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## Introduction

Organic light-emitting diodes (OLEDs) are promising materials for novel flat-panel displays, and solid-state lighting sources.<sup>1–5</sup> Transition metal complexes with effective intersystem crossing have shown great potential for use in phosphorescent OLEDs because they can fully harvest both the electro-generated singlet and triplet excitons to achieve nearly 100% internal quantum efficiency.<sup>6–8</sup> Among these transition metal complexes, phosphorescent iridium(m) complexes have been regarded as the most popular organic electronic materials for the emission layer in the electroluminescent devices, owing to their efficient

## Two novel neutral and ionic Ir(III) complexes based on the same bipolar main ligand: a comparative study of their photophysical properties and applications in solution-processed red organic light-emitting diodes<sup>†</sup>

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Using 4-(5-(4-(dimesitylboranyl)phenyl)pyridin-2-yl)-*N*,*N*-diphenylaniline (**BNpppy**) as a cyclometalated ligand, 1,10-phenanthroline or 2,4-pentanedione (acac) as the ancillary ligand, respectively, two novel iridium(III) complexes (**Ir-1** and **Ir-2**) were successfully synthesized and their photoelectric properties have been investigated in detail. The incorporation of electron-accepting dimesitylboron (Mes<sub>2</sub>B) moieties and electron-donating triphenylamine moieties into iridium(III) complexes has been demonstrated with benign photophysical and electronic properties. The solution-processed OLEDs were fabricated using these two iridium(III) complexes, respectively. The devices of **Ir-2** show good performances compared to those of **Ir-1** with a maximum luminance of 7916 cd m<sup>-2</sup>, a maximum external quantum efficiency (EQE) of 2.48% and a maximum current efficiency of 3.99 cd A<sup>-1</sup>. These results indicate that the introduction of a donor-acceptor type of ligand into transition metal complexes has potential applications in constructing an efficient emitter in OLEDs with excellent performances.

luminescence properties and the facile color tunability.<sup>9–12</sup> Also, it is well known that the introduction of different kinds of ligand into phosphorescent iridium(m) complexes can drastically influence the electrochemical and photophysical properties of iridium(m) complexes.<sup>13–17</sup> Therefore, phosphorescent iridium(m) complexes possess the huge potentiality in developing energy-efficient and high-performing phosphorescent organic light-emitting diodes.

The charge-transport balance is significant for phosphorescent OLEDs doped with iridium(III) complexes. Rational chemical tailoring of the cyclometalated ligand can facilitate the hole and electron transport. As we know, the dimesitylboron (Mes<sub>2</sub>B) moieties have been widely used to construct organic functional optoelectronic materials.<sup>18,19</sup> And they also have been introduced into ligands of transition metal complexes as functional units to improve the corresponding device performance.<sup>20</sup> For example, Wang et al. reported two novel cyclometalated phosphorescent platinum(II) complexes functionalized with dimesitylboryl and developed those complexes as an anion-sensor for fluoride ions.<sup>21</sup> Later on, the red emission phosphorescent bis(5-(dimesitylboryl)-2-phenylpyridinato)iridium-(acac) was reported by Zhou et al., which showed an excellent electroluminescence (EL) performance.<sup>22,23</sup> Besides, the electron acceptor of the boron center can easily facilitate intramolecular



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<sup>†</sup> Electronic supplementary information (ESI) available: Experimental details. <sup>1</sup>H NMR and mass spectra. Extra absorption and emission spectra. See DOI: 10.1039/d0nj02462g



Scheme 1 Synthetic routes of Ir(III) complexes.

charge transfer (CT) in the presence of an electron donor and provide the highly luminescent materials.  $^{24,25}$ 

Herein, we designed and synthesized two novel iridium(III) complexes (Ir-1 and Ir-2) with 4-(5-(4-(dimesitylboranyl)phenyl)pyridin-2-yl)-N,N-diphenylaniline (BNpppy) as the cyclometalated ligand, which is composed of the triphenylamine group and dimesitylboron (Mes<sub>2</sub>B) unit as the electron donor and acceptor, and 1,10-phenanthroline or 2,4-pentanedione (acac) as the ancillary ligand, respectively, as shown in Scheme 1. The results showed that BNpppy exhibits apparent solvatochromism behavior in different solvents. The incorporation of a D-A (donor-acceptor) type N^C chelate ligand into iridium(III) metal complexes can facilitate metal-to-ligand charge transfer (MLCT) transitions, which should be expected to achieve highly efficient phosphorescent iridium(III) complexes. Furthermore, solution-processed OLEDs based on iridium(m) complexes with 2,4-pentanedione as the ancillary ligand also gave a good performance due to their excellent solubility and solid-state stability. In this paper, the synthesis, photophysical properties and electroluminescence properties in OLEDs of both the iridium(III) complexes were investigated.

## Experimental

### General information

4-Bromo-*N*,*N*-diphenylaniline, 5-bromo-2-iodopyridine, 1,4-dibromobenzene,  $IrCl_3 \cdot 3H_2O$ , 1,10-phenanthroline, 2,4-pentanedioneand and all other chemicals were purchased from Shanghai J&K company and used without any further purification. Nuclear magnetic resonance (NMR) (300 MHz, 500 MHz) spectra were recorded at room temperature on a Bruker Ultra shield Plus 300 and 500 Hz instrument, which adopts  $CDCl_3$  or  $(CD_3)_2SO$  as the solvent, and TMS as the internal standard. Infrared spectra were recorded on a Bruker Tensor 27 spectrometer. Mass spectra were obtained on a Bruker autoflex MALDI-TOF/TOF mass spectrometer. Ultraviolet-Visible absorption spectra were measured by using a Shimadzu Uv-3600 Uv-Vis-NIR spectrophotometer. Emission spectra were recorded on a FL-400PC Spectra spectrophotometer. Thermal gravimetric analysis (TGA) was performed on a PerkinElmer TGA7 thermal analyzer at a heating rate of 10 °C min<sup>-1</sup> under a nitrogen atmosphere. Time-resolved fluorescence spectra of the solutions in dichloromethane (DCM) were recorded using an Edinburgh Instruments (FLS920) spectrometer. To evaluate the performance of the devices, the characteristics of the devices were measured using a Keithley 2400 source meter and a fiber integration sphere (FOIS-1) coupled with a QE65 Pro spectrometer.

#### Synthesis and characterization

Scheme 1 and Scheme S1 in the ESI<sup>†</sup> show the synthetic routes of **BNpppy** ligand and both iridium(m) complexes. All structures of the intermediates and target products were characterized by <sup>1</sup>H NMR and <sup>13</sup>C NMR. **Ir-1** and **Ir-2** were prepared using a typical two-step strategy by the cyclometalation of IrCl<sub>3</sub>·3H<sub>2</sub>O with the **BNpppy** ligand to initially form the chloride-bridged dimers, followed by treatment with 1,10-phenanthroline or 2,4-pentanedione, respectively, to obtain the two iridium(m) complexes.<sup>26</sup> Finally, **Ir-1** and **Ir-2** were obtained as red solids.

Synthesis of  $[(BNpppy)_2Ir(\mu-Cl)_2Ir(BNpppy)_2]$ . A mixture of  $IrCl_3 \cdot 3H_2O$  (70.00 mg, 0.15 mmol), BNpppy (194.00 mg, 0.3 mmol), ethoxyethanol (2.4 mL) and  $H_2O$  (0.8 mL) was placed in an evacuated round bottom flask and stirred for 24 h at 110 °C under a nitrogen atmosphere. After cooling to room temperature, the solution was treated with a large amount of water and ethanol, and then the insoluble was dried to obtain a reddish-brown solid (230.00 mg, yield: 88%).

Synthesis of  $[(BNpppy)_2Ir(1,10-phenanthroline)]^+(PF_6^-)$  (Ir-1). A mixture of  $[(BNpppy)_2Ir(\mu-Cl)_2Ir(BNpppy)_2]$  (182.50 mg, 0.06 mmol), 1,10-phenanthroline (29.70 mg, 0.15 mmol), methanol (2.0 mL) and dichloromethane (4.0 mL) was placed in an evacuated round bottom flask and stirred for 4 h at 45  $^\circ\mathrm{C}$ under a nitrogen atmosphere. Then after cooling to room temperature, KPF<sub>6</sub> was added in five portions, and continued to stir for 2 h at room temperature. The solution was evaporated to dryness with a rotary evaporator, the crude material was purified by column chromatography over silica gel (PE:EA = 15:1) to obtain a reddish brown solid (197.00 mg, yield: 93%). <sup>1</sup>H NMR (300 MHz, DMSO-D<sub>6</sub>):  $\delta$  = 8.90 (d, *J* = 8.0 Hz, 2H), 8.46 (d, *J* = 4.2 Hz, 2H), 8.33 (s, 2H), 8.21–8.13 (m, 2H), 7.91 (s, 4H), 7.77 (d, *J* = 8.6 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 6H), 7.05 (dd, *J* = 18.5, 7.6 Hz, 20H), 6.83 (s, 12H), 6.59 (d, J = 9.0 Hz, 2H), 5.93 (s, 2H), 2.26 (s, 12H), 1.91 (s, 24H); <sup>13</sup>C NMR(126 MHz, DMSO-D<sub>6</sub>):  $\delta$  = 166.26, 151.97, 149.49, 147.07, 146.85, 146.38, 145.52, 144.96, 144.53, 141.46, 140.36, 139.33, 138.87, 138.07, 136.80, 136.19, 136.05, 132.12, 131.60, 129.57, 128.64, 127.55, 126.79, 126.16, 125.49, 124.48, 122.08, 119.27, 114.09, 23.16, 21.09; IR (KBr) v 3059, 3023, 2954, 2919, 2855, 2729, 1723, 1605, 1573, 1574, 1508, 1490, 1475, 1454, 1426, 1374, 1316, 1284, 1236, 1220, 1173, 1152, 1069, 1027, 1014, 1002, 960, 908, 873, 840, 754, 724, 696, 662, 643, 584, 556, 523, 510, 471, 432 cm<sup>-1</sup>; MALDITOF-MS *m/z*: calculated: 1664.723, found: 1663.916; anal. calcd. for C<sub>106</sub>H<sub>92</sub>B<sub>2</sub>IrN<sub>6</sub>: C 76.52, H 5.57, N 5.05. Found: C 76.72, H 5.58, N 5.03.

Synthesis of [(BNpppy)2Ir(acac)] (Ir-2). A mixture of  $[(BNpppy)_2Ir(\mu-Cl)_2Ir(BNpppy)_2]$  (577.90 mg, 0.19 mmol), 2,4-pentanedione (50.10 mg, 0.5 mmol), Na<sub>2</sub>CO<sub>3</sub> (219.40 mg, 2.07 mmol) and ethoxyethanol (12.0 mL) was placed in an evacuated round bottom flask and stirred for 12 h at 85  $^\circ C$  under a nitrogen atmosphere. After cooling to room temperature, the solution was washed with methanol and evaporated to dryness using a rotary evaporator. Then the crude material was purified by column chromatography over silica gel (PE:DCM = 4:1) to obtain a red solid (500.00 mg, yield: 80%). <sup>1</sup>H NMR (500 MHz, DMSO-D<sub>6</sub>):  $\delta$  = 8.53 (s, 2H), 8.03 (d, J = 9.6 Hz, 2H), 7.83 (d, J = 8.6 Hz, 2H), 7.65 (d, J = 8.0 Hz, 4H), 7.58 (d, J = 8.0 Hz, 4H), 7.53 (d, J = 8.5 Hz, 2H), 7.09 (t, J = 7.7 Hz, 8H), 6.89 (s, 20H), 6.32 (d, J = 8.4 Hz, 2H), 5.73 (s, 12H), 5.28 (s, 1H), 2.30 (s, 12H), 2.03 (s, 24H), 1.76 (s, 6H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>):  $\delta$  = 184.72, 166.85, 148.52, 147.73, 147.25, 145.77, 141.68, 140.84, 139.81, 138.78, 137.77, 137.20, 134.32, 131.93, 128.77, 128.26, 125.92, 125.64, 125.41, 124.56, 122.87, 117.47, 113.97, 28.74, 23.49, 21.21. IR (KBr) v 3022, 2952, 2916, 2854, 2729, 1597, 1574, 1546, 1510, 1490, 1476, 1449, 1401, 1375, 1313, 1291, 1273, 1257, 1238, 1218, 1173, 1152, 1138, 1065, 1027, 1015, 958, 872, 846, 823, 804, 752, 724, 695, 668, 635, 585, 574, 560, 511, 470, 420 cm<sup>-1</sup>; MALDITOF-MS m/z: calculated: 1583.699, found: 1583.342; anal. calcd. for C<sub>99</sub>H<sub>91</sub>B<sub>2</sub>IrN<sub>4</sub>O<sub>2</sub>: C 75.13, H 5.80, N 3.54. Found: C 74.91, H 5.82, N 3.55.

### **Results and discussion**

#### The solvatochromism effect of BNpppy

At room temperature, we measured the Uv-Vis absorption spectrum and the fluorescence emission spectrum of **BNpppy**, which was dissolved in CH<sub>2</sub>Cl<sub>2</sub> and the solution concentration was  $10^{-5}$  M. As shown in Fig. S1 in the ESI,<sup>†</sup> its absorption spectrum shows a sharp peak at 300-400 nm, which is mainly on account of the  $\pi$ - $\pi$ \* transition and charge transfer transition in BNpppy. In the emission spectrum, the emission peak wavelength is located at 522 nm and the solution reveals a strong yellow-green emission. At the same time, we also measured the emission spectra of BNpppy in different solvents (cyclohexane, ethyl acetate, tetrahydrofuran, methylene chloride, and acetonitrile), and found that the highest emission peak was located at different wavelengths in different solvents. This means that BNpppy has a distinct behavior of solvatochromism, as shown in Fig. 1, which proves the existence of the intramolecular charge transfer process.

#### Photophysical properties of Ir-1 and Ir-2

The photophysical properties of the iridium(m) complexes in  $CH_2Cl_2$  and thin films were investigated at 298 K, and the photophysical data are listed in Table 1. In the absorption spectra, both the complexes show a full vibronic-structured absorption band at 250–350 nm, which was assigned to the spin-allowed ligand-central  $\pi$ - $\pi$ \* transition.<sup>27</sup> The low-lying



Fig. 1 Normalized emission spectra of **BNpppy** in various solvents ( $10^{-5}$  M). (Inset: Photograph of **BNpppy** in various solvents under a 365 nm UV lamp.)

peak with a shoulder in the region of 400-500 nm can be assigned to the mixture of metal-to-ligand charge transfer (<sup>1</sup>MLCT, <sup>3</sup>MLCT) and intramolecular charge transfer (ICT) transitions.<sup>28</sup> The absorption bands of Ir-1 with 1,10-phenanthroline as the ancillary ligand have a noticeable difference compared with those of Ir-2 that has the ancillary ligand acetylacetonate (acac) (Fig. 2). It suggests that the ancillary ligand variation affects their excited state energy. The emission spectra of Ir-1 and Ir-2 exhibit intense red phosphorescence at 625 nm and 601 nm in CH<sub>2</sub>Cl<sub>2</sub> at room temperature, respectively. To understand these differences in luminescence properties, the theoretical calculations were carried out and the frontier orbital distribution was obtained. As shown in Fig. 3, the lowest unoccupied molecular orbitals (LUMOs) of Ir-1 and Ir-2 were primarily dominated by BNpppy ligands. The highest occupied molecular orbitals (HOMOs) of Ir-1 were mainly located over the auxiliary ligand, but the HOMOs of Ir-2 were mainly located on the main ligands. Furthermore, the spectra of the two complexes were almost the same in both the solution state and the film state, which is attributed to the steric hindrance of the dimesitylboron (Mes<sub>2</sub>B) units suppressing the structural relaxation of the iridium(m) complexes in the solid state. The photoluminescence (PL) quantum yields ( $\Phi_{\rm P}$ ) of **Ir-1** and **Ir-2** were calculated to be 5.8% and 42.9%, respectively, which were measured in degassed CH<sub>2</sub>Cl<sub>2</sub> in a N<sub>2</sub> atmosphere using Ir(ppy)<sub>3</sub> ( $\Phi_{\rm P}$  = 40%) as a standard.<sup>29</sup> The phosphorescence lifetimes  $(\tau)$  for both the iridium(III) complexes are in the range of microseconds, with observed times of 0.185 µs and 1.065 µs in CH<sub>2</sub>Cl<sub>2</sub> solution for Ir-1 and Ir-2, respectively (Table 1 and Fig. S21 in the ESI<sup>+</sup>). This proves that Ir-2 exhibits at higher  $\Phi_{\rm P}$  (42.9%) and for longer  $\tau$  (1.065 µs), in OLEDs which indicates their excellent performance.

#### Electrochemical and thermal properties of Ir-1 and Ir-2

The electrochemical properties of **Ir-1** and **Ir-2** were investigated using cyclic voltammetry (CV) using ferrocene as an internal standard. Both the complexes exhibit a reversible oxidation progress in  $CH_2Cl_2$  (Fig. 4). According to the oxidation potentials, the HOMOs were calculated to be -5.60 eV (**Ir-1**) and -5.45 eV (**Ir-2**). Correspondingly, the LUMOs were calculated to be -3.12 eV (**Ir-1**) and -3.11 eV (**Ir-2**), according to their HOMOs and absorption spectra.<sup>30</sup> In Fig. 4, **Ir-2** shows a good

Table 1 Physical properties of Ir-1 and Ir-2

	$\lambda_{\rm abs} ({\rm nm})$		$\lambda_{\rm em} (\rm nm)$		$\Phi_{\mathrm{p}}$ (%)					
Complex	Sol. <sup>a</sup>	Film <sup>b</sup>	Sol. <sup>a</sup>	Film <sup>b</sup>	Sol. <sup>a</sup>	Film <sup>b</sup>	$\tau^{c}$ (µs)	$HOMO^{d}$ (eV)	$LUMO^{d}$ (eV)	$T_{d}^{e}(^{\circ}C)$
Ir-1	278, 451	325, 450	625	605	5.8	5.96	0.185	-5.60	-3.12	213
Ir-2	310, 421, 480	317, 428, 489	601	610	42.9	5.69	1.065	-5.45	-3.11	189

<sup>*a*</sup> In dilute DCM ( $10^{-5}$  M). <sup>*b*</sup> Films at a quartz substrate. <sup>*c*</sup> Recorded in the degassed DCM solution with a 400 nm light source. <sup>*d*</sup> Determined by cyclic voltammetry and the optical band gap from the absorption spectra. <sup>*e*</sup> Decomposition temperature corresponding to 5% weight loss measured by TGA.



Fig. 2 The normalized absorbance and emission spectra: (a) Ir-1 solution (in CH<sub>2</sub>Cl<sub>2</sub>,  $10^{-5}$  M), (b) Ir-1 thin film, (c) Ir-2 solution (in CH<sub>2</sub>Cl<sub>2</sub>,  $10^{-5}$  M), and (d) Ir-2 thin film.



Fig. 3 The HOMO and LUMO distributions of the Ir-1 and Ir-2 complexes.

redox reversibility, which gives advantages for the complexes applied in electroluminescent devices. As shown in Fig. S22 in the ESI,† the thermal gravimetric analysis (TGA) curves show that the two compounds exhibited good thermal stability. A weight loss of 5% was found at temperatures of 213 °C for **Ir-1** and 189 °C for **Ir-2**. To conveniently design the structure of the electroluminescent device, all these data are summarized in Table 1.

### Solution-processed OLEDs

To investigate the applicability of these bipolar complexes in electroluminescent devices, a series of solution-processed



Fig. 4 Cyclic voltammograms in degassed  $CH_2Cl_2$  (scan rate = 100 mV s<sup>-1</sup>).

OLEDs have been fabricated with the configuration of indium tin oxide (ITO)/polyethylenimine ethoxylated (PEIE)-modified zinc oxide (ZnO, around 20 nm)/CBP: *x* wt% Ir complex (around 57 nm)/bis(dimethyl aniline) phenyl cyclohexane (TAPC, 40 nm)/molybdenum oxide (MoO<sub>x</sub>, 7 nm)/Al (100 nm), in which PEIE-modified ZnO and TAPC layers were used as the electron transport layer and hole transport layer, respectively. The MoO<sub>x</sub>/Al bilayers and ITO were selected as the top electrodes and bottom electrodes in the sequence. Fig. 5 shows the energy level diagram of the HOMO and LUMO levels for the materials



Fig. 5 Energy level diagram of the HOMO and LUMO levels for materials used in OLEDs and their molecular structures.



**Fig. 6** Characteristics of devices (A1–A5): (a) current density–external quantum efficiency (J–EQE), (b) normalized EL spectra, and (c) voltage–current density (V–J) and (d) voltage–luminance (V–L) curves.

investigated in this study as well as their molecular structures. To optimize the electroluminescence efficiency, the emissive layer was prepared by spin-coating a solution of the complex:CBP blend at different concentrations in chloroform. For the OLED fabrication, the details of PEIE-modified ZnO spin-coated onto ITO glass can be found elsewhere.<sup>31</sup> The emissive layer was formed by mixing the **Ir-1/Ir-2** with CBP prepared in chloroform *via* spin-coating onto the ZnO films and then annealing at 60 °C for 20 min. Finally, the TAPC layers and MoO<sub>x</sub>/Al electrode were fabricated *via* vacuum evaporation deposition. The current density–external quantum efficiency (*J*–EQE), EL spectra, voltage–current density (*V*–*J*), and voltage–luminance (*V*–*L*) curves of each device are showed in Fig. 6 and 7. Furthermore, the critical electroluminescence data are summarized in Table S1 in the ESI.<sup>†</sup>

Doping Ir-2 in CBP, with the doping level increasing from device B1 (4 wt%) to B5 (14 wt%), the electroluminescence



**Fig. 7** Characteristics of devices (B1–B5): (a) current density–external quantum efficiency (J–EQE), (b) normalized EL spectra, and (c) voltage–current density (V–J) and (d) voltage–luminance (V–L) curves.

efficiencies of **Ir-2** doped devices reach a maximum at a 14% doping-level. Device B5 showed luminance  $(L_{\text{max}})$  of 7916 cd m<sup>-2</sup> at 16V, current efficiency  $(\eta_{\text{L}})$  of 3.99 cd A<sup>-1</sup>, and external quantum efficiency (EQE) of 2.48% (Fig. 7 and Table S1 in the ESI†). As shown in Fig. 7, the devices A1–A5 for **Ir-1** turned on at a voltage of 6 V, while the optimized device A5 (25 wt%) can only emit a maximum luminance of 983 cd m<sup>-2</sup> at 13 V, and has the highest  $\eta_{\text{L}}$  of 0.50 cd A<sup>-1</sup>, and EQE of 0.28%, which is much poorer in performance than the highly red phosphorescent emitter **Ir-2**. These results can reveal that the OLED using **Ir-2** as the emitter exhibits a much better electroluminescence performance than the one using **Ir-1** as the emitter, which can be attributed to the higher quantum efficiency.

## Conclusions

In summary, we have achieved the design and synthesis of a novel bipolar ligand and its corresponding complexes **Ir-1** and **Ir-2**. The photophysical and electrochemical properties of all these compounds were investigated. The solution-processed OLEDs based on the two iridium(m) complexes were then fabricated by the optimization of the doping concentrations at the emissive layer, and gave a good performance based on the **Ir-2** complex at a 14% doping-level with the maximum EQE, peak luminance, and the highest current efficiency of 2.48%, 7916 cd m<sup>-2</sup>, and 3.99 cd A<sup>-1</sup>, respectively. The good performance can be attributed to the incorporation of donor and acceptor functional groups in the cyclometalated ligand, and these results can provide a deeper insight into the significant improvements in the OLED performance based on these bipolar ligands.

## Conflicts of interest

There are no conflicts to declare.

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