

Electronic Supplementary Information for:

Enhancement of luminescence performance from the alteration of stacking pattern of Pt(II) dendrimers

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Experimental Section

Chemicals

All reactions and manipulations were carried out under argon using standard Schlenk techniques. Chemicals and reagents for chemical synthesis were obtained from commercial sources. Solvents, such as dichloromethane (DCM), tetrahydrofuran (THF), toluene and chlorobenzene were purified and distilled from appropriate drying agents before use. Other reagents were of analytical grade and were used as received. 2,4-diphenylquinoline (**PPQ**), 4-(4-Bromophenyl)-2-phenylquinoline and the ligand **LD1** (Scheme S1) were prepared according to literature methods.^{1,2} The ligand **LC4-D1** and **LC4-D2** (Scheme S1) were synthesized according to the modified procedures.³⁻⁶

Instrumentations

Complex Characterization

The ¹H and ¹³C NMR spectra were recorded in appropriate solvents on Bruker Avance 300/400 MHz NMR spectrometer with chemical shifts (in ppm) relative to tetramethylsilane. Elemental analysis was carried out using a Bio-Rad Co's elemental analytical instrument. MALDI-TOF mass spectra were obtained on an AXIMA CFR MS apparatus (COMPACT). TGA was performed under a flow of nitrogen at a heating rate of 10 °C/min with Perkin-Elmer-TGA 7 thermal gravimetric analyzer.

Physical and electrochemical Measurements

UV-vis absorption and PL spectra were measured on Perkin-Elmer Lambda 35 UV-vis spectrometer and Perkin-Elmer LS 50B spectrofluorometer in aerated solution, respectively. The lifetimes of the samples were obtained by an exponential fit of

emission decay curves recorded on the laser photolysis technique, in which the third harmonic of an Nd:YAG laser (355 nm output and ca. ~3 ns pulse width) was used as the excitation source, coupled with a fast response photomultiplier. The solution PL quantum efficiencies were measured in toluene solution at room temperature against the (ppy)Pt(acac) standard ($\Phi_p=0.15$).⁷

Cyclic voltammetry experiments were performed with an EG&G 283 (Princeton Applied Research) potentiostat/galvanostat system at room temperature. A conventional three-electrode configuration consisting of a Pt working electrode, a Pt counter electrode and an Ag/AgCl reference electrode were used. The solvent in all measurements was DCM and the supporting electrolyte was 0.1 M tetrabutylammonium perchlorate (*n*-Bu₄NClO₄). Ferrocene was added as a calibrant after each set of measurements and all potential reported were quoted with reference to the ferrocene/ferrocenium (Fc/Fc⁺) couple at a scan rate of 100 mV·s⁻¹.

Crystal Structure Determination

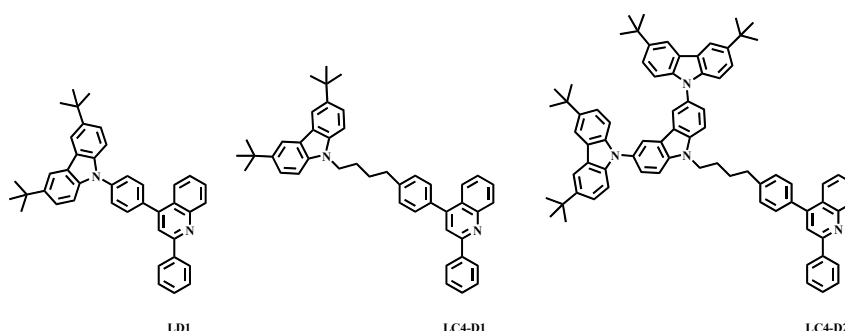
Crystals of **D1-2**, **C4-D1-2** and **(PPQ)Pt(acac)** were obtained by slow evaporation of a DCM/MeOH solution at room temperature. The crystal data and details of data collection and refinement were summarized in Table S1. The single-crystal X-ray diffraction experiments were carried out using a Bruker Smart APEX diffractometer with CCD detector and graphite monochromator, Mo K α radiation ($\lambda = 0.71073$ Å). The intensity data were recorded with ω scan mode (187 K). Lorentz, polarization factors were made for the intensity data and absorption corrections were performed using SADABS program.⁸ The crystal structure was determined using the SHELXTL program and refined using full matrix least squares.⁹ All non-hydrogen atoms were assigned with anisotropic displacement parameters, whereas hydrogen

atoms were placed at calculated positions theoretically and included in the final cycles of refinement in a riding model along with the attached carbons.

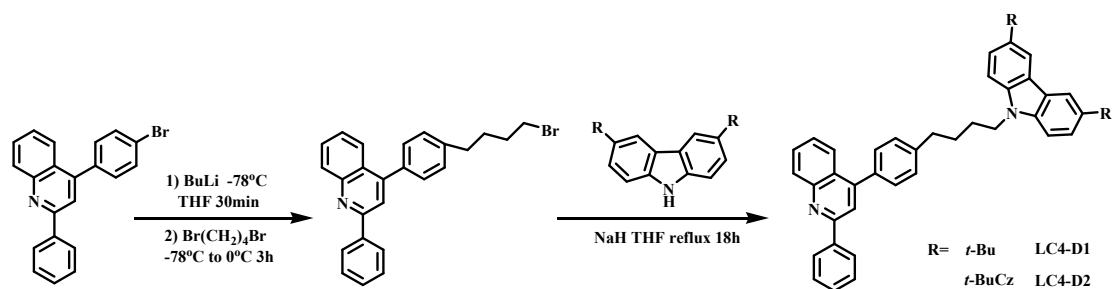
OLED Fabrication and Measurements

The OLEDs were fabricated with a structure of ITO/PEDOT:PSS (50 nm)/emissive layer (CBP:4% Pt(II) dendrimer) (30 nm)/TPCz (60 nm)/LiF (1 nm)/Al (100 nm). The PEDOT:PSS and emissive layers (chlorobenzene was used as the solvent) were spin-coated in sequence onto the pre-cleaned and UV-ozone treated ITO substrate, respectively, followed by thermal evaporation of the TPCz (60 nm) and LiF (1 nm)/Al (100 nm) structure in vacuum chamber at a base pressure of less than 4×10^{-4} Pa. The current-density-voltage and brightness-voltage curves of the devices were measured using a Keithley 2400 source meter with a calibrated silicon photodiode. The EL spectra and CIE coordinates were recorded using the PR650 spectra colorimeter. All of the experiments and measurements were carried out at room temperature under ambient conditions.

Synthesis and Characterization



Scheme S1. Molecular structures of the ligands **LD1**, **LC4-D1** and **LC4-D2**.



Scheme S2. Synthesis of the ligands **LC4-D1** and **LC4-D2**.

Preparations of Ligand LC4-D1 and LC4-D2

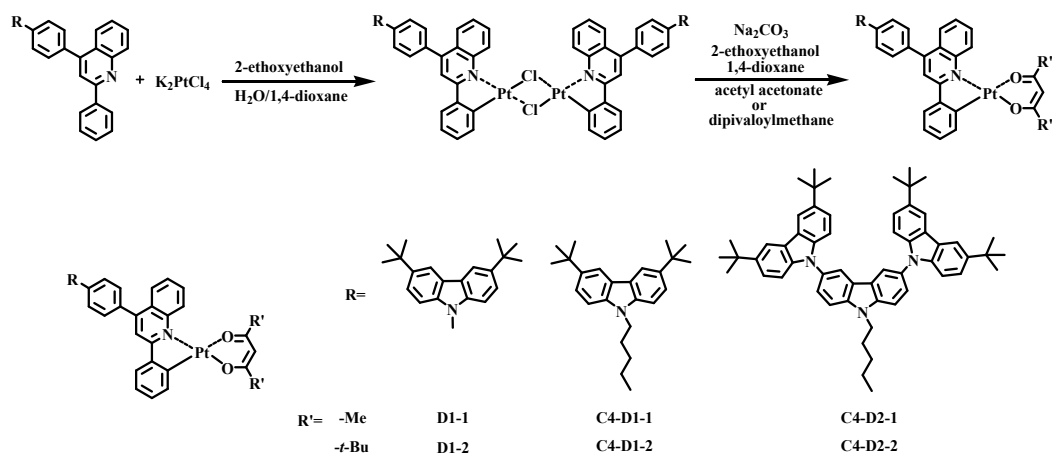
4-(4-(4-bromobutyl)phenyl)-2-phenylquinoline: To a stirred solution of 4-(4-bromophenyl)-2-phenylquinoline (10 mmol) in THF (200 mL) under an argon atmosphere, *n*-butyllithium (1.1 eq., 2.5 M in hexane) was added dropwise at -78 °C and then the mixture was stirred for 30 min. To this mixture was added 4.8 mL of 1,4-dibromobutane (4.0 eq.) and the temperature was allowed to rise slowly to room temperature. After stirring for 3 h, the reaction mixture was hydrolyzed with water. The aqueous phase was extracted with diethyl ether (3×40 mL), the combined organic phase were dried over Na₂SO₄ and concentrated. The residue obtained was purified by column chromatography on silica gel using petroleum (PE)/ethyl acetate (EA) (20:1, v/v) as the eluent, yield: 80%. ¹H NMR (400 MHz, CDCl₃, ppm): δ 8.21 (d, *J* = 7.2 Hz, 3H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.83 (s, 1H), 7.75 (t, *J* = 7.6 Hz, 1H), 7.56-7.46 (m, 6H), 7.38 (d, *J* = 8.0 Hz, 2H), 3.48 (t, *J* = 6.4 Hz, 2H), 2.78 (t, *J* = 7.2 Hz, 2H), 2.04-1.97 (m, 2H), 1.95-1.85 (m, 2H).

LC4-D1: Under an argon atmosphere, a suspension of 95% sodium hydride (35 mmol) and 3,6-di-*t*-butylcarbazole (9.54 mmol) in THF (40 mL) was stirred at room temperature for 15 min, then heated to reflux for 30 min. After cooled to room temperature, a solution of 4-(4-(4-bromobutyl)phenyl)-2-phenylquinoline (7.95 mmol) in anhydrous THF (40 mL) was added to the above anion solution, and stirred 30 min

at room temperature. The green reaction mixture obtained was heated to reflux for 18 h, during which it turned brown. The cooled mixture was quenched with distilled water, and extracted with diethyl ether (3×40 mL). The organic phase was dried over anhydrous Na₂SO₄ and concentrated. The residue was purified by column chromatography on silica gel using the mixture of PE and EA (50:3, v/v) as the eluent to give pure product, yield: 89%. ¹H NMR (300 MHz, CDCl₃, ppm): δ 8.26 (d, *J* = 6.3 Hz, 1H), 8.19 (d, *J* = 6.3 Hz, 2H), 8.12 (d, *J* = 1.5 Hz, 2H), 7.93 (d, *J* = 8.1 Hz, 1H), 7.81 (s, 1H), 7.74 (t, *J* = 7.2 Hz, 1H), 7.56-7.45 (m, 8H), 7.34-7.28 (m, 4H), 4.32 (t, *J* = 6.9 Hz, 2H), 2.74 (t, *J* = 7.5 Hz, 2H), 2.00 (quint, *J* = 6.9 Hz, 2H), 1.82 (quint, *J* = 7.5 Hz, 2H), 1.46 (s, 18H).

LC4-D2: The procedure was similar to that for ligand **LC4-D1**, except that 3,6-di-*t*-butyl-9-(3-(3,6-di-*t*-butylcarbazol-9-yl)carbazol-6-yl)carbazole was used in place of 3,6-di-*t*-butylcarbazole, yield: 50%. ¹H NMR (300 MHz, CDCl₃, ppm): δ 8.20-8.16 (m, 9H), 7.95 (d, *J* = 8.1 Hz, 2H), 7.83 (s, 1H), 7.67 (s, 4H), 7.54-7.47 (m, 6H), 7.45-7.38 (m, 6H), 7.27 (d, *J* = 7.2 Hz, 4H), 4.56 (t, *J* = 6.9 Hz, 2H), 2.87 (t, *J* = 7.5 Hz, 2H), 2.19 (quint, *J* = 6.9 Hz, 2H), 1.97 (quint, *J* = 7.5 Hz, 2H), 1.45 (s, 36H).

General Procedure for Preparations of Pt(II) Dendrimers and (PPQ)Pt(acac)



Scheme S3. Synthetic route and structures of the Pt(II) dendrimers.

Pt(II) dendrimers and **(PPQ)Pt(acac)** were synthesized according to the literature procedures.^{7, 10} The mixture of K₂PtCl₄ and 2.5 equiv of the corresponding ligand (**LD1**, **LC4-D1**, **LC4-D2** and **PPQ**) in 2-ethoxyethanol/H₂O (3:1, v/v) and 1,4-dioxane were heated to 60 °C for 48 h. The solvents were removed under vacuum to give the dimeric intermediate, which was used directly without further purification. The suspension of dimer, acetyl acetonate (Hacac) or dipivaloylmethane (Hdpm) (3 equiv.) and anhydrous Na₂CO₃ (5 equiv.) in 2-ethoxyethanol and 1,4-dioxane were heated and stirred at 80 °C for 48 h. The resulting mixture was poured into water and extracted with DCM. The combined organic layers were washed with water and dried over anhydrous Na₂SO₄. After the volatiles were completely removed under vacuum, the residue was purified by column chromatography on silica gel using DCM/PE (1:2, v/v) as the eluent to afford the pure product.

D1-1: yield: 70%. ¹H NMR (300 MHz, CDCl₃, ppm): δ 9.61 (d, *J* = 8.2 Hz, 1H), 8.18 (s, 2H), 7.98 (d, *J* = 8.1 Hz, 1H), 7.84-7.79 (m, 6H), 7.66 (d, *J* = 7.5 Hz, 1H), 7.65 (d, *J* = 7.5 Hz, 1H), 7.58 (d, *J* = 7.5 Hz, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.52 (s, 4H), 7.17 (t, *J* = 7.5 Hz, 1H), 5.60 (s, 1H), 2.07 (s, 6H), 1.49 (s, 18H). ¹³C NMR (75 MHz, CDCl₃, ppm): δ 185.9, 184.6, 169.7, 150.7, 149.9, 146.8, 143.7, 140.4, 139.5, 139.4, 136.3, 131.2, 131.0, 130.4, 129.7, 127.1, 127.0, 126.3, 125.3, 124.2, 124.1, 124.0, 117.3, 116.8, 109.6, 102.2, 35.2, 32.4, 28.8, 27.6. Anal. Calcd for C₄₆H₄₄N₂O₂Pt: C, 64.85; H, 5.21; N, 3.29. Found: C, 65.25; H, 4.87; N, 3.00%. MALDI-TOF (*m/z*): 852.3 [M+H]⁺.

D1-2: yield: 39%. ¹H NMR (300 MHz, CDCl₃, ppm): δ 9.74 (d, *J* = 8.7 Hz, 1H), 8.18 (s, 2H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.87 (d, *J* = 8.3 Hz, 2H), 7.80-7.76 (m, 5H), 7.67 (d, *J* = 7.5 Hz, 1H), 7.58 (d, *J* = 7.2 Hz, 1H), 7.53 (d, *J* = 0.9 Hz, 4H), 7.27 (d, *J*

= 7.2 Hz, 1H), 7.18 (td, $J = 7.5, 0.9$ Hz, 1H), 5.94 (s, 1H), 1.50 (s, 18H), 1.34 (s, 9H), 1.32 (s, 9H). ^{13}C NMR (151 MHz, CDCl_3 , ppm): δ 194.3, 192.8, 168.3, 149.1, 148.6, 145.3, 142.3, 139.7, 138.0, 137.9, 134.9, 129.8, 129.7, 129.3, 128.2, 126.3, 125.6, 125.4, 124.7, 123.7, 122.7, 122.6, 115.9, 115.3, 108.2, 91.6, 41.2, 40.0, 33.7, 30.9, 27.7, 27.5. Anal.Calcd for $\text{C}_{52}\text{H}_{56}\text{N}_2\text{O}_2\text{Pt}$: C, 66.72; H, 6.03; N, 2.99. Found: C, 66.46; H, 6.07; N, 2.91%. MALDI-TOF (m/z): 936.4 $[\text{M}+\text{H}]^+$.

C4-D1-1: yield: 24%. ^1H NMR (300 MHz, CDCl_3 , ppm): δ 9.53 (d, $J = 8.7$ Hz, 1H), 8.12 (d, $J = 1.8$ Hz, 2H), 7.84 (dd, $J = 8.4, 1.2$ Hz, 1H), 7.76-7.71 (m, 2H), 7.70 (s, 1H), 7.57 (dd, $J = 7.8, 0.9$ Hz, 1H), 7.52 (dd, $J = 8.7, 2.1$ Hz, 2H), 7.49-7.43 (m, 3H), 7.35-7.29 (m, 4H), 7.23 (td, $J = 7.5, 1.2$ Hz, 1H), 7.13 (td, $J = 7.5, 1.2$ Hz, 1H), 5.58 (s, 1H), 4.33 (t, $J = 6.9$ Hz, 2H), 2.74 (t, $J = 7.5$ Hz, 2H), 2.04 (s, 3H), 2.03 (s, 3H), 1.99 (quint, $J = 7.5$ Hz, 2H), 1.81 (quint, $J = 6.9$ Hz, 2H), 1.46 (s, 18H). ^{13}C NMR (75 MHz, CDCl_3 , ppm): δ 185.4, 184.1, 169.2, 151.1, 143.0, 141.6, 139.9, 139.0, 135.1, 130.4, 129.9, 129.4, 129.2, 128.8, 126.5, 126.3, 126.1, 124.8, 123.8, 123.3, 122.7, 116.8, 116.4, 108.0, 101.8, 43.0, 35.5, 34.7, 32.1, 29.0, 28.8, 28.4, 27.3. Anal.Calcd for $\text{C}_{50}\text{H}_{52}\text{N}_2\text{O}_2\text{Pt}$: C, 66.14; H, 5.77; N, 3.09. Found: C, 66.08; H, 5.44; N, 2.73%. MALDI-TOF (m/z): 908.3 $[\text{M}^++\text{H}]$.

C4-D1-2: yield: 43%. ^1H NMR (300 MHz, CDCl_3 , ppm): δ 9.67 (d, $J = 8.7$ Hz, 1H), 8.12 (d, $J = 1.5$ Hz, 2H), 7.84 (d, $J = 7.8$ Hz, 2H), 7.74-7.69 (m, 2H), 7.58 (dd, $J = 7.4, 0.9$ Hz, 1H), 7.53 (dd, $J = 8.4, 1.8$ Hz, 2H), 7.49-7.45 (m, 3H), 7.35-7.29 (m, 4H), 7.24 (td, $J = 7.5, 1.2$ Hz, 1H), 7.14 (td, $J = 7.2, 0.6$ Hz, 1H), 5.91 (s, 1H), 4.33 (t, $J = 7.2$ Hz, 2H), 2.74 (t, $J = 7.2$ Hz, 2H), 2.00 (quint, $J = 7.5$ Hz, 2H), 1.82 (quint, $J = 6.9$ Hz, 2H), 1.46 (s, 18H), 1.32 (s, 9H), 1.29 (s, 9H). ^{13}C NMR (151 MHz, CDCl_3 , ppm): δ 194.3, 192.7, 168.2, 149.9, 148.5, 145.4, 141.9, 140.5, 139.5, 137.9, 134.1, 129.5, 129.2, 128.3, 128.0, 127.7, 126.1, 125.5, 125.1, 124.9, 123.6, 122.5, 122.2,

121.7, 115.7, 115.3, 106.9, 91.6, 41.9, 41.2, 39.9, 34.4, 33.6, 31.0, 27.8, 27.7, 27.4.

Anal. Calcd for $C_{56}H_{64}N_2O_2Pt$: C, 67.79; H, 6.50; N, 2.82. Found: C, 68.01; H, 6.82; N, 2.60%. MALDI-TOF (m/z): 992.4 [M+H]⁺.

C4-D2-1: yield: 45%. ¹H NMR (300 MHz, CDCl₃, ppm): δ 9.52 (d, *J* = 8.7 Hz, 1H), 8.19 (s, 2H), 8.14 (d, *J* = 1.5 Hz, 4H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.73 (dd, *J* = 7.5, 0.9 Hz, 1H), 7.69-7.65 (m, 6H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.48 (d, *J* = 8.1 Hz, 2H), 7.44-7.37 (m, 7H), 7.30 (d, *J* = 8.7 Hz, 4H), 7.21 (td, *J* = 7.2, 1.2 Hz, 1H), 7.09 (td, *J* = 7.65, 0.9 Hz, 1H), 5.56 (s, 1H), 4.54 (t, *J* = 6.6 Hz, 2H), 2.86 (t, *J* = 7.5 Hz, 2H), 2.20-2.12 (m, 2H), 2.04 (s, 3H), 2.03 (s, 3H), 2.00-1.92 (m, 2H), 1.44 (s, 36H). ¹³C NMR (151 MHz, CDCl₃, ppm): δ 184.3, 183.0, 168.1, 149.9, 148.4, 145.4, 141.7, 141.4, 139.2, 138.9, 134.3, 129.4, 128.9, 128.8, 128.4, 128.1, 127.7, 125.6, 125.5, 125.3, 124.9, 124.7, 123.6, 122.7, 122.5, 122.4, 122.0, 118.4, 115.7, 115.1, 108.8, 108.0, 100.7, 42.4, 34.4, 33.7, 31.0, 28.0, 27.8, 27.3, 26.2. Anal. Calcd for $C_{82}H_{82}N_4O_2Pt$: C, 72.92; H, 6.12; N, 4.15. Found: C, 72.93; H, 6.20; N, 4.01%. MALDI-TOF (m/z): 1349.6 [M+H]⁺.

C4-D2-2: yield: 43%. ¹H NMR (300 MHz, CDCl₃, ppm): δ 9.67 (d, *J* = 9.0 Hz, 1H), 8.21 (s, 2H), 8.16 (s, 4H), 7.86 (d, *J* = 4.2 Hz, 1H), 7.84 (d, *J* = 3.3 Hz, 1H), 7.71 (d, *J* = 9.0 Hz, 2H), 7.67 (s, 4H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 2H), 7.46-7.39 (m, 7H), 7.32 (d, *J* = 8.7 Hz, 4H), 7.24 (t, *J* = 8.1 Hz, 1H), 7.11 (t, *J* = 7.2 Hz, 1H), 5.92 (s, 1H), 4.56 (t, *J* = 6.6 Hz, 2H), 2.88 (t, *J* = 7.5 Hz, 2H), 2.19 (quint, *J* = 7.2 Hz, 2H), 1.97 (quint, *J* = 7.2 Hz, 2H), 1.46 (s, 36H), 1.33 (s, 9H), 1.29 (s, 9H). ¹³C NMR (151 MHz, CDCl₃, ppm): δ 194.3, 192.7, 168.2, 149.8, 148.5, 145.4, 141.7, 141.4, 139.5, 139.2, 138.6, 134.3, 129.5, 129.3, 128.9, 128.5, 128.0, 127.7, 126.1, 125.5, 125.2, 124.8, 124.7, 123.6, 122.5, 122.4, 122.3, 122.0, 118.4, 115.7, 115.1, 108.8, 108.0, 91.6, 42.4, 41.2, 39.9, 34.4, 33.6, 31.0, 28.0, 27.8, 27.7, 27.5, 26.3.

Anal.Calcd for $C_{88}H_{94}N_2O_2Pt$: C, 73.67; H, 6.60; N, 3.90. Found: C, 73.28; H, 6.95; N, 3.96%. MALDI-TOF (m/z): 1433.7 [M+H]⁺.

(PPQ)Pt(acac): yield: 66%. ¹H NMR (300 MHz, CDCl₃, ppm): δ 9.56 (d, $J = 8.7$ Hz, 1H), 7.82 (d, $J = 8.4$ Hz, 1H), 7.78-7.72 (m, 3H), 7.60-7.54 (m, 6H), 7.48 (td, $J = 7.4, 0.9$ Hz, 1H), 7.24 (td, $J = 7.8, 1.5$ Hz, 1H), 7.14 (td, $J = 7.0, 0.9$ Hz, 1H), 5.58 (s, 1H), 2.06 (s, 3H), 2.05 (s, 3H). ¹³C NMR (75 MHz, CDCl₃, ppm): δ 185.8, 184.5, 169.6, 151.6, 149.8, 146.8, 140.3, 138.0, 130.9, 130.3, 129.7, 129.6, 129.4, 129.2, 127.1, 127.0, 126.8, 126.4, 124.2, 117.2, 102.2, 28.8, 27.6. Anal.Calcd for $C_{26}H_{21}NO_2Pt$: C, 54.35; H, 3.68; N, 2.44. Found: C, 54.37; H, 3.37; N, 2.04%. MALDI-TOF (m/z): 575.1 [M+H]⁺.

Table S1. Summary of the crystal data and structure refinement.

	D1-2	C4-D1-2	(PPQ)Pt(acac)
Empirical formula	C ₅₂ H ₅₆ N ₂ O ₂ Pt	C ₅₆ H ₆₄ N ₂ O ₂ Pt	C ₂₆ H ₂₁ NO ₂ Pt
Formula weight	936.08	1077.11	574.53
Temperature (K)	185(2)	185(2)	185(2)
Cryst size (mm)	0.26×0.12×0.08	0.35×0.23×0.09	0.36×0.25×0.09
Cryst syst	Triclinic	Monoclinic	Monoclinic
Space group	<i>P</i> -1	<i>P</i> 2/ <i>c</i>	<i>P</i> 2(1)/ <i>n</i>
<i>a</i> (Å)	10.1108(4)	12.5676(8)	14.3583(10)
<i>b</i> (Å)	10.6323(4)	29.5883(19)	7.6478(5)
<i>c</i> (Å)	20.9287(8)	13.6576(9)	18.9808(13)
<i>α</i> (deg)	94.0210(10)	90.0	90.0
<i>β</i> (deg)	99.3170(10)	99.0920(10)	101.6610(10)
<i>γ</i> (deg)	97.3480(10)	90.0	90.0
<i>V</i> (Å³)	2192.44(15)	5014.8(6)	2040.6(2)
<i>Z</i>	2	4	4
Dcaled (g cm⁻³)	1.418	1.427	1.870
<i>μ</i> (mm⁻¹)	3.242	2.948	6.899
<i>F</i> (000)	952	2200	1112
<i>θ</i> rang (deg)	1.94-26.02	1.64-26.04	1.63-26.04
no. of reflns collected	11888	31630	11714
no. of unique reflns	8411	9865	4029
<i>R</i>_{int}	0.0125	0.0496	0.0354
no. of params	590	577	335
R1 [<i>I</i> > 2.0σ(<i>I</i>)]	0.0273	0.0565	0.0280
wR2 (all data)	0.0731	0.1615	0.0547
GOF on <i>F</i>²	1.005	1.000	1.013

Table S2. Electrochemical performance of Pt(II) dendrimers.

	HOMO ^[a]	LUMO ^[a]	ΔE ^[b]		HOMO ^[a]	LUMO ^[a]	ΔE ^[b]
D1-1	-5.06	-2.96	2.10	D1-2	-5.46	-2.96	2.50
C4-D1-1	-5.08	-2.91	2.17	C4-D1-2	-5.41	-2.92	2.49
C4-D2-1	-5.18	-2.93	2.25	C4-D2-2	-5.33	-2.93	2.40

[a] Measured in DCM at room temperature with 0.1 mol·L⁻¹ *n*-Bu₄NClO₄ as supporting electrolyte; scanning rate: 100 mV·s⁻¹; values are reported vs. Fc⁺/Fc. [b] $\Delta E = \text{LUMO} - \text{HOMO}$.

Table S3. Selected bond lengths (Å) and angles (deg) for dendrimers **D1-2**, **C4-D1-2** and **(PPQ)Pt(acac)**.

		D1-2	C4-D1-2	(PPQ)Pt(acac)
Bond lengths (Å)	Pt-C(1)	1.959(3)	1.983(8)	1.961(5)
	Pt-N(1)	2.046(3)	2.030(6)	2.054(4)
	Pt-O(1)	2.099(2)	2.111(6)	2.114(3)
	Pt-O(2)	1.988(2)	1.996(5)	2.005(3)
Bond angles (°)	C(1)-Pt-O(2)	90.1(1)	89.8(3)	88.8(3)
	O(1)-Pt-O(2)	88.6(0)	88.1(2)	88.6(0)
	C(1)-Pt-N(1)	80.5(4)	80.6(3)	81.6(5)
	O(1)-Pt-N(1)	100.6(3)	101.4(2)	101.4(9)
	C(1)-Pt-O(1)	177.9(1)	176.7(3)	177.0(3)
	N(1)-Pt-O(2)	169.7(8)	169.8(3)	169.7(7)
Torsion angles (°)	C(5)-C(6)-C(7)-N(1)	12.16	5.10	2.85
	C(9)-C(10)-C(15)-C(14)	5.80	3.17	5.22
	C(8)-C(9)-C(21)-C(26)	65.71	45.01	51.77
Dihedral angles (°)	PtC(1)N(1) and PtO(1)O(2)	4.44	4.14	2.09
	PtC(1)O(2) and PtN(1)O(1)	4.60	4.70	2.30
Mean deviation from plane (Å)	C(1)N(1)O(2)O(1)	0.0222	0.0083	0.0005
Deviation of Pt atom from plane (Å)	C(1)N(1)O(2)O(1)	0.0523	0.0534	0.0274

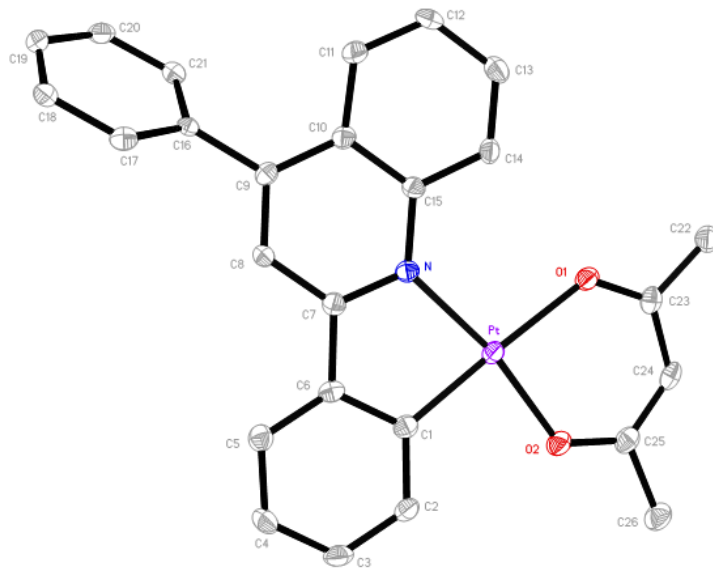
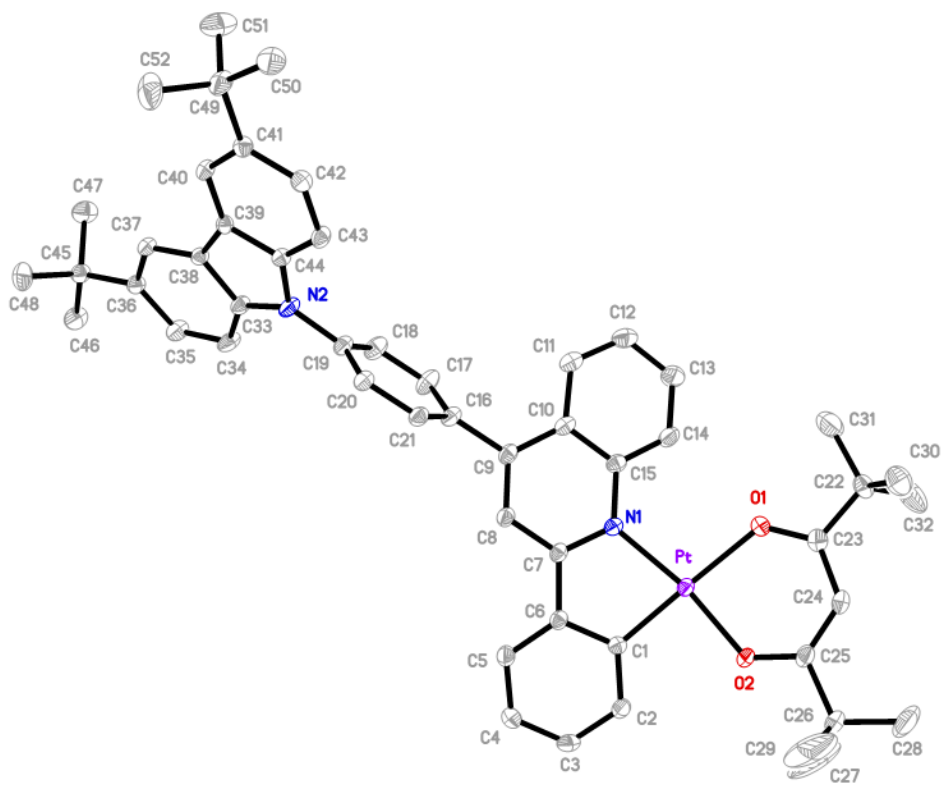


Figure S1. Perspective view of complex **D1-2** (top) and **(PPQ)Pt(acac)** (bottom) with thermal ellipsoids shown at the 30% probability level limit (hydrogen atoms have been omitted for clarity).

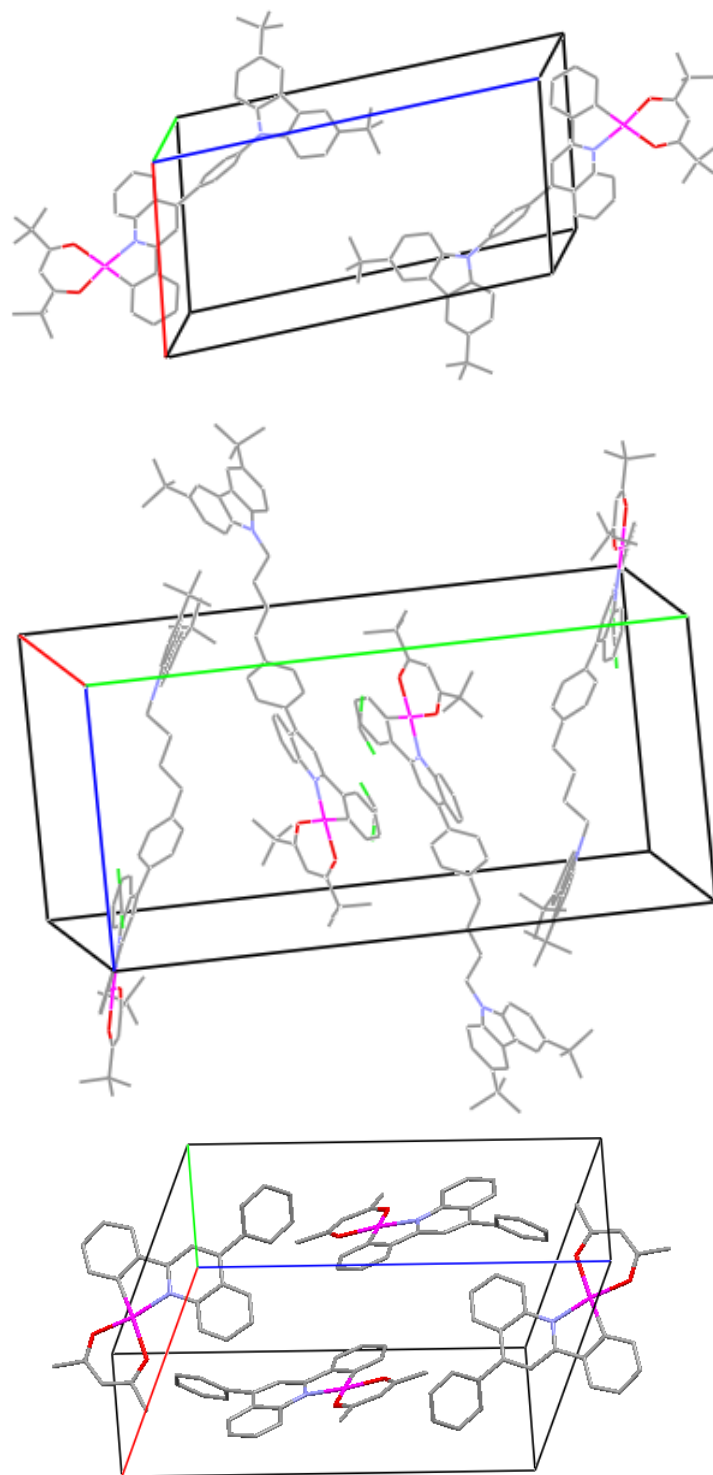


Figure S2. The packing diagram of complex **D1-2** (top), **C4-D1-2** (middle) and **(PPQ)Pt(acac)** (bottom) in a crystal cell (hydrogen atoms have been omitted for clarity).

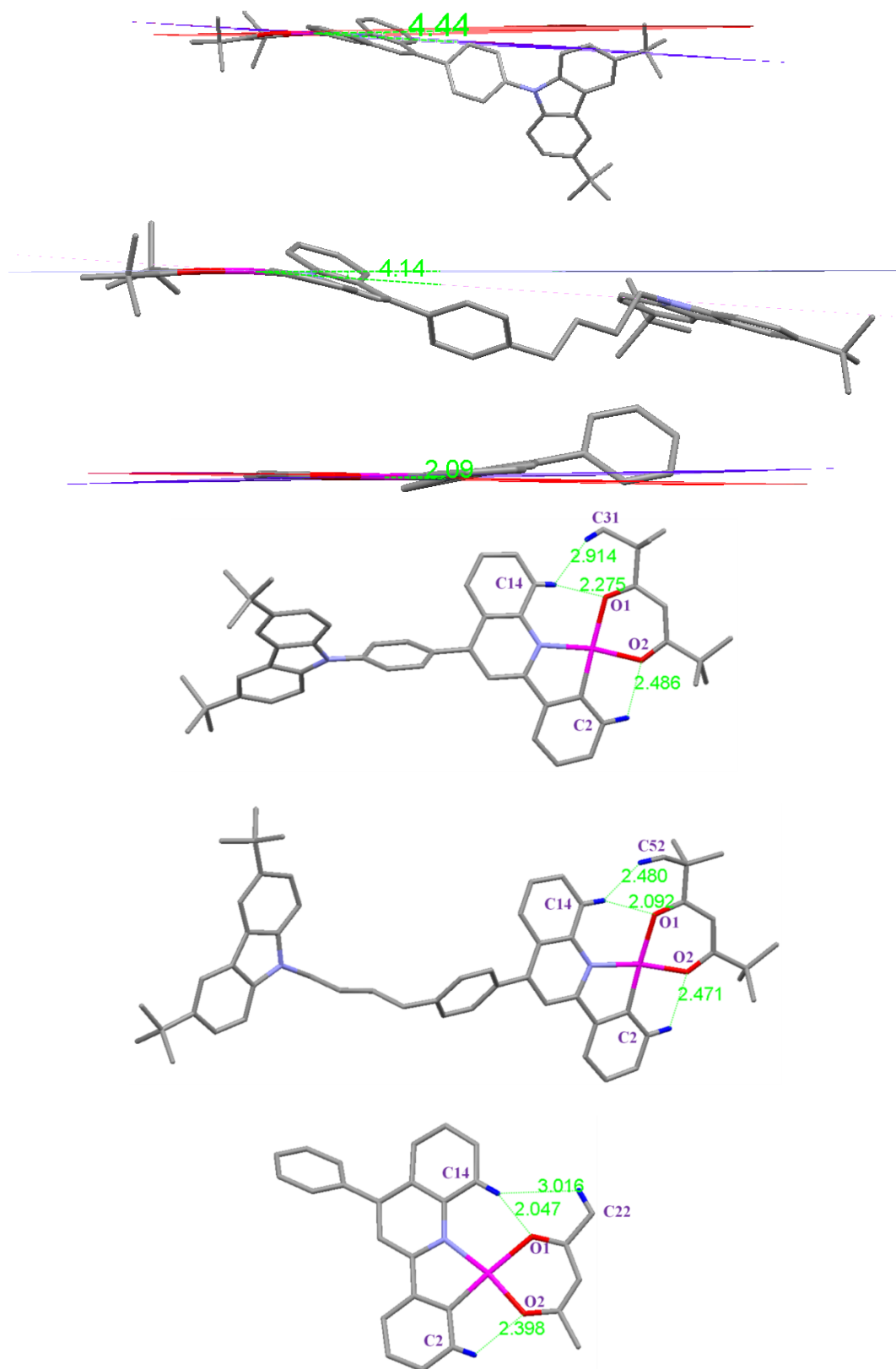


Figure S3. The dihedral angles ($^{\circ}$) of the planes PtC(1)N(1) and PtO(1)O(2) and atoms distances for complex D1-2 and C4-D1-2 (hydrogen atoms have been omitted for clarity).

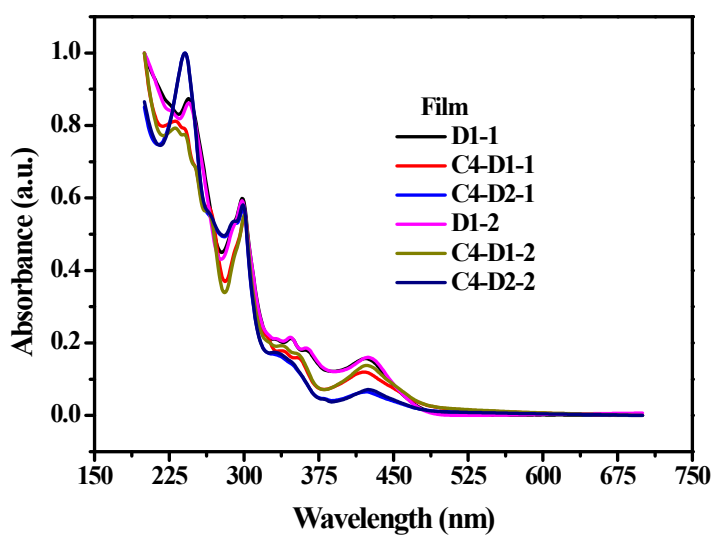
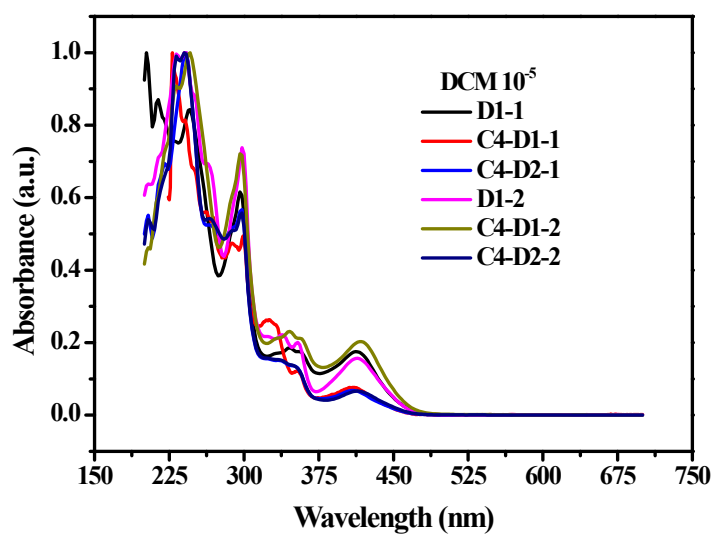


Figure S4. Absorption spectra of the Pt(II) dendrimers in DCM solution (10^{-5} M, top) and neat films (bottom).

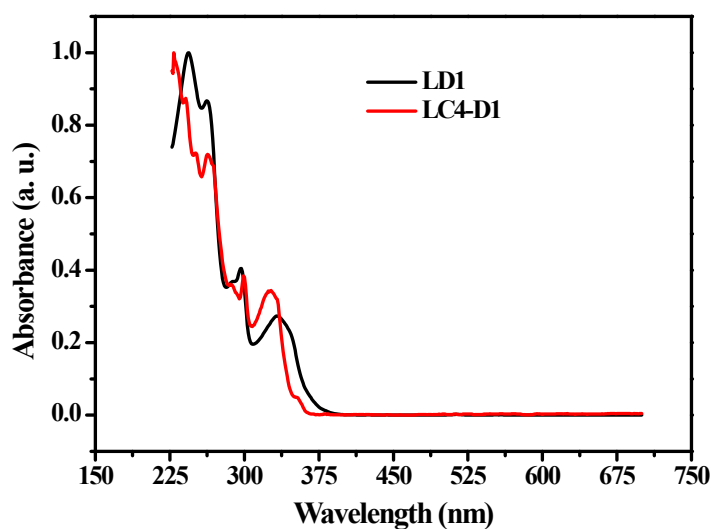


Figure S5. Absorption spectra of the ligands **LD1** and **LC4-D1** in DCM solution (10^{-5} M).

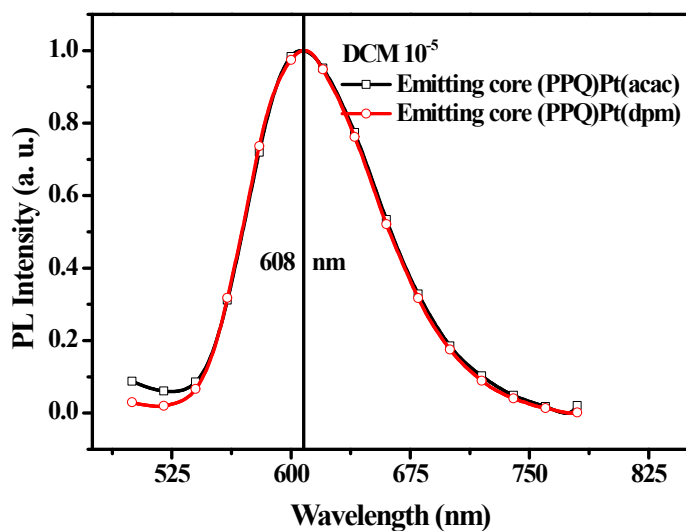


Figure S6. PL spectra of the emitting cores **(PPQ)Pt(acac)** and **(PPQ)Pt(dpm)** in DCM solution (10^{-5} M).

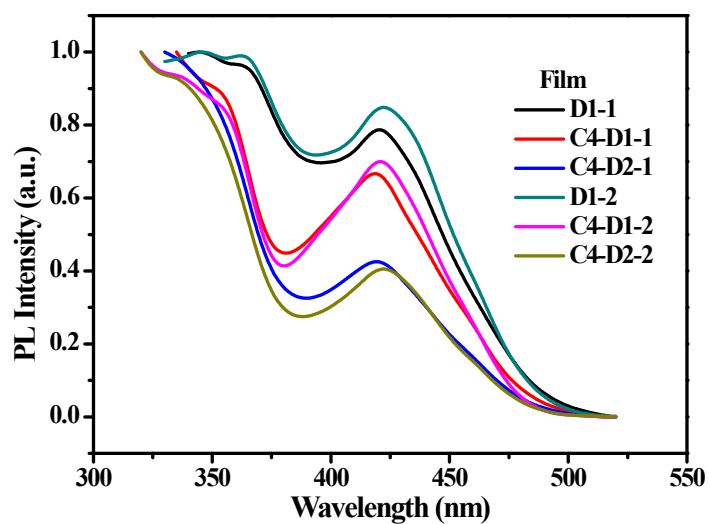
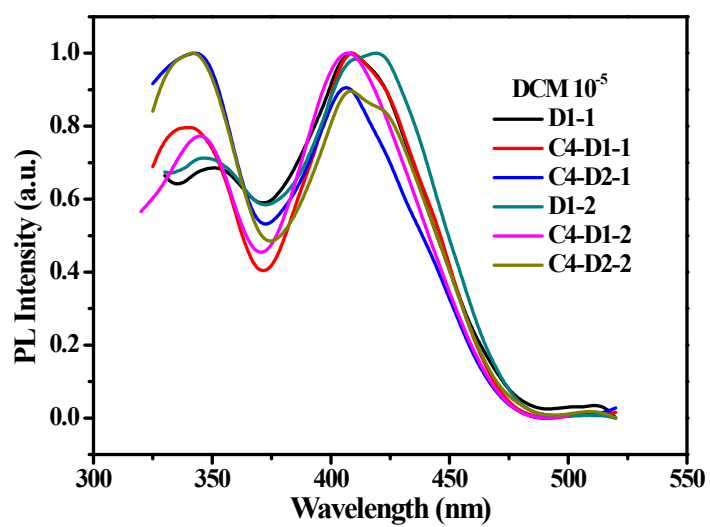


Figure S7. PL excitation spectra of the Pt(II) dendrimers in DCM solution (10^{-5} M, top) and neat films (bottom) at the maximum PL peak.

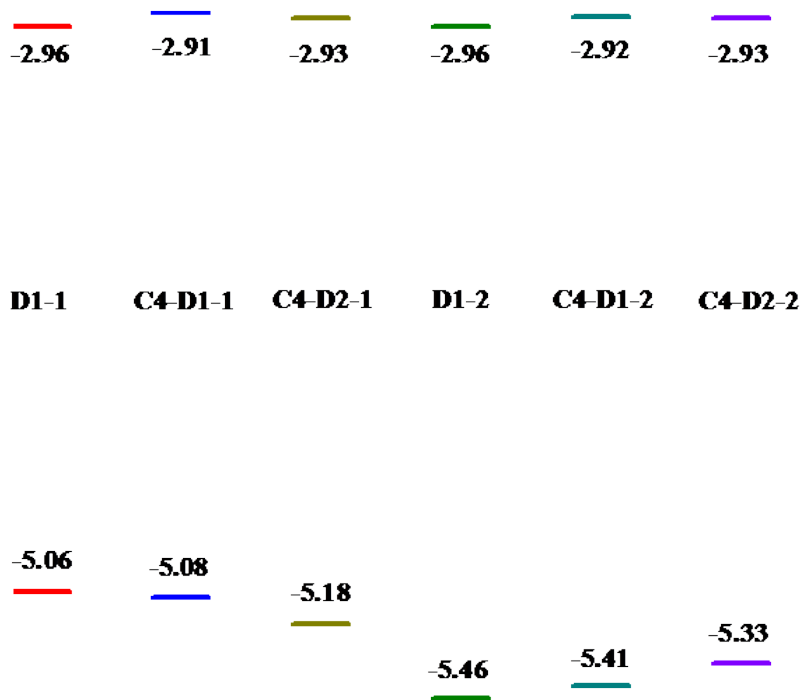


Figure S8. Diagram of the energy levels for Pt(II) dendrimers.

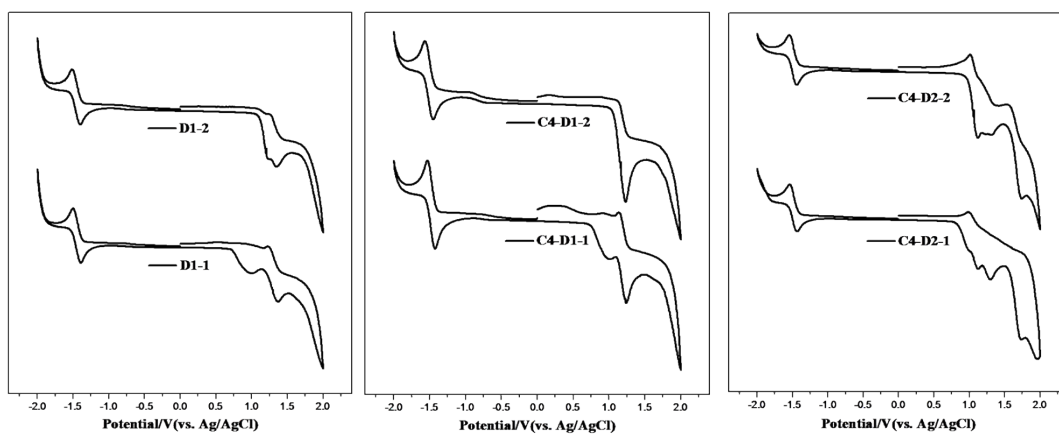


Figure S9. Cyclic voltammograms of the Pt(II) dendrimers.

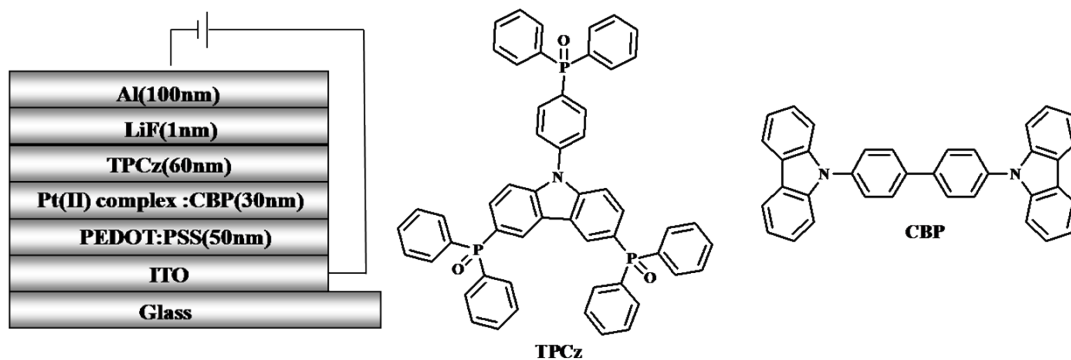


Figure S10. Multilayer structure of the devices and the molecular structure of the TPCz and CBP used in fabricating the EL devices.

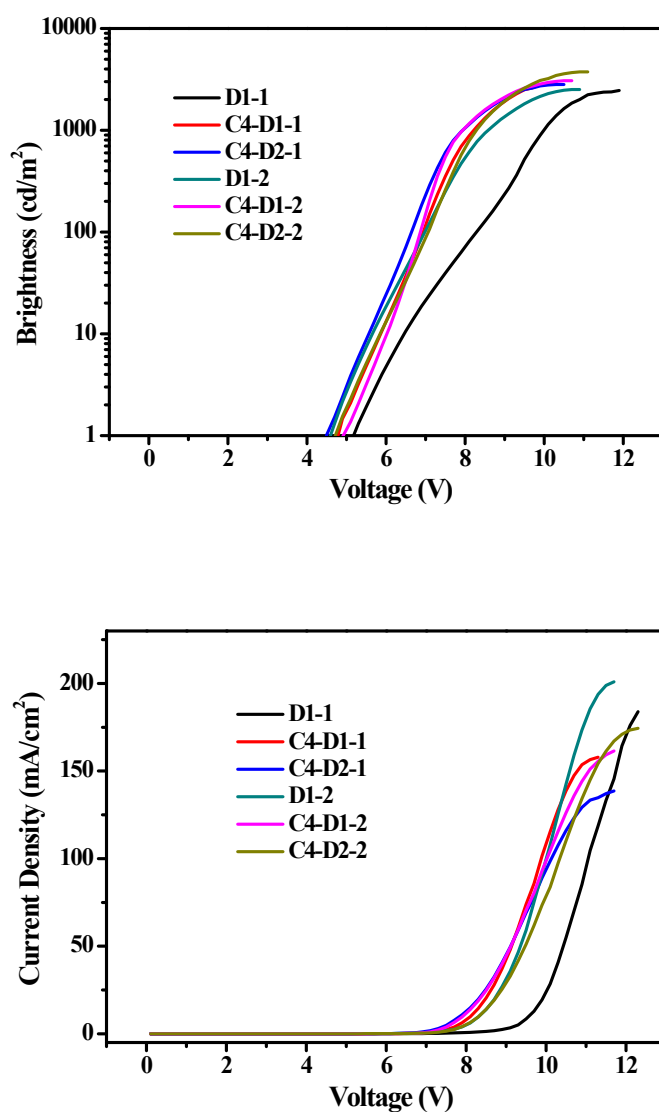


Figure S11. Voltage-brightness (top)/current density (bottom) characteristics for OLEDs using the Pt(II) dendrimers.

Reference

- [1] J. Ding, J. Gao, Q. Fu, Y. Cheng, D. Ma, L. Wang, *Synth. Metal.* 2005, **155**, 539.
- [2] J. Ding, J. Lu, Y. Cheng, Z. Xie, L. Wang, X. Jing, F. Wang, *Adv. Funct. Mater.* 2008, **18**, 1.
- [3] F. Brisse, G. Durocher, S. Gauthier, D. Gravel, R. Marqds, C. Vergelati, B. Zelent, *J. Am. Chem. Soc.* 1986, **108**, 6597.
- [4] D. Gravel, S. Gauthier, F. Brisse, S. Raymond, M. Damboise, P. Messier, B. Zelent, G. Duroch, *Can. J. Chem.* 1990, **68**, 908.
- [5] H. Cao, Y. Fujiwara, T. Haino, Y. Fukazawa, C.-H. Tung, Y. Tanimoto, *Bull. Chem. Soc. Jpn.* 1996, **69**, 2801.
- [6] V. B. Kurteva, A. G. Santo, C. A. M. Afonso, *Org. Biomol. Chem.* 2004, **2**, 514.
- [7] J. Brooks, Y. Babayan, S. Lamansky, P. I. Djurovich, Irina Tsyba, R. Bau, M. E. Thompson, *Inorg. Chem.* 2002, **41**, 3055.
- [8] R. H. Blessing, *Acta Cryst., Sect. A: Found. Crystallogr.* 1995, **51**, 33.
- [9] G. M. Sheldrick, *SHELXTL, Version 5.1*, Bruker Analytical X-ray System. Inc.: Madison, WI 1997.
- [10] H. Li, J. Ding, Z. Xie, Y. Cheng, L. Wang, *J. Organomet. Chem.* 2009, **694**, 2777.