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# Electronic Supplementary Information

Towards high performance solution-processed orange organic lightemitting devices: precisely-adjusting properties of Ir(III) complexes by reasonably engineering the asymmetric configuration with second functionalized cyclometalating ligands

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## **General information**

Commercial chemicals were directly used without purification. The <sup>13</sup>C NMR and <sup>1</sup>H NMR spectra were measured in CDCl<sub>3</sub> on a Bruker Avance 400 MHz spectrometer. Mass spectral (MS) were measured on the WATERS I-Class VION IMS QTof equipment. The thermogravimetric analyses were conducted on a NETZSCH STA 409C instrument under N<sub>2</sub> at a heating rate of 20 K min<sup>-1</sup>. UV-vis absorption spectra were measured on a HITACHI U-3010 spectrophotometer. PL spectra and emission lifetimes were recorded on an Edinburgh Instruments Ltd (FLSP920) fluorescence spectrophotometer. The solution PLQYs were measured at room temperature using fac-( $Ir(ppy)_3$ ) (PLQY = 0.97) as the reference standard.<sup>1</sup> Cyclic voltammetry curves were recorded on a Princeton Applied Research (PARSTAT 2273, Advanced Electrochemical System) equipment in CH<sub>3</sub>CN solutions containing *n*-Bu<sub>4</sub>NPF<sub>6</sub> (0.1 M) as the supporting electrolyte under a N<sub>2</sub> atmosphere, and internal calibrated with ferrocene/ferrocenium (Fc/Fc<sup>+</sup>) couple. The HOMO and LUMO levels were calculated on the basis of the onset of oxidation potential  $(E_{ox})$  and reduction potential  $(E_{red})$  according to  $E_{\text{HOMO}} = -(E_{\text{ox}} + 4.8) \text{ eV} \text{ and } E_{\text{LUMO}} = -(E_{\text{red}} + 4.8) \text{ eV}.$ 

## X-ray diffraction investigation

The single crystals of Ir(III) complexes **SIrS** and **SIrB** were cultivated by slowly diffusing their CHCl<sub>3</sub> solutions into hexane at room temperature. The X-ray diffraction data were collected using a Rigaku Saturn 724 diffractometer on a rotating anode (Mo-K radiation, 0.71073 Å) at 173 K. The structure was solved and refined by the direct method using SHELXS-2015 and refined with Olex2.<sup>2-4</sup>

### **Theoretical computation**

Density functional theory (DFT) and time dependent-DFT (TD-DFT) calculations were carried out for theoretical analysis. <sup>5, 6</sup> Non-metal atoms of C, H, N, O, and S were calculated using B3LYP/6-31G (d, p) basis set. The Ir atom was calculated using B3LYP/LanL2DZ basis set. The excitation properties were calculated by TD-DFT method based on optimized  $S_0$  geometries. The NTOs were calculated based on optimized  $T_1$  geometries. All calculations were carried out by using the Gaussian 09 program.<sup>7</sup>

# Charge mobility measurements

Hole-only and electron-only devices were fabricated in a configuration of ITO/MoO<sub>3</sub> (3 nm)/poly(ethylenedioxythiophene): poly(styrenesulfonate) (PEDOT:PSS) (20 nm)/Ir(III) complex (40 nm)/PEDOT: PSS (20 nm)/MoO<sub>3</sub> (3 nm)/Al (100 nm) and ITO/LiF (3 nm)/Ir(III) complex (40 nm)/LiF (3 nm)/Al (100 nm), respectively. The charge mobilities of these Ir(III) complexes were determined using the space-charge-limited current (SCLC) method by fitting current density–voltage (J-V) curves based on the Mott-Gurney law.

$$J = \frac{9\varepsilon_r \varepsilon_0 \mu V^2}{8d^3} \tag{1}$$

In the equation (1), *J* is the current density,  $\varepsilon_r$  is the relative dieletiric constant,  $\varepsilon_0$  is the permittivity of the free space ( $\varepsilon_0 = 8.85 \times 10^{-12}$  F m<sup>-1</sup>),  $\mu$  is the carrier mobility, *V* is the applied voltage, and *d* is the thickness of the film. Usually, the relative dieletiric constants of organic semiconductor materials are in the range from 2 to 4, thus the average dielectric constant  $\varepsilon_r = 3$  is used for calculations.

#### **OLED** fabrication and measurements

The ITO glass substrates were pre-cleaned and exposed to ultraviolet-ozone for *ca*. 10 min. Then PEDOT:PSS was spin-coated on the surface of ITO glass substrates to form a holeinjection layer, followed by the annealing at 120 °C for 30 min in the air. Emissive layers were form by spin-coating the chloroform solutions containing the TCTA host material doped with the Ir(III) complexes at different doping levels on the surface of the PEDOT:PSS layer, followed by annealing at 60 °C for 10 min. Other functional layers of TPBI, LiF, and Al cathode were deposited under vacuum condition. The operation voltages and efficiencies of the resultant devices were tested with the Keithley 2602 and Source Meter. The EL spectra were recorded with a PR650 Spectra Scan spectrometer. All measurements were carried out under ambient conditions.

Synthesis of ligand L-S



**Compound 1** To a solution (60 mL) of CH<sub>3</sub>COOH containing thianthrene (6.50 g, 30.0 mmol) at 0 °C, Br<sub>2</sub> (5.76g, 36.0 mmol) was added slowly with a dropping funnel. After the

addition of Br<sub>2</sub>, the reaction mixture was heated to 80 °C and stirred for 5 h. Then, after cooled to room temperature, the reaction mixture was washed with NaHSO<sub>3</sub> solution, and extracted with CH<sub>2</sub>Cl<sub>2</sub> several times. The combined organic layers were dried and concentrated before the purification on a silica column. The resultant product was obtained with 83.5% yield (7.35 g). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 7.63 (d, *J* = 2.0 Hz, 1H), 7.49–7.46 (m, 2H), 7.35–7.31 (m, 2H), 7.27–7.24 (m, 2H).

**Compound 2** To a mixture of compound 1 (2.00 g, 6.78 mmol), CH<sub>3</sub>COOH (60 mL), and CH<sub>2</sub>Cl<sub>2</sub> (25 mL), H<sub>2</sub>O<sub>2</sub> (30 %, 15 mL) was added before the reaction mixture was stirred at room temperature for 1 h. Then, the reaction mixture was heated at 90 °C for 36 h. After cooled to room temperature, the reaction mixture was poured into water (100 mL) and extracted with CH<sub>2</sub>Cl<sub>2</sub> several times. The combined organic layers were dried and concentrated before the purification on a silica column. The resultant product was obtained with 51.0% yield (1.24 g). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 8.37 (d, *J* = 1.6 Hz, 1H), 8.27–8.23 (m, 2H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.96–7.94 (m, 1H), 7.87–7.83 (m, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 140.69, 139.33, 139.07, 138.19, 136.71, 133.98, 133.88, 129.05, 128.82, 127.48, 126.16, 126.08.

**Compound 3** Under a N<sub>2</sub> atmosphere, the reaction mixture containing compound **2** (2.40 g, 6.70 mmol), potassium acetate (3.30 g, 33.7 mmol), Pd(dppf)Cl<sub>2</sub> (0.48 g, 0.66 mmol), *bis*(pinacolato)diboron (2.60 g, 10.0 mmol), and dioxane (50 mL) was stirred at 100 °C for 12 h. After cooled to room temperature, the reaction mixture was poured into water (50 mL) and extracted with  $CH_2Cl_2$  several times. The combined organic layers dried over anhydrous

 $Mg_2SO_4$ . After the removal of solvent, the residue was washed with petroleum ether several times and used as a reagent in the next synthesis step without further purification.

Ligand L-S Under a N<sub>2</sub> atmosphere, compound **3** (1.50 g, 3.60 mmol), 2-bromopyridine (0.62 g, 4.00 mmol), and Pd(PPh<sub>3</sub>)<sub>4</sub> (0.42 g, 0.36 mmol) were added to the mixture of THF (30 mL) and 2 M K<sub>2</sub>CO<sub>3</sub> (20 mL). The reaction mixture was heated to 110 °C and stirred for 12 h. After cooled to room temperature, the reaction mixture was poured into water (100 mL) and extracted with CH<sub>2</sub>Cl<sub>2</sub> several times. The combined organic layers were dried and concentrated before the purification on a silica column. The ligand was obtained with 62.5% yield (0.81 g). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 8.88 (d, *J* = 1.2 Hz, 1H), 8.77 (d, *J* = 4.4 Hz, 1H), 8.49 (dd, *J* = 1.2, 8.4 Hz, 1H), 8.34 (d, *J* = 8.0 Hz, 1H), 8.30–8.27 (m, 2H), 7.87–7.83 (m, 4H), 7.41–7.37 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 153.02, 150.36, 144.72, 139.98, 139.63, 138.87, 137.37, 133.73, 133.68, 131.39, 126.66, 126.03, 125.98, 124.27, 124.19, 121.13.

Synthesis of ligand L-N



Under a N<sub>2</sub> atmosphere, a mixture of 3-bromo-9-ethyl-carbazole (2.74 g, 10.0 mmol), 2-(tributylstannyl)pyridine (3.70 g, 10.0 mmol), Pd(PPh<sub>3</sub>)<sub>4</sub> (0.56 g, 0.5 mmol), and toluene (45 mL) heated to 110 °C and stirred for 12 h. Then, the reaction mixture was cooled to room temperature, and the solvent was removed. The residual was purified on a silica column to the

target product (1.44 g, 53.1%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 8.78 (s, 1H), 7.73 (d, J = 4.8 Hz, 1H), 8.19 (d, J = 7.6 Hz, 1H), 8.14 (d, J = 8.8 Hz, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.77 (t, J = 7.6 Hz, 1H), 7.51–7.48 (m, 2H), 7.43 (d, J = 8.0 Hz, 1H), 7.26 (t, J = 7.2 Hz, 1H), 7.20 (t, J = 6.0 Hz, 1H), 4.41 (q, J = 7.2 Hz, 2H), 1.47 (t, J = 7.2 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 158.31, 149.56, 140.53, 140.33,136.69, 130.41, 125.84, 124.78, 123.39, 123.26, 121.14, 120.68, 120.22, 119.16, 119.12, 108.62, 108.55.

Ligands L-B and L-O were synthesized according to our previously studies.<sup>8,9</sup>



# General procedure for synthesizing Ir(III) complexes

Under a N<sub>2</sub> atmosphere, a mixture solution of THF and H<sub>2</sub>O (3:1, v/v) (30 mL), organic ligand **L-S** or **L-N** or **L-O** or **L-B** (1.0 eqv.), organic ligand **L-S** (1.0 eqv.), and IrCl<sub>3</sub>·nH<sub>2</sub>O (1.0 eqv.) was heated to 110 °C. The reaction mixture was stirred for ~ 12 h, and cooled to room temperature. Then, the mixture was extracted with CH<sub>2</sub>Cl<sub>2</sub> three times. The combined organic layers were dried and concentrated. Under a N<sub>2</sub> atmosphere, the residue and thallium(I) acetylacetonate (1.0 eqv.) were dissolved in CH<sub>2</sub>Cl<sub>2</sub> (20 mL), and the reaction mixture was stirred for  $\sim 8$  h at room temperature. After filtered, the filtrate was concentrated and purified on self-made silica TLC to give the titled Ir(III) complexes.

SIrS (Yield, 38.3%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 8.48 (d, J = 5.6 Hz, 2H),
8.29 (s, 2H), 8.18–8.14 (m, 4H), 8.07–8.01 (m, 4H), 7.73–7.67 (m, 4H), 7.49 (t, 6.93 (s, 2H),
5.30 (s, 1H), 1.82 (s, 6H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 185.62, 157.65, 150.24,
148.77, 143.42, 139.26, 139.13, 137.01, 133.27, 133.17, 132.23, 129.23, 125.74, 125.34,
124.79, 120.98, 119.87, 103.77, 28.41. ESI-MS (*m/z*): (M+Na)<sup>+</sup>, 1027.0064.

**SIFN** (Yield, 20.4%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 8.69 (d, J = 5.6 Hz, 1H), 8.38 (d, J = 5.6 Hz, 1H), 8.28 (d, J = 6.0 Hz, 2H), 8.11 (d, J = 4.0 Hz, 2H), 8.06–8.01 (m, 2H), 7.98–7.95 (m, 2H), 7.84 (t, J = 7.6 Hz, 1H), 7.65–7.63 (m, 2H), 7.43 (t, J = 6.4 Hz, 1H), 7.30 (t, J = 8.0 Hz, 1H), 7.22–7.15 (m, 3H), 7.10 (t, J = 7.6 Hz, 1H), 5.88 (s, 1H), 5.28 (s, 1H), 3.88 (q, J = 9.6 Hz, 2H), 1.83 (s, 3H), 1.81 (s, 3H) , 1.23 (t, J = 7.2 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 185.22, 185.09, 168.54, 150.56, 149.06, 147.74, 140.45, 139.51, 139.44, 137.91, 137.75, 136.60, 135.70, 132.98, 132.87, 130.37, 129.78, 125.60, 124.96, 124.50, 123.93, 123.76, 120.83, 120.04, 119.52, 119.14, 118.96, 118.64, 111.02, 108.28, 100.70, 37.09, 28.65, 28.55, 13.43. ESI-MS (m/z): (M)<sup>+</sup>, 919.1318.

SIrO (Yield, 33.5%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 8.50 (d, J = 5.2 Hz, 1H),
8.35 (d, J = 5.6 Hz, 1H), 8.25 (s, 1H), 8.18 (d, J = 6.4 Hz, 1H), 8.09 (d, J = 8.4 Hz, 1H), 7.83–
7.80 (m, 3H), 7.73–7.71 (m, 2H), 7.48 (d, J = 8.8 Hz, 1H), 7.29 (t, J = 6.4 Hz, 1H), 7.26–7.18 (m, 3H), 7.04 (t, J = 7.2 Hz, 1H), 6.89 (d, J = 7.6 Hz, 2H), 6.42 (d, J = 6.8 Hz, 1H), 5.61 (d, J = 1.6 Hz, 1H), 5.25 (s, 1H), 1.84 (s, 3H), 1.77 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm)

185.14, 185.08, 167.45, 165.13, 161.80, 158.25, 155.84, 150.71, 148.70, 147.84, 146.50,
140.43, 139.47, 137.98, 137.91, 136.43, 133.13, 132.98, 130.57, 129.70, 129.43, 125.59,
125.50, 125.08, 124.01, 123.51, 121.43, 121.22, 120.15, 119.40, 118.73, 111.00, 100.69,
28.59, 28.52. ESI-MS (*m/z*): (M)<sup>+</sup>, 894.1039.

**SIrB** (Yield, 20.9%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 8.58 (d, *J* = 4.2 Hz, 1H), 8.36 (s, 1H), 8.23 (s, 1H), 8.14 (dd, *J* = 3.2, 6.4 Hz, 1H), 8.08–8.03 (m, 2H), 7.91–7.84 (m, 3H), 7.69 (dd, *J* = 3.2, 6.4 Hz, 1H), 7.62 (d, *J* = 7.6 Hz, 1H), 7.35 (t, *J* = 6.4 Hz, 1H), 7.11 (s, 1H), 6.86 (d, *J* = 7.6 Hz, 1H), 6.84 (s, 4H), 6.71 (t, *J* = 7.2 Hz, 1H), 6.10 (d, *J* = 7.2 Hz, 1H), 5.11 (s, 1H), 2.30 (s, 6H), 2.09 (s, 12H), 1.80 (s, 3H), 1.22 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 185.39, 184.75, 170.05, 165.31, 162.12, 155.35, 150.52, 148.80, 145.12, 144.10, 140.99, 140.46, 139.70, 139.46, 137.95, 136.67, 132.97, 132.89, 132.74, 130.48, 130.08, 129.87, 128.56, 125.59, 125.29, 125.01, 124.01, 122.08, 120.19, 119.43, 118.49, 100.75, 28.38, 27.81, 23.59, 21.25. ESI-MS (*m/z*): (M)<sup>+</sup>, 1050.2563.





Fig. S2 MS spectra of SIrN.







Fig. S4 MS spectra of SIrB.

Compound	SIrS·2CHCl <sub>3</sub>	SIrB·2CHCl <sub>3</sub>	
CCDC No.	1882275	1882276	
formula	C <sub>39</sub> H <sub>27</sub> IrN <sub>2</sub> O <sub>10</sub> S <sub>4</sub> ,2(CHCl <sub>3</sub> )	C <sub>51</sub> H <sub>46</sub> BIrN <sub>2</sub> O <sub>6</sub> S <sub>2</sub> ,2(CHCl <sub>3</sub> )	
M (g mol <sup>-1</sup> )	1242.80	1288.76	
crystal system	Monoclinic	Triclinic	
space group	P21/c	P-1	
<i>a</i> (Å)	14.218(5)	13.614(4)	
<i>b</i> (Å)	21.349(7)	14.015(4)	
<i>c</i> (Å)	15.308(5)	15.677(4)	
α (°)	90.00	81.078(12)	
β (°)	96.210(7)	79.523(12)	
γ (°)	90.00	67.633(10)	
$V(Å^3)$	4619(3)	2707.8(12)	
Ζ	4	2	
$D_{calcd}$ (g cm <sup>-3</sup> )	1.787	1.581	
$\mu$ (mm <sup>-1</sup> )	3.477	2.889	
F(000)	2448	1288	
$\theta$ range (°)	1.441 to 27.494	1.578 to 27.533	
reflections collected	36190	37159	
independent reflections	10566	12360	
R <sub>int</sub>	0.0599	0.0467	
$R (I > 2\sigma(I))$	R1 = 0.0868, wR2 = 0.1341	R1 = 0.0456, wR2 = 0.0928	
R (all data)	R1 = 0.1018, $wR2 = 0.1398$ $R1 = 0.0491$ , $wR2 = 0.0000$		
Goodness-of-fit on F <sup>2</sup>	1.269	1.082	

Table S1 Crystallographic data of SIrS·2CHCl<sub>3</sub> and SIrB·2CHCl<sub>3</sub>



Fig. S5 TGA curves of complexes SIrS, SIrN, SIrO, and SIrB.



Fig. S6 EL performance of devices A1-D1: (a) EL spectral, (b) J - V - L characteristics, (c) curves of EQE vs luminance, and (d) curves of CE and PE vs luminance.



Fig. S7 EL performance of devices A3-D3: (a) EL spectral, (b) J - V - L characteristics, (c) curves of EQE vs luminance, and (d) curves of CE and PE vs luminance.

Emitter	EQE <sub>max</sub> (%)	CE <sub>max</sub> (cd A <sup>-1</sup> )	PE <sub>max</sub> (lm W <sup>-1</sup> )	Ref.	Publishing year
SIrO	18.7	50.6	37.6	This work	
SIrB	23.2	66.5	56.0	This work	
Ir-G2	21.0	54.2	21.6	10	2012
(3Phbt) <sub>2</sub> Ir(acac)	-	17.2	-	11	2013
(EtPy) <sub>2</sub> Ir(acac)	11.2	13.4	5.9	12	2013
(CF3BT-CF3P)2Ir(acac)	-	10.5	3.0	13	2014
Ir(Flpy-CF <sub>3</sub> ) <sub>3</sub>	25.2	74.6	97.2	14	2015
(impy) <sub>2</sub> Ir(tmd)	6.1	16.3	-	15	2015
Ir(dmppm) <sub>2</sub> (dmd)	12.0	27.2	21.5	16	2016
<i>m</i> -LIrpic	17.1	43.9	23.0	17	2016
<i>m</i> -CF <sub>3</sub> DPQIr-HT	21.64	52.16	24.56	18	2017
IrO1	17.4	45.8	24.5	19	2018
Ir(Flpy-CF <sub>3</sub> ) <sub>2</sub> acac	23.7	62.1	80.4	20	2018

Table S2 Efficiencies of representative solution-processed orange OLEDs

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