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A promising phosphorescent iridium complex with fluorine substituents: Synthesis, crystal structure, photo- and electro-luminescence performance

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ABSTRACT

In this paper, we report a phosphorescent Ir(III) emitter of Ir(acac-F6)(F-BT)₂, where acac-F6 = 1,1,1,5,5,5-hexafluoropentane-2,4-dione and F-BT = 2-(2-fluorophenyl)benzo[d]thiazole, including its crystal structure, electronic nature, photophysical characteristics, thermal and electrochemical properties. Data suggest that Ir(acac-F6)(F-BT)₂ is a promising emitter with high quantum yield of 0.19 and good thermal stability, along with its proper energy levels for charge carrier transportation. Electroluminescence (EL) devices using Ir(acac-F6)(F-BT)₂ as emitter are also fabricated, and their electroluminescence performances are investigated in detail. The optimal EL device shows a maximum luminance of 27,000 cd/cm² and a peak current efficiency of 8.7 cd/A.

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1. Introduction

Recently, the synthesis of luminescent transition metal complexes has attracted much attention due to their favorable optical and electrical properties, making them in general perfect candidates for electro-optical applications such as organic light-emitting diodes (OLEDs), solar cells, and optical sensors [1,2]. For OLED application which is believed to be a promising candidate for the next generation display technology, organometallic complexes possessing heavy transition metal cores are highly desired [3,4]. The strong spin–orbit coupling effectively promotes intersystem crossing as well as enhances the subsequent emissive decay from triplet excited state to ground state, facilitating strong phosphorescence by harvesting both singlet and triplet excitons within OLEDs. Since the internal quantum efficiency can theoretically be achieved as high as 100%, these heavy-metal containing emitters are thus superior to fluorescent ones in OLED applications [5].

In this series, phosphorescent Ir(III) complexes are particularly promising because of their favorable short excited state lifetimes, well-suited energy levels, thermal stability, and environmental inertness. The strong appeal and desire for better emitters, along with the need for a deeper understanding on the correlation between structural processes and photophysical properties, has pushed a continuous progress in the design of phosphorescent Ir(III)

complexes. In exploring high efficiency phosphorescent emitters and moving towards materials with the required color gamut for full color displays, a good harvest of high-performance Ir(III) complexes covering the whole visible region has been achieved, and the correlation between cyclometalated ligand structures and emission character is well established [6–8]. For example, Thompson and coworkers report neutral cyclometalated ligands and their corresponding Ir(III) and Pt(II) complexes for OLED applications, serving as phosphorescent emitters [9,10]. Grushin et al. developed a series of fluorine-containing phosphorescent emitters whose emission colors can be finely controlled by modulating the structures and positions of substituents of ligands, and it seems that fluorine atom is highly effective on improving the electroluminescence (EL) performance of emitters [11].

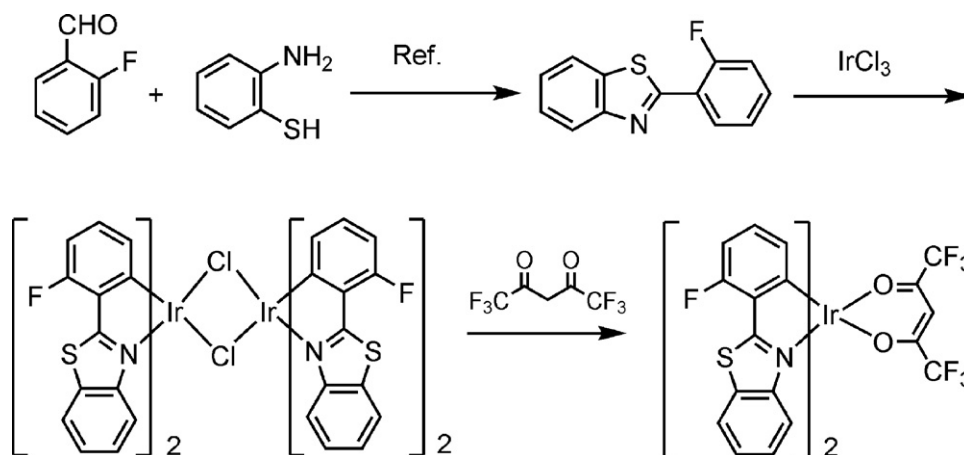
Enlightened by above reports, we intend to incorporate fluorine substituents into both C[^]N cyclometalated ligand and auxiliary ligand, hoping to develop a new phosphorescent emitter with high EL performance. In this paper, we report a phosphorescent Ir(III) emitter of Ir(acac-F6)(F-BT)₂, where acac = 1,1,1,5,5,5-hexafluoropentane-2,4-dione and F-BT = 2-(2-fluorophenyl)benzo[d]thiazole, including its crystal structure, electronic nature, photophysical characteristics, thermal and electrochemical properties. OLEDs using Ir(acac-F6)(F-BT)₂ as emitter are also fabricated, and their EL performances are investigated.

2. Experimental

A synthetic procedure for Ir(acac-F6)(F-BT)₂ is shown in Scheme 1. 2-Aminathiophenol, 2-fluorobenzaldehyde,

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Scheme 1. A synthetic route for $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$.

1,1,1,5,5,5-hexafluoropentane-2,4-dione (acac-F6), *p*-toluenesulfonic acid monohydrate, $\text{IrCl}_3 \cdot 3\text{H}_2\text{O}$, 4,4',4''-tris[methyl-phenyl(phenyl)amino]-triphenylamine (*m*-MTDATA), 4,4'-*N,N'*-dicarbazole-biphenyl (CBP), 4,4'-bis[*N*-(1-naphthyl)-*N*-phenylamino]biphenyl (NPB), tris(8-hydroxy-quinoline)aluminum (Alq_3), LiF, and 4,7-diphenyl-1,10-phenanthroline (BPhen) were purchased from Aldrich Chemical Co. and used without further purifications. Organic solvents, including 2-ethoxyethanol, 1,2-dichloroethane, ethanol, CH_2Cl_2 , and CHCl_3 , were purified through standard procedures.

2.1. Synthesis of $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$

2-(2-Fluorophenyl)benzo[*d*]thiazole (F-BT). The mixture of 10 mmol of 2-aminathiophenol, 10 mmol of 2-fluorobenzaldehyde, 1 mmol of *p*-toluenesulfonic acid monohydrate, and 20 mL of CHCl_3 was heated to reflux under N_2 atmosphere for 24 h. After cooling, the mixture was poured into cold water and extracted with CH_2Cl_2 . After the evaporation of solvent, the residue was purified by recrystallization from hot ethanol to give the desired product as yellow solid. ^1H NMR (CDCl_3 , 300 MHz) δ [ppm]: 7.33 (d, $J=7.5$ Hz, 1H), 7.35 (d, $J=7.0$ Hz, 1H), 7.54 (d, $J=8.5$ Hz, 1H), 7.51 (m, 1H), 7.93 (d, $J=8.5$ Hz, 1H), 8.11 (m, 1H), 8.22 (m, 2H).

$\text{Ir}(\text{acac-F6})(\text{F-BT})_2$. The mixture of 1 mmol of $\text{IrCl}_3 \cdot 3\text{H}_2\text{O}$, 2 mmol of F-BT, 20 mL of 2-ethoxyethanol, and 5 mL of H_2O was heated to reflux for 48 h. After cooling, 5 mL of H_2O was added into the mixture to precipitate orange solid which was then washed with ethanol and hexane. The dried product was mixed with 3 mmol of anhydrous sodium carbonate, 25 mL of 2-ethoxyethanol, and 3 mmol of acac-F6. The mixture was heated to reflux for 16 h. After cooling, 5 mL of H_2O was added to precipitate orange red solid which was collected by filtration. The crude product was chromatographed to give the desired product as orange needles. ^1H NMR (CDCl_3) δ [ppm]: 5.54 (s, 1H), 6.15 (d, $J=7.3$ Hz, 2H), 6.62 (d, $J=10$ Hz, 2H), 6.69 (d, $J=8.0$ Hz, 2H), 7.48 (m, 4H), 7.90 (m, 2H), 8.25 (m, 2H). Anal. Calcd for $\text{C}_{31}\text{H}_{15}\text{F}_8\text{IrN}_2\text{O}_2\text{S}_2$: C 43.51, H 1.77, N 3.27. Found: C 43.35, H 1.91, N 3.48. Its identity was further confirmed by single crystal XRD.

2.2. Fabrication of OLEDs

EL devices using $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ as the emitter were fabricated by resistive heating method under a chamber pressure of $\sim 3 \times 10^{-4}$ Pa onto a clean glass that was pre-coated with a layer of indium tin oxide (ITO). Prior to use, the ITO surface was cleaned by sonication in detergent solution, water, and ethanol sequen-

tially. After being blown dry with nitrogen, the ITO substrates (resistivity $< 30 \Omega$, active area = 4 mm^2) were treated with oxygen plasma for 1 min before being loaded into the vacuum chamber. LiF and Al were used as the electron injection layer and the cathode, respectively. The thicknesses of deposited layers and the evaporation speed of individual materials were monitored in vacuum with quartz crystal monitors.

2.3. Measurements and methods

Density functional theory (DFT) and singlet excitation calculations using time-dependent density functional theory (TD-DFT) were performed on $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ at RB3PW91/SBKJ level. The initial geometry was obtained from its single crystal. All computations were finished by GAMESS software package.

Single crystal data were collected on a Siemens P4 single-crystal X-ray diffractometer with a Smart CCD-1000 detector and graphite-monochromated Mo $\text{K}\alpha$ radiation, operating at 50 kV and 30 A at 298 K. All hydrogen atoms were calculated. Luminescence decay data were obtained with a 355 nm light generated from the Third-Harmonic-Generator pumped, using pulsed Nd:YAG laser as the excitation source. The Nd:YAG laser possesses a line width of 1.0 cm^{-1} , pulse duration of 10 ns and repetition frequency of 10 Hz. A Rhodamine 6G dye pumped by the same Nd:YAG laser was used as the frequency-selective excitation source. All photoluminescence (PL) spectra were measured with a Hitachi F-4500 fluorescence spectrophotometer. UV-vis absorption spectra were recorded using a Shimadzu UV-3101PC spectrophotometer. Luminescence quantum yield was determined by the method of Demas and Crosby with quinine sulfate in 1.0 M sulfuric acid ($\Phi=0.546$) as the reference standard [12]. ^1H NMR spectra were obtained with a Varian INOVA 300 spectrometer. Elemental analysis was performed on a Carlo Erba 1106 elemental analyzer. Cyclic voltammetry measurements were conducted on a voltammetric analyzer (CH Instruments, Model 620B) with a polished Pt plate as the working electrode, Pt mesh as the counter electrode, and a commercially available saturated calomel electrode (SCE) as the reference electrode, with a scan rate of 0.1 V/s. The voltammograms were recorded in CH_3CN solutions with $\sim 10^{-3}$ M sample and 0.1 M tetrabutylammonium hexafluorophosphate (TBAPF_6) as the supporting electrolyte. In order to precisely calculate the energy levels of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), the offset potentials are determined by the point of intersection of the tangential lines near the beginning part of the redox peaks. Prior to each electrochemical measurement, the solution was purged

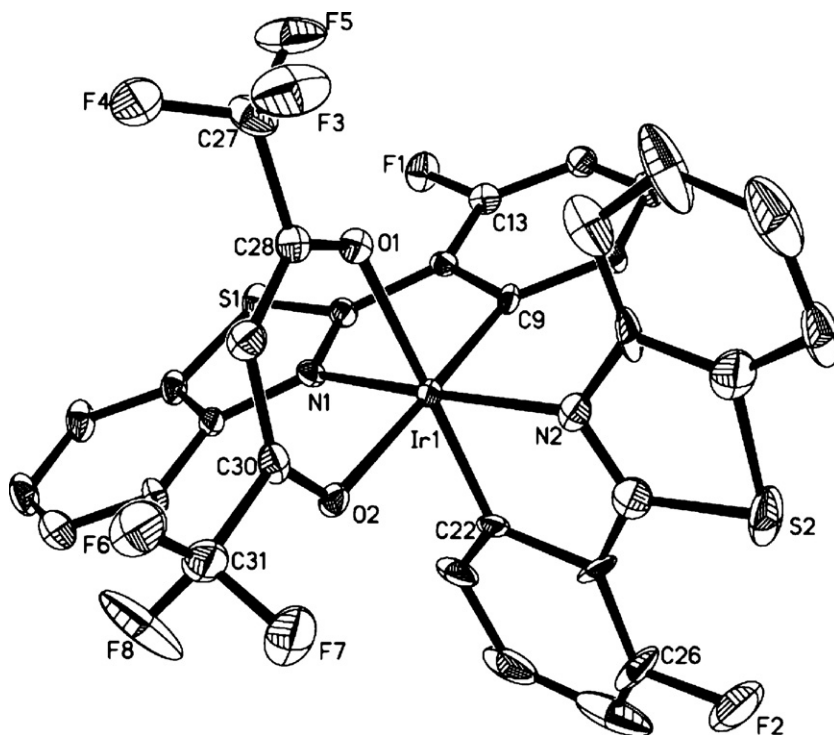


Fig. 1. Crystal structure of $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$. All hydrogen atoms are not shown for a clear view.

with nitrogen for ~10–15 min to remove the dissolved O_2 gas. EL spectra were measured by a PR650 spectrascan spectrometer. The luminance–current–voltage characteristics were recorded simultaneously with the measurement of EL spectra by combining the spectrometer with a Keithley 2400 source meter. All measurements were carried out in the air at room temperature without being specified.

3. Results and discussion

3.1. Molecular structure of $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$

3.1.1. Geometric structure

The crystal structure of $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ is shown in Fig. 1, along with the selected geometric parameters summarized in Table 1. It is found that the Ir(III) center localizes in a distorted octahedral environment by two chelating ligands of F-BT with *trans*-N,N and *cis*-C,C dispositions in addition to a bidentate monoanionic ligand of acac. $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ molecules crystallize in monoclinic system with double molecules per unit cell. The Ir–C bond length values are close to the literature values for bis-cyclometalated acac complexes [13]. The Ir–N bond length values are longer than the corresponding ones of Ir–C, suggesting a weaker interaction between coordinated N atom and Ir(III) center. The Ir–O bond length values are even longer than both Ir–C and Ir–N ones, indi-

cating a more weaker σ -donation of acac ligand to Ir(III) center compared with that of aromatic ring carbon. In addition, slight variations are found for Ir–O bond lengths, and the Ir–O bond lengths indicate a slight structural *trans*-effect of the phenyl group. The similar C–O bond lengths, however, suggest that the –1 charge of acac ligand is delocalized over both O atoms. The two F-BT ligands are mirror images of each other with respect to the symmetry plane passing Ir(III) center and bisecting the ancillary ligand of acac. The C–Ir–N ($\sim 81^\circ$) and O–Ir–O ($\sim 86.7^\circ$) bite angles indicate that the coordination sphere around the Ir(III) center is not so crowded due to the small ligand of acac-F6. This decreased steric hindrance may be positive to suppress the geometric relaxation in $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ excited state.

In addition, it is also observed that there is inter-molecular π -stacking within solid state $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ due to the large coplanar conjugation planes from F-BT fragment, as shown by Fig. 2. As for solid $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$, every two F-BT planes are bonded head-to-head due to the π - π attraction between F-BT planes, and the two rings align exactly parallel to each other with a dihedral angle of 0° and a distance of 3.393 Å, which confirms that there is face-to-face π - π stacking between the two F-BT planes. This inter-molecular π -stacking within solid state $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ actually increases π - π attraction and allows solid $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ molecules to take a more organized geometry.

3.1.2. Electronic structure

With the crystal structure on hand, we perform a TD-DFT calculation, which has been proved to be an effective tool for geometric and electronic natures of transition metal complexes, on $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ to explore its electronic structure [14]. As shown by Table 2, HOMO of $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ demonstrates a predominant Ir d character, admixed with large contributions from F-BT fragment. While, its LUMO is essentially π^* orbital localized on the diamine ligand of F-BT, with very slim contributions from Ir atom and acac moiety. The onset electronic transition corresponds to a transition from HOMO to LUMO, and is thus assigned as a character

Table 1

Selected geometric parameters of $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ obtained from single crystal XRD.

Bond length (Å)		Bond angle ($^\circ$)	
Ir–C(9)	1.982	C(9)–Ir–N(1)	81.05
Ir–N(1)	2.050	N(2)–Ir–C(22)	81.59
Ir–N(2)	2.079	O(1)–Ir–O(2)	86.72
Ir–C(22)	1.979	C(22)–Ir–C(9)	90.79
Ir–O(1)	2.143	C(22)–Ir–N(1)	95.05
Ir–O(2)	2.162	C(22)–Ir–O(2)	90.84

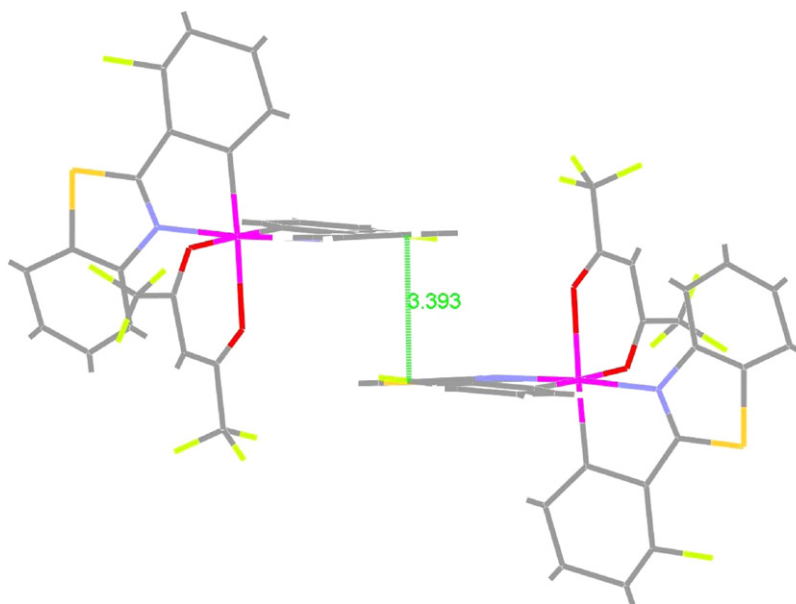


Fig. 2. Graphic presentation of inter-molecular π -stacking within solid state $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$.

of metal-to-ligand-charge-transfer {MLCT [$d(\text{Ir}) \rightarrow \pi^*(\text{F-BT})$]}. The onset electronic transition energy of 2.668 eV (465 nm) is so close to $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ onset 0–0 transition of 474 nm shown in Fig. 3, confirming the correctness of TD-DFT calculation.

3.2. Photophysical property of $\text{Ir}(\text{acac})(\text{F-BT})_2$

3.2.1. UV–vis absorption

Fig. 3 shows the UV–vis absorption spectrum of $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ in CH_2Cl_2 solution with a concentration of 1×10^{-4} mol/L. The absorption spectrum is composed of a strong absorption band with multiple peaks of 210 nm, 266 nm and 330 nm, respectively, and a broad weak band from 350 nm to 600 nm. The energy and extinction coefficient of the two strong absorption bands are comparable to those of free F-BT ligand reported by literature [15]. Hereby, these features are assigned to the spin-allowed $\pi \rightarrow \pi^*$ transition of F-BT ligand. $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ demonstrates both singlet MLCT ($^1\text{MLCT}$) and triplet MLCT ($^3\text{MLCT}$) absorption bands in the low energy region from 350 nm to 600 nm. According to the previous report [9], these weak bands located at long wavelengths have been assigned to the MLCT transitions of iridium complexes. Thus, the broad absorption shoulders at 474 and 495 nm observed for $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ are likely to be ascribed to the absorption for $^1\text{MLCT}$ and $^3\text{MLCT}$. The intensity of the $^3\text{MLCT}$ transition is close to that of $^1\text{MLCT}$, suggesting that the $^3\text{MLCT}$ transition is strongly allowed by an effective mixing of singlet–triplet with higher lying spin-allowed

transitions on the cyclometalated ligand [9]. Considering that the effective mixing in iridium complexes depends on the participation of Ir(III) electrons in frontier molecular orbitals, this mixing is facilitated by the large donation of iridium center to HOMO and LUMO, as revealed by Table 2.

3.2.2. PL spectrum and quantum yield

Fig. 3 also shows the PL spectrum of $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ in CH_2Cl_2 solution with a concentration of 1×10^{-4} mol/L. Clearly, the emission spectrum exhibits a gauss-liked emission band peaking at 528 nm with a FWHM of only 73 nm, without giving any vibronic progressions, suggesting a charge transfer emissive character. It is observed that the low energy absorption band around 600 nm overlaps with the emission peak, suggesting a slight geometric relaxation that occurs in the excited state. Unlike the multiple emission peaks of other ppy-based Ir(III) complexes, only one emission peak is detected for $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$, indicating that the emission comes from only one emissive center. Combined with DFT calculation results listed above, the emissive state is thus assigned as a $^3\text{MLCT}$ one.

PL quantum yield, which is defined as the ratio of the number of photons emitted to the number of photons absorbed, is an important parameter for emitters and can be determined according to the following expression:

$$\phi_s = \phi_r \left(\frac{B_r}{B_s} \right) \left(\frac{n_s}{n_r} \right)^2 \left(\frac{D_s}{D_r} \right) \quad (1)$$

Table 2

Calculated percentage composition of frontier molecular orbitals and the first five singlet excitations of $\text{Ir}(\text{acac-F6})(\text{F-BT})_2$ calculated at RB3PW91/SBKJC level.

	Energy (eV)	Ir	Composition (%)	
			F-BT	acac-F6
LUMO + 2 (126)	−2.261	11.9	80.1	8.0
LUMO + 1 (125)	−2.373	4.8	93.1	2.1
LUMO (124)	−2.476	5.6	32.2	62.2
HOMO (123)	−5.919	35.8	52.8	11.4
HOMO − 1 (122)	−6.338	43.5	46.6	10.0
$S_0 \rightarrow S_1$	2.668	123 $\rightarrow$ 124(95.3)		
$S_0 \rightarrow S_2$	2.861	123 $\rightarrow$ 125(86.0) & 123 $\rightarrow$ 126(8.3)		
$S_0 \rightarrow S_3$	2.980	123 $\rightarrow$ 126(84.9) & 123 $\rightarrow$ 125(7.0)		
$S_0 \rightarrow S_4$	3.062	122 $\rightarrow$ 124(94.1)		
$S_0 \rightarrow S_5$	3.197	122 $\rightarrow$ 125(74.8) & 122 $\rightarrow$ 126(15.7)		

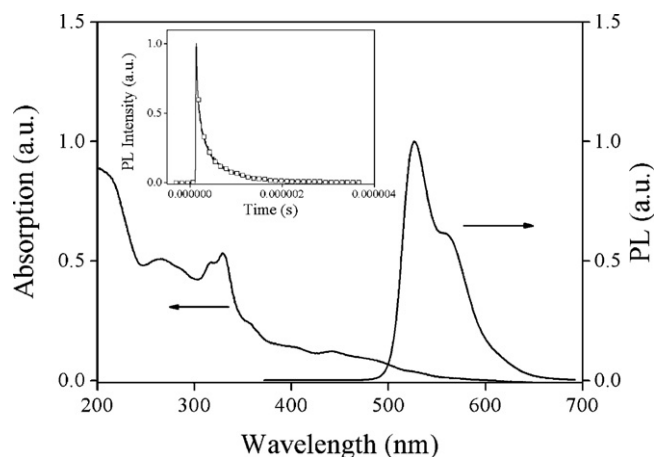


Fig. 3. Absorption and PL spectra of Ir(acac-F6)(F-BT)₂. Inset: PL decay data of Ir(acac-F6)(F-BT)₂.

where the subscripts *s* and *r* refer to sample and reference standard solution respectively, *n* is refractive index of the solvent, *D* is the integrated intensity, and Φ is luminescence quantum yield. The quantity *B* is calculated by $B = 1 - 10^{-AL}$, where *A* is the absorption coefficient at the excitation wavelength and *L* is the optical length. PL quantum yield of Ir(acac-F6)(F-BT)₂ is measured to be as high as 0.19, making itself a promising emitter for OLED applications.

3.2.3. Excited state lifetime

The emission owns an excited state lifetime of 0.29 μs in CH₂Cl₂ solution with a concentration of 1×10^{-4} mol/L, confirming the presence of a triplet state emissive character. Combined with the TD-DFT calculation result mentioned above, we come to a conclusion that the emission of Ir(acac-F6)(F-BT)₂ originates from ³MLCT excited state. The potential surface crossing (PSC) from higher $\pi \rightarrow \pi^*$ state to lower MLCT state of Ir(acac-F6)(F-BT)₂ is then analyzed by the measurement of its excited state lifetime. As shown by the inset of Fig. 3, the PL emission follows a single exponential decay pattern. In general, the observation of effective excitation band in $\pi \rightarrow \pi^*$ state absorption region and the shorter decay lifetime from $\pi \rightarrow \pi^*$ state than those from the lower MLCT state can suggest an efficient PSC from the higher $\pi \rightarrow \pi^*$ state to the lower MLCT state. As shown in Fig. 3, there is a strong absorption at $\pi \rightarrow \pi^*$ state region, suggesting an effective mixing of singlet-triplet and consequently high efficiency ³MLCT radiation. And this component assignment is consistent with the DFT result and Ir(acac-F6)(F-BT)₂'s high PL quantum yield mentioned above.

3.3. Thermal and electrochemical property of Ir(acac-F6)(F-BT)₂

Thermogravimetric analysis of Ir(acac-F6)(F-BT)₂ is shown in Fig. 4. Here, thermal decomposition temperature (*T*_{dec}) is defined as the temperature when the sample loses 5% of its initial weight. *T*_{dec} of Ir(acac-F6)(F-BT)₂ is measured to be 174 °C. This high decomposition temperature suggests that Ir(acac-F6)(F-BT)₂ is thermally stable enough to experience device construction through vacuum deposition. At 180 °C, Ir(acac-F6)(F-BT)₂ begins to lose weight obviously, with two regions of weight loss upon higher temperatures. The first gradual weight loss with an endothermic process from 200 to 280 °C is due to the liberation of acac-F6 ligand, which may be caused by the contribution from F-BT liberation. When the temperature increases to 300 °C, Ir(acac-F6)(F-BT)₂ begins to dramatically disassociate, which can be assigned to the thermal release of two cyclometalated F-BT ligand.

Cyclic voltammetry is used to investigate the electrochemical behavior of Ir(acac-F6)(F-BT)₂ and subsequently to evaluate

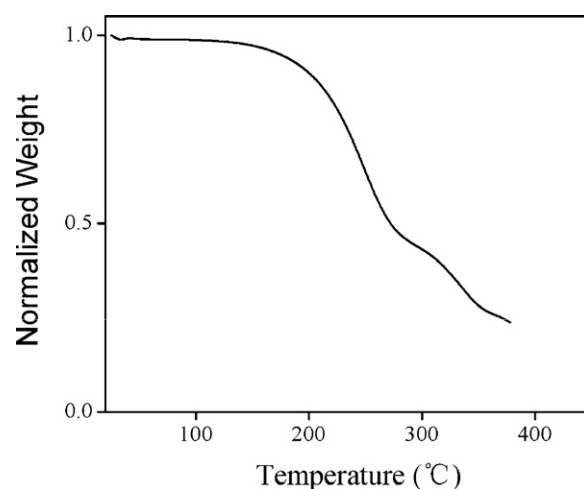


Fig. 4. TGA curve of Ir(acac-F6)(F-BT)₂.

its energy level. The oxidation and reduction potentials of Ir(acac-F6)(F-BT)₂ are measured to be 1.31 V and −1.32 V, respectively. The energy levels of HOMO and LUMO are calculated from the onset oxidation (*E*_{onset(Ox)}) and reduction (*E*_{onset(Red)}) potentials with the formula of $E_{\text{HOMO}} = -4.74 - E_{\text{onset(Ox)}}$ and $E_{\text{LUMO}} = -4.74 - E_{\text{onset(Red)}}$ (−4.74 V for SCE with respect to the zero vacuum level) [16]. The calculations give the *E*_{HOMO} of −6.05 V and the *E*_{LUMO} of −3.42 V for Ir(acac-F6)(F-BT)₂, respectively. The energy gap between *E*_{HOMO} and *E*_{LUMO} is calculated to be 2.63 eV, and this value is so close to the calculated onset electronic transition energy of 2.668 eV mentioned above. Those proper energy levels make Ir(acac-F6)(F-BT)₂ convenient to take the doping device structure for OLED applications.

3.4. Electroluminescence performance of Ir(acac-F6)(F-BT)₂

Considering Ir(acac-F6)(F-BT)₂'s excellent performances, including its high PL quantum yield, short excited state lifetime, good thermal stability, and proper HOMO/LUMO energy levels, we select Ir(acac-F6)(F-BT)₂ as a dopant to investigate its potential application in the field of OLED. In our initial work, we use a classic device structure of ITO/*m*-MTDATA (30 nm)/NPB (20 nm)/CBP:dopant (30 nm)/BPhen (15 nm)/Alq₃ (30 nm)/LiF (0.8 nm)/Al (300 nm), where *m*-MTDATA serves as a hole-injection layer, NPB is a hole-transporting layer, BPhen and Alq₃ are employed as an exciton-blocking layer and an electron-transporting layer, respectively.

Fig. 5 shows the EL spectra of devices at a driving voltage of 12 V upon various dopant concentrations from 4 wt% to 16 wt%. When the dopant concentration is as low as 4%, a weak emission originated from NPB peaking at 430 nm is observed, indicating that excess electrons are injected into NPB layer. Upon even higher dopant concentrations, NPB emission decreases and emission from Ir(acac-F6)(F-BT)₂ becomes dominant. In addition, the emission spectrum shows a slight red shift tendency to 550 nm compared with that of pure Ir(acac-F6)(F-BT)₂ due to the intermolecular action between emitter and host, which is consistent with previous report [17].

Fig. 6 depicts the current density versus luminance characteristics of the four EL devices. It can be seen that luminance increase dramatically with increasing current density. The 12 wt% EL device shows a maximum luminance of 27,000 cd/m². The current efficiency versus current density characteristics of the four EL devices suggest that the maximum current efficiency is achieved as high as 8.7 cd/A by the 12 wt% EL device. The current efficiency

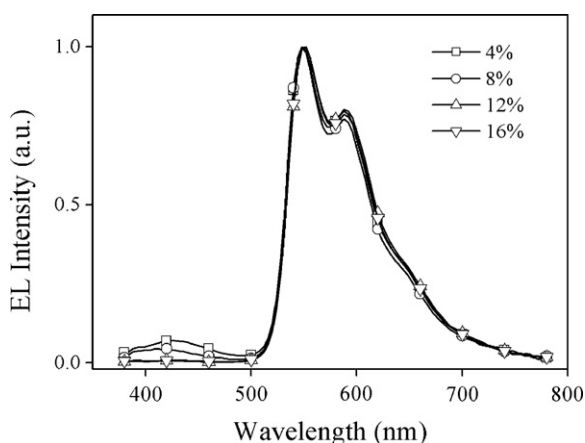


Fig. 5. EL spectra of devices at 8 V upon various dopant concentrations from 4 wt% to 16 wt%.

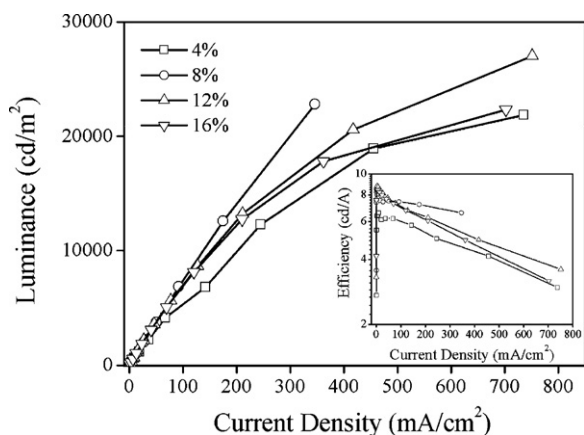


Fig. 6. Current density and luminance characteristics of the four EL devices.

of all EL devices decreases with increasing current density, owing to the triplet–triplet (T–T) and triplet–polar (T–P) annihilations [18]. Above data suggest that the optimal dopant concentration is 12 wt%, and further efforts need to be done to suppress the severe T–T and T–P annihilations. This finding may be helpful for future design of phosphors.

4. Conclusion

In this paper, we report a phosphorescent Ir(III) emitter of Ir(acac-F6)(F-BT)₂, including its crystal structure, electronic nature, photophysical characteristics, thermal and electrochemical properties. Data suggest that Ir(acac-F6)(F-BT)₂ is a promising emitter

with high quantum yield of 0.19 and good thermal stability, along with its proper energy levels for charge carrier transportation. OLEDs using Ir(acac-F6)(F-BT)₂ as emitter are also fabricated, and their electroluminescence performances are investigated in detail. The optimal EL device shows a maximum luminance of 27,000 cd/cm² and a peak current efficiency of 8.7 cd/A. The current efficiency of all EL devices decreases with increasing current density, owing to the triplet–triplet (T–T) and triplet–polar (T–P) annihilations [18]. Data suggest that the optimal dopant concentration is 12 wt%, and further efforts need to be done to suppress the severe T–T and T–P annihilations. In addition, it seems that the introduction of excess fluorine substituents into emitter is harmful for thermal stability. This find may be helpful for future design of phosphors.

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