Supporting Information

Photoluminescence and electroluminescence of iridium(III) complexes with 2',6'-bis(trifluoromethyl)-2,4'-bipyridine and 1,3,4-oxadiazole/1,3,4-thiadiazole derivatives ligands

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Table S1. Parameters associated with the single crystal diffraction data collection for **Ir1**

	Ir1
Formula	$C_{39}H_{18}F_{15}IrN_6O_2$
Formula weight	1079.79
T (K)	296(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	11.6755(5)
b (Å)	13.7860(5)
c (Å)	24.0468(9)
α (deg)	90.00
β (deg)	93.2230(10)
γ (deg)	90.00
V (Å^3)	3864.4(3)
Z	4
ρ_{calcd} (g/cm^3)	1.856
μ (Mo Kα) (mm^{-1})	3.573
F (000)	2088
Range of transm factors (deg)	1.70-25.01
Reflns collected	21215
Unique(R_{int})	6808(0.0243)
$R_1{}^a$, $wR_2{}^b$ [I > 2s(I)]	0.0240, 0.0579
$R_1{}^a$, $wR_2{}^b$ (all data)	0.0306, 0.0604
GOF on F^2	1.093
CCDC number	1455234

$R_1{}^a = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $wR_2{}^b = [\Sigma w(F_o{}^2 - F_c{}^2)^2/\Sigma w(F_o{}^2)]^{1/2}$

GOF = $[(\Sigma w|F_o| - |F_c|)^2/(N_{obs} - N_{param})]^{1/2}$.

Table S2. The table of selected bond lengths and angles of **Ir1.**

Selected Bond	Bond Length (Å)	Selected Angle	Bond Angle (°)
Ir(1)-C(1)	2.038(3)	C(13)-Ir(1)-C(1)	95.70(13)
Ir(1)-C(13)	2.034(3)	C(13)-Ir(1)-N(4)	105.23(12)
Ir(1)-N(2)	2.098(3)	C(1)-Ir(1)-N(4)	80.66(12)
Ir(1)-N(4)	2.044(3)	C(13)-Ir(1)-N(6)	80.72(13)
Ir(1)-N(6)	2.045(3)	C(1)-Ir(1)-N(6)	103.74(12)
Ir(1)-O(1)	2.102(2)	N(4)-Ir(1)-N(6)	172.38(11)
		C(13)-Ir(1)-N(2)	93.05(12)
		C(1)-Ir(1)-N(2)	169.25(11)
		N(4)-Ir(1)-N(2)	91.04(11)
		N(6)-Ir(1)-N(2)	83.81(11)
		C(13)-Ir(1)-O(1)	172.22(12)
		C(1)-Ir(1)-O(1)	84.90(11)
		N(4)-Ir(1)-O(1)	82.53(11)
		N(6)-Ir(1)-O(1)	91.59(11)
		N(2)-Ir(1)-O(1)	87.23(10)

Table S3. Electrochemical data of **Ir1** and **Ir2**.

Complex	E_{ox} (V) [a]	E_{red}(V)	HOMO(eV) [b]	LUMO(eV)	E_g(eV)
Ir1	0.96	-1.40	-5.59	-2.84	2.75
Ir2	0.89	-1.40	-5.57	-3.09	2.48

[a] Oxidation potential measured in solution at 50 mV/s.

[b] The HOMO energy levels were calculated from the equation: HOMO (eV) = E_{ox}-$E^{+}_{Fc/Fc}$ + 4.8.

Table S4. Percentage distributions of HOMO and LUMO in **Ir1** and **Ir2**.

Complex	Orbital	Energy/eV (Calculated)	E_{gap}/eV (Calculated)	Composition (%)		
				Ir	BTBP	LX
Ir1	HOMO	-5.566	3.370	14.70	5.36	79.95
	LUMO	-2.196		1.94	69.39	28.67
Ir2	HOMO	-5.544	3.186	15.02	5.23	79.65
	LUMO	-2.357		0.96	9.23	89.81