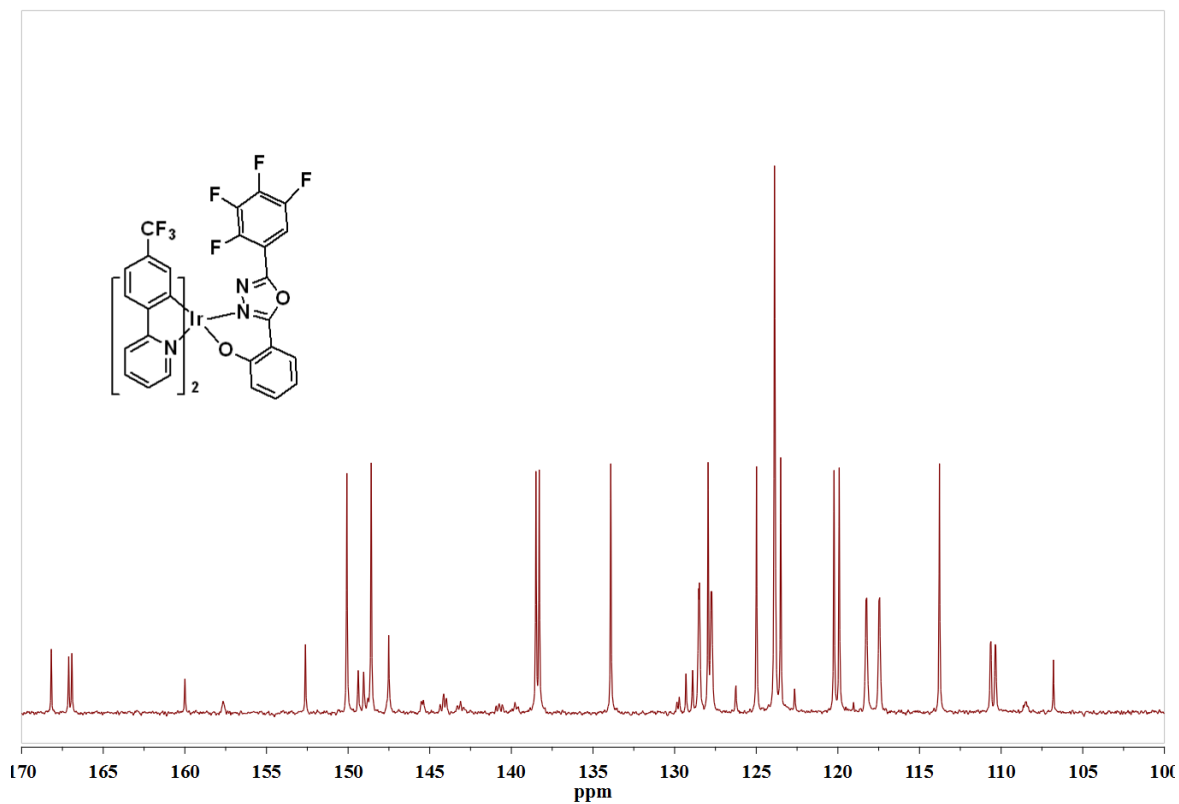
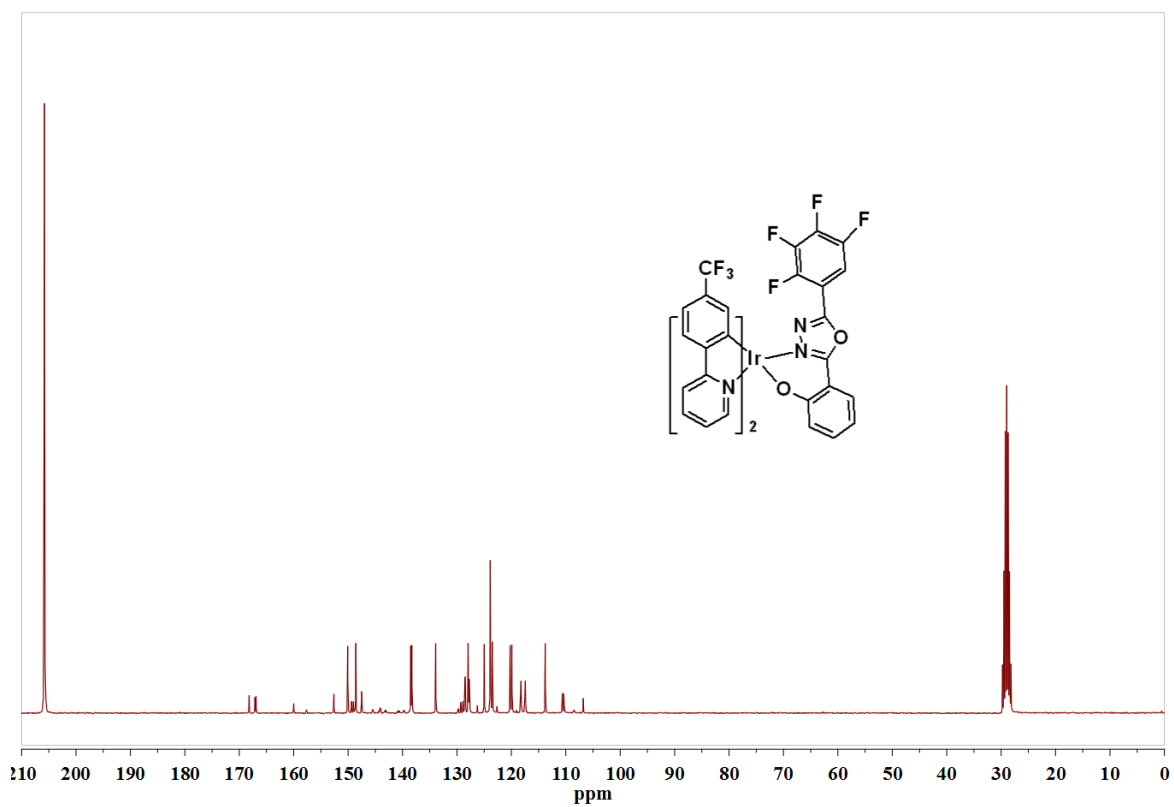
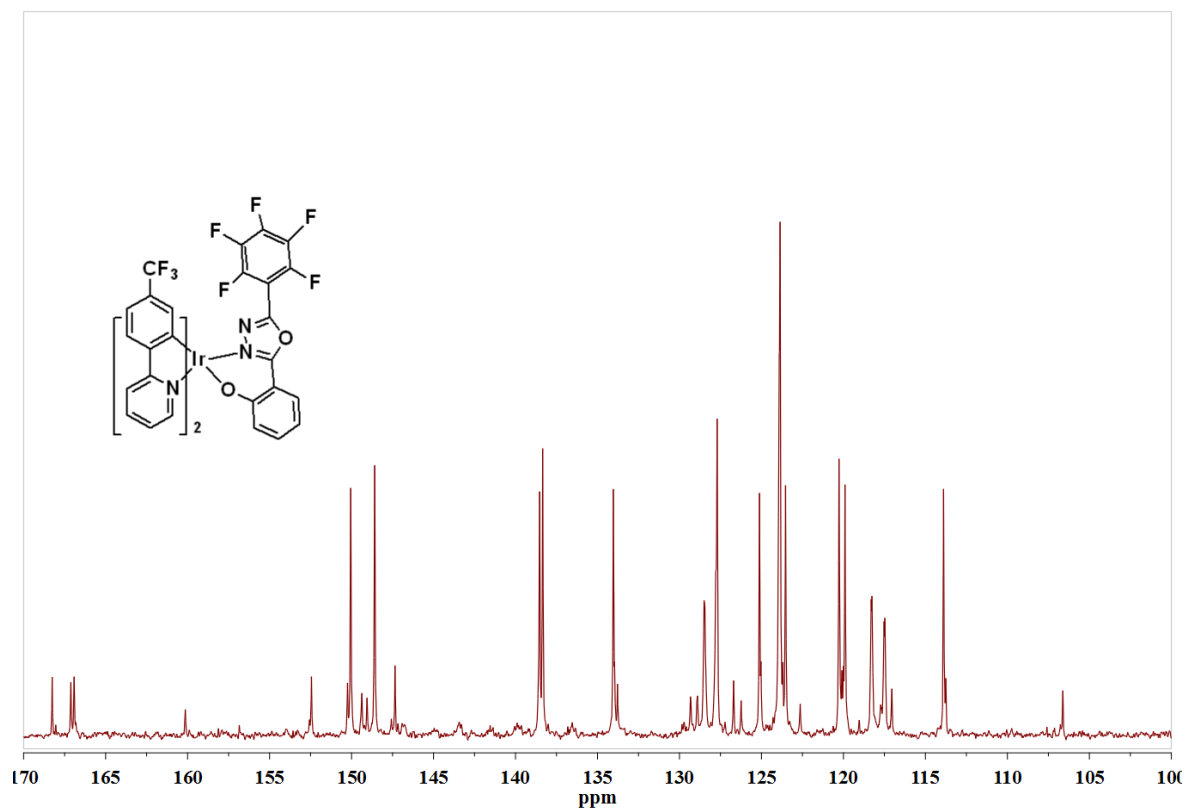
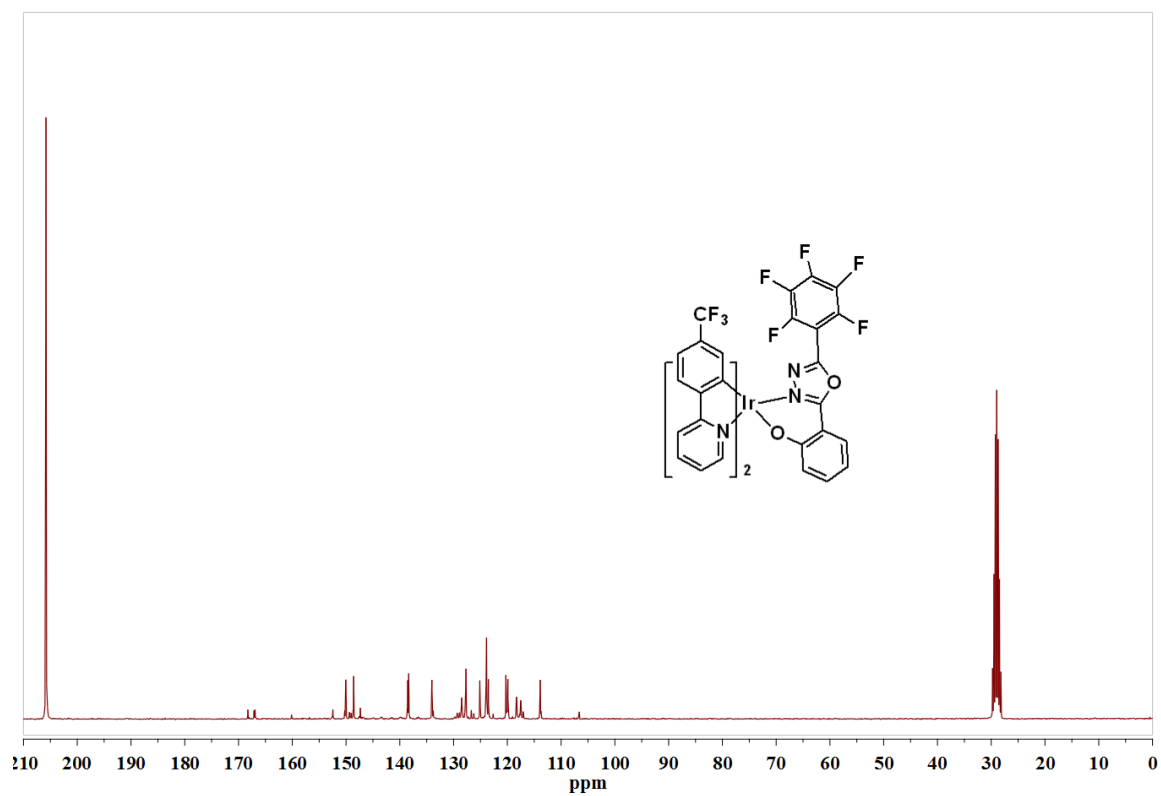


Fig. S5 The ^{13}C -NMR spectra of **Ir2** in acetone- d_6 .



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Fig. S6 The ^{13}C -NMR spectra of **Ir3** in acetone- d_6 .



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Fig. S7 The ^{13}C -NMR spectra of Ir4 in acetone- d_6 .