Notes

A Multifunctional Platinum-Based Triplet Emitter for OLED Applications[#]

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Summary: The synthesis of a novel trifunctional Pt(II) cyclometalated complex in which the hole-transporting (HT), electron-transporting (ET), and electroluminescent (EL) components are integrated into a single molecule is accomplished, and this complex can be sublimed and used for the fabrication of neat emissive layer electrophosphorescent devices.

Since the breakthrough on a multilayer configuration for small molecule organic electroluminescent (EL) devices,[1] this research field has come under intense scrutiny on account of its huge market share in next-generation flat-panel display technology.[2] The current focus and challenge for high-efficiency organic light-emitting devices (OLEDs) lie in the optimization of EL cell structures[2c,3] and the use of electrophosphorescence.[4] While the sophisticated multilayer configuration consisting of the hole-transporting (HT), the electron-transporting (ET), and the EL layers is frequently used to achieve a balanced injection and transport of holes and electrons, fabrication of multilayer devices is often tedious, difficult, and more expensive than single-layer devices. In view of this, recent work has proliferated particularly in single-layer dendrimer[5] and polymer[6] phosphorescent OLEDs (PHOLEDs), which rival those from multilayer devices in performance. However, only a few reports are available for single-layer PHOLEDs using low-molecular-weight d^6 metal-organic compounds of Ru(II), Os(II), Re(I), and Ir(III) that, in the majority of cases, are solution-processed along with a polymer matrix by spin coating.[7] Although examples of multilayer PHOLEDs based on heavy metal complexes of Ir(III) and Pt(II) as dopants are known[4] and these complexes were only used primarily as emitters rather than as multifunctional chromophores, there is no report of simple neat emissive layer PHOLEDs fabricated from *neutral* multifunctional small molecule d^8 metal complexes. Here, we describe the synthesis and light-emitting properties of a novel trifunctional cyclometalated Pt(II) complex in which the HT, ET, and EL functional groups are integrated into one molecule. This new complex is stable with respect to sublimation and

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Scheme 1. Synthesis of New Trifunctional Platinum(II) Complex 4

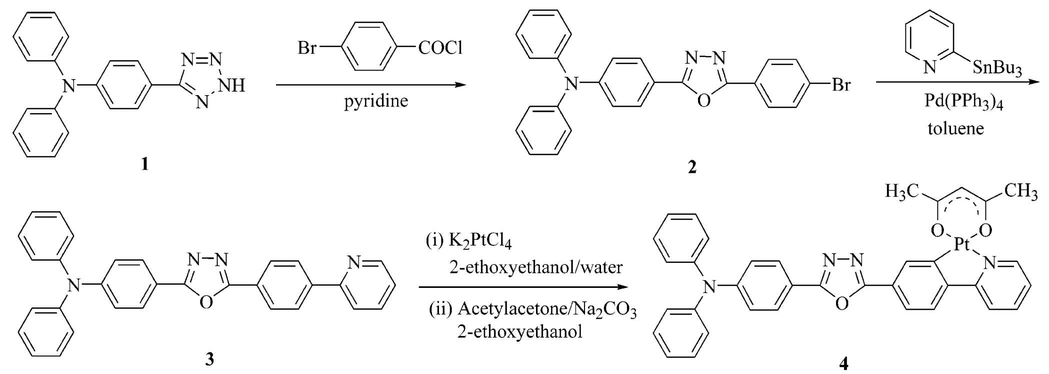

Table 1. Photophysical, Redox, and Thermal Data for 3 and 4

	absorption (298 K)	emission (298 K)						
	λ_{abs}/nm[a] CH_2Cl_2	λ_{em}/nm CH_2Cl_2	λ_{em}/nm film	Φ[b]	$\tau/\mu s$	T_{decomp}/°C[c]	E_{ox}/V[d]	E_{red}/V[d]
3	294 (5.81) 368 (5.85)	451	489	0.70	4.2×10^{-3}	456 ± 5	+0.66	−1.65
4	294 (4.90) 372 (4.86)	471, 533, 570	550, 590, 668	0.02	24.4	370 ± 5	+0.62	−1.71

[a] Log ϵ values are shown in parentheses. [b] Relative to quinine sulfate in 0.1 N H_2SO_4 ($\Phi = 0.54$), $\lambda_{ex} = 360$ nm. [c] Onset temperature. [d] 0.1 M $[Bu_4N]PF_6$ in CH_2Cl_2, scan rate 100 mV s^{-1}, vs Fc/Fc^+ couple.

thus is suitable for vacuum deposition in PHOLED fabrication.

The key compound in this study is ligand **3**, which is obtained from 4-tetrazoyltriphenylamine **1**[3a] by a two-step reaction. Compound **1** reacts with 4-bromobenzoyl chloride to give **2**, which can then undergo Stille coupling with 2-(tributylstannyl)pyridine to afford **3**. The design rationale of **3** is that it possesses both HT triphenylamine and ET oxadiazole groups, while the 2-phenylpyridine unit serves as a cyclometalating site. Metal complex **4** can be synthesized by reaction of K_2PtCl_4 with **3** followed by treatment with acetylacetone in the presence of a base (Scheme 1).[4e] Purification by preparative TLC afforded **4** as an air-stable orange crystalline solid in high purity. All new compounds were fully characterized by NMR spectroscopy and FABMS. The crystal structure of **4** was determined (Figure 1) in which the four-coordinate Pt core adopts a square-planar geometry. The oxadiazole ring and the Pt square plane differ from coplanarity only by 8.6°. The lattice is highlighted by the presence of dimeric Pt···Pt stacking interactions (ca. 3.350 Å) between adjacent molecules, and this metal–metal interaction is notably shorter than those observed for other monocyclometalated $\pi-\pi$ stacked Pt(II) complexes containing a simpler 2-phenylpyridine moiety in the literature,[8] where the smallest Pt···Pt length reported is 3.528 Å.[8c] Both **3** and **4** exhibit high thermal stabilities, and their onset decomposition temperatures are 456 and 370 °C, respectively (Table 1). In addition, **4** was observed to sublime before its decomposition temperature was reached. For **3**, two intense absorption bands are observed at 294 and 368 nm, which are attributed to the $\pi-\pi^*$ transitions associated with the N–Ar and $N-C_6H_4-X$ fragments.[9] Similar data were observed by Low et al. in the spectra of $Ar_2N-C_6H_4-X$ species near 300 and 350 nm. An analogous ligand system containing a 2,2′-bipyridyl unit also shows absorption features at 316 and 388 nm.[7e] The absorption spectrum of **4** in CH_2Cl_2 features two intense bands at 294 and 372 nm due to the $\pi-\pi^*$ ligand-centered (LC) component in the optical transition. These assignments were also supported by DFT calculations, and the contour plots depicted in Figure 2 show that the highest occupied molecular orbital (HOMO) is basically triphenylamine-based and the lowest unoccupied molecular orbital (LUMO) predominantly corresponds to the π orbitals of the 2-(2-phenylpyridine)-1,3,4-oxadiazole group. The HOMO−1 level contains substantial contribution from the Pt's d orbital character. Both **3** and **4** are good light-emitters in fluid solution and in the solid state at 298 K. The luminescence spectrum of **3** is dominated by LC $^1(\pi\pi^*)$ transitions at 451 nm ($\Phi = 0.70$, $\tau = 4.2$ ns). For **4**, it shows three emission peaks at 471, 533, and 570 nm at 298 K ($\Phi = 0.02$, $\tau = 24.4\ \mu s$, monitored at 533 nm). The structured luminescence and microsecond radiative decay lifetimes for the low-lying bands are in line with emission arising from a ^{3}LC excited state in **4**.[8a] Consistent with the X-ray structural data, examination of the emission behavior of **4** in CH_2Cl_2 and in the solid state suggests the presence of solid-state aggregates in thin films (see Table 1).

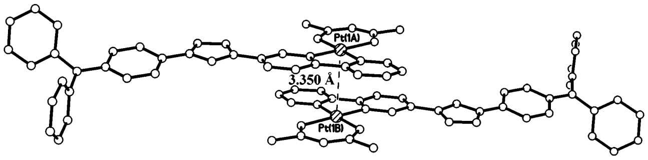

Figure 1. X-ray crystal structure of **4** showing the dimeric Pt···Pt stacking interactions. Selected bond lengths (Å) and angles (deg): Pt–C 1.921(13), Pt–N 1.955(11), Pt–O 1.991(9) and 2.088(9); C–Pt–N 80.9(5), O–Pt–O 91.7(3).

The ligand redox properties are affected by cyclometalation. Complex **4** is both easier to oxidize and harder to reduce when compared to **3**. Both compounds exhibit reversible oxidation processes at $E_{1/2} = +0.66$ and $+0.62$ V (vs Fc/Fc^+), respectively, that are tentatively assigned

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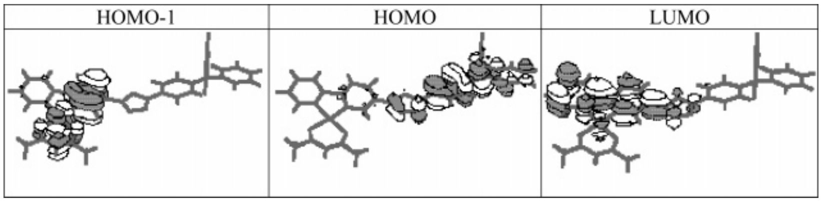

Figure 2. Contour plots of the highest occupied (HOMO−1 and HOMO) and lowest unoccupied (LUMO) molecular orbitals for **4**.

to the oxidation of the triphenylamine moiety. Cathodic sweeps show an irreversible wave at −1.65 and −1.71 V for **3** and **4**, respectively, presumably due to reduction of the oxadiazole ring.[3a,10] The reduction of the 2-phenylpyridyl group is not apparent within the solvent window. The HOMO and LUMO levels of **4** can be estimated by taking −4.8 eV as the HOMO level for the Fc/Fc$^+$ couple with respect to the vacuum level.[11] The HOMO and LUMO levels for **4** were found to be −5.42 and −3.09 eV, respectively (i.e., HOMO−LUMO gap of ca. 2.33 eV), which match closely with the energy levels for copper phthalocyanine (CuPc, −5.2 eV) and Ca (−2.9 eV). The LUMO level of **4** is lower than that of 2-(4-biphenylyl)-5-(4-*tert*-butylphenyl)-1,3-4-oxadiazole (PBD, −2.4 eV),[2c] one of the most widely used ET/HB (hole-blocking) materials and comparable to that of tris(8-hydroxylquinoline)aluminum (Alq$_3$, −3.0 eV). The HOMO level of **4** is also close to that of *N*,*N*′-diphenyl-*N*,*N*-bis-(1-naphthyl)-1,1-biphenyl-4,4-diamine (NPD, −5.5 eV), showing its good HT ability. Our data can be compared to the poorer ET property associated with [Pt(acac)(L)] (acac = acetylacetonate, LH = 2-phenylpyridine), showing a more negative reduction potential of −2.39 V.[8a] Complex **4** is thus expected to display bipolar character, typical of some organic EL materials.[3a]

The sublimability and multifunctional nature of **4** render it a suitable candidate for PHOLED structures. A bilayer vacuum-deposited device of ITO/CuPc(15 nm)/**4**(90 nm)/Ca(30 nm)/Al(100 nm) was fabricated where a single active layer of **4** as the neat emissive film was obtained by vacuum evaporation and sandwiched between two bilayer electrodes (ITO/CuPc as the anode and Ca/Al as the cathode). The CuPc layer serves only as the hole-injecting layer. This neat emissive layer device exhibits strong orange-yellow EL at 538 and 578 nm (CIE coordinates: $x = 0.52$, $y = 0.47$ for forward bias) with a low turn-on voltage at around 6 V. The EL spectrum resembles its corresponding PL spectrum from thin film (Figure 3 and its inset) and shows a weak aggregate shoulder at 648 nm due to contribution from its excimer.[8a,12] The EL spectra for this OLED exhibit no significant change with variation of operating bias voltages. The device reached a maximum luminous efficiency of 1.2 cd/A, and a luminance (L) of 1065 cd/m^2 was obtained at 14 V, which appears to perform better than that for the related 2-phenylpyridine derivative fabricated in a complicated multilayer configuration.[4j] It is also worthwhile to compare the device performance with single-layer EL devices fabricated using Ru^{II} and Re^{I} diimine complexes with similar ligands, which showed a maximum brightness of 730 cd/m^2.[7e] At a brightness of 100 cd/m^2, our device showed a luminous efficiency of 0.6 cd/A at 9.5 V.

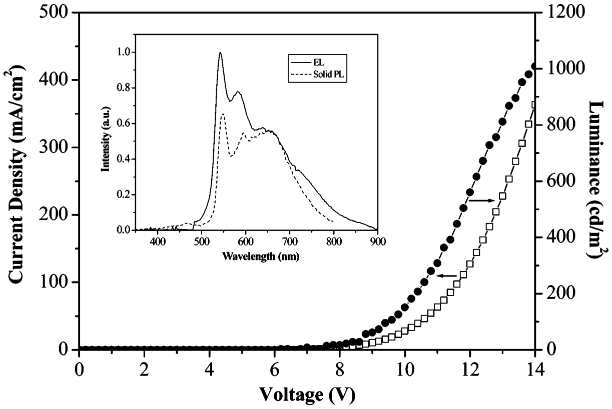

Figure 3. Current density−luminance-voltage curves for the PHOLED device using **4** (inset: EL and solid PL spectra).

In summary, we have demonstrated the synthesis, optical and redox properties, and OLED applications of a novel multifunctional Pt(II) complex combining the triplet-emitting and hole- and electron-transporting groups into one molecule, and it can act as an efficient dopant-free electrophosphorescent emitter. In contrast to most previously reported Pt(II) emitters with simpler cyclometalating ligands that are usually fabricated in multilayer configurations, a simpler small molecule device architecture can be achieved in this work. Future efforts on functionalizing the ligand substituents to fine-tune both device color and efficiency should stimulate a broad spectrum of interest within the realm of OLEDs.

Experimental Section

General Comments. All reactions were carried out under a nitrogen atmosphere using standard Schlenk techniques. Solvents were predried and distilled from appropriate drying agents. All reagents and chemicals, unless otherwise stated, were purchased from commercial sources. NMR spectra were measured in CDCl$_3$ on a JEOL EX270 or a Varian Inova 400 MHz FT-NMR spectrometer, with ^{1}H and ^{13}C NMR chemical shifts quoted relative to TMS. FAB mass spectra were recorded on a Finnigan MAT SSQ710 mass spectrometer. Thermal analyses were performed with a Perkin-Elmer DTA-7 thermal analyzer.

Preparation of 2. A mixture of **1** (0.72 g, 2.30 mmol), 4-bromobenzoyl chloride (0.50 g, 2.30 mmol), and dry pyridine (8 mL) was stirred and heated under reflux for 36 h. After being cooled to room temperature (rt), the mixture was added to CH$_2$Cl$_2$ (80 mL), washed with water (20 mL × 3), and dried over anhydrous MgSO$_4$, and the solvent was removed by rotary evaporation. The product was purified by column chromatography on silica using CH$_2$Cl$_2$ as the eluent to furnish a pale yellow powder of **2** in 62% yield (0.67 g). ^{1}H NMR (CDCl$_3$): δ

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8.00−7.97 (m, 2H, Ar−H), 7.94−7.91 (m, 2H, Ar−H), 7.68−7.65 (m, 2H, Ar−H), 7.36−7.31 (m, 4H, Ar−H), 7.19−7.09 (m, 8H, Ar−H). ^{13}C NMR ($CDCl_3$): δ 164.77, 163.23, 151.04, 146.53, 132.34, 129.59, 128.14, 128.02, 126.06, 125.71, 124.45, 123.00, 120.92, 115.64 (Ar). FABMS (*m/z*): 468 [M^+]. Anal. Calcd for $C_{26}H_{18}N_3BrO$: C 66.68, H 3.87, N 8.97. Found: C 66.48, H 3.65, N 8.74.

Preparation of 3. A mixture of 2-(tributylstannyl)pyridine (0.32 g, 0.88 mmol), **2** (0.41 g, 0.88 mmol), $Pd(PPh_3)_4$ (0.05 g, 0.043 mmol), and toluene (10 mL) was stirred and heated to 110 °C under a nitrogen atmosphere for 50 h. Upon cooling to rt, the solvent was removed under reduced pressure and the product was column chromatographed over silica gel using CH_2Cl_2/ethyl acetate (5:1, v/v) to afford a yellow powder of **3** (0.20 g, 48%). ^{1}H NMR ($CDCl_3$): δ 8.75−8.72 (m, 1H, Ar−H), 8.24−8.15 (m, 4H, Ar−H), 7.99−7.94 (m, 2H, Ar−H), 7.82−7.79 (m, 2H, Ar−H), 7.36−7.27 (m, 5H, Ar−H), 7.19−7.09 (m, 8H, Ar−H). ^{13}C NMR ($CDCl_3$): δ 164.54, 163.64, 155.87, 150.85, 149.76, 146.49, 141.98, 136.82, 129.49, 127.95, 127.34, 127.07, 125.59, 124.31, 124.26, 122.73, 120.97, 120.69, 115.88 (Ar). FABMS (*m/z*): 467 [M^+]. Anal. Calcd for $C_{31}H_{22}N_4O$: C 79.81, H 4.75, N 12.01. Found: C 79.70, H 4.48, N 11.92.

Preparation of 4. A mixture of **3** (0.10 g, 0.21 mmol), K_2PtCl_4 (0.04 g, 0.10 mmol), 2-ethoxyethanol (6 mL), and water (2 mL) was stirred under a nitrogen atmosphere and heated to 80 °C for 16 h. After cooling to rt, the mixture was added to water (20 mL), and the precipitate was washed with water (20 mL × 4) and dried at 50 °C in a vacuum. The precipitate was then treated with acetylacetone (0.03 mL, 0.3 mmol) and Na_2CO_3 (0.106 g, 1.0 mmol) in 2-ethoxyethanol (8 mL) at 100 °C under nitrogen for 16 h. After the removal of all volatile components, the compound was purified by column chromatography on silica using CH_2Cl_2 as the eluent to afford **4** as a yellow solid (0.04 g, 50%). ^{1}H NMR ($CDCl_3$): δ 9.03−9.01 (d, 1H, Ar−H), 8.27−8.26 (d, 1H, Ar−H), 7.97−7.80 (m, 4H, Ar−H), 7.67−7.64 (d, 1H, Ar−H), 7.54−7.51 (d, 1H, Ar−H), 7.36−7.26 (m, 4H, Ar−H), 7.19−7.10 (m, 9H, Ar−H), 5.50 (s, 1H, CH), 2.06−2.02 (d, 6H, CH_3). ^{13}C NMR ($CDCl_3$): δ 185.64, 184.12, 166.81, 164.30, 150.65, 147.64, 147.37, 146.60, 139.28, 138.19, 129.48, 128.09, 127.85, 126.33, 125.54, 124.18, 123.51, 123.01, 122.27, 121.96, 121.16, 119.01, 116.36 (Ar), 102.56 (CH), 28.29, 27.35 (CH_3). FABMS (*m/z*): 760 [M^+]. Anal. Calcd for $C_{36}H_{28}N_4O_3Pt$: C 56.91, H 3.71, N 7.37. Found: C 56.76, H 3.55, N 7.16.

X-ray Crystallography. Intensity data were collected at 293 K using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) on a Bruker Axs SMART 1000 CCD diffractometer. The collected frames were processed with the SAINT program and an absorption correction (SADABS) was applied to the reflections. The structure was solved and refined by full-matrix least-squares analyses on F^2 using the SHELXTL program.[13] Hydrogen atoms were generated in their idealized positions, and all non-hydrogen atoms were refined anisotropically.

Selected crystal data of **4**: $C_{36}H_{28}N_4O_3Pt{\cdot}H_2O$, $M_r = 777.73$, monoclinic, space group $P2_1/c$, $a = 19.827(9)$ Å, $b = 13.692(6)$ Å, $c = 11.835(6)$ Å, $\beta = 97.041(10)°$, $V = 3189(3)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.620$ g cm^{-3}, $\mu = 4.446$ mm^{-1}, $F(000) = 1536$, 15 455 reflections measured, 5589 unique ($R_{int} = 0.1077$), final R1 = 0.0603 and wR2 = 0.1329 for 2932 observed reflections with $I > 2\sigma(I)$.

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Supporting Information Available: Text giving experimental procedures for photophysical and electrochemical measurements, DFT study and OLED device fabrication, the ORTEP plot of **4** showing the atom-numbering scheme and a CIF file containing X-ray data for **4**. This material is available free of charge via the Internet at http://pubs.acs.org.

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