# Fast Synthesis of the Iridium (Iii) Complexes At Room Temperature for High-Performance Oled<sub>s</sub>

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Abstract: Organic light-emitting devices (OLEDs) have attracted much attention due to their advantages of low driving voltage, high brightness and high efficiency. They have broad application prospects in solid-state lighting and flat panel display. Among the emitters used in OLEDs, the Iridium(III) complexes have been widely applied due to their tunable emission energy, excellent chemical stability and high photoluminescent efficiency. But for the preparation of most Ir(III) complexes, the last reaction process is always kept at high temperature for a long time, which would inevitably increase the manpower and cost. Therefore, it is important to find suitable ligands which can form phosphorescent complexes at room temperature efficiently. In this paper, a sulfur atom containing ligand of N,N-diisopropyl dithiocarbamate was prepared and used as an ancillary ligand for red and green Ir(III) complexes with 4-(4-(trifluoromethyl)phenyl)quinazoline and 2-[4-(trifluoromethyl)phenyl]pyridine as the cyclometalated ligands, respectively. Both complexes were synthesized at room temperature in few minutes and also show good device performances. Respectively, the red OLED shows a maximum luminance above 26000 cd m-2 and an EQEmax of 15.30%. and the green device displays a Lmax above 33466 cd m-2 with an EQEmax of 25.17%. These results suggest that the sulfur containing Ir(III) complexes have potential application in OLEDs with reduced cost

#### 1. Introduction

# 1.1 Concept of Electroluminescence and Advantage of Organic Light-Emitting Diode (Oled).

Electroluminescence (EL) is a process by which photons are generated when the excess electron—hole pairs are created by an electric current caused by an externally applied bias. And the organic light-emitting diode (OLED) is the device which can realize the EL process. Nowadays, the display market is predominated by LCD (liquid crystal display). But LCD has its weaknesses like slow response time, requirement for the background light, high cost of energy, narrow viewing angle and instability to high temperatures, which provides the chance for the rise of OLEDs. Currently, OLED has taken quite a place in the mobile display market and also begun expanding their presence to TVs market and lighting with a near-30-year development, including the potential for flexible screen.

# 1.2 Working Mechanism of Oled

The typical electroluminescence device consists of glass substrate, transparent anode, electron hole transport layer, emissive layer, and cathode, etc.

#### 1.3 Emitters for Oled Devices

As emitters in OLED, there are mainly three types of materials (Figure 1). After the birth, excitons in organic molecules come to the singlet excited state  $(S_1, S_2...)$  from the ground state  $(S_0)$ . Meanwhile, the instable high-state excitons drop back to the minimum excited state  $S_1$  by internal conversion, and the electrons in state  $S_1$  have the possibility of reaching the triplet state with the least energy  $T_1$  by intersystem crossing. If the electron goes back to  $S_0$  (electronic ground

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state) from  $S_1$  in the form of electromagnetic radiation, the material gives out fluorescence. What's more, according to Statistical theory of electron spin and quantum chemistry, the proportion of singlet excitons and triplet excitons turns out to be 1:3. But because in most of the molecules, the triplet excitons are prohibited from going back to the ground state or giving out phosphorescence (they would turn into heat), which cause the maximum efficiency of OLED device to nearly 25%.

If the electron goes back from T<sub>1</sub> to S<sub>0</sub>, phosphorescence would take place. However, due to the fact that the spin direction of the electron on S<sub>0</sub> varies from that on the T<sub>1</sub>, phosphorescence couldn't be obtained because of forbidden transition generally. But in complexes with the heavy-metal center, the existence of heavy-metal atoms causes spin-orbital coupling (SOC), making the prohibited triplet able to give phosphorescence and improving the efficiency of the device to 100%. At present, the cyclometalated Iridium(III) complexes have attracted great attention because of their tunable emission energy, excellent chemical stability and high photoluminescent efficiency<sup>[1,2,3,4,5,6,7]</sup>. For the commercial OLED products, the green and red emitters are Ir(III) complexes. But in comparison with extensively studied Ir(III)-based red and green phosphorescent complexes, the efficient blue emitters are limited due to their high lying energy level and long triplet state lifetime, and the performances of blue OLEDs are still not satisfactory. Therefore, achieving stable and highly efficient blue phosphorescent Ir(III) complexes and their corresponding devices still remains a significant challenge with low device operation lifetime.

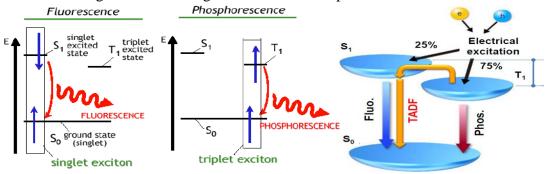


Fig.1 The Luminescence Mechanisms of Three Type Materials<sup>[8,9,10,11]</sup>

# 1.4 The Development of Ir(Iii) Complex

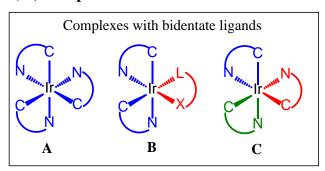


Fig.2 Different Coordination Types of Neutral Ir(Iii) Phosphorescent Complexes (C^n: Main Ligand, l^X: Ancillary Ligand).

As mentioned in the Figure 2, the phosphorescent Ir(III) complexes adopt a disordered octahedral geometry with six coordination bonds. For complexes with structures A-C, three monovalent bidentate ligands are used to form homoleptic (A) complex with same organometallic ligands and heteroleptic (B and C) complexes with different ligands. Normally, Ir(III) complexes used in OLEDs are divided into three main groups depending on the light they give off when exerted with electric current: green, red and blue Ir(III) complexes (some examples are listed in Figure 3). Since the emitting properties of the Ir(III) phosphors are mainly determined by the triplet metal-to-ligand charge transfer state (<sup>3</sup>MLCT) and/or triplet ligand centered charge transfer state (<sup>3</sup>LC), the energy levels and the ligand field strength of the organometallic ligands are essential for the emission color, band width, decay time and quantum yields, etc.

The research on the green complexes were done the earliest because they always show higher brightness and efficiency than the other two kinds. The most widely and intensively studied green Ir(III) complex is fac-Ir(ppy)<sub>3</sub> whose application in the organic electrophosphorescent device was first reported by Thompson and Forrest et al. in 1999<sup>[12,13,14]</sup>. Due to the proper ligand filed strength and energy level of ppy derivatives, many efficient green homoleptic Ir(III) phosphors have been developed in the past years. But the synthesis of homoleptic Ir(III) is complicated due to the high synthesis temperature and mixed products of fac/mer-Ir(ligand)3, which were difficult to be separated. Therefore, most work were focusing on the heteroleptic Ir(III) complexes with different ancillary ligands. The most widely used and intensively studied ancillary ligand is acetyl acetone (acac), such as  $Ir(ppy)_2(acac)^{[15,16,17,18,19,20,21,22,23]}$ . Since the acac ligand does not exert significant influence on the frontier molecular orbitals, the photophysical properties of the heteroleptic phosphors with acac ancillary ligand are mainly determined by the main organometallic ligands. In 2011, Zheng Youxuan group reported a novel ancillary ligand tetraphenylimidodiphosphinate (tpip) with large steric hindrance and the corresponding phosphor Ir(tfmppy)2(tpip) has good electron mobility<sup>[24]</sup>. Consequently, the device efficiency can be enhanced and the efficiency roll-off effect can be suppressed.

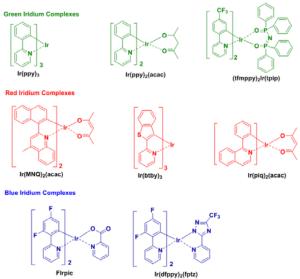


Fig.3 The Examples of Some Iridium(Iii) Complexes with Green, Red and Blue Colors.

Red Ir(III) complexes come after the green ones. In order to achieve long wavelength emission, the phosphors should have small HOMO/LUMO energy band gap, which guarantees the low emissive excited state energy. The widely-used molecular design approaches are increasing the conjugated structure of the organometallic ligand by fused aromatic rings and introducing electron-rich aromatic moieties into the ligand, such as the complexes of Ir(btby)3, Ir(MNQ)2(acac) and Ir(piq)2(acac)[17,22,23].

But in comparison with extensively studied Ir(III)-based red and green phosphorescent complexes, the efficient blue emitters are limited due to their high lying energy level and long triplet state lifetime, and the performances of blue OLEDs are still not satisfactory. As the most famous sky-blue emitter, FIrpic benefits from not only the fluorine substituents on the ppy main ligand but also the pic ancillary ligand with high ligand field strength. By replacing pic by 1,2,4-triazole pyridine, Ir(dfppy)<sub>2</sub>(fptz) derivatives were also widely investigated<sup>[25,26,27]</sup>. Therefore, achieving stable and highly efficient blue phosphorescent Ir(III) complexes and their corresponding devices still remains a significant challenge with low device operation lifetime.

# 1.5 The Research Target of This Work

As mentioned before, the Ir(III) complexes are the most important emitters for OLEDs, and the demand for this precious substance is huge in the industrialization of product. In order to speed up the process of OLEDs industrialization, cost reduction is also important. But for the preparation of

most Ir(III) complexes, the last reaction process is always to reflux the  $[(C^N)_2 Ir(\mu-Cl)]_2$  chloride-bridged dimmer with cyclometalated or ancillary ligands at high temperature (110 °C) for a long time (> 2 h), which would inevitably increase the manpower and cost. It is important, but difficult to find suitable ligands which can form phosphorescent complexes at room temperature efficiently to reduce the cost of OLEDs industrialization significantly.

Meanwhile, four-membered ring structures of Ir(III) complexes with sulfur atoms in the ancillary ligands are rarely studied in OLEDs, and there is no new progress in the research of the Ir(III) complexes containing the four-membered ring based on Ir-S-C-S backbone. Furthermore, the Hard-Soft-Acid-Base (HSAB) theory is widely used to judge the stability of the metal complexes and also to explain the reaction mechanism. The central theme of this theory is that when all other factors are the same, the "soft" acid with the "soft" alkali and the "hard" acid with the "hard" alkali react more quickly and form strong bonds. Based on this theory, the central Iridium atom and sulfur ion can be classified as soft acid and base, respectively, thus the bonding speed of complexes is fast and the formed compounds are stable. Therefore, in this paper we synthesize two red and green Ir(III) complexes at room temperature in several minutes with the sulfur-containing ligands.

# 2. Rapid Synthesis of a Red Iridium(Iii) Complex with Four-Membered Ir-s-C-s Chelating ring At Room Temperature

### 2.1 Experimental

All chemical reagents are purchased commercially without purification. NMR is measured in Bruker AM 400M, molecular masses of the ligands are measured by ESI-MS (LCQ fleet, Thermo Fisher Scientific). Molecular mass of the complex is measured on MALDI-TOF-MS. Elemental analyses of the percentage of carbon, nitrogen and oxygen are completed on Elementar Vario MICRO analyzer. Thermal analysis is tested on DSC 823e analyzer (METTLER). Absorption and emission spectra are measured respectively on UV-3100 and Hitachi F-4600. Lifetime for the complex is tested in normal temperature and anaerobic system, using Edinburgh Instruments FLS-960. Electrochemistry statistics are measured on MPI-A multifunctional electrochemistry and chemical luminance instrument with tetrabutylammonium hexafluorophosphate as supporting electrolyte, ferrocene as external standard, glassy carbon electrode as electrode, platinum wire electrode as the opposite electrode, and Ag/AgNO3 electrode as the reference electrode. Quantum efficiency of the solution is calculated by comparing the strength of the emission peak of the sample and the standard *fac*-Ir(ppy)3 in the formula below:

$$\Phi_s = \Phi_{std}(\frac{I_s}{I_{std}}) \left(\frac{A_{std}}{A_s}\right) \left(\frac{\eta_s}{\eta_{std}}\right)^2$$

### 2.2 Results and Discussion

#### 2.2.1 Analysis of the Structure of Irred Single Crystal.

The single crystal was obtained by vacuum sublimation and X-ray diffraction measurements was carried out. The ellipsoid structure is shown in Figure 4.

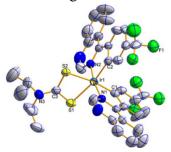


Fig.4 The Ellipsoid Structure of the Complex Irred (Hydrogen Omitted), (Ccdc No. 1832357) .Ellipsoids Are Drawn At 50% Probability Level.

The expected octahedral coordination geometry is formed with Iridium atoms as the center which has six coordination sites. Structurally, in *Irred*, two coordination C atoms of main quinazoline ligands are on one side of the Iridium atom, causing the [C1-Ir-C2] angle less than 90 degrees, while two N atoms form a straight line on both sides of the Iridium atom. The *Irred* has octahedral coordination geometry around Iridium center by three chelating ligands with *cis*-C-C and *trans*-N-N dispositions in which the N-Ir-N angles is almost 175°. Two coordination S atoms and two coordination C atoms form a planar quadrilate-like structure. The four-membered Ir-S-C-S backbone could cause significantly acute S-Ir-S bite angle compared with the larger five-membered or six-membered heterocycles based on such as pic, acac derivatives. It also illustrates that -1 charge of dithiocarbamate is scattered over both sulfur atoms. The two coordinated S atoms of ancillary ligand reside in the equatorial plane *trans* to the metalated atoms. From the above analysis, this compact and tensile bonding mode is well understood.

# 2.2.2 Thermogravimetric Analysis

The thermal stability of *Irred* values a lot for organic electroluminescent devices. By thermogravimetry (TG) method, we measured the thermal property of the Ir(III) complex. The TG curve in the Figure 5 (5% wt weight loss) is as high as 384°C, which indicates that the introduction of sulfur atoms in ancillary ligand can strongly affect the decomposition temperature of complex. Moreover, the high decomposition temperature of the complex indicates that it could be used in OLEDs.

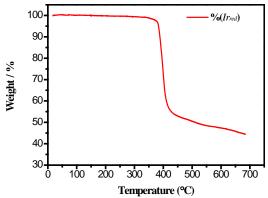


Fig.5 The Decomposed Temperature (5% Wt Weight Loss)

# 2.2.3 Photophysical Property of Irred

As shown in Figure 6, the UV-Vis absorption and emission spectra of *Irred* were measured in the dichloromethane solution (without oxygen) with a concentration of  $5 \times 10^{-5}$  mol/L. And, the relevant data are listed in Table 1.

The intense absorption bands below 400 nm arise from the spin-allowed intraligand  $\pi \to \pi^*$  transitions, and the relatively weak bands in the visible region (400-630 nm) can be assigned to the mixed  $^1$ MLCT and  $^3$ MLCT (metal-to-ligand charge-transfer) states, or LLCT (ligand-to-ligand charge-transfer) transition through strong spin-orbit coupling of Iridium atom.

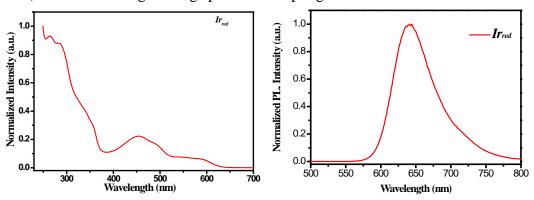


Fig.6 The Absorption Spectrum (Left) and Emission Spectrum of Irred (Right).

Table 1 the Photophysical Properties of Irred.

		$T_{\rm d}$	Absorption	Emission	□ 298 K	□ P	$E_{\mathrm{T}}$	HOMO/LUMO
		$(^{\circ}C)^{a}$	$(\square \ nm)^b$	$(\square_{\max} nm)^b$	$(\mu s)^b$	(%) <sup>c</sup>	$(eV)^d$	$(eV)^e$
	Irred	384	263/285/453/592	641	1.41	58.3	2.04	-5.44/-3.19

<sup>a)</sup>  $T_d$ : decomposition temperature (with 5% mass loss); <sup>b)</sup> Determination at room temperature in dichloromethane solution (without oxygen), with a solution concentration of  $5\times10^{-5}$  mol/L; <sup>c)</sup> Determination at room temperature with fac-Ir(ppy) as a reference material ( $\Phi$ = 0.40) in dichloromethane solution; <sup>d)</sup> The cyclic voltammetry curve and UV-Vis absorption spectrum were calculated with ferrocene as internal standard.

The PL quantum yield of *Irred* was measured as 58.3%. In addition, the lifetime of *Irred* is in the microsecond range (1.41  $\mu$ s), which is indicative of the phosphorescent origin for the excited states in the case.

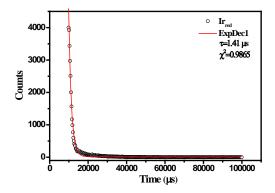


Fig.7 Lifetime Curve of Irred.

# 2.2.4 Electrochemistry and the Theoretical Calculation

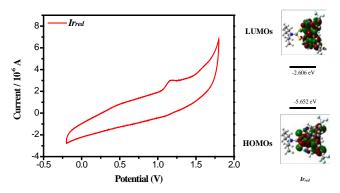


Fig.8 Cyclic Voltammetric Curve of Irred (Left) and Orbital Electron Density Distributions of Homo/Lumo (Right).

The HOMO/LUMO level values of the complex matter a lot to the design of OLEDs. In order to measure the HOMO/LUMO energy levels of *Irred*, the electrochemical properties of the complex were studied by cyclic voltammetry in dichloromethane solution (without oxygen) with ferrocene as external standard and saturated potassium chloride calomel electrode as reference electrode. As shown in Figure 8 (left), the cyclic voltammetric curve of *Irred* shows a strong oxidation peak, but the reduction peak is not obvious, displaying that the redox process of complex is irreversible. According to the peak value of oxidation with the equation of  $E_{\text{HOMO}} = (E_{\text{OX}} + 4.8) \text{ eV}$ , the HOMO level is calculated as -5.44 eV. Based on the HOMO level and spectral bandgap, the LUMO level is calculated to be -3.49 eV.

Table 2 the Electronic Cloud Density Distributions of Irred

Complex	Orbital	Energy/eV (Calculated)	Energy/eV	Composition (%)		
			(experimental)	Main ligand	Ir	Ancillary Ligand
Irred	HOMO	-5.65	-5.44	47.9	39.42	12.67
	LUMO	-2.61	-3.19	94.35	3.45	2.20

#### 2.2.5 Oled Performances

To illustrate their electroluminescence (EL) properties, typical OLED using the complex as an emitter was fabricated with ITO / HAT-CN (dipyrazino[2,3-f:2',3'-h]quinoxaline-2,3,6,7,10,11-hexacarbonitrile, 6 nm) / HAT-CN (0.2 wt%): TAPC (di-[4-(N,N-ditolylamino) phenyl]cyclohexane, 50 nm) / Irred (3 wt%): 2,6DCzPPy (2,6-bis(3-(carbazol-9-yl)phenyl)pyridine, 10 nm) / Tm3PyP26PyB (1,3,5-tris(6-(3-(pyridin-3-yl)phenyl)pyridin-2-yl) benzene, 60 nm) / LiF (1 nm) / Al (100 nm) is named as Dev1.

#### 2.3 Conclusion

Due to the sulfur atoms in the dithioformate ancillary ligand, a red Ir(III) complex with 4-(4-trifluoromethylphenyl)quinazoline as main ligand was synthesized at room temperature in few minutes. The single crystal analysis confirmed its molecular structure. Theoretical calculations show that the HOMO-level electron clouds of the complex mainly distribute in the main ligands quinoxaline and d orbital of the Ir atom, and the LUMO-level electron clouds mainly distribute in the main ligand. The emission peak reaches 641 nm with a quantum efficiency in the solution of 58.3%, and the lifetime of the excited state is also in microsecond order. The complex has 4-(4-trifluoromethylphenyl)quinazoline electron-withdrawing electron-donating group and iisopropylamine group, which means that it has bipolar ability, thus largely improving the device efficiency and reducing the efficiency roll-off. Using this complex as emitter, the single-layer OLED shows good performances with a  $L_{\text{max}}$  above 26000 cd m<sup>-2</sup>, a  $\eta_{\text{c,max}}$  of 9.81 cd A<sup>-1</sup> and an EQE<sub>max</sub> of 15.30%. From the above discussion, we can find out that with the sulfur containing dithioformate ligand can synthesize the Ir(III) complex efficiently and reduce the cost.

# 3. Rapid Synthesis of a Green Iridium(Iii) Complex with Four-Membered Ir-s-C-s Chelating ring At Room Temperature

# 3.1 Experimental

#### 3.1.1 Reagents Needed:

2,4-*bis*(trifluoromethyl)phenylboronic acid, 2-bromopyridine, diisopropylamine, LiOH•H<sub>2</sub>O, benzene, carbon disulfide, IrCl<sub>3</sub>, anhydrous THF, 2-ethoxyethanol (EtOCH<sub>2</sub>CH<sub>2</sub>OH) and Pd(PPh<sub>3</sub>)<sub>4</sub>.

#### 3.2 Results and Discussion

# 3.2.1 Analysis of the Structure of Single Irgreen Crystal.

The single crystal was obtained by vacuum sublimation and X-ray diffraction measurements was carried out..

# 3.2.2 Thermogravimetric Analysis

the thermal stability of the complex is very important to the OLED operation. From the DSC curve in Figure 9 it's clear that the melting point of Irgreen is 323 °C. In the TG curve (right), its thermal decomposition temperatures ( $T_d$ , corresponding to 5% weight loss) is 334°C. The two figures show the thermal stability of Irgreen is very good, and it has potential in OLED service.

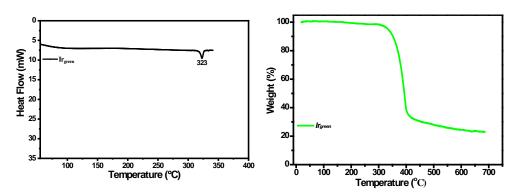


Fig. 9 Dsc (Left) and Tg (Right) Curves of Irgreen.

# 3.2.3 Electrochemistry and the Theoretical Calculations

In order to determine the HOMO/LUMO levels of *Irgreen*, the electrochemical property of *Irgreen* was investigated by cyclic voltammetry in deaerated CH<sub>2</sub>Cl<sub>2</sub>, relative to an internal ferrocenium/ferrocene reference (Fc<sup>+</sup>/Fc) (Figure10). According to the equation of  $E_{\text{HOMO}} = -(E_{\text{ox}} - E_{\text{Fc/Fc+}} + 4.8)$  eV, the HOMO energy level ( $E_{\text{HOMO}}$ ) of *Irgreen* was obtained. Based on the  $E_{\text{HOMO}}$  and optical band gap calculated by the equation of  $\Delta E_{\text{bandgap}} = 1240/\lambda_{\text{abs-onset}}$ , the LUMO energy level was also obtained.

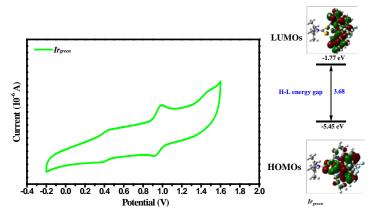


Fig.10 Cyclic Voltammogram Curve of Irgreen (Left) and Molecular Orbital Diagram for the Homo/Lumo of the Complex Calculated in Ch<sub>2</sub>cl<sub>2</sub> (Right).

#### 3.2.4 Oled Performance

Since the OLED device with single emissive layer has been examined before, in this section we would mainly discuss the OLED with double emissive layers with the configuration of ITO / HAT-CN (dipyrazino[2,3-f:2',3'-h]quinoxaline-2,3,6,7,10,11-hexacarbonitrile, 5 nm) / (di-[4-(N,N-ditolylamino)phenyl]cyclohexane, 50 nm) Irgreen (x wt%) **TCTA** 2,6DCzPPy (4,4',4"-tris(carbazol-9-yl)triphenylamine, nm) Irgreen wt%) (2,6-bis(3-(carbazol-9-yl)phenyl)pyridine, **TmPvPB** (1,3,5-tri[(3-pyridyl)-phen-3-yl]benzene, 50 nm) / LiF (1 nm) / Al (100 nm) named as Dev2. As shown in Figure 22, the materials of HAT-CN and LiF served as hole- and electron-injecting interface modified materials, respectively. The bipolar material 2,6DCzPPy and the hole-transporting material TCTA were chosen as host materials, respectively. The stepwise changed HOMO energy levels of TAPC (-5.5 eV), TCTA (-5.7 eV) and 2,6DCzPPy (-6.1 eV) are beneficial for the hole injection and transport. Similarly, it is also beneficial for the injection and transport of electrons owing to the gradual changed LUMO energy levels of TmPyPB (-2.7 eV), 2,6DCzPPy (-2.6 eV) and TCTA (-2.4 eV). Additionally, the triplet state (2.34) of the Irgreen is within the 2,6DCzPPy, which is helpful to inhibit the energy reversion from the guest to the host. Thus, holes and electrons will be distributed in more balanced emissive layers and the exciton recombination zone is expected to be broadened. Furthermore, the HOMO energy level of TmPyPB is 0.6 eV lower than that of 2,6DCzPPy and the LUMO energy level of TAPC is 0.6 eV higher than that of TCTA, which would result in well conformed exciton (hole-electron pair) within emissive layers and the triplet exciton quenching avoided effectively.

The electroluminescence (EL) spectrum, current density (*J*)-voltage (*V*)-luminance (*L*), current efficiency ( $\eta_c$ ) and power efficiency ( $\eta_p$ ) versus luminance, and EQE as a function of luminance characteristics of the device are displayed

The Dev 2 ( $\Phi_P$  of *Irgreen* is 71.6%) at a doping concentration of 8 wt% shows good EL performances with the maximum luminance ( $L_{max}$ ) above 33466 cd m<sup>-2</sup>, the peak current efficiency ( $\eta_{c,max}$ ) of 86.81 cd A<sup>-1</sup>, the peak power efficiency ( $\eta_{p,max}$ ) of 59.85 lm W<sup>-1</sup> and a maximum external quantum efficiency (EQE<sub>max</sub>) of 25.17% with CIE coordinates of (0.253, 0.634).

Table 3 El Performances Of the Device.

Device	V <sub>turn-on</sub> <sup>a)</sup>	$L_{ m max}$	$\eta_{ m c,max}$	$\eta_{ m ext,max}$	$\eta_{ m p,max}$	$\eta_c^{b)}$	$\eta_{\rm ext}^{\rm b)}$	CIE <sup>c)</sup>
	(V)	(cd m <sup>-2</sup> )	(cd A <sup>-1</sup> )	(%)	(lm W <sup>-1</sup> )	(cd A <sup>-1</sup> )	(%)	(x, y)
Dev 2	3.1	33466	86.81	25.17	59.85	86.18	24.92	(0.253, 0.634)

<sup>&</sup>lt;sup>a)</sup> Applied voltage recorded at a luminance of 1 cd m<sup>-2</sup>; <sup>b)</sup> Recorded at 10000 cd m<sup>-2</sup>; <sup>c)</sup> Measured at driving voltage of 5 V.

#### 3.3 Conclusion

Due to the sulfur atoms in the dithioformate ancillary ligand, a green Ir(III) complex with 2-[4-(trifluoromethyl)phenyl]pyridine as main ligand was synthesized at room temperature in five minutes. The single crystal analysis confirmed its molecular structure. Theoretical calculations show that the HOMO-level electron clouds of the complex mainly distribute in the main ligands quinoxaline and d orbital of the Ir atom, and the LUMO-level electron clouds mainly distribute in the main ligand. The emission peak reaches 513 nm with a quantum efficiency in the solution of 71.6%, and the lifetime of the excited state is also in microsecond order. Using this complex as emitter, the OLED with double emissive layers shows good performances with a  $L_{\text{max}}$  above 33466 cd m<sup>-2</sup>, a  $\eta_{\text{c,max}}$  of 86.81 cd A<sup>-1</sup> and an EQE<sub>max</sub> of 25.17%. From the above discussion, we can find out that with the sulfur containing dithioformate ligand can be used as a potential ligand for synthesis of the Ir(III) complex efficiently and reduce the cost.

#### 4. Conclusions

In summary, with use of dithioformate ancillary ligand containing sulfur atoms, we successfully constructed versatile Iridium complexes rapidly at room temperature. By synthesizing these complexes at room temperature in mere minutes, costs of the OLEDs are successfully reduced. More interestingly, we showed the Basic thermal, photophysical, structural properties and the performance in devices. Since the high capabilities of these four-membered-ring complexes, it is reasonable to speculate that these multifunctional material might find potentials in the area of display.

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