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Synthesis and characterization of phosphorescent cyclometalated iridium complexes containing 2,5-diphenylpyridine based ligands

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A series of phosphorescent cyclometalated iridium complexes with 2,5-diphenylpyridine-based ligands has been synthesized and characterized to investigate the effect of the simple ligand modification on photophysics, thermostability and electrochemistry. The complexes have the general structure $(C^N)_2Ir(acac)$, where C^N is a monoanionic cyclometalating ligand [e.g. 2,5-diphenylpyridyl (dppy), 2,5-di(4-methoxyphenyl)pyridyl (dmoppy), 2,5-di(4-ethoxyphenyl)pyridyl (deoppy) and 2,5-di(4-ethylphenyl)pyridyl (deppy)]. The absorption, emission, cyclic voltammetry and thermostability of the complexes were systematically investigated. The $(dppy)_2Ir(acac)$ has been characterized using X-ray crystallography. Calculation on the electronic ground state of $(dppy)_2Ir(acac)$ was carried out using B3LYP density functional theory. The highest occupied molecular orbital (HOMO) level is a mixture of Ir and ligand orbitals, while the lowest occupied molecular orbital (LUMO) is predominantly dppy ligand-based. Electrochemical studies showed the oxidation potentials of $(dmoppy)_2Ir(acac)$, $(deoppy)_2Ir(acac)$, $(deppy)_2Ir(acac)$ were smaller than that of $(ppy)_2Ir(acac)$, while the oxidation potential of $(dppy)_2Ir(acac)$ was larger relative to $(ppy)_2Ir(acac)$. The 10% weight reduction temperatures of these complexes were above that of $(ppy)_2Ir(acac)$. All complexes exhibited intense green photoluminescence, which has been attributed to MLCT triplet emission. The maximum emission wavelengths in CH_2Cl_2 at room temperature were in the range 531–544 nm, which is more red-shifted than that of $(ppy)_2Ir(acac)$. Copyright © 2005 John Wiley & Sons, Ltd.

KEYWORDS: cyclometalated iridium complex; Suzuki cross coupling reaction; phosphorescent emitting material; single crystal structure

INTRODUCTION

In recent years, the cyclometalated iridium complexes have been extensively investigated because of their high luminescence quantum yields applicable to organic light emitting devices (OLEDs).[1–8] The strong spin–orbit coupling of iridium atom allows for efficient intersystem crossing between singlet and triplet states, which can lead to a high quantum yield of emission from the triplet state.[1,2,9] One of the best phosphorescent green materials is *fac*-tris(2-phenylpyridine)iridium [Ir(ppy)₃] which exhibits high quantum efficiency.[2,10] More recently, a green device with internal quantum efficiency of nearly 100% has also been reported with the use of bis(2-phenylpyridinato) Ir(III) (acetylacetonate) [(ppy)₂Ir(acac)] as a phosphorescent dopant.[11] The complexes based on Ir(ppy)₃ and (ppy)₂Ir(acac) skeleton have such a simple molecular structures and excellent luminescent properties that many efforts are still focusing on chemical modification of this type of complex for better luminescent performance.[3,6,12–16]

In this paper we report on the simple colour tuning of photoluminescence, changing the different substituents on

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the 5-position of pyridyl ring and the 4′-position of phenyl ring based on (ppy)$_2$Ir(acac). Substitution in these positions of 2-phenylpyridine is supposed to bring about a fine tuning of the HOMO and emitting ^{3}MLCT states with a subsequent impact on the properties of photophysics, thermostability and electrochemistry.

EXPERIMENTAL

2,5-Dibromopyridine, phenyl boronic acid, 4-methoxyphenyl boronic acid, 4-ethoxyphenyl boronic acid, 4-ethylphenyl boronic acid and IrCl$_3 \cdot n$H$_2$O were from Aldrich, and used without further purification. All procedures were carried out in an inert gas atmosphere despite the air stability of the compounds. ^{1}H-NMR spectra were recorded on a Bruker Avance 300 MHz instrument. Elemental analyses were performed on a VarioEL III CHNS instrument. Mass spectra (FAB) were recorded on a JMS-700 double focusing mass spectrometer (Jeol, Tokyo, Japan). Absorption spectra were measured on UV–vis–NIR scanning spectrophotometer. Photoluminescence (PL) spectra were measured with a F-4500 Fluorescence Spectrometer. Thermo-gravimetric analysis (TGA) was performed by a TGA 2950 thermal analyser (TA Co.) under a nitrogen stream with a scanning rate of 10 °C/min.

Electrochemistry

Cyclic voltammetry experiments were performed with an MCP-1 electrochemical analyser (JiangFen Co., China). All measurements were carried out at room temperature with a conventional three-electrode configuration consisting of a platinum working electrode, a platinum wire auxiliary electrode and an Ag–AgCl reference electrode. The $E_{1/2}$ values were determined as 0.5 ($E_p^a + E_p^c$), where E_p^a and E_p^c are the anodic and cathodic peak potentials, respectively. All potentials reported were not corrected for the junction potential. The solvent was CH$_2$Cl$_2$ and the supporting electrolyte was 0.1 M tetra(n-butyl)ammonium hexafluorophosphate.

X-ray crystallography

The intensity data for (dppy)$_2$Ir(acac) were collected at room temperature ($T = 296$ K) on a Bruker Smart Apex II CCD diffractometer with graphite-monochromated Mo–Kα radiation ($\lambda = 0.71073$ Å). Data were corrected for Lorentz and polarized (LP) factors and absorption was applied by using the SADABS program. The structure was solved by direct methods and refined by full-matrix least-squares refinement on F^2 using the SHELXTL-97 program package.[17] All non-hydrogen atoms were refined anisotropically, and hydrogen

Table 1. Crystal data and structure refinement for (dppy)$_2$Ir(acac)

Empirical formula	C39 H31 Ir N2 O2
Formula weight	751.86
Temperature	296 K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P $\bar{1}$
Unit cell dimension	$a = 8.422(2)$ Å $\alpha = 94.843(4)°$
	$b = 13.565(4)$ Å $\beta = 106.199(4)°$
	$c = 14.249(4)$ Å $\gamma = 93.026(4)°$
Volume	1552.6(7) Å^3
Z	2
Density (calculated)	1.608 mg/m^3
Absorption coefficient	4.337 mm^{-1}
F(000)	744
Crystal size	$0.24 \times 0.16 \times 0.21$ mm^3
Theta range for data collection	2.01–28.86°
Index ranges	$-11 \leq h \leq 11, -17 \leq k \leq 16, -11 \leq l \leq 19$
Reflections collected	9500
Independent reflections	7088 [R(int) = 0.0162]
Completeness to theta = 29.09°	98.0%
Maximum and minimum transmission	0.6241 and 0.4225
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	7088/0/399
Goodness-of-fit on F^2	1.046
Final R indices [$I > 2\text{sigma}(I)$]	$R_1 = 0.0286, wR_2 = 0.0735$
R indices (all data)	$R_1 = 0.0361, wR_2 = 0.0768$
Largest differential between peak and hole	1.396 and -0.802 e Å^{-3}

atoms were placed at calculated positions and refined using a riding model with C–H distances in the range 0.93–0.96 Å and U_{iso} (H) = $1.2U_{eq}$ (C) or 1.5 U_{eq}(methyl C). A summary of crystal data and refinement parameters is given in Table 1.

General procedure for the synthesis of 2,5-diphenylpyridine based ligands

2,5-Diphenylpyridine (Hdppy), 2,5-di(4-methoxyphenyl) pyridine (Hdmoppy), 2,5-di(4-ethoxyphenyl)-pyridine (Hdeoppy) and 2,5-di(4-ethylphenyl)pyridine (Hdeppy) were obtained from the reaction of 2,5-dibromopyridine and the corresponding phenyl boronic acids by a similar procedure,[18,19] so a detailed description is provided only for Hdppy.

Synthesis of Hdppy

2,5-Dibromopyridine (19.5 g, 0.0821 mol), phenyl boronic acid (30 g, 0.246 mol), 10% Pd(0)/C (27 g, 0.0123 mol), PPh$_3$ (13 g) and 2 M Na$_2$CO$_3$ 150 ml were heated in 100 ml 1,2-dimethoxyethane to reflux for 50 h. The mixture was then cooled, dichloromethane (100 ml) and water (100 ml) added to dilute the solution, filtered to remove Pd/C, and then transferred to a separating funnel. The organic layer was separated and the aqueous phase was extracted with dichloromethane (3 × 100 ml). The combined organic layer was washed with water (3 × 100 ml), dried over MgSO$_4$, filtered, and the filtrate evaporated under reduced pressure. The residue was chromatographed using *n*-hexane/dichloromethane (1 : 1) as eluent to afford the white powders in 53% yield. ^{1}HNMR (CDCl$_3$) δ (ppm): 8.84 (s, 1H), 7.93 (d, 2H), 7.80 (d, 1H), 7.50 (d, 2H), 7.30 (m, 6H). Anal. found: C, 88.63; H, 5.444; N, 5.974. Calcd: C, 88.31; H, 5.627; N, 6.060. MS (FAB): m/e 230.9 (M$^+$)

Hdmoppy

White powders. Yield: 60%. ^{1}HNMR (CDCl$_3$) δ (ppm): 8.86 (s, 1H), 8.00 (d, 2H), 7.87 (d, 1H), 7.71 (d, 1H), 7.55 (d, 2H), 7.00 (d, 4H), 3.87 (s, 6H). Anal. found: C, 78.65; H, 5.772; N, 4.701. Calcd: C, 78.35; H, 5.842; N, 4.811. MS (FAB): *m/e* 291.1 (M$^+$).

Hdeoppy

White powders. Yield: 55%. ^{1}HNMR (CDCl$_3$) δ (ppm): 8.86 (s, 1H), 7.97 (d, 2H), 7.87 (d, 1H), 7.70 (d, 1H), 7.53 (d, 2H), 7.00 (d, 4H), 4.09 (s, 4H), 1.45 (t, 6H). Anal. found: C, 79.23; H, 6.475; N, 4.277. Calcd: C, 79.00; H, 6.583; N, 4.388. MS (FAB): *m/e* 319.1 (M$^+$).

Hdeppy

White powders. Yield: 78%. ^{1}HNMR (CDCl$_3$) δ (ppm): 8.83 (s, 1H), 7.80 (m, 3H), 7.60 (d, 1H), 7.40 (d, 2H), 7.20 (d, 4H), 2.60 (m, 4H), 1.22 (t, 6H). Anal. found: C, 88.06; H, 7.167; N, 4.737. Calcd: C, 87.80; H, 7.317; N, 4.878. MS (FAB): *m/e* 287.2 (M$^+$).

General procedure for the synthesis of iridium complexes

The (C^N)$_2$Ir(acac) was obtained in two steps using standard method.[12] These iridium complexes were prepared by similar
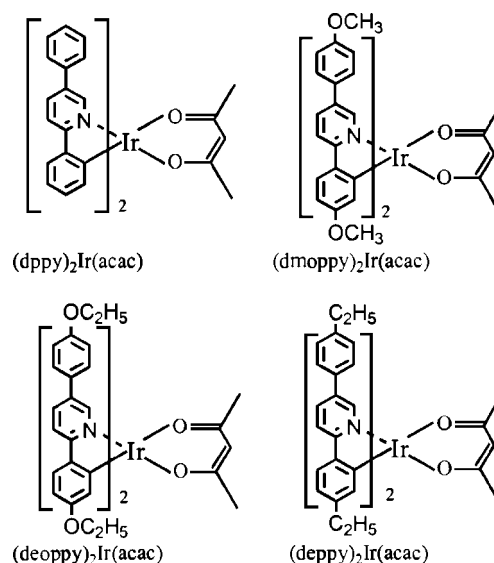
Figure 1. Ir complexes and their abbreviations in this study.

procedures, therefore only the synthesis of (dppy)$_2$Ir(acac) is presented in detail. The complexes used in this study are illustrated in Fig. 1.

Synthesis of (dppy)$_2$Ir(acac)

Iridium(III) bis(2,5-diphenylpyridinato-N,C$^{2'}$)acetylacetonate: a mixture of 1.00 g (2.835 mmol) IrCl$_3$ · nH$_2$O, 1.31 g (5.670 mmol) of Hdppy, 80 ml 2-ethoxyethanol, and 20 ml water was refluxed at 120 °C for 24 h. After cooling to room temperature, the chloride-bridged dimer was isolated by addition of water followed by filtration and methanol wash. The dimer was not further characterized and was used directly in subsequent reaction. A mixture of 1.75 g (1.273 mmol) of the dimer, 0.32 g (3.182 mmol) acetylacetone, 1.2 g Na$_2$CO$_3$ and 100 ml 2-ethoxyethanol was refluxed for 16 h. After down to room temperature, the solvent was removed by vacuum, and the crude orange product was washed with methanol to remove any unreacted acetylacetone. The orange (dppy)$_2$Ir(acac) was afforded in 55% yield with train sublimation. ^{1}HNMR (CDCl$_3$) δ (ppm): 8.82 (s, 2H), 7.96 (m, 4H), 7.65–7.41 (m, 12H), 6.82 (m, 4H), 6.36 (d, 2H), 5.27 (s, 1H), 1.80 (s, 6H). Anal. found: C, 62.51; H, 3.933; N, 3.760. Calcd: C, 62.30; H, 4.126; N, 3.727. MS (FAB): *m/e* 751.2 (M$^+$).

(dmoppy)$_2$Ir(acac)

Iridium(III)bis[2,5-di(4-methoxyphenyl)pyridinato-N,C$^{2'}$] acetylacetonate (yellow powders, yield 50%). ^{1}HNMR (CDCl$_3$) δ (ppm): 8.57 (s, 2H), 8.17 (m, 4H), 7.71 (m, 6H), 7.13 (d, 4H), 6.44 (d, 2H), 5.58 (s, 2H), 5.32 (s, 1H), 3.57 (s, 12H), 1.76 (s, 6H). Anal. found: C, 59.31; H, 4.409; N, 2.977. Calcd: C, 59.22; H, 4.478; N, 3.214. MS (FAB): *m/e* 871.4 (M$^+$).

(deoppy)₂Ir(acac)

Iridium(III)bis[2,5-di(4-ethoxyphenyl)pyridinato-N,C²′]acetylacetonate (yellow powders, yield 61%). ¹HNMR (CDCl₃) δ (ppm): 8.57 (s, 2H), 8.18 (m, 4H), 7.67 (m, 6H), 7.11 (d, 4H), 6.42 (d, 2H), 5.57 (s, 2H), 5.32 (s, 1H), 4.10 (m, 4H), 3.75 (m, 4H), 1.75 (s, 6H), 1.37 (t, 6H), 1.11 (t, 6H). Anal. found: C, 60.40; H, 4.901; N, 3.005. Calcd: C, 60.82; H, 5.104; N, 3.019. MS (FAB): *m/e* 927.2 (M⁺).

(deppy)₂Ir(acac)

Iridium(III)bis[2,5-di(4-ethylphenyl)pyridinato-N,C²′]acetylacetonate (orange powders, yield 40%). ¹HNMR (CDCl₃) δ (ppm): 8.70 (s, 2H), 7.80 (m, 4H), 7.49–6.90 (m, 10H), 6.57 (d,2H), 6.08 (s, 2H), 5.14 (s, 1H), 2.67 (m, 4H), 2.30 (m, 4H), 1.70 (s, 6H), 1.27 (t, 6H), 0.94 (t, 6H). Anal. found: C, 64.94; H, 5.441; N, 3.110. Calcd: C, 65.28; H, 5.479; N, 3.240. MS (FAB): *m/e* 863.2 (M⁺).
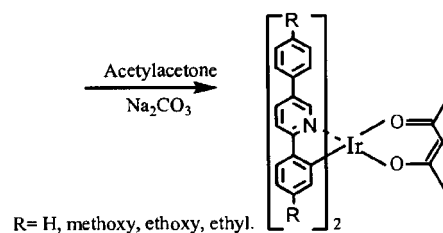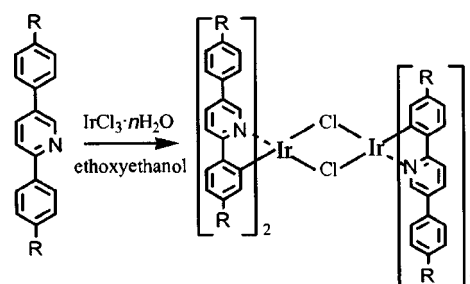
RESULTS AND DISCUSSION

Synthesis of the materials

The synthesis of ligands was carried out using the palladium charcoal-catalysed Suzuki–Miyaura coupling reaction, as illustrated in Scheme 1. Compared with air-sensitive and expensive homogeneous palladium catalysts, palladium charcoal can be safely handled and removed by simple filtration, and the palladium metal can be recovered and reused. The synthesis of the bis-cyclometalated iridium complexes involved two steps. First, cyclometalated Ir(III) *m*-chlorobridged dimers were synthesized by the reacting IrCl₃ · *n*H₂O and 2,5-diphenylpyridine or its derivatives.[20] Then, the dimers were reacted with acetylacetone in 2-ethoxyethanol to afford yellow products in 40–61% yields. These are shown in Scheme 2.

Crystal structure of (dppy)₂Ir(acac)

Single crystals of (dppy)₂Ir(acac) were grown from sublimation and characterized using crystallography. The ORTEP drawing of the complex is shown in Fig. 2. Selected parameters of the molecular structure are listed in Table 2. The complex has a distorted octahedral coordination geometry around the iridium atom and the two nitrogen atoms of

Scheme 1.

Scheme 2.
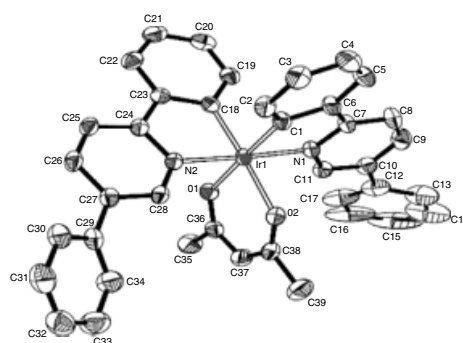
Figure 2. ORTEP diagram of (dppy)₂Ir(acac).

Table 2. Comparison of structural parameters of experimental values from X-ray diffraction with DFT calculation of (dppy)₂Ir(acac)

Parameters	Experimental	Calculated
Ir(1)–N(1)	2.036(3) Å	2.0530 Å
Ir(1)–N(2)	2.031(3) Å	2.0548 Å
Ir(1)–C(1)	1.984(4) Å	2.0091 Å
Ir(1)–C(18)	1.994(4) Å	2.0093 Å
Ir(1)–O(1)	2.159(3) Å	2.1940 Å
Ir(1)–O(2)	2.150(3) Å	2.1920 Å
N(1)–Ir(1)–N(2)	175.88(11)°	177.01°
N(1)–Ir(1)–C(1)	80.35(14)°	80.86°
N(2)–Ir(1)–C(18)	80.82(15)°	80.84°
N(1)–Ir(1)–O(1)	95.46(12)°	94.23°
C(18)–Ir(1)–O(1)	92.45(12)°	91.13°
O(1)–Ir(1)–O(2)	87.82(11)°	85.43°
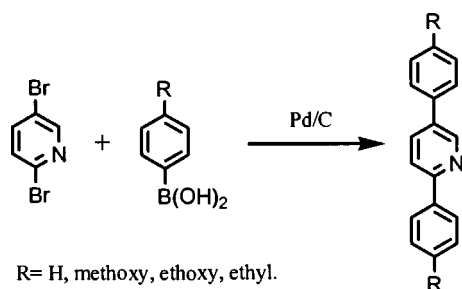
dppy ligands exhibit *cis*-C–C and *trans*-N–N chelate dispositions. The Ir–C bonds [Ir–C$_{av}$ = 1.989(4) Å] are shorter than the Ir–N bonds [Ir–N$_{av}$ = 2.034(3) Å]. The Ir–C bonds of (dppy)$_2$Ir(acac) are shorter than that of (ppy)$_2$Ir(acac) [Ir–C, 2.003 (9) Å], while the Ir–N and Ir–O bonds (Ir–O$_{av}$ = 2.155 Å) are longer than the value of the latter [Ir–N, 2.010(9) Å; Ir–O, 2.146(6) Å].[3] The N(1)–Ir(1)–N(2) [175.88(11)°], C(1)–Ir(1)–N(1) [80.35(14)°], C(18)–Ir(1)–N(2) [80.82(15)°], N(1)–Ir(1)–O(1) [95.46(12)°], C(18)–Ir(1)–O(1) [92.45(12)°] and O(1)–Ir(1)–O(2) [87.82(11)°] bond angles are typical for cyclometalates and *β*-diketonate derivatives of Ir.[3,21,22] There are slight deviations possibly due to introduction of a phenyl ring into the 5-position of 2-phenylpyridine. All other features appear to be normal.
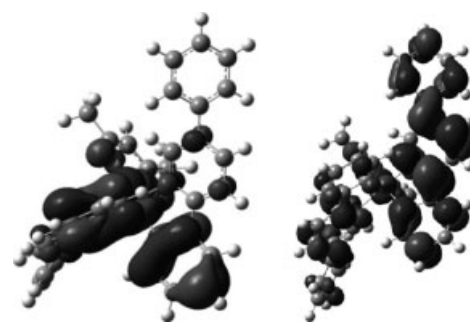
DFT calculations

DFT calculation on the electronic ground state of (dppy)$_2$Ir(acac) was carried out at the B3LYP/LANL2DZ level.[23,24] A similar approach has been used to investigate properties of Ir(ppy)$_3$ and (ppy)$_2$Ir(acac).[25] The HOMO and LUMO energies were determined using minimized singlet geometries to approximate the ground state. The results of the optimized structure for (dppy)$_2$Ir(acac) are summarized in Table 2, and compared with X-ray diffraction studies. The calculated Ir–C$_{av}$ bond length of 2.009 Å was 0.02 Å longer than experimental value. The Ir–N$_{av}$ bond length of 2.054 Å and Ir–O$_{av}$ bond length of 2.193 Å were 0.020 and 0.038 Å longer than measured values. The calculated values for C–Ir–N, N–Ir–N, N–Ir–O, O–Ir–O chelate angles were consistent with the corresponding experimental values determined in the X-ray structure of (dppy)$_2$Ir(acac).

The HOMO and LUMO levels are shown in Fig. 3. The HOMO (−4.88 eV) consisted of a mixture of 2-phenyl of dppy ligand, Ir orbitals while the LUMO (−1.67 eV) was mostly on one dppy ligand and partly on another.

Thermal stability

In the vacuum deposition process, OLED materials should be stable even at high temperatures (300–400 °C), because the decomposition products may contaminate the OLED and lead to poor device performance. The decomposition temperature was determined by a TGA thermal analyser under a nitrogen

Figure 3. Density functional theory calculation (DFT) of HOMO (left) and LUMO (right) for (dppy)$_2$Ir(acac).

stream with a scanning rate of 10 °C/min. The 10% weight loss temperature ($\Delta T_{10\%}$) of these new iridium complexes was in the range 351–381 °C, while the value of (ppy)$_2$Ir(acac) was 340 °C. This indicates that these complexes containing 2,5-diphenylpyridine-based ligands have relative high thermal stability. As the chain of conjugated bonds increases in length of the ligand, the thermostability of iridium complexes rises. (dppy)$_2$Ir(acac) has a high decomposition temperature ($\Delta T_{10\%}$ = 381 °C), but incorporation of the alkyl chain on dppy ligands results in the lowering of thermostability, see Table 3.

Cyclic voltammetric studies

The electrochemical properties of these complexes were characterized using cyclic voltammetry; the redox data are given in Table 3. All studied complexes showed reversible oxidation waves in the range 755–828 mV vs Ag/AgCl, which can be attributed to the oxidation of the iridium(III). No reduction waves were measured in the complexes up to −3.0 V. The oxidation wave value of (dppy)$_2$Ir(acac) with an electron-withdrawing group (phenyl) was 828 mV, which was higher than that of (ppy)$_2$Ir(acac) (810 mV, in this measurement condition), while the (dmoppy)$_2$Ir(acac), (deoppy)$_2$Ir(acac) and (deppy)$_2$Ir(acac), containing electron-donating groups (alkyl, alkoxy), had lower values (755–793 mV) relative to that of (dppy)2Ir(acac). Therefore, incorporating the electron-withdrawing group on the phenylpyridine gave an increase

Table 3. Absorption, emission, TGA and Redox properties of Ir(III) complexes

Complexes	Absorption, λ^a (nm) (log ε)	λ_{em}^b (nm)	redox (mV),^{c} $E_{1/2}^{ox}$	TGA (°C)^d
(dppy)$_2$Ir(acac)	282 (4.74), 296 (4.72), 375 (3.86), 426 (3.71), 474 (3.66)	544	828	381
(deppy)$_2$Ir(acac)	287 (4.73), 301 (4.76), 317 (4.71), 382 (3.96), 428 (3.77), 464 (3.73)	542	755	366
(dmoppy)$_2$Ir(acac)	316 (4.84), 378 (4.23), 420 (4.03), 442 (3.98)	531	793	353
(deoppy)$_2$Ir(acac)	260 (4.55), 318 (4.79), 381 (4.23), 443 (3.92)	534	784	351

^{a} Measured in CH$_2$Cl$_2$ solution at a concentration of 10^{-5} mol/l.
^{b} Measured in CH$_2$Cl$_2$ solution at 298 K.
^{c} Measured in CH$_2$Cl$_2$ at a concentration of 10^{-3} M and a scan rate of 80 mV s^{-1}; values are reported relative to Ag/AgCl.
^{d} The temperature listed is at point of 10% weight loss.

in the oxidation potential, while introduction of electron-donating groups into the ligand led to a decreased value. This is consistent with our DFT calculation; the HOMO orbitals of (dppy)$_2$Ir(acac) are the mixture of Ir with dppy, and incorporation of substituents on cyclometalated ligands has been shown to affect the oxidation potential of the iridium ion.

Photophysical properties

Absorption and room-temperature emission spectra were recorded for all of the complexes, as shown in Figs 4 and 5, respectively. The data are summarized in Table 3.

The intense absorption bands around 300 nm can be assigned to spin allowed $^1(\pi-\pi^*)$ transitions, and the bands in the range 400–440 nm corresponded to spin allowed metal–ligand charge transfer band (^{1}MLCT). Weak absorption at 440–500 nm was assigned to the formally spin-forbidden ^{3}MLCT transition, similar to reported value of (ppy)$_2$Ir(acac).[3]
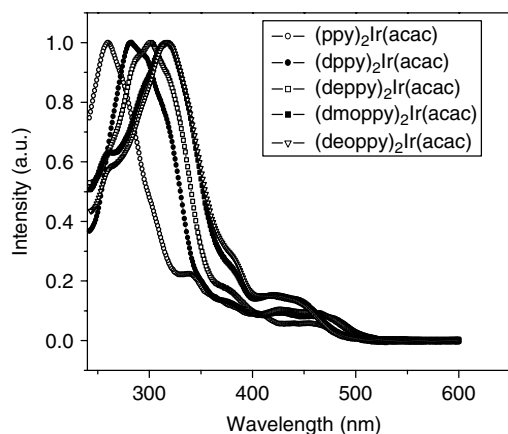
Figure 4. Absorption spectra for (dppy)$_2$Ir(acac), (deppy)$_2$Ir(acac), (dmoppy)$_2$Ir(acac), (deoppy)$_2$Ir(acac) and (ppy)$_2$Ir(acac) complexes in CH$_2$Cl$_2$ solution.
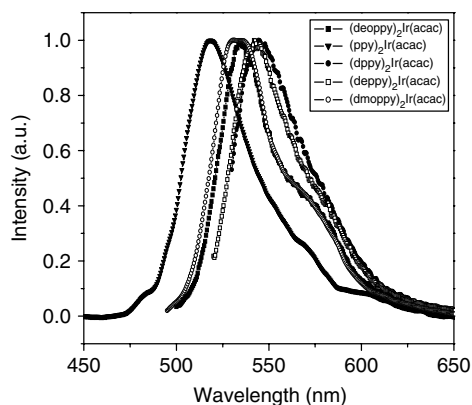
Figure 5. Emission spectra for (dppy)$_2$Ir(acac), (deppy)$_2$Ir(acac), (dmoppy)$_2$Ir(acac), (deoppy)$_2$Ir(acac) and (ppy)$_2$Ir(acac) complexes in CH$_2$Cl$_2$ solution at room temperature.

The peak wavelength is sensitive not only to the property but also to the position of the substituents.[6] By changing the substituents and their position, the peak wavelength of phosphorescent emissions can be tuned. In (dppy)$_2$Ir(acac), incorporation of an electron-withdrawing group (phenyl) on the 5-position of the pyridyl of 2-phenylpyridine in (ppy)$_2$Ir(acac) lowers the LUMO level, reduces the gap between HOMO and LUMO level, and hence a 26 nm red shift is observed compared with that of (ppy)$_2$Ir(acac) (518nm).[3,25] According to our DFT calculation, substitution of an electron-donating group (alkyl, alkoxy) onto the 4-position of the 2-phenyl ring of dppy ligand in (dppy)$_2$Ir(acac) seems to raise both the LUMO and HOMO levels, resulting in no change in the emission spectrum; however, incorporation of these groups on the 4′-position of the 5-phenyl ring raises the LUMO level slightly, and hence results in the blue shift of the emission bands by 2, 10 and 13 nm for (deppy)$_2$Ir(acac), (deoppy)$_2$Ir(acac) and (dmoppy)$_2$Ir(acac), respectively, compared with (dppy)$_2$Ir(acac) (544 nm). It was observed that the alkyl group affects only slightly the tuning of the emission, while the alkoxy groups have relatively larger effect. These data indicate the possibility of predicating the emission wavelengths depending on the substituents of iridium complexes containing 2,5-diphenylpyridine based ligands.

CONCLUSION

In summary, we have synthesized new bis-cyclometalated iridium complexes containing 2,5-diphenylpyridine-based ligands. Tuning of the emission of these complexes was carried out by simple ligand modification. This work gives a pathway to predicate the emission wavelengths depending on the nature of the substituents of iridium complexes. These complexes are easily prepared, have good thermostability and sublimable, making them good candidates for use in OLEDs.

SUPPLEMENTARY MATERIAL

Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC no. 271509 for complex (dppy)$_2$Ir(acaac). Copies of this information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge CB2 IEZ, UK (Fax: +44 1223 336033; email: deposit@ccdc.cam.ac.uk or http: www.ccdc.cam.ac.uk). Supplementary Information includes tables of collection parameters, distances, angles and coordinates for the structure.

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