



Synthesis and characterization of a new iridium(III) complex with bulky trimethylsilylxylylene and applications for efficient yellow-green emitting phosphorescent organic light emitting diodes

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ABSTRACT

We designed and synthesized a new iridium(III) complex with phenylpyridine ligands containing a bulky trimethylsilylxylylene, 5-(2,5-dimethyl-4-(trimethylsilyl)phenyl)-2-phenylpyridine, by Suzuki coupling reaction and characterized using various spectroscopic studies. Nuclear magnetic resonance studies show its structure to be that of a facial isomer. Thermogravimetric analysis and differential scanning calorimetry studies show its higher thermal stability ($\Delta T_{5\%}$) of 638 K with a glass transition temperature of 425 K. It shows the photoluminescence emission at 532 nm in solution with the band gap energy of 2.56 eV. The new iridium(III) complex as dopant in phosphorescent organic light emitting diodes exhibits the yellow-green emission at 532 nm as it effectively hinders aggregation formation in the solid state at a dopant concentration of 6%, resulting in higher device efficiencies of 12.7% and 45.7 cd/A. The results show that the new iridium complex could be useful in white organic light emitting diodes for the lighting applications.

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1. Introduction

Since organic light emitting diodes (OLEDs) were demonstrated first by Tang and Van Slyke, tremendous efforts have been made in the field of OLEDs. OLEDs have many advantages such as low power consumption, wide viewing angle, fast response time, compactness and light weight for display and solid state lighting applications [1–4]. Compared to the fluorescent OLEDs, the performance of the phosphorescent OLEDs is significantly improved because both singlet and triplet excitons generated can be harvested for light emission [5]. Since then, phosphorescent OLED materials and devices have been intensively studied for higher device performances. Among the various phosphorescent materials, iridium complexes remain as efficient phosphorescent emitters in OLEDs because of their relatively short life-times and high quantum efficiencies. The emission wavelength of iridium complexes can be fine-

tuned by the introduction of substituent groups having different electronic effects or leading to variations in the conjugation system of ligands [6–13]. The highly efficient white OLEDs (WOLEDs) have recently been demonstrated using three-colour (red, green and blue) phosphorescent materials in which the most commonly used green-emitting phosphorescent iridium complex, fac-tris(2-phenylpyridine)iridium [Ir(ppy)₃], was employed for the green emission with peak emission around 510 nm [14,15]. WOLEDs employing Ir(ppy)₃ as a phosphorescent dopant emitter for the green emission exhibit a lack of emission intensity in the yellow-green region, which influences the colour purity of the devices [14,15]. Fluorescent dyes, such as 5,6,11,12-tetraphenylnaphthacene (rubrene) (peak at 560 nm) and 4-(dicyanomethylene)-2-*t*-butyl-6-(1,1,7,7-tetramethyljulolidyl-9-enyl)-4*H*-pyran (DCJTb) (peak at 568 nm), which were sensitized by the phosphorescent Ir(ppy)₃ complex, have been utilized for yellow-green emission in efficient WOLEDs suitable for the lighting applications [16,17].

Phosphorescent emitter materials having high thermal stability, high vapour pressure, good solubility, and a wide range of emission colours are useful in both solution-processed- and vacuum-deposited- OLED devices for display and lighting applications. The

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substitution of methyl groups on the ppy ligands of green-emitting Ir(ppy)₃ has considerable influence on photophysical, electrochemical and electroluminescence properties, in particular colour tuning up to yellow-green emission [9]. The substitution of Triarylsilyl moieties showed high chemical stability and improved solubility, resulting in improved device performances [18]. However, the triarylsilyl derivatives possess some drawbacks such as lower yield, difficulties in synthesis and low vapour pressure. We have reported that the trimethylsilyl functional groups confer such attributes as higher vapour pressure, thermal stability (high T_g), good solubility and steric bulk via higher volume [7]. Iridium(III) complexes with trimethylsilyl groups also showed yellowish-green electroluminescence (524 nm) with higher device efficiencies of 39.2 cd/A and 17.3 lm/W.

In this study, we designed and synthesized a new iridium(III) complex with phenylpyridine ligands containing a bulky trimethylsilylxylylene, 5-(2,5-dimethyl-4-(trimethylsilyl)phenyl)-2-phenylpyridine [Ir(dmtppy)₃], suitable for lighting applications. The introduction of a bulky, twisted trimethylsilylxylylene on pyridine ring of Ir(ppy)₃ is expected to effectively hinder the aggregation formation as well as tune the emission colour, red-shifted, to yellow-green, suitable for lighting applications.

2. Experimental

2.1. Materials

All experiments were performed under dry N₂ atmosphere using standard Schlenk technique. All solvents were freshly distilled over appropriate drying reagents prior to use. All starting materials were purchased from either Aldrich or TCI and were used without further purification.

2.2. Measurements

¹H and ¹³C nuclear magnetic resonance (NMR) spectra were recorded using DRX 300 MHz Bruker spectrometer and chemical shifts in spectra were reported in parts per million (ppm) units with tetramethylsilane as internal standard. Infrared (IR) measurements of the samples were carried out using a Genesis II FT-IR spectrometer. A Jeol JMS-700 mass spectrometer (MS) was used to obtain the high-resolution mass (HR-Mass) spectra of the samples. Thermogravimetric analysis (TGA) was performed under nitrogen using a TA instrument 2025 thermogravimetric analyzer. The sample was heated from 323 K to 1073 K with a heating rate of 283 K per minute. Differential scanning calorimeter (DSC) studies were carried out under nitrogen atmosphere using a TA instrument 2100 differential scanning calorimeter. The sample was heated from 303 K to 523 K with a heating rate of 283 K per minute. UV–visible absorption and photoluminescence (PL) spectra were recorded at room temperature using Perkin Elmer LAMBDA-900 UV/VIS/NIR spectrometer and LS-50B luminescence spectrophotometer, respectively. For the PL efficiency measurements, CBP thin film of 50 nm doped with Ir(dmtppy)₃ (6%) was deposited on the quartz substrate and excited at 325 nm determined from the excitation spectrum of Ir(dmtppy)₃ in solution. Cyclic voltammogram (CV) of the sample was recorded using a Epsilon E3 cyclic voltammeter at room temperature using the conventional three electrode configuration consisting of platinum working electrode, a platinum wire as auxiliary electrode and Ag/AgCl wire as quasi reference electrode. 4,4'-bis[N-(1-naphyl)-N-phenyl-amino] biphenyl (NPB) was used as an internal reference. The cyclic voltammogram was made in one compartment glass cell in methylene chloride containing 1 × 10^{−3} complex and 0.1 M solution of

tetrabutylammonium perchlorate (C₁₆H₃₆ClNO₄) as supporting electrolyte under nitrogen environment at a scan rate of 50 mV s^{−1}.

2.3. Synthesis

2.3.1. (4-Bromo-2,5-dimethylphenyl)trimethylsilane (1)

A solution of 1,4-dibromo-2,5-dimethylbenzene (15 g, 0.43 mol) in tetrahydrofuran (THF) (200 mL) was cooled to 195 K. *n*-BuLi (27.3 mL, 0.68 mol, 2.5 M in hexane) was slowly added dropwise to the above solution. After stirring for 1 h, the solution was cooled down again to 195 K. Then, trimethylsilyl chloride (TMSCl, 8.97 mL, 0.74 mol) was added dropwise and the mixture was allowed to warm to room temperature and stirred overnight. Then, 50 mL of water was added to the above solution. The aqueous phase was extracted three times with 150 mL of ether. The combined organic phase was washed with water (3 × 150 mL) and then dried over MgSO₄. After removal of the solvents, using column chromatography on silica with hexane, the pure product was obtained in 87% yield as colourless oil (12.7 g). ¹H NMR (300 MHz, CDCl₃) ppm: 7.32 (s, 1H), 7.28 (s, 1H), 2.93 (s, 6H), 0.32 (s, 9H). IR (KBr, cm^{−1}): 3150, 1600, 1452, 1412, 730, 650.

2.3.2. 2,5-Dimethyl-4-(trimethylsilyl)phenylboronic acid (2)

An oven-dried, three-necked flask was loaded with (4-bromo-2,5-dimethylphenyl)trimethylsilane (**1**) (11 g, 0.43 mol), in 150 mL of THF under N₂. After cooling down the solution to 195 K, 20.53 mL (2.5 M solution in hexane) of *n*-BuLi (0.51 mol) was added dropwise to the solution. The solution was then allowed to warm up to 263 K and then cooled to 195 K again. 9.40 mL of triethylborate (0.56 mol) was slowly added and the solution warmed up to room temperature and left under N₂ overnight. Then, 50 mL of 2 N HCl was added and the solution was stirred for 30 min before evaporation to drying. The crude product was dissolved in dichloromethane and washed with water. The aqueous phase was extracted three times with 150 mL of dichloromethane. The combined organic layers were evaporated to dryness. The crude product was washed with hexane. The pure product was obtained in 70% yield as a white powder (4g). m.p: 469–471 K. ¹H NMR (300 MHz, CDCl₃) ppm: 7.96 (s, 1H), 7.37 (s, 1H), 2.78 (s, 3H), 2.51 (s, 3H), 1.5 (s, 2H), 0.36 (s, 9H). IR (KBr, cm^{−1}): 3250, 3150, 1600, 1450, 1412, 725.

2.3.3. 5-Bromo-2-phenylpyridine (3)

2,5-Dibromopyridine (4.5 g, 0.19 mol), phenylboronic acid (2.8 g, 0.22 mol) and Pd(PPh₃)₄ (0.66 g, 3 mol%) were dissolved in toluene (60 mL). A solution of 2M K₂CO₃ (20 mL) was added and the mixture was refluxed with stirring for 24 h in the nitrogen atmosphere. After it was cooled, the mixture was poured into 2N HCl and extracted with ether. The organic layer was dried over MgSO₄. The solvent was removed under reduced pressure to give a yellow oil. The crude product was purified by chromatography on silica gel (dichloromethane/hexane, 1/6, v/v) to obtain a white powder (3.07 g, 70%). m.p: 348–349 K. ¹H NMR (300 MHz, CDCl₃) ppm: 8.74 (s, 1H), 7.97–7.94 (d, 2H), 7.88–7.85 (d, 1H), 7.64–7.61 (d, 1H), 7.47–7.44 (q, 3H). IR (KBr, cm^{−1}): 3150, 1690, 1600, 1450, 1350, 625.

2.3.4. 5-(2,5-Dimethyl-4-(trimethylsilyl)phenyl)-2-phenylpyridine (4)

5-Bromo-2-phenylpyridine (**3**) (1.5 g, 0.06 mol), 2,5-dimethyl-4-(trimethylsilyl)phenylboronic acid (1.98 g, 0.07 mol) and Pd(pPh₃)₄ (0.22 g, 3 mol%) were dissolved in toluene (20 mL). A solution of 2M K₂CO₃ (5 mL) was added and the mixture was refluxed with stirring for 24 h under nitrogen. After it was cooled, the mixture was poured into 2N HCl and extracted with ether. The organic layer was dried over MgSO₄. The solvent was removed under reduced pressure to give yellow oil. The crude product was purified by

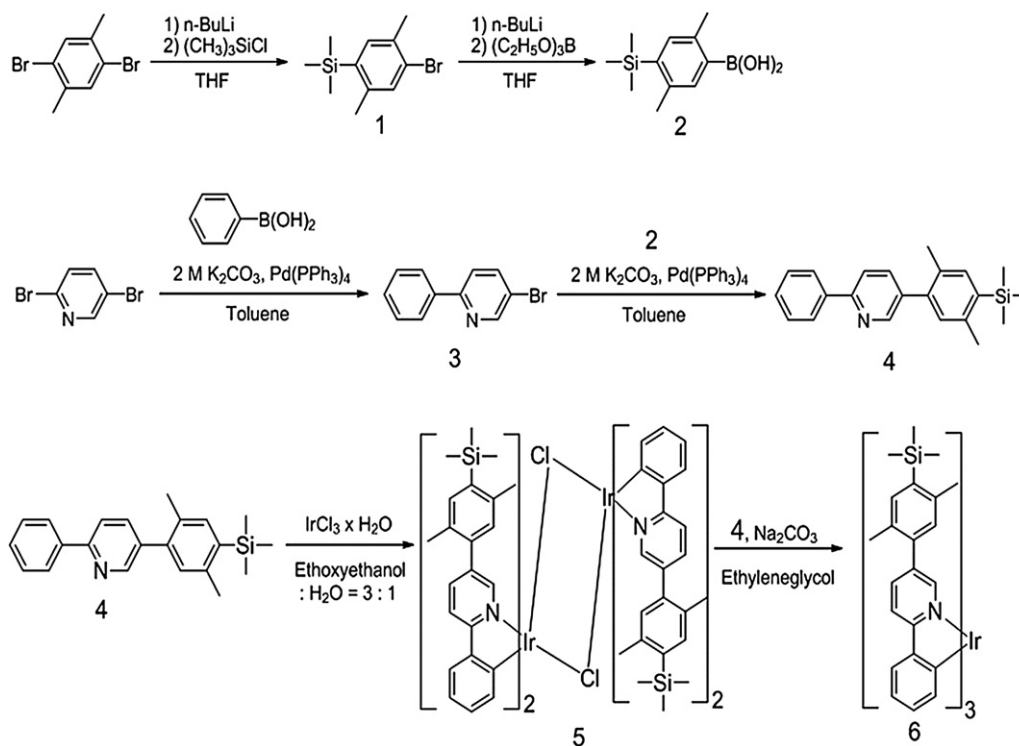


Fig. 1. The synthetic scheme of Ir(dmtppy)₃ complex.

chromatography on silica gel (EtOAc/hexane, 1/10, v/v) to obtain the yellow solid (2.05 g, 96%). m.p.: 350–352 K. ¹H NMR (300 MHz, CDCl₃) ppm: 8.73 (s, 1H), 8.10–8.06 (d, 2H), 7.81–7.78 (q, 2H), 7.53–7.51 (m, 3H), 7.43 (s, 1H), 7.13 (s, 1H), 2.52 (s, 3H), 2.35 (s, 3H), 0.40 (s, 9H). IR (KBr, cm⁻¹): 3150, 1650, 1600, 1475, 1412, 725.

2.3.5. [(dmtppy)₂IrCl]₂ (5)

Iridium trichloride hydrate (0.54 g, 1.81 mmol) and 5-(2,5-dimethyl-4-(trimethylsilyl)phenyl)-2-phenylpyridine (**4**) (1.5 g, 4.52 mmol) were dissolved in a mixture of 2-ethoxyethanol (30 mL) and water (10 mL) and refluxed for 24 h. The solution was cooled to room temperature and 100 mL of water was added to the cooled solution. The resulting yellow precipitate was collected on a glass filter. The precipitate was washed with water and filtered. [(dmtppy)₂IrCl]₂ (1.6 g, 50%).

2.3.6. Ir(dmtppy)₃ (6)

[(dmtppy)₂IrCl]₂ complex (**5**) (0.5 g, 0.28 mmol), 5-(2,5-dimethyl-4-(trimethylsilyl)phenyl)-2-phenylpyridine (**4**) (0.2 g, 0.62 mmol) and K₂CO₃ (0.27 g, 1.96 mmol) were dissolved in ethylene glycol (15 mL) and the mixture was heated to 453 K under nitrogen for 24 h. The reaction mixture was then cooled to room temperature. Then, 150 mL of water was added to the mixture and the solution was extracted with 150 mL of chloroform. The organic layer was dried over MgSO₄. The solvent was removed under reduced pressure, yielding a yellow powder. The crude product was purified by chromatography on silica gel (ethyl acetate/hexane, 1/8, v/v) to obtain a light brown powder (0.12 g, 36%). m.p.: 552–554 K. ¹H NMR (300 MHz, CDCl₃) ppm: 7.92–7.89 (d, 3H), 7.69–7.65 (m, 6H), 7.58–7.55 (d, 3H), 7.21 (s, 3H), 6.97–6.89 (m, 9H), 6.81 (s, 1H), 2.34 (s, 9H), 1.89 (s, 9H), 0.32 (s, 27H). IR (KBr, cm⁻¹): 3150, 1640, 1600, 1475, 1412, 720. ¹³C NMR (300 MHz, CDCl₃): 165.07, 161.14, 147.05, 143.53, 141.18, 138.33, 137.60, 137.16, 136.90, 139.70, 135.19, 131.31, 130.89, 129.85, 124.04, 119.84, 118.30, 22.30, 19.73, -0.18. HR Mass (FAB): *m/z* = 1183.5 [M⁺].

2.4. Device fabrication

Phosphorescent organic light emitting diodes (PHOLEDs) based on Ir(dmtppy)₃ dopant were fabricated by a thermal evaporation process using the following device configuration: indium-tin-oxide (ITO)/1,1-bis[di-4-tolylamino]phenylcyclohexane (TAPC) as hole transport layer (HTL) (40 nm)/(4,4'-N, N'-dicarbazole)biphenyl (CBP) host: x% of Ir(dmtppy)₃ dopant as emissive layer (EML) (30 nm)/2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline (BCP) (10 nm)/tris-(8-hydroxyquinoline)aluminum (Alq₃) (40 nm)/LiF (1 nm)/Al (100 nm). The concentration of Ir(dmtppy)₃ dopant in CBP host was 6% for device A, 12% for device B and 18% for device C.

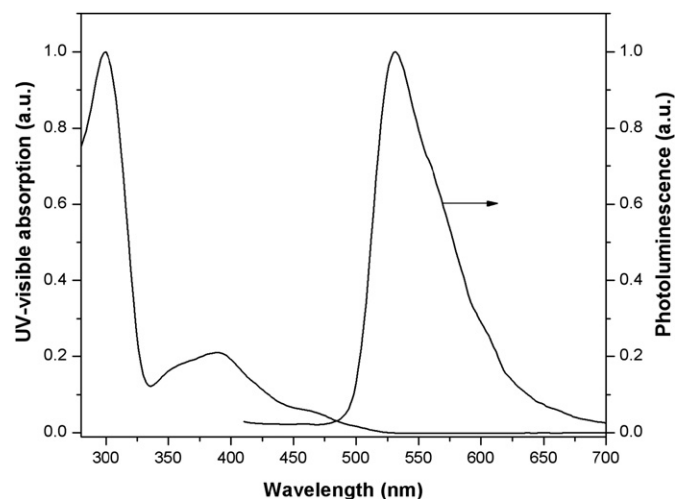


Fig. 2. UV-visible absorption and photoluminescence spectra of Ir(dmtppy)₃ complex in chloroform at room temperature.

Table 1The photophysical and electrochemical properties of Ir(dmtppy)₃ complex.

Absorption ^a λ_{abs} (nm)	Emission λ_{PL} ^b (nm)	PL ^c efficiency (%)	T_d^d/T_g^e (K)	HOMO (eV)	LUMO (eV)	E_g^f (eV)
300,390,470	532	53.1	638/425	5.38	2.82	2.56

^a The major UV–visible absorption peaks are listed.^b Photoluminescence (PL) emission peak measured in chloroform at room temperature.^c PL efficiency of Ir(dmtppy)₃ complex for the dopant concentration of 6% in CBP thin film (50 nm) at an excitation wavelength of 325 nm.^d T_d – Temperature corresponding to 5% weight loss in thermogravimetric analysis.^e T_g – Glass transition temperature from differential scanning calorimetry (DSC) studies.^f E_g – Band gap energy calculated from the equation $E_g = hc/\lambda = 1241/\lambda$, where λ is the edge wavelength (nm) of UV–visible absorption spectrum.

BCP as hole blocking layer (HBL), Alq₃ as electron transport layer (ETL), LiF as electron injection layer and Al as cathode were deposited under a vacuum of 6.6×10^{-5} Pa without breaking the vacuum. Prior to the deposition of organic layers, ITO substrates (anode) were degreased in acetone and IPA followed by the UV–ozone treatment for 10 min. The current density–voltage–luminescence (J – V – L) characteristics of PHOLEDs were carried out using Keithley 2400 source meter and Spectra Colorimeter PR650. The electroluminescence spectra were measured at a driving current of 10 mA/cm^{-2} .

3. Results and discussion

The cyclometalated ligand, 5-(2,5-dimethyl-4-(trimethylsilyl)phenyl)-2-phenylpyridine, was conveniently prepared by Suzuki coupling reaction. Tris-cyclometalated iridium(III) complexes can be prepared from the cyclometalating ligand precursors as depicted in Fig. 1. The tris-cyclometalated complex can be prepared from the appropriate dichloro-bridged dimer, $[(C^N)_2Ir(\mu-Cl)_2Ir(C^N)_2]$, by heating the iridium complex with 2–3 equiv of cyclometalating ligand in ethylene glycol. The dichloro-bridged dimers and compounds are easily prepared from $IrCl_3 \times H_2O$. The obtained yellow-green Ir(dmtppy)₃ was characterized by ¹H nuclear magnetic resonance (NMR), ¹³C NMR, infrared (FT-IR) and high-resolution mass (HR-Mass). From the ¹H & ¹³C NMR studies, the structure of Ir(dmtppy)₃ was found to be *fac*-isomer.

Fig. 2 shows the absorption and photoluminescence spectra of Ir(dmtppy)₃ complex in chloroform (10^{-5} M) at room temperature. In the UV–visible absorption spectrum of the trimethylsilylxylylene-substituted Ir(dmtppy)₃ complex, the absorption below 320 nm is attributed to spin-allowed ligand-centered π – π^* transitions. The absorption band with shoulders in the lower energy region spanning from 356 nm to 500 nm is attributed to spin-allowed and spin-forbidden metal–ligand charge transfer (MLCT) transitions of the iridium(III) complex [19–21]. The spectrum also shows the photoluminescence emission at 532 nm in solution. The photoluminescence efficiency of Ir(dmtppy)₃ complex (6%) doped in CBP thin film at an excitation wavelength of 325 nm was found to be 53.1%. The thermal properties of the Ir(dmtppy)₃ complex were determined by differential scanning calorimeter (DSC) and thermogravimetric analysis (TGA) measurements under the nitrogen atmosphere. TGA data revealed excellent thermal stability and 5%

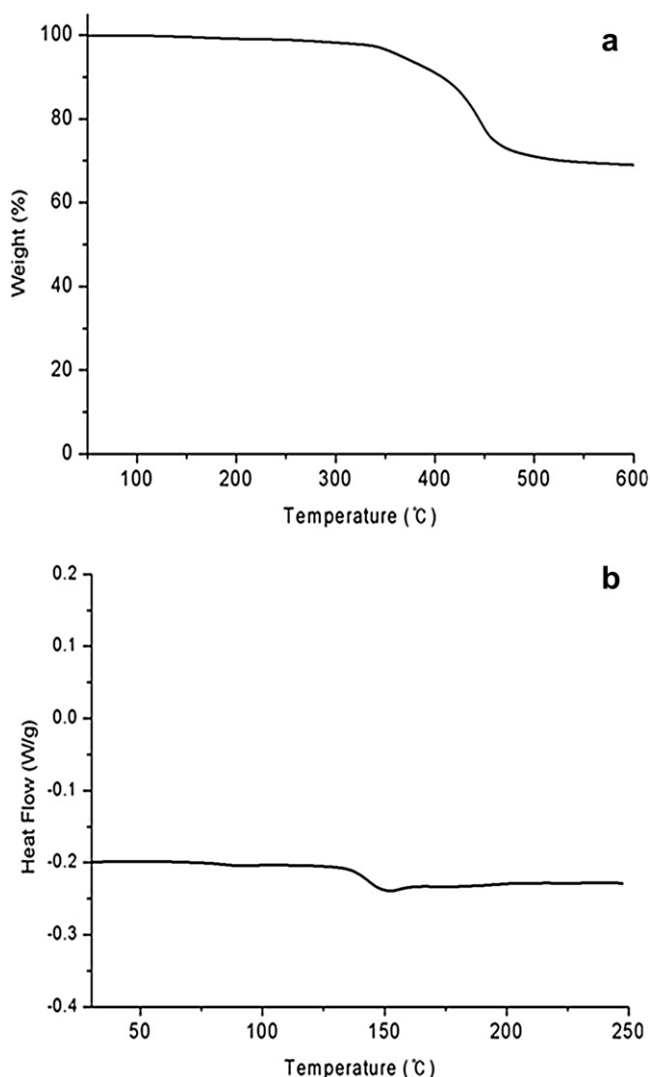


Fig. 3. (a) Thermogravimetric analysis (TGA) and (b) differential scanning calorimeter (DSC) studies of Ir(dmtppy)₃ complex.

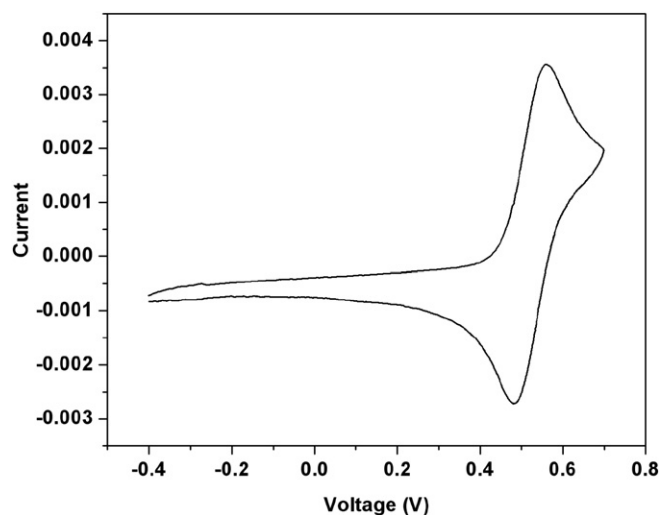


Fig. 4. Cyclic voltammogram of Ir(dmtppy)₃ complex.

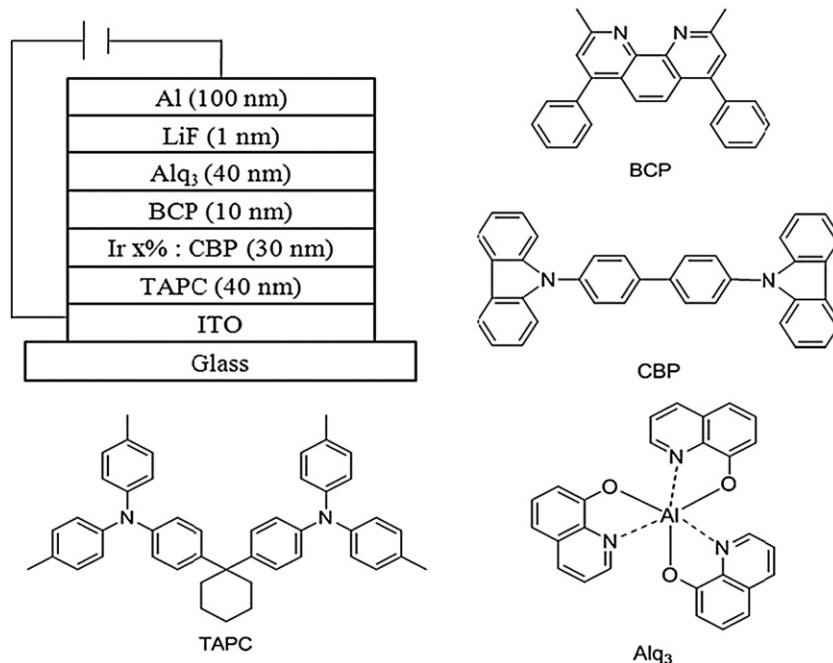


Fig. 5. The device structure and molecular structures of the materials used in the devices.

weight loss at 638 K (Fig. 3a). DSC data of Ir(dmtppy)₃ showed no crystallization peak but a high glass transition temperature (T_g) of 425 K (Fig. 3b) and exists as an amorphous solid that is resistant to crystallization. Amorphous films with high stability and efficiency are usually desirable for OLED applications. The electrochemical properties of the Ir(dmtppy)₃ complex were investigated by cyclic voltammetric (CV) studies, and the CV curve is shown in Fig. 4. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels of the Ir(dmtppy)₃ complex were determined from the electrochemical data and the edge wavelength of the UV–visible absorption spectrum. It shows a band gap energy of 2.56 eV. The photophysical and electrochemical data are summarized in Table 1.

Phosphorescent organic light emitting diodes (PHOLEDs) based on the Ir(dmtppy)₃ dopant were fabricated using the device configuration: ITO/TAPC (40 nm)/CBP doped with a percentage of Ir(dmtppy)₃ (30 nm)/BCP (10 nm)/Alq₃ (40 nm)/LiF/Al. The concentration of Ir(dmtppy)₃ dopant in the CBP host was 6% for device A, 12% for device B and 18% for device C. The molecular structures of materials and the device structure are shown in Fig. 5. TAPC with a higher LUMO energy level of 2.0 eV and BCP with a HOMO energy level of 6.5 eV compared with those (HOMO: 5.9 eV; LUMO: 2.6 eV) of the CBP host were used as a hole transport- and hole blocking- layer

respectively for the effective confinement of charge carriers within the emissive layer (EML) of the device. The energy level diagram for the materials used in the devices is shown in Fig. 6 [10,22,23]. The current density–voltage–luminescence (J – V – L) characteristics of devices A, B and C are shown in Fig. 7. From J – V – L characteristics, device A showed a maximum luminescence of 9189 cd/m² at 9.6 V. The turn-on voltage, which is defined as the applied voltage required to produce a luminescence of 1 cd/m², was observed to be 3.3 V for device A. Fig. 8 shows the current- and external quantum efficiency characteristics of devices A, B and C. Device A showed the maximum external quantum efficiency of 12.7% and current efficiency of 45.7 cd/A. The electroluminescence spectra of the devices A, B and C measured at 10 mA/cm² are shown in Fig. 9. Device A exhibited an electroluminescence (EL) emission peak at 532 nm with CIE colour coordinates of (0.37, 0.60), which is the same as with the PL emission

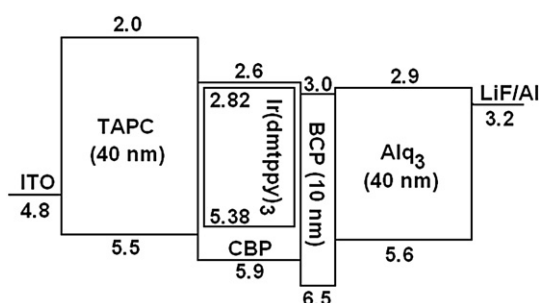


Fig. 6. The energy level diagram of the materials used in the devices.

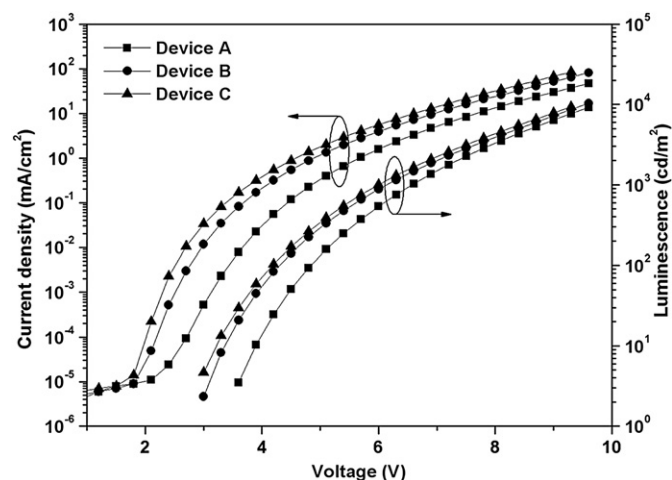


Fig. 7. The current density–voltage–luminescence (J – V – L) characteristics of devices. The doping concentration of Ir(dmtppy)₃ in CBP host as the emissive layer of the device was 6% for device A, 12% for device B and 18% device C.

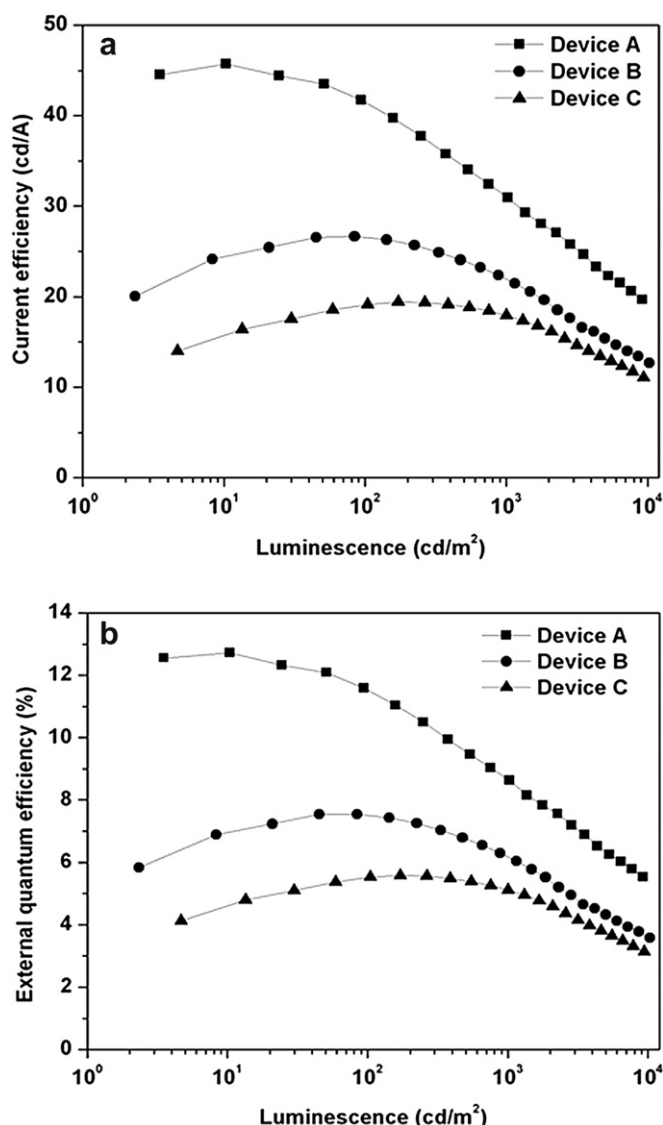


Fig. 8. (a) The current efficiency-current density- and (b) external quantum efficiency-current density- characteristics of the devices. The doping concentration of Ir(dmtppy)₃ in CBP host as the emissive layer of the device was 6% for device A, 12% for device B and 18% device C.

(532 nm) of the Ir(dmtppy)₃ complex in solution. This indicates that the yellow-green EL emission originates from the triplet excited states of the Ir(dmtppy)₃ dopant emitter. This also reveals that the bulky twisted trimethylsilylxylylene- substituted iridium(III) complex effectively hinders aggregation formation in the solid state for the dopant concentration of 6% in CBP. No emission from the host and/or adjacent charge transporting layers was observed, indicating the

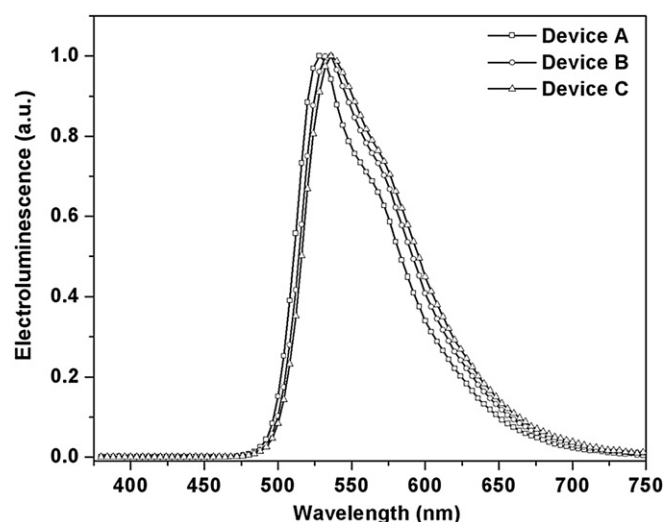


Fig. 9. The electroluminescence spectra of the devices. The doping concentration of Ir(dmtppy)₃ in CBP host as the emissive layer of the device was 6% for device A, 12% for device B and 18% device C.

effective confinement of charge carriers and/or excitons and complete energy transfer from CBP host to Ir(dmtppy)₃ dopant emitter in the EML of the device A.

Device B based on 12% Ir(dmtppy)₃ doped in the CBP host showed a slightly higher current density compared with that of device A (Fig. 7). It exhibited a maximum luminescence of 10310 cd/m² at 9.6 V. The maximum external quantum efficiency of 7.5% and current efficiency of 26.6 cd/A were observed for the device B. It showed an EL emission peak at 534 nm with CIE colour coordinates of (0.39, 0.59). Device C with 18% Ir(dmtppy)₃ dopant in CBP also showed slightly higher current density compared with that of device B. The slightly increasing current density for the increasing dopant concentration in the EML of the device reveals the charge transporting ability of the Ir(dmtppy)₃ complex in the device. A maximum luminescence of 9354 cd/m² was observed for device C. It exhibited a maximum external quantum efficiency of 5.5% and current efficiency of 19.3 cd/A. Device C exhibited an EL emission peak at 538 nm with colour coordinates of (0.40, 0.58). The device performances and EL characteristics of the devices are summarized in Table 2. The electroluminescence emission peak of device C with a dopant concentration of 18% was red-shifted by 6 nm compared with that (532 nm) of device A with a dopant concentration of 6%. The effect of the doping concentration of Ir(dmtppy)₃ molecules on the EL spectra is attributed to the strong dipole–dipole interaction between the dopant molecules due to aggregation formation with an increase in the doping concentration [24]. The results show that the new bulky trimethylsilylxylylene- substituted Ir(dmtppy)₃ complex exhibits yellow-green emission at 532 nm with higher

Table 2

The electroluminescence characteristics of the devices.^a

Device ^b	Doping Concentration(%)	Turn-on ^c (V)	L (cd/m ²)	η_c (cd/A)	η_{ext} (%)	EL ^d (nm)	CIE ^e (x,y)
A	6	3.3	9189	45.7	12.7	532	(0.37, 0.60)
B	12	2.7	10310	26.6	7.5	534	(0.39, 0.59)
C	18	2.7	9354	19.3	5.5	538	(0.40, 0.58)

^a The data for luminescence (L), current efficiency (η_c) and external quantum efficiency (η_{ext}) are the maximum values of the corresponding device.

^b The device structure is ITO/TAPC (40 nm)/CBP doped with concentration (x%) of Ir(dmtppy)₃ as emissive layer (30 nm)/BCP (10 nm)/Alq3 (40 nm)/LiF/Al.

^c The turn-on voltage for all the devices was defined as voltage required to get the luminescence of 1 cd/m².

^d The peak emission wavelength of the EL spectrum of corresponding device at 10 mA/cm².

^e CIE colour coordinates of electroluminescence of the corresponding device.

device efficiencies of 12.7% and 45.7 cd/A and could be useful in white OLEDs.

4. Conclusion

A new iridium(III) complex with phenylpyridine ligands containing bulky trimethylsilylxylylene, Ir(dmtppy)₃, was synthesized by a Suzuki coupling reaction and confirmed using various spectroscopic studies. The thermal, photophysical and electrochemical properties of the Ir(dmtppy)₃ complex were studied using thermogravimetric analysis and differential scanning calorimetry, UV–visible absorption, photoluminescence and cyclic voltametric studies. The phosphorescent organic light emitting diodes based on Ir(dmtppy)₃ complex doped in CBP host exhibits the yellow-green emission at 532 nm with CIE colour coordinates of (0.37, 0.60), which is consistent with PL emission (532 nm) of Ir(dmtppy)₃ complex in solution. This reveals that the bulky, twisted trimethylsilylxylylene-substituted iridium(III) complex effectively hinders aggregation formation in the solid state at 6% doped in CBP, resulting in a higher device external quantum efficiency of 12.7% and current efficiency of 45.7 cd/A. The results show that Ir(dmtppy)₃ dopant could be useful in white organic light emitting diodes for the lighting applications.

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