Journal of Luminescence 203 (2018) 83–89

Contents lists available at ScienceDirect

Journal of Luminescence

journal homepage: www.elsevier.com/locate/jlumin

Synthesis of a novel iridium complex and its exhaustive investigations of photophysics, electrochemistry, luminescent mechanism and electroluminescent performances

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ARTICLE INFO

Keywords:
5-Methyl-2-(2H-1,2,3-triazol-2-yl)benzoic acid
Decarboxylation coordination
Iridium complex
Electroluminescent performance

ABSTRACT

A novel iridium complex [$(dfppy)_2Ir(ttz)$, Ir complex] was synthesized *via* decarboxylic reaction of ancillary ligand with the iridium complex dimer containing dichloro-bridged bond, the decarboxylation-coordination reaction for the synthesis of Ir complex firstly is found. The single crystal structure, thermally stability, UV–vis absorption, photoluminescence, electrochemistry, and electroluminescent performances of the Ir complex were investigated. Blue and orange-red emissions can be observed for the Ir complex in dichloromethane and OLED with low emissive efficiencies, respectively. We explored the reason for the poor emissive performance. In addition, the luminescent mechanism of $(dfppy)_2Ir(ttz)$ was also studied through DFT/TD-DFT calculations.

1. Introduction

For decades, Organic light-emitting diodes (OLED) is strongly focused by the academic and technological circles, because of its special advantages in the field of display. Red, green and blue are three basic colors for a full display. Red and green OLEDs have well fulfilled their practical application due to their high-efficient luminescence [1,2], long-served lifetimes [3] and a little efficiency roll-off under high current density [4,5], but the blue OLED, because of its low emissive efficiency and insufficient blue emission [6–10], restricts the industrialization as a blue-display device for a long term. An OLED's performance largely depends on the fabricated material. So, the development of the blue emissive materials has become an effort aim for material scientists in the field of OLED.

For an organic material as OLED's application, its singlet excition only can be utilized in the process of luminescence due to symmetrically conserved transition rule for electrons. According to the law of quantum statistics, the singlet and triplet excition's proportion is 1:3, thus, the peak quantum efficiency for a pure organic material is 25%, so, a pure organic material usually shows a low-efficient luminescence. In recent years, the thermally activated delayed fluorescent materials (TADFM) have been developed [11,12] due to their comparable luminescent efficiency as iridium complexes. TADFM possesses a small gap (ΔE_{ST}) of singlet and triplet energy level so that the triplet excitons can adversely convert to the singlet state, thus, the triplet excitons can be utilized in the process of radiation. But, the molecular design of TADFM is based on some experiences.

Iridium complex usually reveals high-efficient luminescence due to harvesting the singlet and triplet excitons in the form of triplet-exciton radiative decay. For a homoleptic iridium complex [$Ir(C\hat{}N)_3$] or a heteroleptic iridium complex [$(C\hat{}N)_2Ir$ (LX)], its HOMO mainly distributes on Ir(III) and aromatic ring, LUMO resides on aromatic heterocycte. We can obtain blue emissive iridium complexes through enhancing the gap of HOMO and LUMO. The conjugated degree of ligand, grafted group's type as well as group's position locating on the ligand influence on the gap. Commonly, the ligand with a small conjugated degree usually causes a blue shift for iridium complex's emission.

FIrpic is a commercialized blue emissive material, but the blue deep is deficient. We can obtain some blue emissive materials by modifying its ancillary ligand. Based on this idea, in this work, we changed the ancillary ligand of FIrpic (the picolinic acid) into 5-methyl-2-(2H-1,2,3-triazol-2-yl)benzoic acid. Unfortunately, in the process of the synthesis for this designed iridium complex, the ancillary ligand occurred decarboxylation, so, we obtained $(dfppy)_2Ir(ttz)$. Its crystal structure, optical physics, electrochemistry, thermally stability, luminous mechanism, electroluminescent performances were investigated.

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https://doi.org/10.1016/j.jlumin.2018.06.048
Received 18 April 2018; Received in revised form 3 June 2018; Accepted 15 June 2018
Available online 18 June 2018
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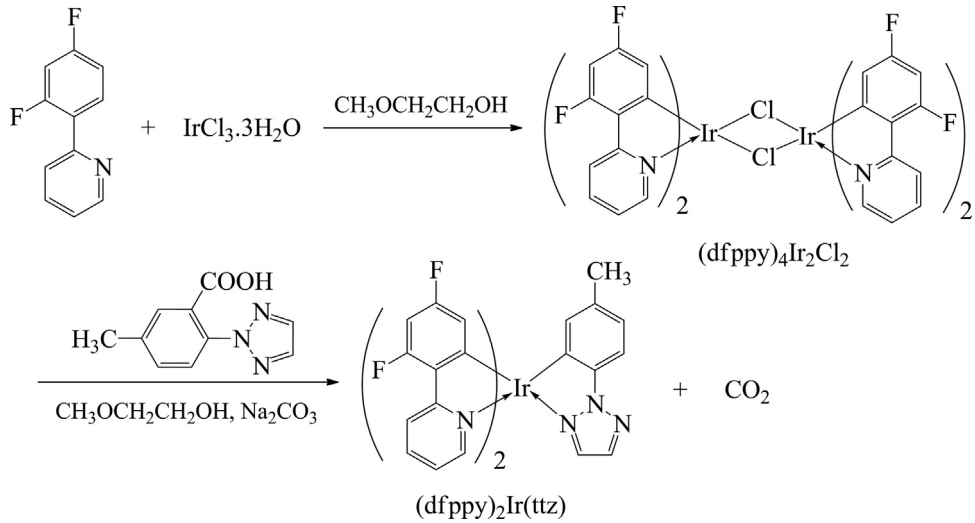

Scheme 1. Synthetic route of $(dfppy)_2Ir(ttz)$.

2. Experimental details

2.1. Synthesis and characterization of $(dfppy)_2Ir(ttz)$

The synthesis route of $(dfppy)_2Ir(ttz)$ is given in the Scheme 1. $(dfppy)_4Ir_2Cl_2$ was synthesized according to the previous literature [13]. A 150 mL of two-neck flask is charged 2.447 g (1.97 mmol) of $(dfppy)_4Ir_2Cl_2$, 1.000 g (4.91 mmol) of 5-methyl-2-(2H-1,2,3-triazol-2-yl)benzoic acid, 1.146 g (10.81 mmol) of Na_2CO_3, 45 mL of 2-methoxyethanol. The content in the flask was magnetically stirred under Ar atmosphere. Thereafter, the reaction mixture was heated up to reflux of 2-methoxyethanol for 10.5 h. During the beginning of the reaction, some bubble can be observed on the surface of the reaction solution, probably suggesting the extrusion of CO_2 apart from the bubble of the boiled 2-methoxyethanol. After the reaction content is cooled to ambient temperature; 2-methoxyethanol was removed by vacuum rotatory evaporation. Distilled water is added to the residue, which was allowed to filtration under reducing pressure, the crude production was washed with distilled water for several times, then dried in a vacuum oven. $(dfppy)_2Ir(ttz)$ was firstly purified by column chromatography [silica gel, V(dichloromethane): V(petroleum ether) = 1.5:1], further purified by gradient-temperature sublimation. 1.609 g (2.20 mmol) of $(dfppy)_2Ir(ttz)$ was obtained as a yellow powder (yield: 56%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (dd, J = 26.2, 6.7 Hz, 3 H), 7.75 – 7.46 (m, 5 H), 7.13 (s, 1 H), 6.93 – 6.75 (m, 3 H), 6.67 (s, 1 H), 6.52 – 6.38 (m, 2 H), 6.02 (dd, J = 7.6, 2.3 Hz, 1 H), 5.84 (dd, J = 9.3, 2.3 Hz, 1 H), 2.20 (s, 3 H). ^{19}F NMR (376 MHz, $CDCl_3$) δ −109.11 (d, J = 10.0 Hz), −109.18 (d, J = 9.6 Hz), −110.43 (d, J = 9.8 Hz), −111.31 (d, J = 10.2 Hz). ESI-MS (m/z), calcd. for $C_{31}H_{20}F_4IrN_5$: 732.14 [M + H$^+$]; found: 731.77. Elemental analysis, calcd. for $C_{31}H_{20}F_4IrN_5$: C 50.95, H 2.76, N 9.58; found: C 50.75, H 2.67, N 10.02.

2.2. Single crystal culture

About 15 mg of $(dfppy)_2Ir(ttz)$ was added to a 10 mL of glass bottle, dissolved with an appropriate amount of CH_2Cl_2, then, carefully dropwise added pure water up to about 0.8 cm of water layer to be formed, finally, about 3 equiv. of absolute ethyl alcohol relative to the water by volume was dropwise added. The glass bottle was imprecisely closed by a rubber plug, the solvents slowly evaporated, after ten days; some small crystals suiting to single crystal test were evolved.

2.3. Instruments and measurements

^{1}H NMR and ^{19}F NMR spectra were recorded on a Bruker-400 MHz nuclear magnetic resonance spectrometer, for ^{19}F NMR test, the resonating frequency is 376 MHz. ESI-MS was performed on a ThermoFisher mass spectrometer (model: LTQ XL). Elemental analysis was carried out on a Perkin Elmer 2400 elemental analyzer. The single crystal measurement was performed on a BRUCKER SMART APEX-CCD diffractometer equipped with a graphite-monochromatic MoKa radiation (λ = 0.71073 Å) at 296(2) K. A total of 35,714 reflections were collected in the range of 1.826° ≤ θ ≤ 25.050° by using a φ-ω scan mode with 4492 ones [R(int) = 0.0563]. The data was corrected by SADABS program. The structure was solved by direct methods with SHELXS-97 and refined by full-matrix least-squares method on F^2 with SHELXL-97. The final refinement gave R1 = 0.0240 and wR2 = 0.0569. The thermogravimetric analysis (TGA) was carried out by a PerkinElmer TGA7 and Shimadzu-DT-40 thermal analysers at a heating rate of 10 °C/min from 30 °C to 800 °C under N_2. The absorption spectrum of $(dfppy)_2Ir(ttz)$ dissolved in CH_2Cl_2 was obtained by using Perkin Elmer Lambda-35 UV–vis spectrometer. The photoluminescent spectrum of $(dfppy)_2Ir(ttz)$ dissolved in CH_2Cl_2 was recorded by using an FLsp920 fluorescence spectrophotometer (xenon lamp) with 2.5 nm excitation and emission slits. The absolute photoluminescent quantum yield in CH_2Cl_2 (~1.00×10^{-4} mol/L) was obtained in an Absolute PL Quantum Yield Spectrometer with an integrating sphere setup C11347 from Hamamatsu Photonics using scan mode, and CH_2Cl_2 was used as blank reference. The phosphorescent lifetime of $(dfppy)_2Ir(ttz)$ dissolved in CH_2Cl_2 (~1.00×10^{-4} mol/L) was measured in a Steady State and Transient State Fluorescence Spectrometer (model: FLS980, manufacturer: Edinburgh instruments UK). The electrochemical property of this iridium complex was tested by using CHI760 electrochemical workstation under Ar. $(dfppy)_2Ir(ttz)$ dissolved in CH_3CN (~3.00×10^{-3} mol/L). Platinum plate was used as working electrode, Pt wire as auxiliary electrode, Ag wire as reference electrode, $(n\text{-}C_4H_9)_4NPF_6$ as supporting electrolyte (0.1 mol/L) and ferrocene as internal standard. Prior to the measurement, Ar was purged into the solution for 5 min. The cyclic voltammogram was recorded at a scan rate of 50 mV/s.

2.4. Computation methods

The ground state for $(dfppy)_2Ir(ttz)$ was optimized by using the density functional theory (DFT) at the RB3LYP level, while the triplet excited state was obtained by time-dependent DFT (TD-DFT) at the

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