Supporting Information

Tetradentate Pt[O^N^C^N] Complexes with Peripheral Diarylamino Substituents for High-Performance and Stable Green Organic Light-Emitting Diodes with LT_{95} of 17140 h at 1000 cd m^{-2}

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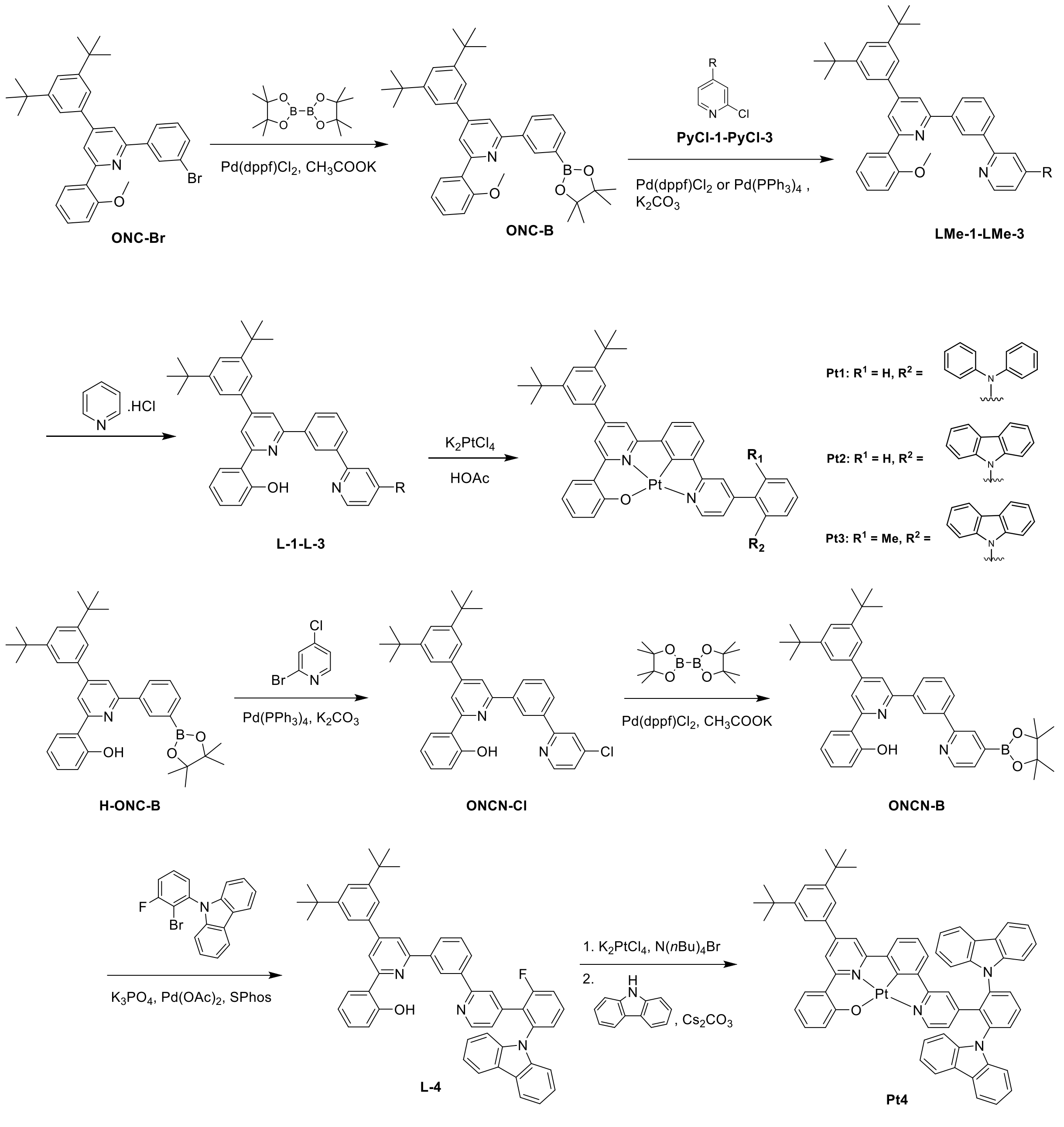
Experimental section

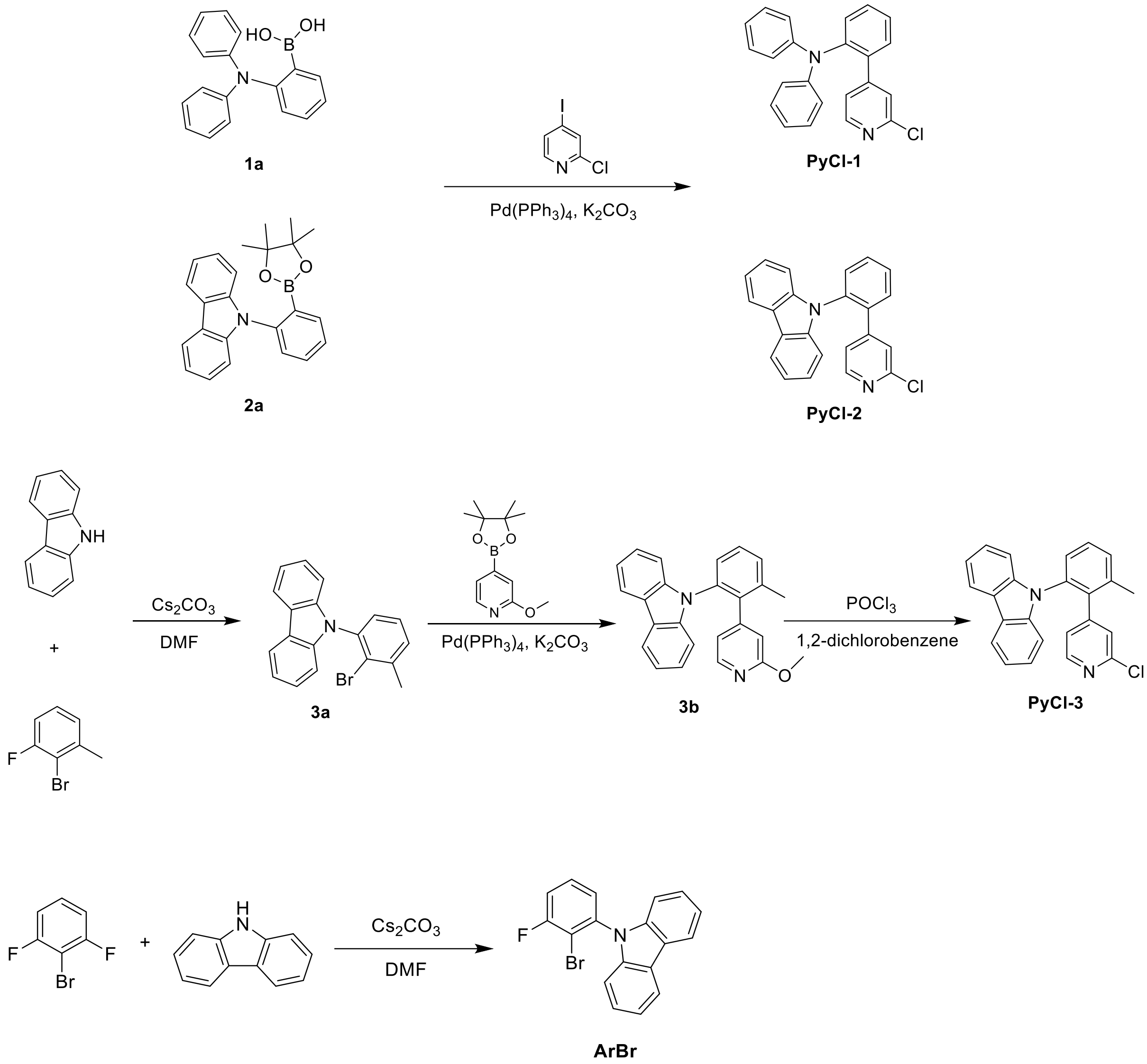
Materials and Instrumentation

All commercially available chemicals were used as received. Compounds **ONC-Br** and **H-ONC-B** were synthesized according to literature procedures.[S1] ^{1}H and ^{13}C NMR spectroscopic study was conducted with a Bruker Avance 400, DRX-500 or Avance 600 FT-NMR spectrometer using tetramethylsilane (TMS; $\delta = 0$ ppm) as internal standard. HRMS (ESI) spectra were measured on a Bruker Q-Tof Maxis II mass spectrometer. UV-visible absorption spectra were obtained using a Hewlett-Packard 8453 A diode array spectrophotometer. Electrochemical cyclic voltammetry was performed with a Princeton Applied Research Model 273A potentiostat/galvanostat coulometer with a three-electrode cell system using glassy carbon as working electrode, platinum wire as counter electrode, SCE as reference electrode. The ferrocene/ferrocenium redox couple was used for potential calibration. Elemental analyses were conducted at the Institute of Chemistry of the Chinese Academy of Sciences, Beijing. Emission spectra of complexes in solutions and films were recorded on a Horiba Fluorolog-3 spectrophotometer. Solutions for photophysical studies were degassed by five freeze-pump-thaw cycles using a high vacuum line prior to measurement. The thin films of the complex doped in mCP were prepared by vapor-deposition under vacuum. Photoluminescence quantum yields of the Pt complexes in solutions and films were measured with Hamamatsu C11347 Quantaurus-QY Absolute PL quantum yields measurement system. The radiative decay lifetime measurements were performed on a Hamamatsu C16361 Compact Fluorescence Lifetime Spectrometer. Nanosecond time-resolved emission (TRE) and nanosecond transient absorption (ns-TA) measurements were performed on a LP920-KS laser flash photolysis spectrophotometer (Edinburgh Instruments Ltd). The excitation source was a Q-switched Nd:YAG laser system and the laser excitation wavelength (λ_{ex}) used was 355 nm. Solution samples were prepared in the same way as for the steady-state photophysical measurements. Data were processed with a PC plugin controlled by the software L900. Femtosecond time-resolved absorption (fs-TA) spectra were recorded by an Ultrafast Systems HELIOS transient absorption spectrometer. The samples were excited by a 400 nm pump beam (the second harmonic of the fundamental 800 nm generated from a Ti:sapphire regenerative amplifier laser system) in a 2 mm path-length cuvette with magnetic stirring, and were probed by a white light continuum pulse generated from a sapphire pumped by the 800 nm laser. The temporal delay of probe to pump pulse was varied by a computer controlled optical delay line. The fs-TA signals were collected by a monochromator and detected with an air-cooled CCD detector.

Synthesis



Scheme S1. Synthetic route of complexes **Pt1–Pt4**.



Scheme S2. Synthesis of the substituted pyridyl chlorides and substituted aryl bromide.

Synthesis of 2-(2-chloropyridin-4-yl)-N,N-diphenylaniline (PyCl-1). A mixture of **1a** (3.4 g, 11.8 mmol), 2-chloro-4-iodopyridine (4.3 g, 18.0 mmol), $Pd(PPh_3)_4$ (1.3 g, 1.12 mmol), K_2CO_3 (4.9 g, 35.5 mmol) in dioxane/H_2O (100 mL/20 mL) was refluxed overnight under N_2 atmosphere. After cooling to room temperature, water (50 mL) was added and the mixture was extracted with dichloromethane (3 × 100 mL). The extracts were combined, washed with water and dried over anhydrous sodium sulfate. After the solvent was removed under reduced pressure, the residue was purified by chromatography on slica gel using hexane/ethyl acetate (v/v = 15/1) as eluent to give **PyCl-1** as a white solid (2.9 g, 69%). ^{1}H NMR (400 MHz, $CDCl_3$, 25°C): δ/ppm = 8.11 (d, J = 5.1 Hz, 1H, ArH), 7.44-7.40 (m, 1H, ArH), 7.32 (d, J = 8.1Hz, 1H, ArH), 7.28 (d, J = 4.0 Hz, 2H, ArH), 7.13-7.05 (m, 6H, ArH), 6.89-6.84 (m, 6H, ArH).

Synthesis of 9-(2-(2-chloropyridin-4-yl)phenyl)-9H-carbazole (PyCl-2). The procedure was similar to that of PyCl-1 except that **2a** (7.5 g, 20.3 mmol) was used instead of **1a**. Yield: 6.0 g (83%, white solid). ^{1}H-NMR (400MHz, $CDCl_3$, 25°C): δ/ppm = 8.05 (d, J = 8.0 Hz, 2H, ArH), 7.84 (d, J = 4.0 Hz, 1H, ArH), 7.65-7.62 (m, 3H, ArH), 7.55-7.53 (m, 1H, ArH), 7.29 (t, J = 8.0 Hz, 2H, ArH), 7.20 (t, J = 8.0 Hz, 2H, ArH), 7.08 (s, 1H, ArH), 7.00 (d, J = 8.0 Hz, 2H, ArH), 6.64 (d, J = 4.0 Hz, 1H, ArH). ^{13}CNMR (100MHz, $CDCl_3$, 25°C): δ/ppm = 151.4, 149.4, 149.2, 140.9, 137.0, 135.0, 131.0, 130.8, 130.3, 129.3, 126.0, 123.3, 123.0, 121.1, 120.4, 120.1, 109.5.

Synthesis of 9-(2-bromo-3-methylphenyl)-9H-carbazole (3a). A mixture of carbazole (3.3 g, 19.7 mmol), 2-bromo-1-fluoro-3-methylbenzene (7.6 g, 40.2 mmol), Cs_2CO_3 (13.0 g, 39.9 mmol) and DMF (30 mL) was stirred at 150 °C under nitrogen for 12 h. After cooling to room temperature, water (100 mL) was added and the mixture was extracted with dichloromethane (3 × 100 mL). The extracts were combined, washed with water and dried over anhydrous sodium sulfate. After the solvent was removed under reduced pressure, the residue was purified by chromatography on slica gel using hexane/ethyl acetate (v/v = 30/1) as eluent to give **3a** as a white solid (3.3 g, 50%). ^{1}H NMR (400 MHz, $CDCl_3$, 25°C): δ/ppm = 8.15 (d, J = 7.7 Hz, 2H), 7.42-7.37 (m, 4H), 7.32-7.24 (m, 3H), 7.05 (d, J = 8.1 Hz, 2H), 2.56 (s, 3H).

Synthesis of 9-(2-(2-methoxypyridin-4-yl)-3-methylphenyl)-9H-carbazole (3b). A mixture of **3a** (4.6 g, 13.7 mmol), 2-methoxy-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine (6.5 g, 27.6 mmol), $Pd(PPh_3)_4$ (1.6 g, 1.39 mmol), K_2CO_3 (3.8 g, 27.4 mmol) in toluene/ethanol/H_2O (25 mL/7.5 mL/10 mL) was refluxed overnight under N_2 atmosphere. After cooling to room temperature, water (50 mL) was added and the mixture was extracted with dichloromethane (3 × 50 mL). The extracts were combined, washed with water and dried over anhydrous sodium sulfate. After the solvent was removed under reduced pressure, the residue was purified by chromatography on silica gel using hexane/ethyl acetate (v/v = 20/1) as eluent to give **3b** as a white solid (3.2 g, 64%). ^{1}H NMR (400 MHz, $CDCl_3$, 25°C): δ/ppm = 7.98 (d, J = 7.7 Hz, 2H), 7.69 (d, J = 5.1 Hz, 1H), 7.50-7.47 (m, 2H), 7.32-7.24 (m, 3H), 7.16 (t, J = 7.3 Hz, 2H), 7.05 (s, br, 2H), 6.44 (d, *J* = 5.1 Hz, 1H), 6.41 (s, 1H), 3.63 (s, 3H), 2.26 (s, 3H).

Synthesis of 9-(2-(2-chloropyridin-4-yl)-3-methylphenyl)-9H-carbazole (PyCl-3). A solution of **3b** (2.9 g, 8.0 mmol) in dichlorobenzene/$POCl_3$ (45 mL / 10 mL) was stirred at 100 ºC for 12 h. After cooling to room temperature, the mixture was slowly added to a solution of NaOH (1M, 50 mL) and stirred for 30 min. Then the mixture was extracted with ethyl acetate (3 × 50 mL), washed with water and dried over anhydrous sodium sulfate. After the solvent was removed under reduced pressure, the residue was purified by chromatography on slica gel using hexane/ethyl acetate (v/v = 30/1) as eluent to give **PyCl-3** as a white solid (2.1 g, 72%). ^{1}H NMR (400 MHz, $CDCl_3$, 25ºC): *δ*/ppm = 7.99 (d, *J* = 7.7 Hz, 2H), 7.87 (d, *J* = 5.1 Hz, 1H), 7.57-7.49 (m, 2H), 7.37-7.31 (m, 3H), 7.19 (t, *J* = 7.4 Hz, 2H), 7.02-6.97 (m, 3H), 6.71 (d, *J* = 4.4 Hz, 1H), 2.27 (s, 3H).

Synthesis of 9-(2-bromo-3-fluorophenyl)-9H-carbazole (ArBr). A mixture of 2-bromo-1,3-difluorobenzene (57.9 g, 300 mmol) and carbazole (16.7 g, 100 mmol) was dissolved in dimethylformamide (400 mL). The solution was stirred under r.t. for 5 mins and then cesium carbonate (65.2 g, 200 mmol) was added. The mixture was heated to reflux for 12 h and the solvent was vaporized under reduced pressure. The residue was suspended in water (500 mL) and extracted with dichloromethane (3 × 200 mL). The combined organic layer was washed with brine (2 × 200 mL) and vaporized under vacuum. The product was purified through a silica gel column (330 g, eluent: hexane/DCM (v/v) = 30/1 to 15/1) and collected as a white solid (31.1 g, isolated yield: 91%). 1H NMR (500 MHz, CD_2Cl_2, 25ºC): δ/ppm = 8.18 (dt, *J* = 7.7, 1.0 Hz, 2H), 7.56 (td, *J* = 8.2, 5.9 Hz, 1H), 7.43 (ddd, *J* = 8.3, 7.2, 1.2 Hz, 2H), 7.41 – 7.35 (m, 2H), 7.32 (td, *J* = 7.5, 1.0 Hz, 2H), 7.10 (d, *J* = 0.9 Hz, 1H), 7.08 (d, *J* = 0.9 Hz, 1H).

Synthesis of ONC-B. A mixture of **ONC-Br** (5.28 g, 10.0 mmol), bis(pinacolato)diboron (1.2 equivalents) and potassium acetate (1.5 equivalents) in dioxane (50 mL) was stirred overnight at 90 ºC under N_2 atmosphere. After cooling to room temperature, the solution was poured into cold water and the resulting mixture was extracted with CH_2Cl_2 (3 × 50 mL). The combined organic layers were washed with water and dried over anhydrous $MgSO_4$, and the volatiles were removed under reduced pressure. The crude product was then purified by recrystallization in methanol to give **ONC-B** as a white solid. Isolated yield: 80%; ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): *δ*/ppm = 8.4 (s, 1H), 8.30 (d, *J* = 7.6 Hz, 1H), 8.05 (d, *J* = 7.6 Hz, 1H), 8.01 (s, 1H), 7.89-7.87 (m, 2H), 7.54-7.50 (m, 4H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.15 (t, *J* = 7.6 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 3.91 (s, 3H), 1.42 (s, 18H), 1.37 (s, 12H).

Synthesis of LMe-1. A mixture of **PyCl-1** (4.8 g, 13.5 mmol), **ONC-B** (9.3 g, 16.2 mmol), $Pd(PPh_3)_4$ (1.5 g, 1.3 mmol), K_2CO_3 (4.6 g, 33.3 mmol) in dioxane/H_2O (50 mL/10 mL) was refluxed overnight under N_2 atmosphere. After cooling to room temperature, water (50 mL) was added and the mixture was extracted with dichloromethane (3 × 100 mL). The extracts were combined, washed with water and dried over anhydrous sulfate. After the solvent was removed under reduced pressure, the residue was purified by chromatography on slica gel using hexane/ethyl acetate (v/v = 10/1) as eluent to give **LMe-1** as a white solid (9.4 g, 91%). ^{1}H NMR (400 MHz, $CDCl_3$, 25°C): *δ*/ppm = 8.47-8.44 (m, 2H, ArH), 8.18 (d, *J* = 7.7 Hz, 1H, ArH), 8.06-8.04 (m, 2H, ArH), 7.85-7.81 (m, 2H, ArH), 7.54-7.51 (m, 5H, ArH), 7.43-7.29 (m, 5H, ArH), 7.16-7.12 (m, 2H, ArH), 7.07-7.01 (m, 5H, ArH), 6.86 (d, *J* = 8.1 Hz, 4H, ArH), 6.77 (t, *J* = 7.2 Hz, 2H, ArH), 3.91 (s, 3H, OMe), 1.41 (s, 18H, *t*-Bu).

Synthesis of LMe-2. The procedure was similar to that of **LMe-1** except that **PyCl-2** (4.5 g, 12.7 mmol) was used instead of **PyCl-1**. Yield: 7.8 g (80%, white solid). ^{1}H-NMR (400MHz, $CDCl_3$, 25°C): *δ*/ppm = 8.32 (d, *J* = 4.0 Hz, 1H, ArH), 8.19 (s, 1H, ArH), 8.08 (d, *J* = 8.0 Hz, 1H, ArH), 8.04-8.02 (m, 2H, ArH), 7.94 (d, *J* = 8.0 Hz, 2H, ArH), 7.76-7.73 (m, 2H, ArH), 7.67-7.64 (m, 2H, ArH), 7.59-7.55 (m, 4H, ArH), 7.42-7.36 (m, 2H, ArH), 7.34 (m, 1H, ArH), 7.27-7.22 (m, 3H, ArH), 7.15-7.09 (m, 3H, ArH), 7.05 (d, *J* = 8.0 Hz, 3H, ArH), 6.91 (d, *J* = 8.0 Hz, 1H, ArH), 3.91 (s, 3H, OCH_3), 1.42 (s, 18H, *t*-Bu). ^{13}CNMR (100MHz, $CDCl_3$, 25°C): *δ*/ppm = 157.4, 157.3, 155.9, 151.5, 150.4, 149.4, 146.9, 141.2, 140.7, 139.4, 139.1, 138.9, 135.0, 131.7, 131.1, 130.4, 130.2, 129.9, 129.6, 129.3, 128.8, 128.0, 127.2, 126.0, 125.6, 123.1, 122.9, 122.5, 121.9, 121.1, 120.9, 120.4, 119.9, 119.7, 117.9, 111.7, 109.6, 55.9, 35.3, 31.8.

Synthesis of LMe-3. The procedure was similar to that of **LMe-1** except that **PyCl-3** (2.5 g, 6.8 mmol) was used instead of **PyCl-1**. Yield: 5.0 g (94%, white solid). ^{1}H NMR (400 MHz, $CDCl_3$, 25°C): *δ*/ppm = 8.26 (d, *J* = 4.8 Hz, 1H), 8.19 (s, 1H), 8.10- 8.04 (m, 3H), 7.89 (d, *J* = 7.3 Hz, 2H), 7.78 (s, 1H), 7.54-7.51 (m, 5H), 7.43-7.38 (m, 3H), 7.31-7.26 (m, 3H), 7.19-7.04 (m, 7H), 6.86 (d, *J* = 4.0 Hz, 1H), 3.91 (s, 3H), 2.32 (s, 3H), 1.42 (s, 18H).

Synthesis of L-1. A mixture of **LMe-1** (4.9 g, 6.4 mmol) and pyridine hydrochloride (50 g) was stirred at 190 °C for 5 h under N_2 atmosphere. After cooling to room temperature, water (100 mL) was added, and the mixture was extracted with dichloromethane (3 × 100 mL). The extracts were combined, washed with water and dried over anhydrous sulfate. After the solvent was removed under reduced pressure, the residue was purified by chromatography on slica gel using hexane/ethyl acetate (v/v = 8/1) as eluent to give **Pt-1** as a light yellow solid (4.1 g, 85%). ^{1}H NMR (400 MHz, $CDCl_3$, 25°C): *δ*/ppm = 8.47 (d, *J* = 4.8 Hz, 1H, ArH), 8.36 (s, 1H, ArH), 8.03 (s, 2H, ArH), 7.95 (d, *J* = 7.3 Hz, 1H, ArH), 7.87 (d, *J* = 8.1 Hz, 1H, ArH), 7.83 (s, 1H, ArH), 7.61-7.58 (m, 3H, ArH), 7.53 (d, *J* = 1.1 Hz, 2H, ArH), 7.45-7.31 (m, 5H, ArH), 7.13-6.96 (m, 7H, ArH), 6.87 (d, *J* = 7.7 Hz, 4H, ArH), 6.76 (t, *J* = 7.3 Hz, 2H, ArH), 1.43 (s, 18H, *t*-Bu).

Synthesis of L-2. The procedure was similar to that of **L-1** except that **LMe-2** (7.8 g, 10.2 mmol) was used instead of **LMe-1**. Yield: 6.4 g (84%, light yellow solid). ^{1}H-NMR (400MHz, $CDCl_3$, 25ºC): δ/ppm = 8.37 (d, J = 4.0 Hz, 1H, ArH), 8.05-8.04 (m, 2H, ArH), 7.97-7.93 (m, 4H, ArH), 7.78-7.76 (m, 1H, ArH), 7.73 (s, 1H, ArH), 7.69-7.67 (m, 2H, ArH), 7.62-7.58 (m, 2H, ArH), 7.54 (s, br, 2H, ArH), 7.43 (t, J = 6.0 Hz, 1H, ArH), 7.36 (t, J = 8.0 Hz, 1H, ArH), 7.31 (s, 1H, ArH), 7.29-7.23 (m, 3H, ArH), 7.13-7.07 (m, 5H, ArH), 7.00-6.96 (m, 2H, ArH), 1.45 (s, 18H, t-Bu). ^{13}CNMR (100MHz, $CDCl_3$, 25ºC): δ/ppm = 160.2, 157.8, 156.6, 155.2, 152.9, 151.9, 149.6, 147.0, 141.2, 139.8, 138.9, 138.8, 138.5, 135.0, 131.5, 131.1, 130.4, 130.3, 129.3, 127.9, 127.6, 126.4, 126.0, 125.5, 123.6, 123.1, 121.8, 121.2, 120.3, 119.9, 119.7, 119.3, 118.8, 118.7, 118.4, 116.4, 109.7, 35.4, 31.8.

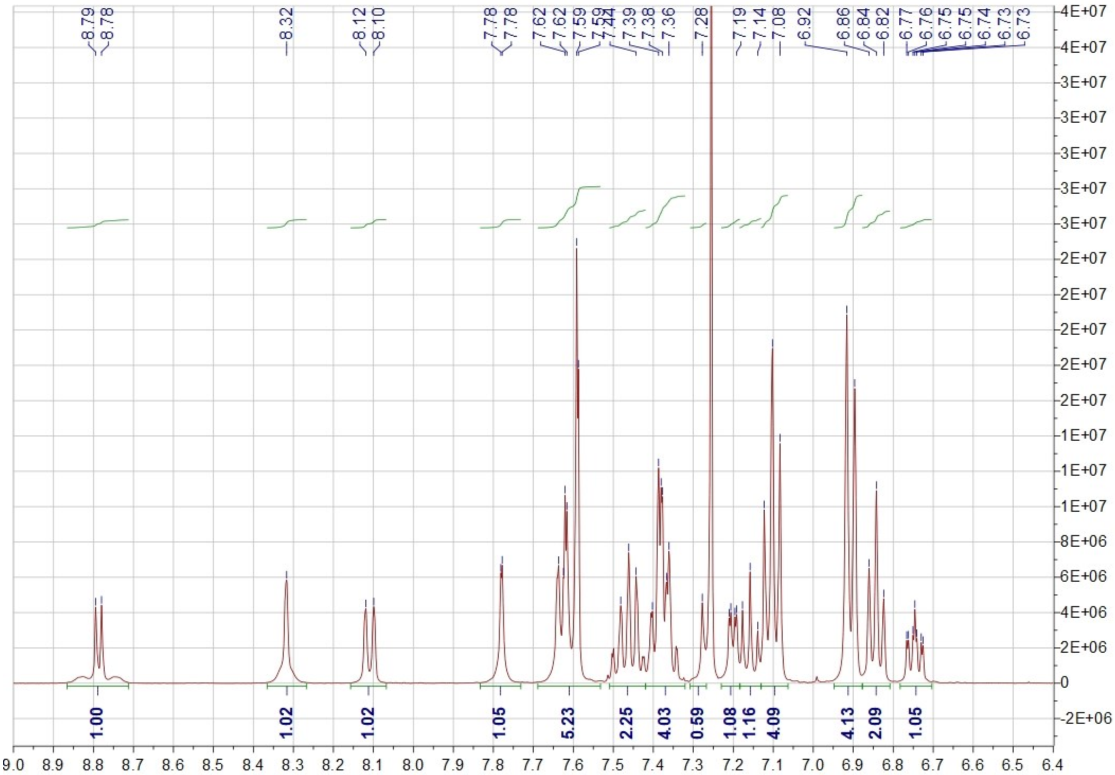
Synthesis of L-3. The procedure was similar to that of **L-1** except that **LMe-3** (5.0 g, 6.6 mmol) was used instead of **LMe-1**. Yield: 4.6 g (94%, white solid). ^{1}H NMR (400 MHz, $CDCl_3$, 25ºC): δ/ppm = 8.28 (d, *J* = 5.1 Hz, 1H), 8.02 (d, *J* = 13.2 Hz, 2H), 7.96-7.91 (m, 2H), 7.87 (d, *J* = 7.7 Hz, 2H), 7.73 (s, 1H), 7.61 (s, 1H), 7.57-7.52 (m, 4H), 7.44-7.39 (m, 2H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.26-7.16 (m, 5H), 7.08-6.95 (m, 5H), 6.92 (d, *J* = 4.4 Hz, 1H), 2.33 (s, 3H), 1.43 (s, 18H).

Synthesis of ONCN-Cl. A solution of **H-ONC-B** (30.9 g, 55 mmol), 2-bromo-4-chloropyridine (31.8 g, 165 mmol) and potassium carbonate (30.4 g, 220 mmol) in tetrahydrofuran (300 mL) and water (100 mL) was degassed under Argon bubbling for 20 mins. Then, tetrakis(triphenylphosphine)palladium(0) (1.27 g, 1.10 mmol) was added and the mixture was heated to reflux for 24 h. After cooling, the organic phase was separated, and the aqueous phase was extracted with dichloromethane (3 × 50 mL). The combined organic phase was washed with brine (3 × 200 mL) and dried over sodium sulphate. The product was purified through a silica gel column chromatography (eluent: hexane/ethyl acetate (v/v) = 20/1 to 6/1) and collected as yellow solid (26.7 g, yield: 89%). ^{1}H NMR (400 MHz, $CDCl_3$, 25ºC) δ/ppm = 14.75 (s, 1H), 8.63 (dd, *J* = 5.3, 0.6 Hz, 1H), 8.57 (t, *J* = 1.8 Hz, 1H), 8.13 – 8.08 (m, 2H), 8.05 (d, *J* = 1.5 Hz, 1H), 7.95 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.89 (d, *J* = 1.3 Hz, 1H), 7.84 (dd, *J* = 2.0, 0.6 Hz, 1H), 7.67 (t, *J* = 7.8 Hz, 1H), 7.61 (t, *J* = 1.8 Hz, 1H), 7.53 (d, *J* = 1.8 Hz, 2H), 7.36 (ddd, *J* = 8.6, 7.2, 1.6 Hz, 1H), 7.30 (dd, *J* = 5.3, 1.9 Hz, 1H), 7.09 (dd, *J* = 8.2, 1.2 Hz, 1H), 6.98 (ddd, *J* = 8.3, 7.2, 1.3 Hz, 1H), 1.43 (s, 18H).

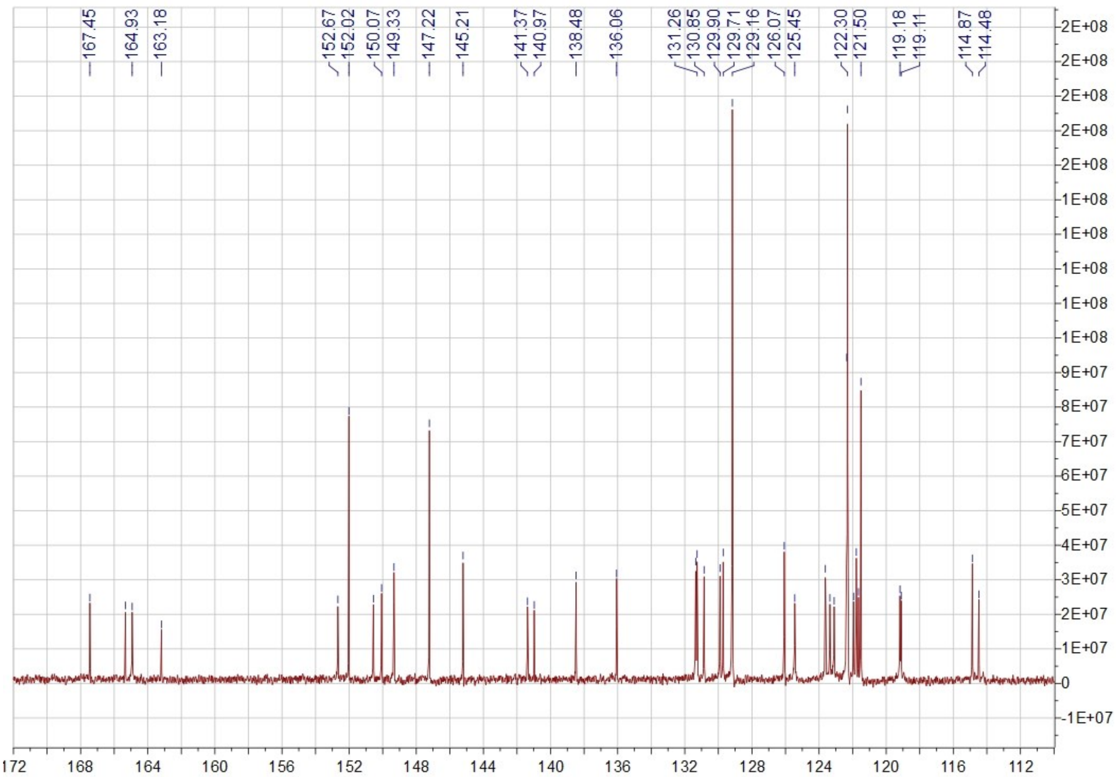
Synthesis of ONCN-B. A suspension of **ONCN-Cl** (5.47 g, 10 mmol), bis(pinacolato)diboron (2.79 g, 11 mmol) and potassium acetate (2.94 g, 30 mmol) in anhydrous toluene (60 mL) was degassed under Argon bubbling for 20 mins. Then, [1,1′-bis(diphenylphosphino)ferrocene]dichloropalladium(II) (0.5 mmol, 366 mg) was added and the mixture was heated to reflux for 36 h. After cooling to room temperature, the mixture was filtered through celite and the filtrate was concentrated with silica gel. The product was purified through a silica gel column chromatography (eluent: hexane/ethyl acetate (v/v) = 5/1 to 1/1) and collected as brown solid (5.19 g, 81%). ^{1}H NMR (400 MHz, $CDCl_3$, 25ºC) δ/ppm = 14.86 (s, 1H), 8.77 (dd, *J* = 4.6, 1.2 Hz, 1H), 8.61 (t, *J* = 1.9 Hz, 1H), 8.21 – 8.15 (m, 2H), 8.11 (ddd, *J* = 7.8, 2.0, 1.1 Hz, 1H), 8.06 (d, *J* = 1.4 Hz, 1H), 7.97 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.94 (d, *J* = 1.4 Hz, 1H), 7.66 (dd, *J* = 14.6, 6.8 Hz, 1H), 7.63 – 7.60 (m, 2H), 7.56 (d, *J* = 1.8 Hz, 2H), 7.37 (ddd, *J* = 8.5, 7.1, 1.5 Hz, 1H), 7.09 (dd, *J* = 8.2, 1.3 Hz, 1H), 6.98 (ddd, *J* = 8.3, 7.2, 1.2 Hz, 1H), 1.44 (d, *J* = 1.4 Hz, 18H), 1.39 (s, 12H).

Synthesis of L-4. A mixture of **ONCN-B** (6.55 g, 10 mmol), **ArBr** (4.08 g, 12 mmol), and potassium phosphate tribasic (6.37 g, 30 mmol) was dissolved in tetrahydrofuran (90 mL) and water (30 mL). The mixed solution was degassed under argon bubbling for 5 mins, then palladium acetate (45 mg, 0.2 mmol) and SPhos (205 mg, 0.5 mmol) were added. The mixture was heated to reflux for 24 h and cooled to r.t.. The aqueous layer was extracted with dichloromethane (3 × 20 mL) and the combined organic phase was washed with brine (3 × 50 mL). The mixed organic phase was dried over anhydrous magnesium sulphate and vaporized under vacuum. The product was purified through a silica gel column (330 g, eluent: hexane/EA (v/v) = 50/1 to 7/1) and collected as a yellow solid (6.9 g, isolated yield: 90%). ^{1}H NMR (500 MHz, CD_2Cl_2, 25°C) δ/ppm = 14.59 (s, 1H), 8.38 (dd, *J* = 5.0, 0.8 Hz, 1H), 8.12 (d, *J* = 1.4 Hz, 1H), 8.08 (t, *J* = 1.9 Hz, 1H), 8.03 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.97 – 7.92 (m, 3H), 7.79 (d, *J* = 1.4 Hz, 1H), 7.69 (td, *J* = 8.2, 6.0 Hz, 1H), 7.65 (t, *J* = 1.8 Hz, 1H), 7.60 (d, *J* = 1.8 Hz, 2H), 7.51 – 7.42 (m, 3H), 7.36 (ddd, *J* = 8.5, 7.1, 1.6 Hz, 1H), 7.32 (d, *J* = 1.6 Hz, 1H), 7.27 (tdd, *J* = 8.5, 6.9, 1.4 Hz, 3H), 7.17 – 7.10 (m, 4H), 7.08 (dt, *J* = 5.1, 1.7 Hz, 1H), 7.04 (dd, *J* = 8.2, 1.3 Hz, 1H), 6.99 (ddd, *J* = 8.3, 7.2, 1.3 Hz, 1H), 1.45 (s, 18H).

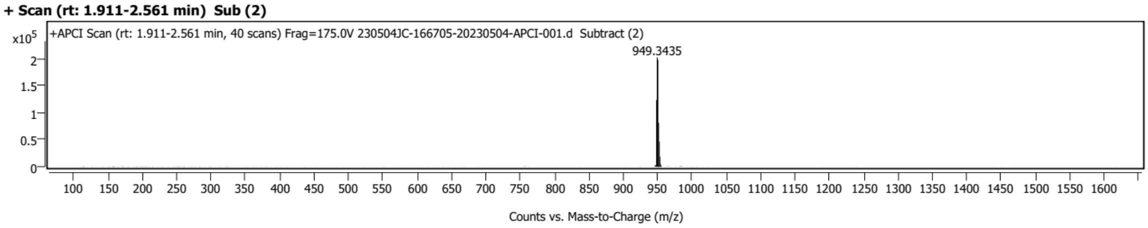
Synthesis of Pt1. A mixture of **L-1** (1.0 g, 1.32 mmol), K_2PtCl_4 (0.66 g, 1.59 mmol), tetrabutylammonium bromide (50 mg) and acetic acid (50 mL) was refluxed for 48 h under N_2 atmosphere. After cooling to room temperature, water (50 mL) was added. Then the resulting mixture was filtered, and the solids were washed with methanol. The collected solids were purified by chromatography on silica gel using hexane/dichloromethane (v/v = 1/3) as eluent to give **Pt1** as an orange solid (0.70 g, 50%). ^{1}H NMR (400 MHz, $CDCl_3$, 25°C): *δ*/ppm = 8.79 (d, *J* = 5.8 Hz, 1H), 8.32 (s, 1H), 8.11 (d, *J* = 7.9 Hz, 1H), 7.78 (d, *J* = 1.4 Hz, 1H), 7.64-7.59 (m, 5H), 7.50-7.44 (m, 2H), 7.43-7.34 (m, 4H), 7.28-7.26 (m, 1H), 7.20 (dd, *J* = 1.7, 5.8 Hz, 1H), 7.16 (t, *J* = 7.6 Hz, 1H), 7.12-7.08 (m, 4H), 6.91 (d, *J* = 7.9 Hz, 4H), 6.84 (t, *J* = 7.2 Hz, 2H), 6.75 (ddd, *J* = 1.8, 6.3, 8.3 Hz, 1H), 1.44 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): *δ*/ppm = 167.45, 165.32, 164.93, 163.18, 152.67, 152.01, 150.56, 150.06, 149.33, 147.22, 145.21, 141.37, 140.97, 138.47, 136.06, 131.35, 131.27, 130.85, 129.90, 129.71, 129.16, 126.07, 125.44, 123.62, 123.35, 123.10, 122.35, 122.30, 121.94, 121.78, 121.65, 121.50, 119.18, 119.10, 114.87, 114.48, 35.17, 31.59. ESI-MS: *m*/*z* 949.3435 $[M+H]^+$. Anal. Calcd for $C_{54}H_{47}N_3OPt$: C, 68.34; H, 4.99; N, 4.43. Found:C, 68.11; H, 4.99; N, 4.44.



[1]H NMR spectrum (400 MHz) of **Pt1** in $CDCl_3$ (aromatic region).



[13]C NMR spectrum (101 MHz) of **Pt1** in $CDCl_3$ (aromatic region).

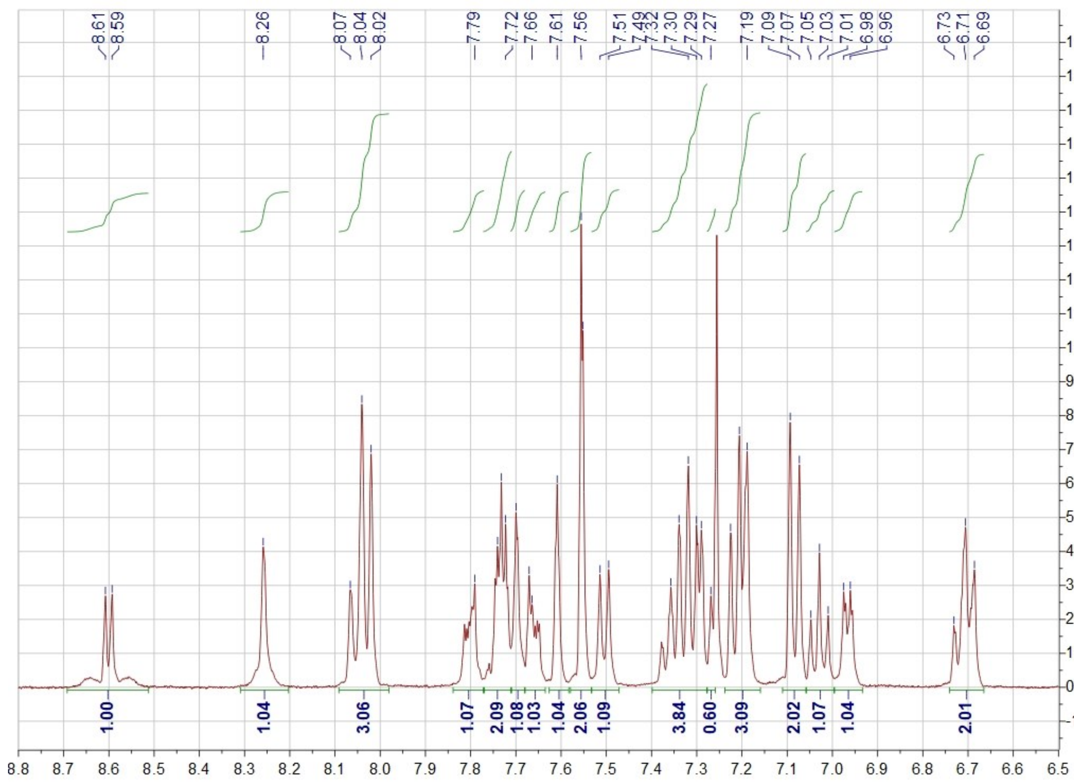


Spectrum Peaks

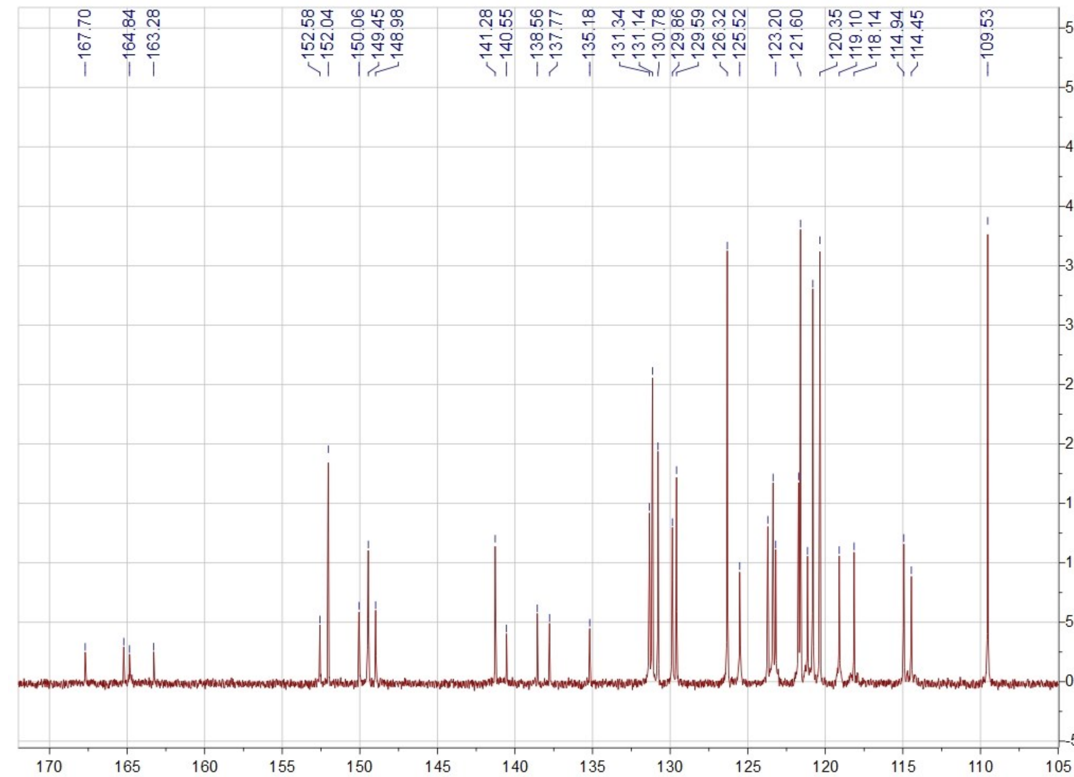
m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
946.3312	1	2688	1.34					
947.3305	1	2095	1.04					
948.3405	1	122873	61.03					
949.3435	1	201344	100.00					
950.3451	1	197218	97.95					
951.3474	1	80995	40.23					
952.3477	1	46094	22.89					
953.3497	1	18312	9.10					
954.3526	1	5003	2.49					

HRMS results of **Pt1**.

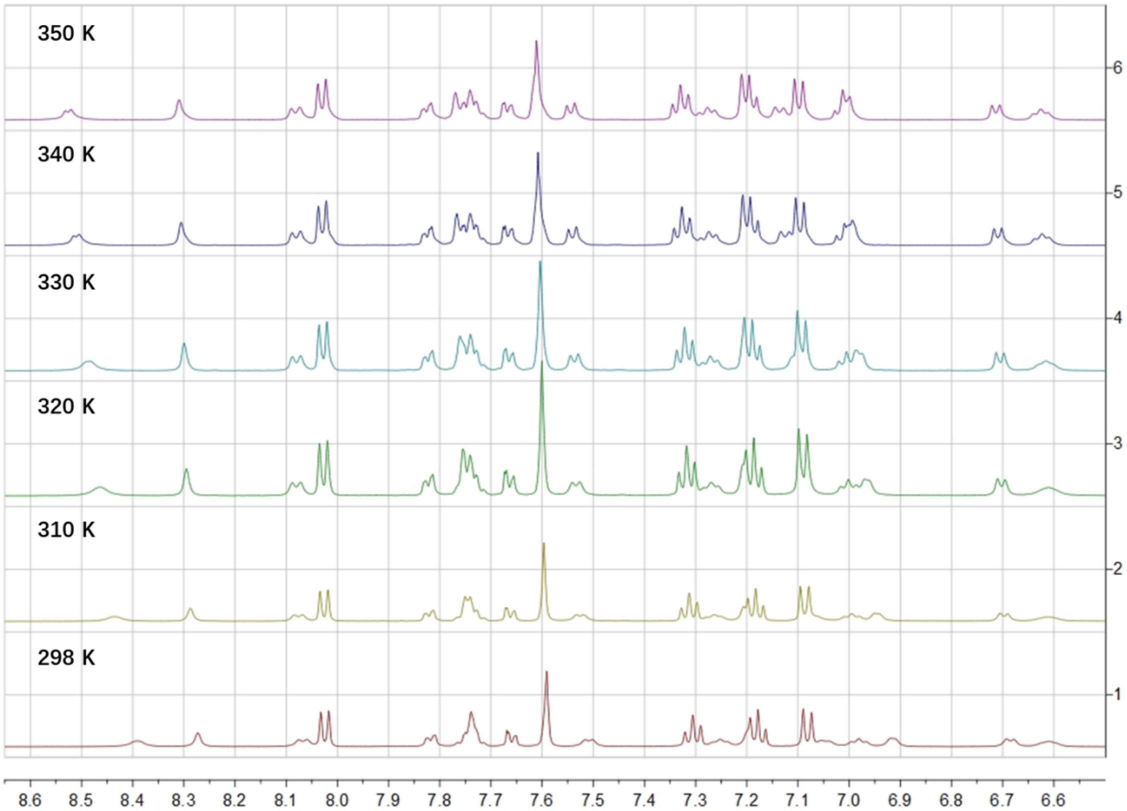
Synthesis of Pt2. The procedure was similar to that of **Pt1** except that **L-2** (2.0 g, 2.6 mmol) was used instead of **L-1**. Yield: 1.5 g (60%, orange solid). ^{1}H-NMR (400 MHz, $CDCl_3$, 25ºC): δ/ppm = 8.60 (d, *J* = 4.0 Hz, 1H, ArH), 8.25 (s, 1H, ArH), 8.04 (t, *J* = 8.0 Hz, 3H, ArH), 7.81-7.79 (m, 1H, ArH), 7.74-7.72 (m, 2H, ArH), 7.69 (s, 1H, ArH), 7.67-7.65 (m, 1H, ArH), 7.60 (s, 1H, ArH), 7.55 (s, 2H, ArH), 7.50 (d, *J* = 8.0 Hz, 1H, ArH), 7.38-7.28 (m, 4H, ArH), 7.25-7.18 (m, 3H, ArH), 7.08 (d, *J* = 8.0 Hz, 2H, ArH), 7.02 (t, *J* = 8.0 Hz, 1H, ArH), 6.96 (d, *J* = 4.0 Hz, 1H, ArH), 6.73-6.68 (m, 2H, ArH), 1.43 (s, 18H, *t*-Bu). ^{13}C NMR (101 MHz, $CDCl_3$, 25ºC): δ/ppm = 167.73, 165.52, 164.87, 163.31, 152.60, 152.06, 150.08, 149.48, 149.01, 141.30, 140.57, 138.59, 137.80, 135.21, 131.36, 131.17, 130.80, 129.89, 129.61, 126.34, 125.54, 123.73, 123.40, 123.22, 121.75, 121.62, 121.17, 120.83, 120.37, 119.13, 118.17, 114.96, 114.47, 109.56, 35.52, 31.96. ESI-MS: *m*/*z* 947.3278 $[M+H]^+$. Anal. Calcd for $C_{54}H_{45}N_3OPt$: C, 68.48; H, 4.79; N, 4.44. Found: 67.93; H, 4.75; N, 4.92.



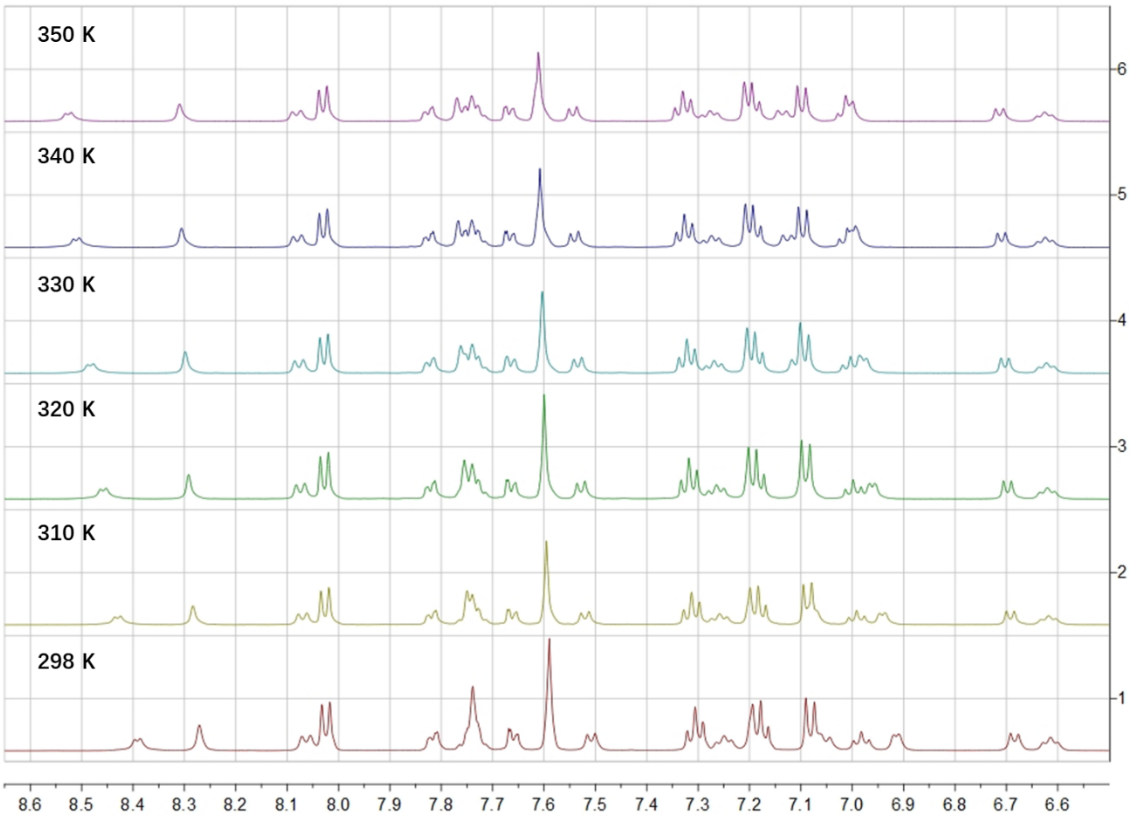
^{1}H NMR spectrum (400 MHz) of **Pt2** in $CDCl_3$ (aromatic region).



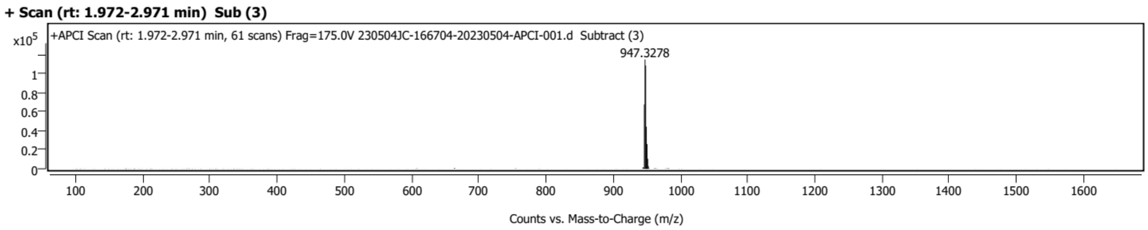
^{13}C NMR spectrum (101 MHz) of **Pt2** in $CDCl_3$ (aromatic region).



Variable temperature ^{1}H NMR spectra recorded in 1,2-dichloroethane-D_4 from 298 to 350 K (heating).



Variable temperature ^{1}H NMR spectra recorded in 1,2-dichloroethane-D4 from 350 to 298 K (cooling).

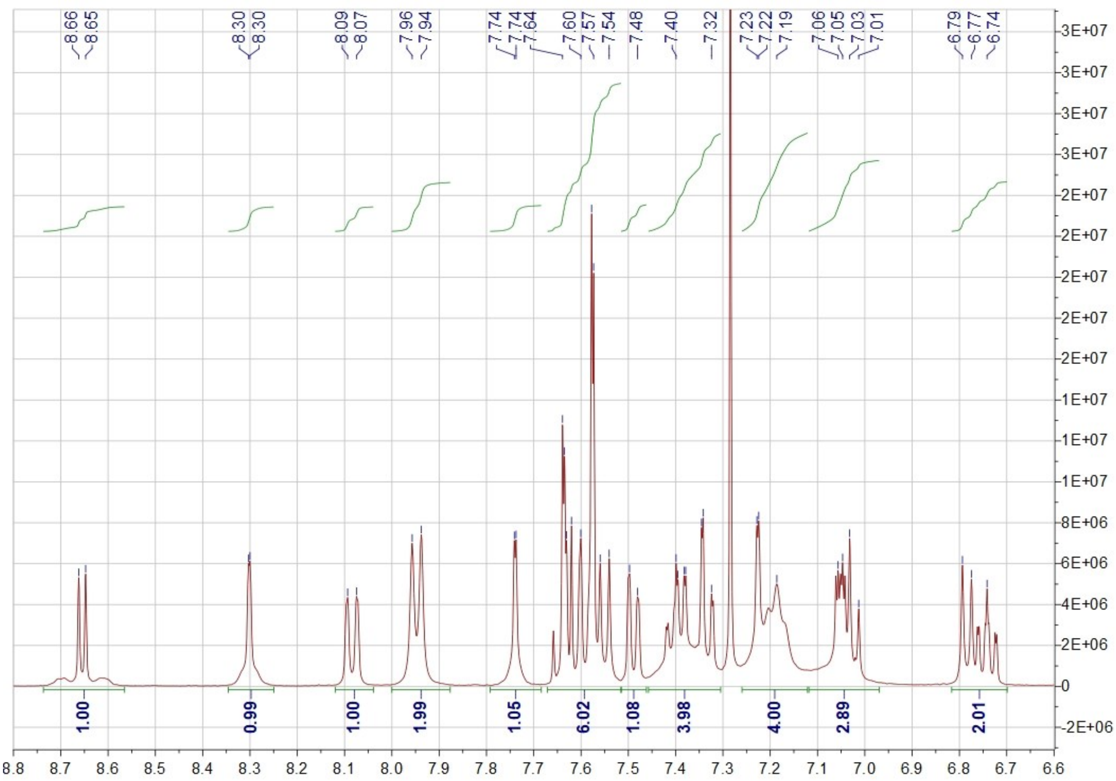


Spectrum Peaks

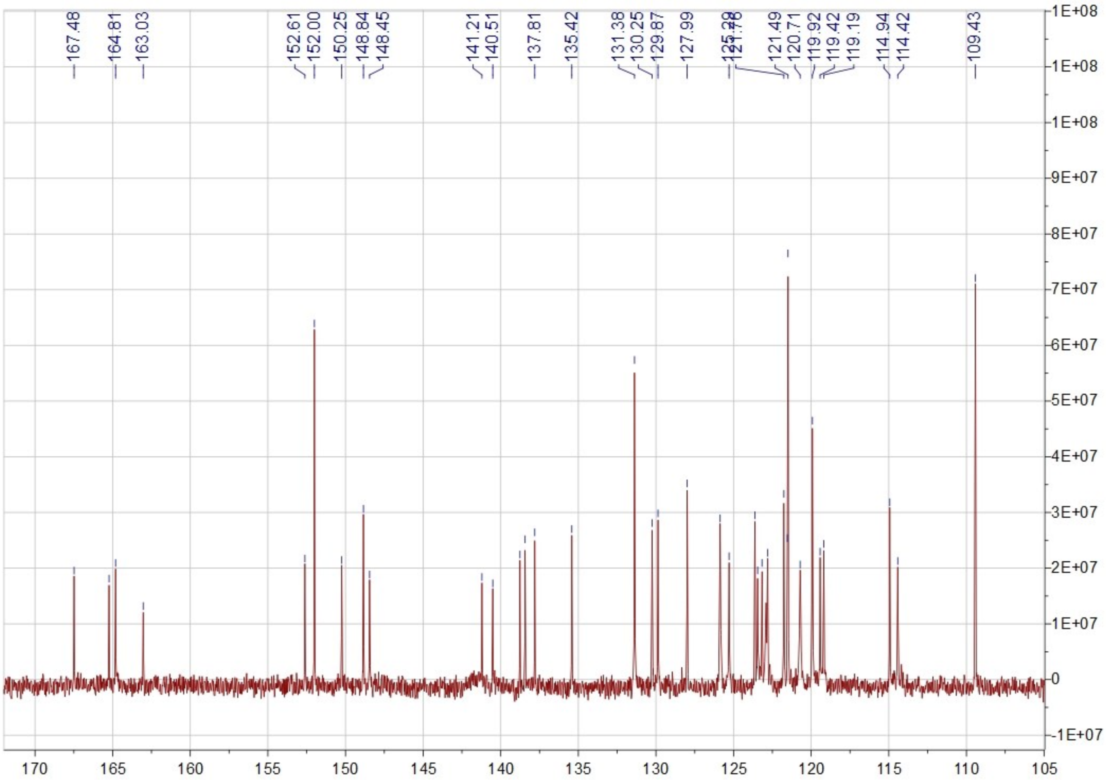
m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
944.3225	1	1574	1.37					
946.3249	1	67694	58.83					
947.3278	1	115060	100.00					
948.3292	1	108638	94.42					
949.3315	1	44313	38.51					
950.3321	1	26038	22.63					
951.3339	1	10563	9.18					
952.3378	1	2847	2.47					

HRMS results of **Pt2**.

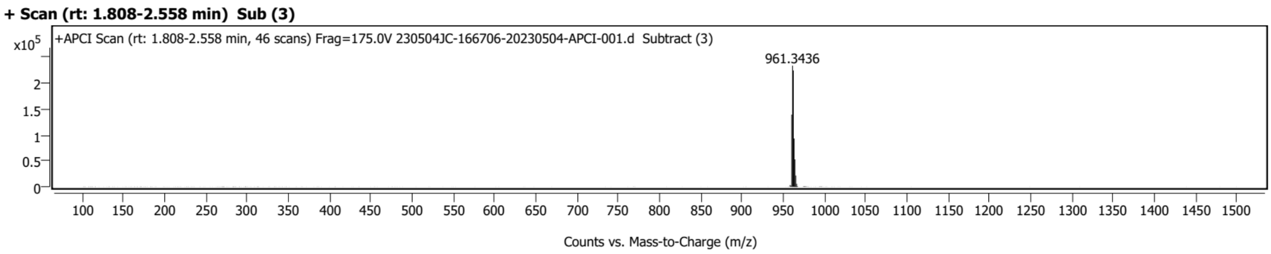
Synthesis of Pt3. The procedure was similar to that of **Pt1** except that **L-3** (1.0 g, 1.3 mmol) was used instead of **L-1**. Yield: 0.74 g (59%, orange solid). ^{1}H NMR (400 MHz, $CDCl_3$, 25ºC): δ/ppm = 8.65 (d, J = 5.9 Hz, 1H), 8.30 (d, J = 1.1 Hz, 1H), 8.08 (d, J = 7.4 Hz, 1H), 7.95 (d, J = 7.6 Hz, 2H), 7.74 (d, J = 1.5 Hz, 1H), 7.66-7.54 (m, 6H), 7.49 (d, J = 7.6 Hz, 1H), 7.42-7.32 (m, 4H), 7.23-7.19 (m, 4H), 7.10-6.98 (m, 3H), 6.79-6.72 (m, 2H), 2.39 (s, 3H), 1.45 (s, 18H, *t*-Bu). ^{13}C NMR (101 MHz, $CDCl_3$, 25 ºC): δ/ppm = 167.48, 165.23, 164.81, 163.03, 152.61, 152.00, 150.24, 148.84, 148.45, 141.21, 140.51, 138.76, 138.43, 137.81, 135.42, 131.38, 130.25, 129.87, 127.99, 125.86, 125.29, 123.63, 123.45, 123.17, 122.90, 122.81, 121.76, 121.54, 121.49, 120.71, 119.92, 119.42, 119.19, 114.94, 114.42, 109.43, 35.31, 31.56, 20.81. ESI-MS: *m*/*z* 961.3436 [M+H]$^+$. Anal. Calcd for $C_{55}H_{47}N_3OPt$: C, 68.74; H, 4.93; N, 4.37. Found: C, 68.45; H, 4.92; N, 4.36.



^{1}H NMR spectrum (400 MHz) of **Pt3** in $CDCl_3$ (aromatic region).



^{13}C NMR spectrum (101 MHz) of **Pt3** in $CDCl_3$ (aromatic region).



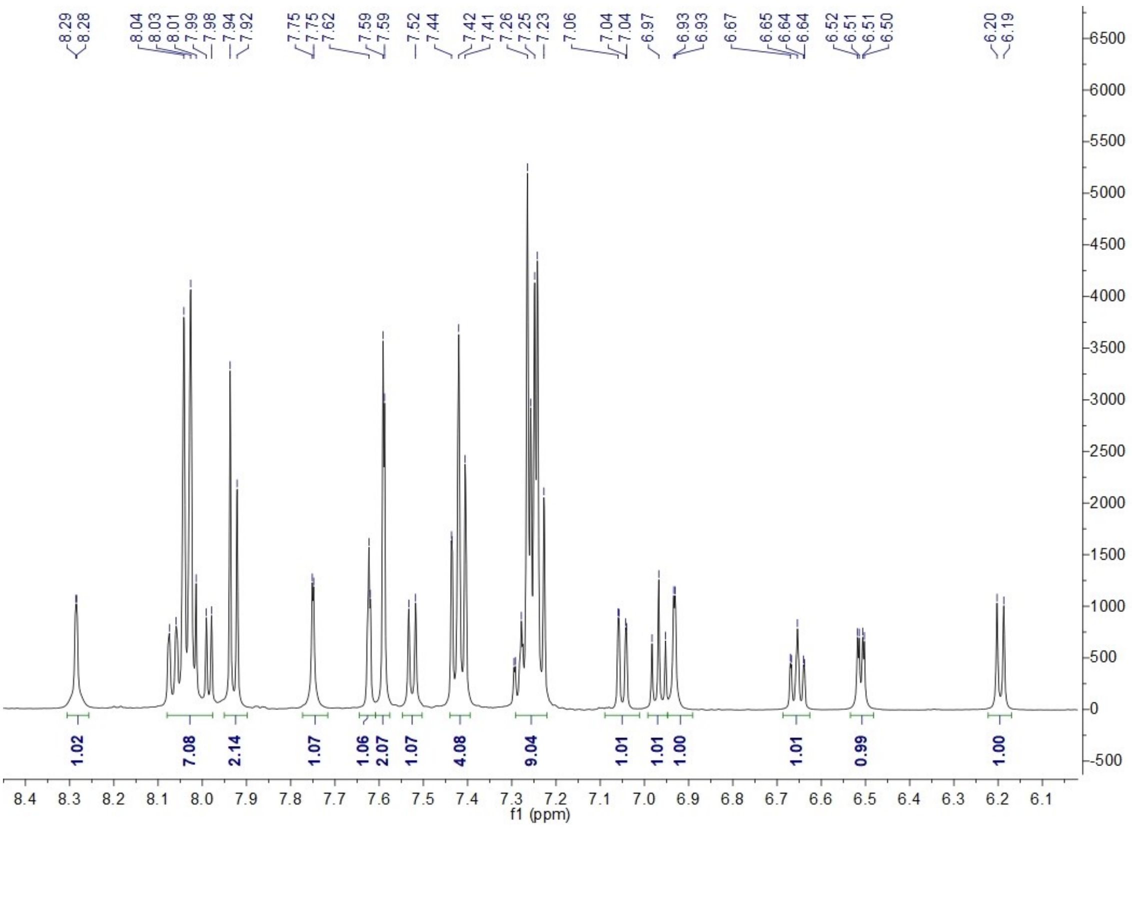
Spectrum Peaks

m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
958.3382	1	2997	1.28					
960.3407	1	139489	59.54					
961.3436	1	234296	100.00					
962.3451	1	224941	96.01					
963.3473	1	93208	39.78					
964.3478	1	52893	22.58					
965.3496	1	21593	9.22					
966.3523	1	5680	2.42					

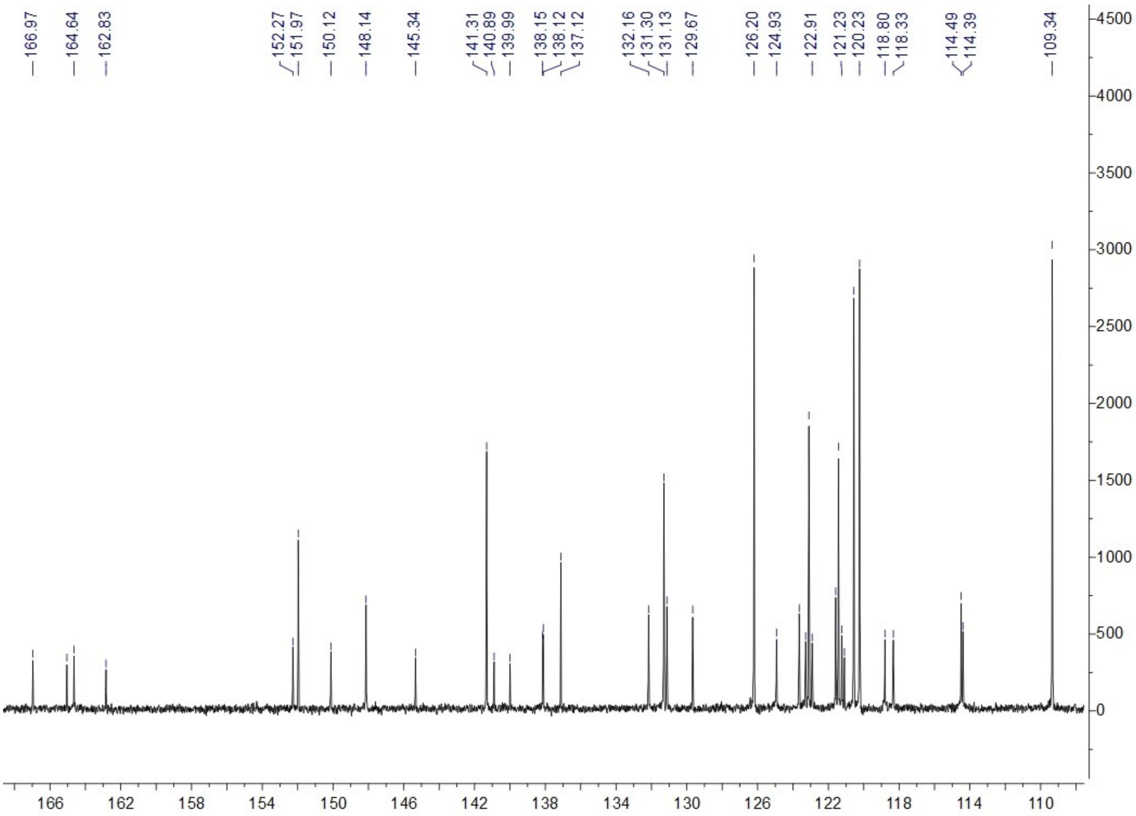
HRMS results of **Pt3**.

Synthesis of Pt4. Potassium tetrachloroplatinate(II) (623 mg, 1.5 mmol) was grinded from a dark red crystal to a pink powder. The grinded potassium tetrachloroplatinate(II) powder and tetrabutylammonium bromide (323 mg, 1 mmol) were added to acetic acid (100 mL) and water (1 mL). Then a solution of ligand 7 (772 mg, 1 mmol) in chloroform (10 mL) was added to the previous suspension. Subsequently, the mixture was heated to reflux under vigorous stir for 12 h in an argon atmosphere and the solvent was removed under reduced pressure. The residue was suspended in water (100 mL) and extracted with dichloromethane (3 × 30 mL). The combined organic phase was washed with brine (2 × 30 mL) and dried under anhydrous magnesium sulphate.

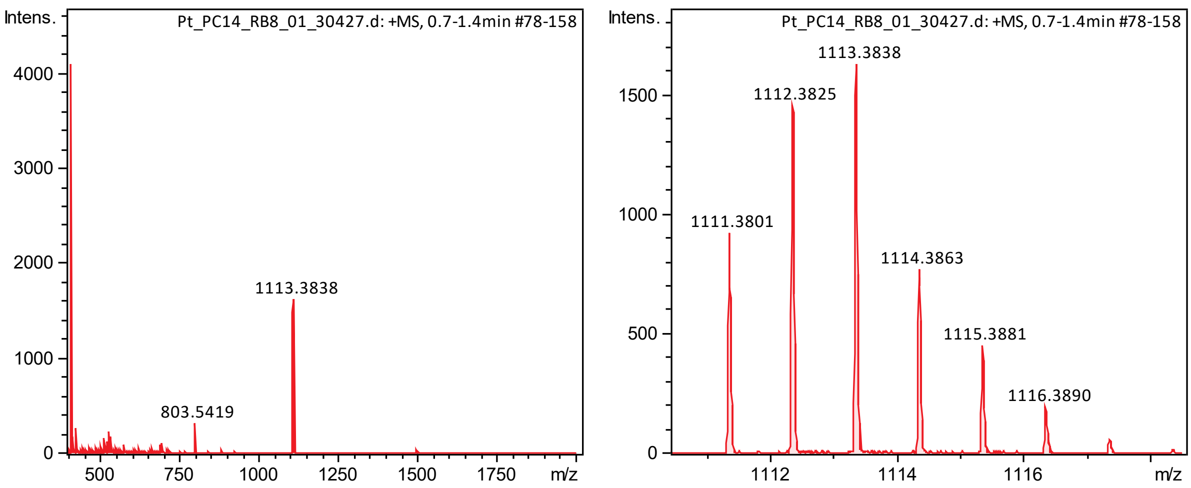
The solvent was vaporized under vacuum and the residue (a dark red solid) was directly used for the next step. Carbazole (251 mg, 1.5 mmol) and cesium carbonate (978 mg, 3 mmol) were dissolved in anhydrous dimethylformamide (100 mL). The mixture was heated to 80ºC and the dark red solid obtained from the previous step was added. Then, the suspension was heated to reflux for 2 hours and cooled to r.t.. The residue was poured to dichloromethane (300 mL) and the organic phase was washed with water (3 × 500 mL) and brine (2 × 300 mL). Then, the organic phase was dried under magnesium sulphate and vaporized under vacuum. The product was separated through a silica gel column (120 g, eluent: hexane/DCM (v/v) = 10/1 to 2/1), which is further purified by recrystallization in hexane/DCM = 45 mL/5 mL (50ºC to r.t., in darkness, 5 h) and collected as a bright yellow solid (902 mg, isolated yield: 81%). ^{1}H NMR (500 MHz, CD_2Cl_2, 25ºC): δ/ppm = 8.29 (d, *J* = 1.8 Hz, 1H), 8.09 – 7.97 (m, 7H), 7.93 (d, *J* = 7.9 Hz, 2H), 7.75 (d, *J* = 1.8 Hz, 1H), 7.62 (d, *J* = 1.8 Hz, 1H), 7.59 (d, *J* = 1.8 Hz, 2H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.42 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 4H), 7.30 – 7.22 (m, 9H), 7.05 (dd, *J* = 8.5, 1.4 Hz, 1H), 6.97 (t, *J* = 7.7 Hz, 1H), 6.93 (d, *J* = 2.0 Hz, 1H), 6.65 (ddd, *J* = 8.2, 6.6, 1.5 Hz, 1H), 6.51 (dd, *J* = 5.9, 2.0 Hz, 1H), 6.20 (d, *J* = 7.6 Hz, 1H), 1.42 (s, 18H). ^{13}C NMR (126 MHz, CD_2Cl_2, 25ºC): δ/ppm = 166.99, 165.06, 164.67, 162.85, 152.29, 151.99, 150.14, 148.15, 145.36, 141.37, 141.33, 140.91, 140.01, 138.17, 138.13, 137.13, 132.18, 131.31, 131.14, 129.68, 126.21, 124.95, 123.66, 123.30, 123.16, 123.12, 122.93, 121.60, 121.45, 121.25, 121.11, 120.60, 120.57, 120.25, 118.82, 118.34, 114.51, 114.41, 109.36, 34.96, 31.19. ESI-MS: *m/z* 1113.3838 $[M+H]^+$. Anal. Calcd for $C_{66}H_{52}N_4OPt$: C, 71.27; H, 4.71; N, 5.04. Found: C, 70.78; H, 4.72; N, 4.86.



^{1}H NMR spectrum (500 MHz) of **Pt4** in CD_2Cl_2 (aromatic region).



^{13}C NMR spectrum (126 MHz) of **Pt4** in CD_2Cl_2 (aromatic region).



HRMS results of **Pt4**.

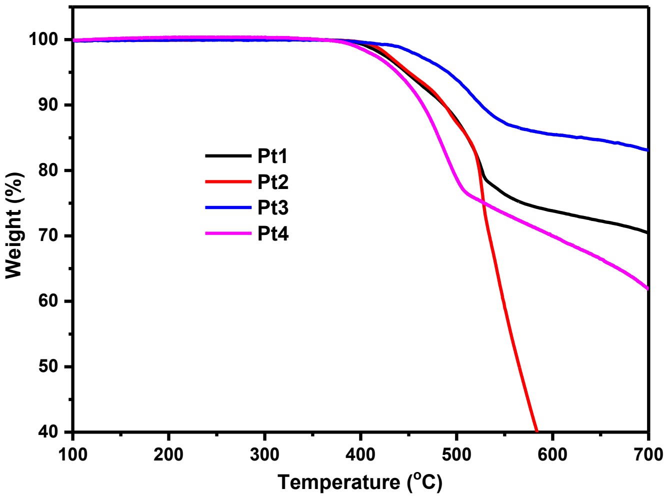


Figure S1. TGA thermograms of **Pt1–Pt4**.

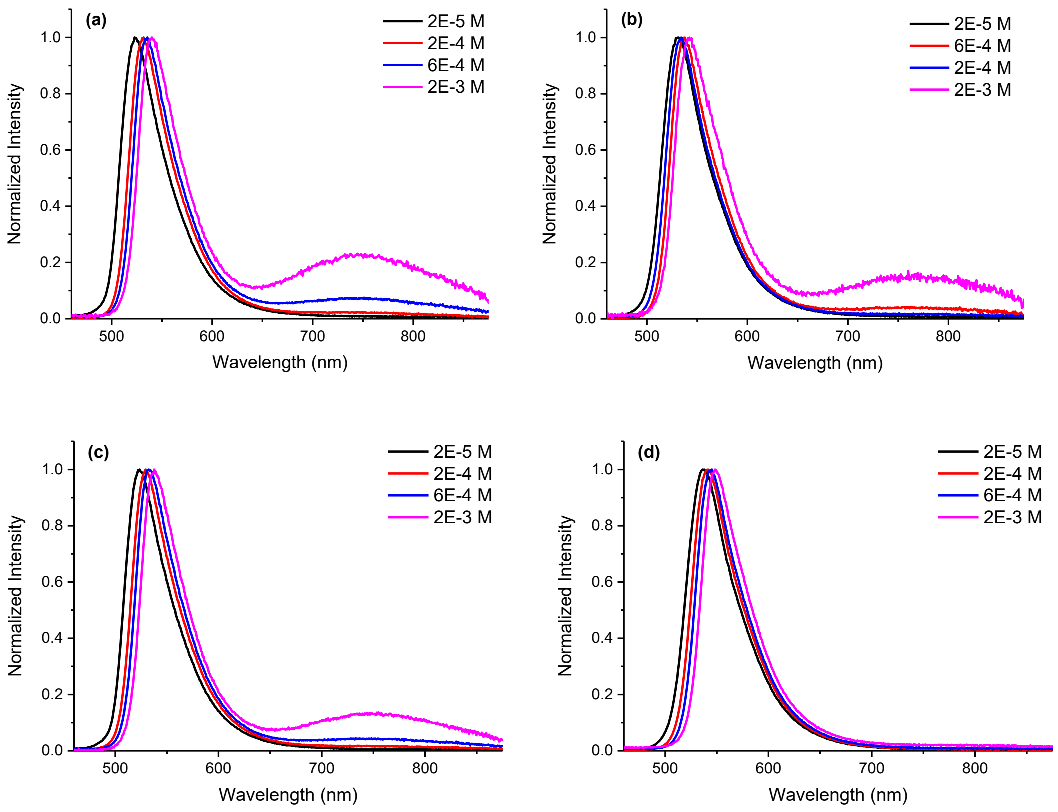


Figure S2. Emission spectra of (a) **Pt1**, (b) **Pt2**, (c) **Pt3** and (d) **Pt4** in toluene at different concentrations.

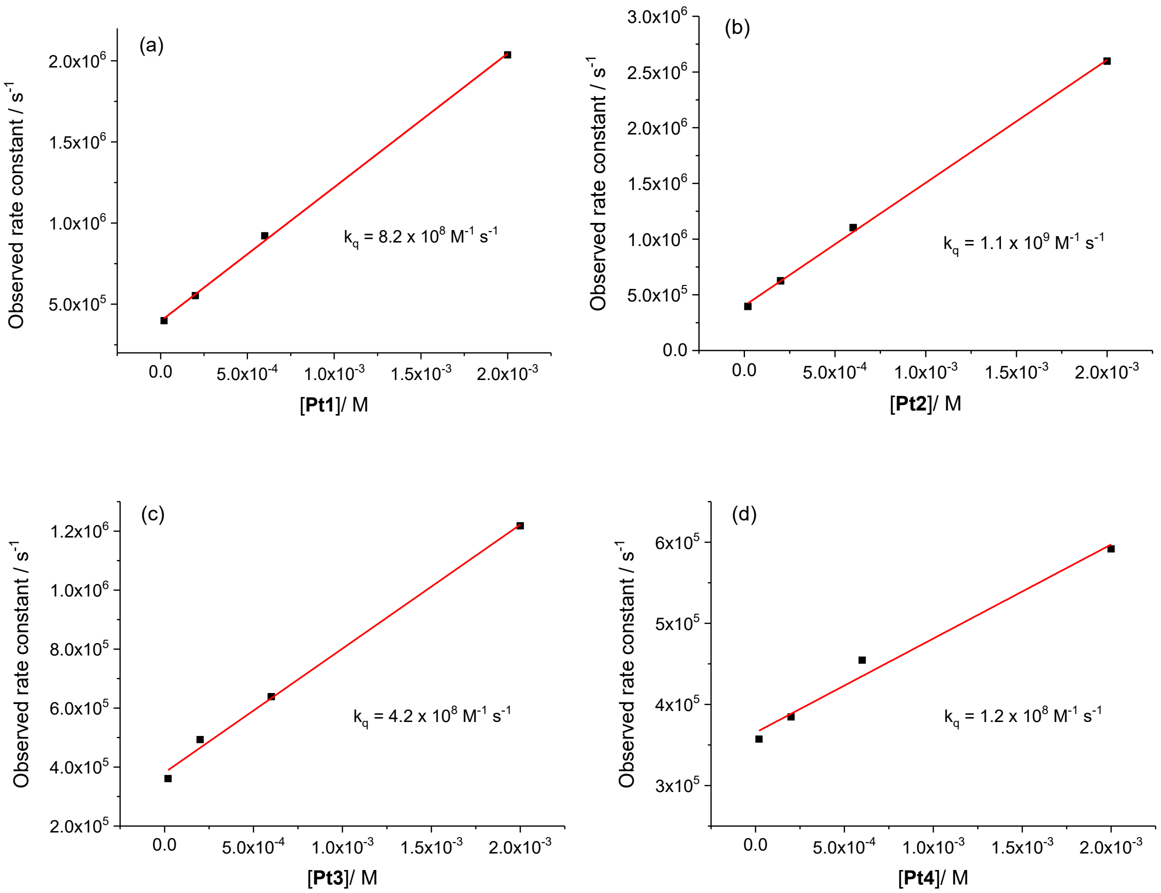
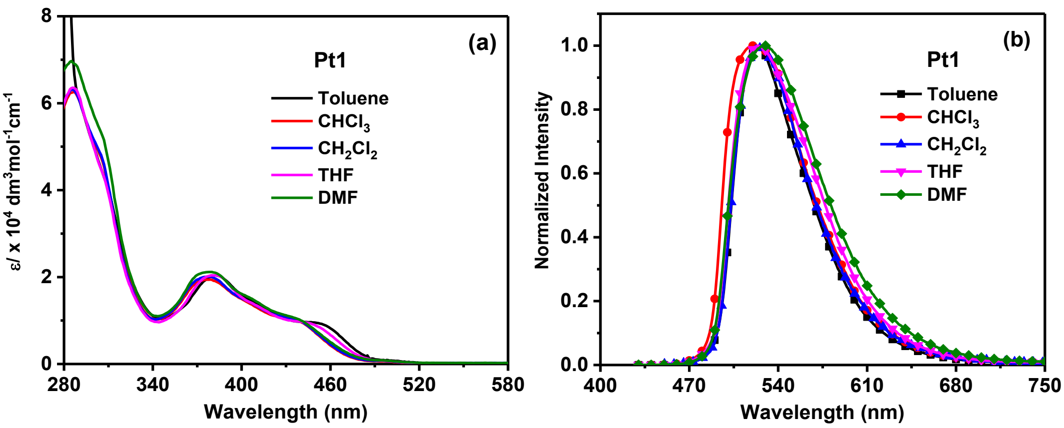


Figure S3. Stern-Volmer plot of (a) **Pt1**, (b) **Pt2**, (c) **Pt3** and (d) **Pt4** in toluene.



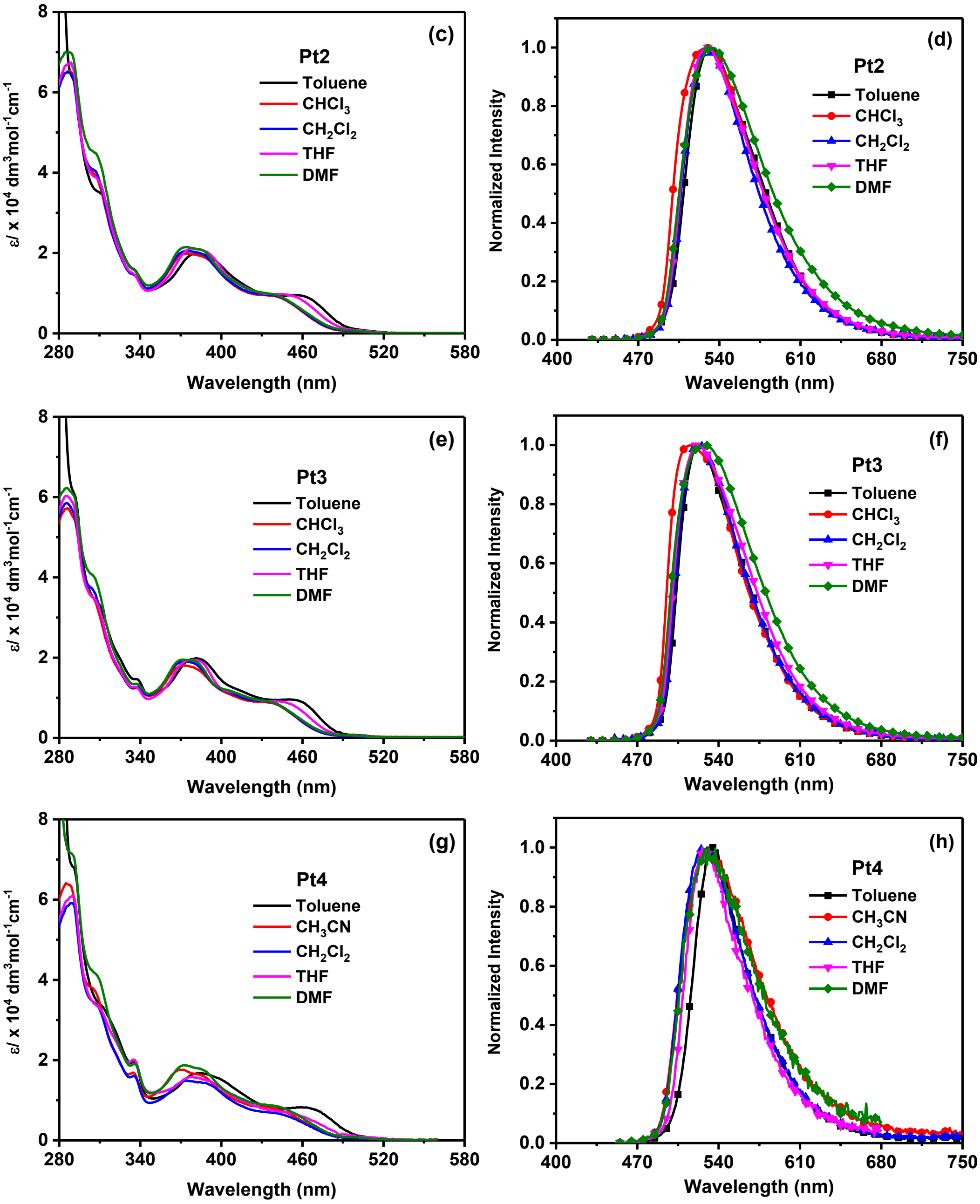


Figure S4. (a, c, e, g) UV-vis absorption spectra and (b, d, f, h) emission spectra of **Pt1–Pt4**, respectively, in different solvents (2×10^{-5} M).

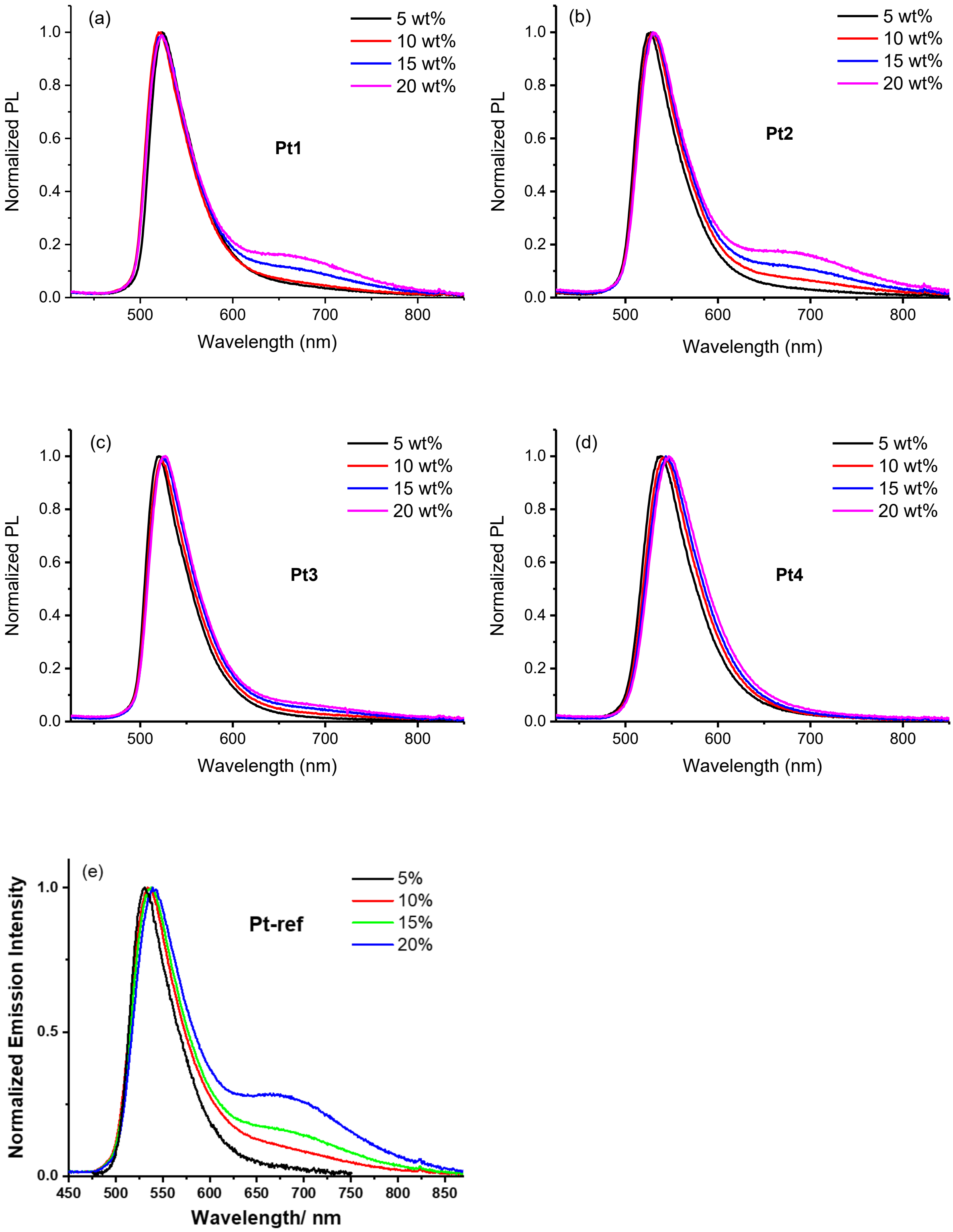


Figure S5. Emission spectra of (a) **Pt1**, (b) **Pt2**, (c) **Pt3**, (d) **Pt4** and (e) **Pt-ref** in mCP thin films with different doping concentration (5–20 wt%).

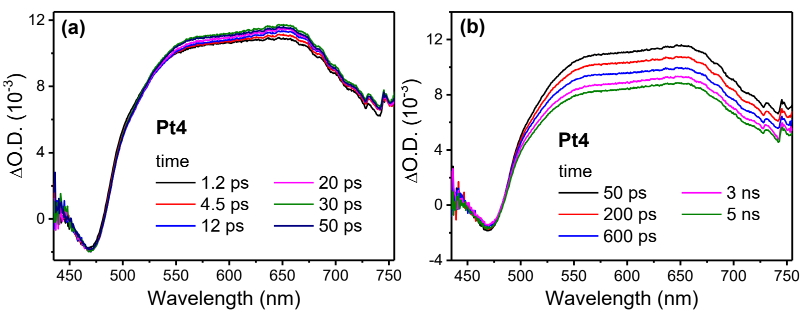


Figure S6. Temporal evolution of fs-TA of **Pt4** (a) from 1.2 ps to 50 ps, and (b) from 50 ps to 5 ns in toluene upon 400 nm excitation.

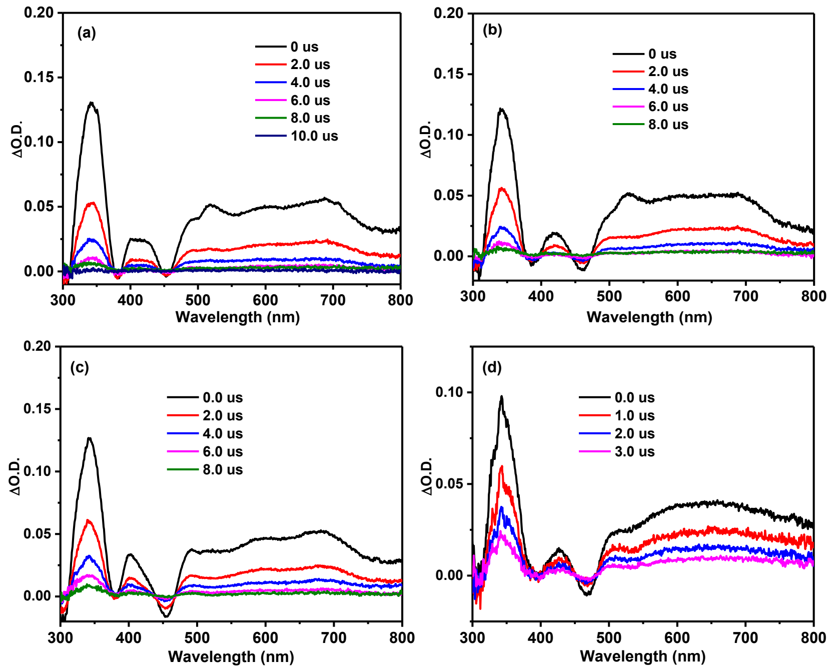


Figure S7. Time-resolved transient absorption (ns-TA) spectra of (a) **Pt1**, (b) **Pt2**, (c) **Pt3** and (d) **Pt4** in toluene (2×10^{-5} M).

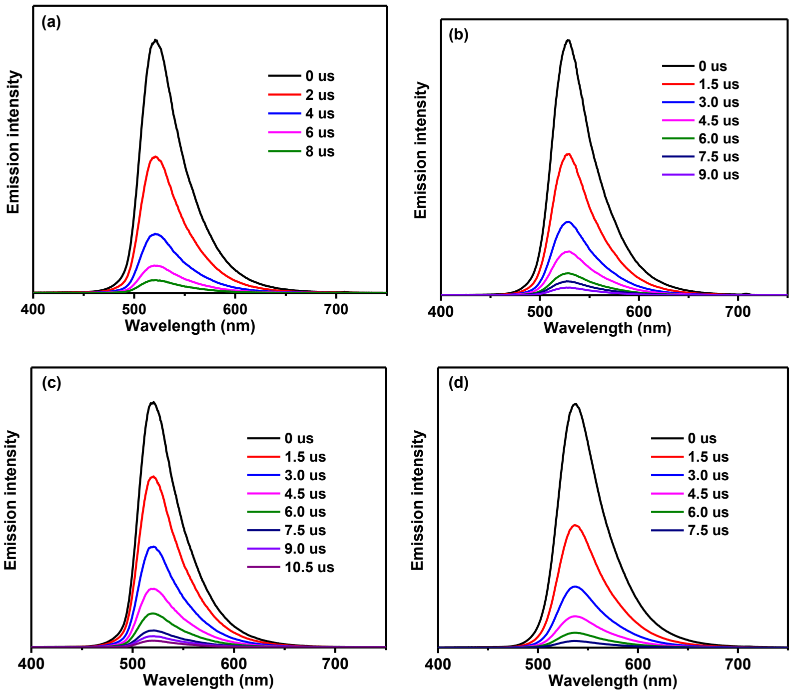


Figure S8. Time-resolved emission spectra of (a) **Pt1**, (b) **Pt2**, (c) **Pt3** and (d) **Pt4** in toluene (2×10^{-5} M).

Computational Details

All geometric optimization, potential energy surface scan and frequency analysis calculations at DFT/PBE0-D3BJ level were performed using Gaussian 16 (revision C.01) program package.[S2] The ECP60MWB[S3] basis set was used for Pt atom, and 60 core electrons were replaced with the corresponding pseudopotential. The 6-31G(d,p) basis set was used for all non-metal atoms. The solvation effect of bulk toluene environment was simulated with SMD (solvation model based on density) model.[S4] The optimized structures were confirmed to be true minima since no imaginary frequencies were observed.

To account for large spin-orbit coupling (SOC) and relativistic effects induced by Pt center, the SOC-TDDFT/PBE0[S5] calculations with the zero-order regular approximation (ZORA) Hamiltonian,[S6] in connection with segmented all-electron relativistically contracted (SARC) basis sets SARC-ZORA-TZVP[S7,S8] for the central Pt atom and ZORA-def2-TZVP[S3,S7] for all other atoms, were performed using ORCA (release 5.0.3) program package.[S9] The solvent effect was included using the SMD model. The SOC-TDDFT/PBE0 calculations took 25 lowest scalar relativistic singlet and triplet excitations into accounts, resulting in totally 100 SOC states. Before the consideration of SOC induced mixing of the singlet and triplet states, main orbital transitions involve in the $T_1 \rightarrow S_0$ transition of **Pt1–Pt4** are summarized in Table S1. Due to the SOC effect, the T_1 state is split into three sublevels in the absence of an external field, which is referred to as the zero-field splitting (ZFS). The radiative rate constant k_r^i and radiative lifetime τ_i from sublevel T_1^i ($i = 1, 2, 3$) to S_0 state is given by[S10]

$$k_r^i = \frac{1}{\tau_i} = \frac{4\alpha_0^3}{3t_0}\left(\Delta E_{S_0-T_1^i}\right)^3 \sum_{\sigma\in\{x,y,z\}} \left|M_\sigma^i\right|^2, \quad (1)$$

where $t_0 = (4\pi\varepsilon_0)^2\hbar^3/(m_e e^4)$, α_0 is the fine structure constant, $\Delta E_{S_0-T_1^i}$ is the transition energy, and M_σ^i is the transition dipole moment. The oscillator strength f_{osc}^i of the transition $T_1^i \rightarrow S_0$ is defined as[S11]

$$f_{osc}^i = \frac{2m_e}{3\hbar^2}\Delta E_{S_0-T_1^i} \sum_{\sigma\in\{x,y,z\}} \left|M_\sigma^i\right|^2. \quad (2)$$

According to the Stickler-Berg relationship,[S11] the radiative rate k_r^i (or lifetime τ_i) was multiplied (or divided) by the squared refractive index of toluene ($n = 1.496$).

The overall observed phosphorescence rate constant k_r and radiative lifetime τ form T_1 state, assuming the Boltzmann distribution of the sublevels, is given by

$$k_r = \frac{1}{\tau} = \frac{k_r^1 + k_r^2\exp\left(-\frac{\Delta E_{1,2}^{ZFS}}{k_B T}\right) + k_r^3\exp\left(-\frac{\Delta E_{1,3}^{ZFS}}{k_B T}\right)}{1 + \exp\left(-\frac{\Delta E_{1,2}^{ZFS}}{k_B T}\right) + \exp\left(-\frac{\Delta E_{1,3}^{ZFS}}{k_B T}\right)}. \quad (3)$$

Here, $\Delta E_{i,j}^{ZFS}$ is the zero-field splitting between the sublevels i and j. The high-temperature limit ($k_B T \gg \Delta E_{i,j}^{ZFS}$) of Eq. (3) can be cast to

$$k_r = \frac{1}{\tau} \approx \frac{1}{3}\sum_{i=1}^{3} k_r^i. \quad (4)$$

To estimate the nonradiative decay rate constant (k_{nr}) from T_1 to S_0 state based on the Marcus theory

$$k_{nr} = \frac{2\pi}{\hbar}\frac{|H_{SOC}|^2}{\sqrt{4\pi\lambda k_B T}}\exp\left(-\frac{\left(\lambda + \Delta E_{S_0-T_1}\right)^2}{4\lambda k_B T}\right), \quad (5)$$

we further computed the optimized structures of the T_1 state for complexes **Pt1**–**Pt4** (Figure S9). Here, H_{SOC} is the SOC matrix element between S_0 and T_1 state, λ and $\Delta E_{S_0-T_1}$ are total reorganization energy and the energy difference between the S_0 and T_1 states at their optimized structures. It is obvious that the structural distortion from optimized T_1 to S_0 state is marginally small (root-mean-square difference < 0.3 Å), and the energy difference between optimized T_1 and S_0 structures at the ground state is < 4 kcal/mol for all complexes. The inner-sphere reorganization energies of **Pt1**–**Pt4** are computed to be <1400 cm^{-1}, while the $\Delta E_{S_0-T_1}$ are over 18000 cm^{-1} (Table S2). By assuming that the outer-sphere reorganization energy is of similar magnitude as inner-sphere reorganization energy, the k_{nr} is negligibly small as compared to the radiative rate constant. This is in line with high photoluminescent quantum yield (close to 1) observed in the experiment. The emission bandwidth is also anticipated to be small due to the small difference between optimized S_0 and T_1 state structures.

Table S1. Contributions from the main molecular orbital transitions to the T_1 state. The percentages are computed as the squared amplitudes that constitute the TDDFT wave function.

Complex	Orbital transition	Contribution
Pt1	HOMO→LUMO	63.8%
	HOMO→LUMO+2	10.2%
Pt2	HOMO→LUMO	66.3%
	HOMO→LUMO+2	9.3%
Pt3	HOMO→LUMO	65.1%
	HOMO→LUMO+2	8.6%
Pt4	HOMO→LUMO	66.0%
	HOMO→LUMO+2	9.2%

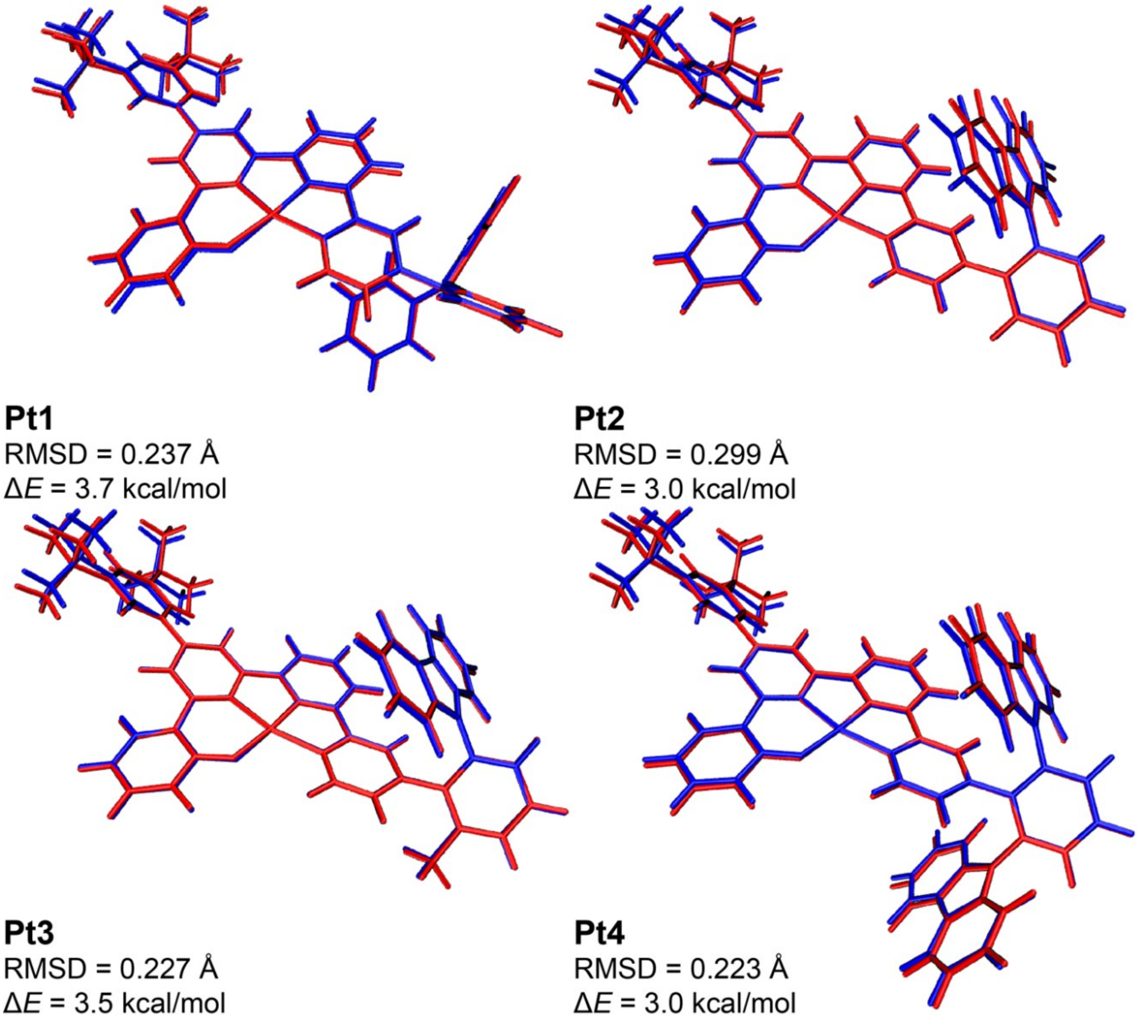


Figure S9. Comparison between optimized S_0 (in blue) and T_1 (in red) state structures for complexes **Pt1**–**Pt4**. The root-mean-square difference (RMSD) and the energy difference between two structures at the S_0 state (ΔE) are also listed.

Table S2. Computed inner-sphere reorganization energies (λ) and adiabatic energy gaps ($\Delta E_{S_0-T_1}$) for complexes **Pt1**–**Pt4**.

	λ (cm^{-1})	$\Delta E_{S_0-T_1}$ (cm^{-1})
Pt1	1371	18719
Pt2	1065	18605
Pt3	1249	18739
Pt4	1098	18518

OLED fabrication and characterization

OLEDs were fabricated in a Kurt J. Lesker SPECTROS vacuum deposition system with a base pressure of 10^{-8} mbar. In the vacuum chamber, organic materials were thermally deposited in sequence at a rate of ~0.1 nm s^{-1}. The doping process in the emitting layer was realized by co-deposition technology. Afterwards, LiF (1.2 nm) and Al (100 nm) were thermally deposited at rates of 0.03 and 0.2 nm s^{-1}, respectively. Film thicknesses were determined in situ by calibrated oscillating quartz-crystal sensors. EL spectra, J-L-V characteristics, CIE coordinates, EQE, CE and PE were measured using a Keithley 2400 source-meter and an absolute external quantum efficiency measurement system (C9920-12, Hamamatsu Photonics). All devices were characterized at room temperature without encapsulation. The device structure for **Pt1–Pt3**-OLEDs is ITO/HAT-CN (5 nm)/TAPC (40 nm)/mCBP (5 nm)/Pt emitter: mCBP (25 nm)/PPF (10 nm)/TmPyPb (40 nm)/LiF (1.2 nm)/Al (100 nm). The device structure for **Pt4**-OLEDs is ITO/HAT-CN (10 nm)/BPBPA (80 nm)/NBP-BC (5 nm)/**Pt4**: RH (40 nm)/HB (5 nm)/ZADN: Liq (35 nm)/Yb (1 nm)/Ag (100 nm).

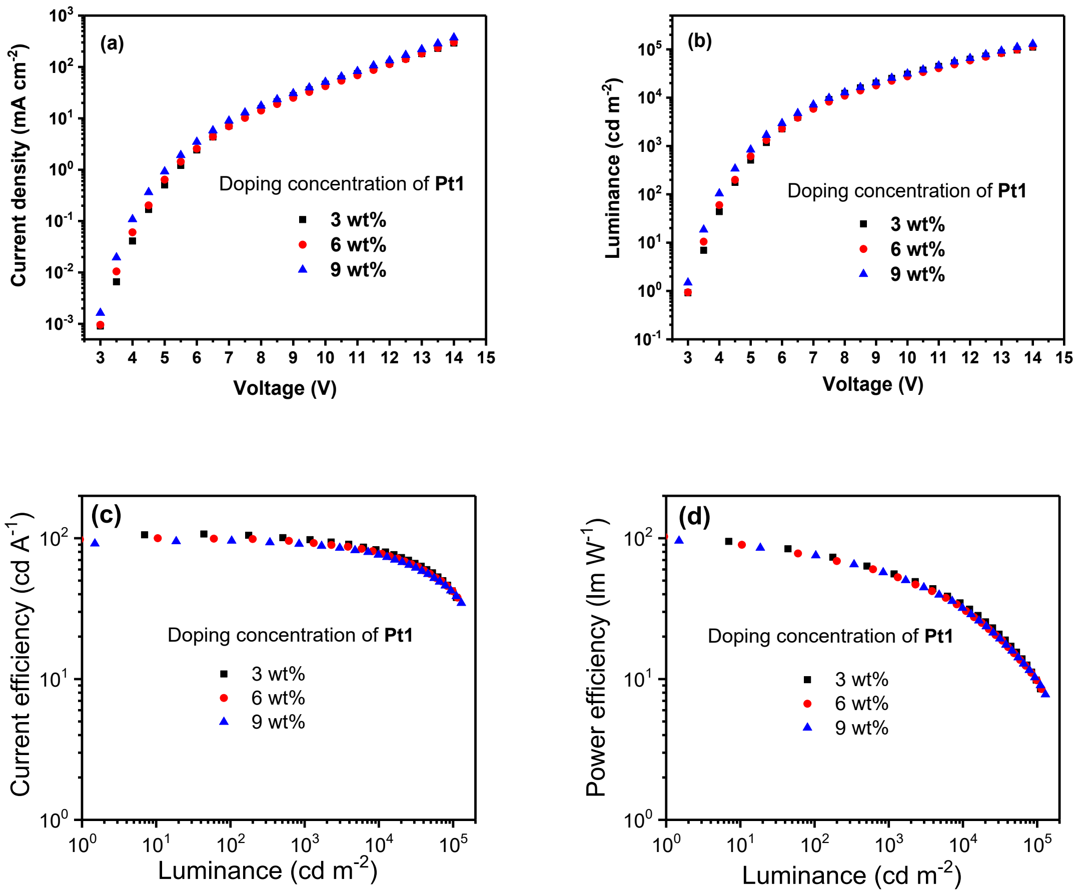


Figure S10. (a) Current density-voltage, (b) luminance-voltage, (c) current efficiency-luminance, and (d) power efficiency-luminance characteristics of the OLEDs based on **Pt1** with different doping concentrations.

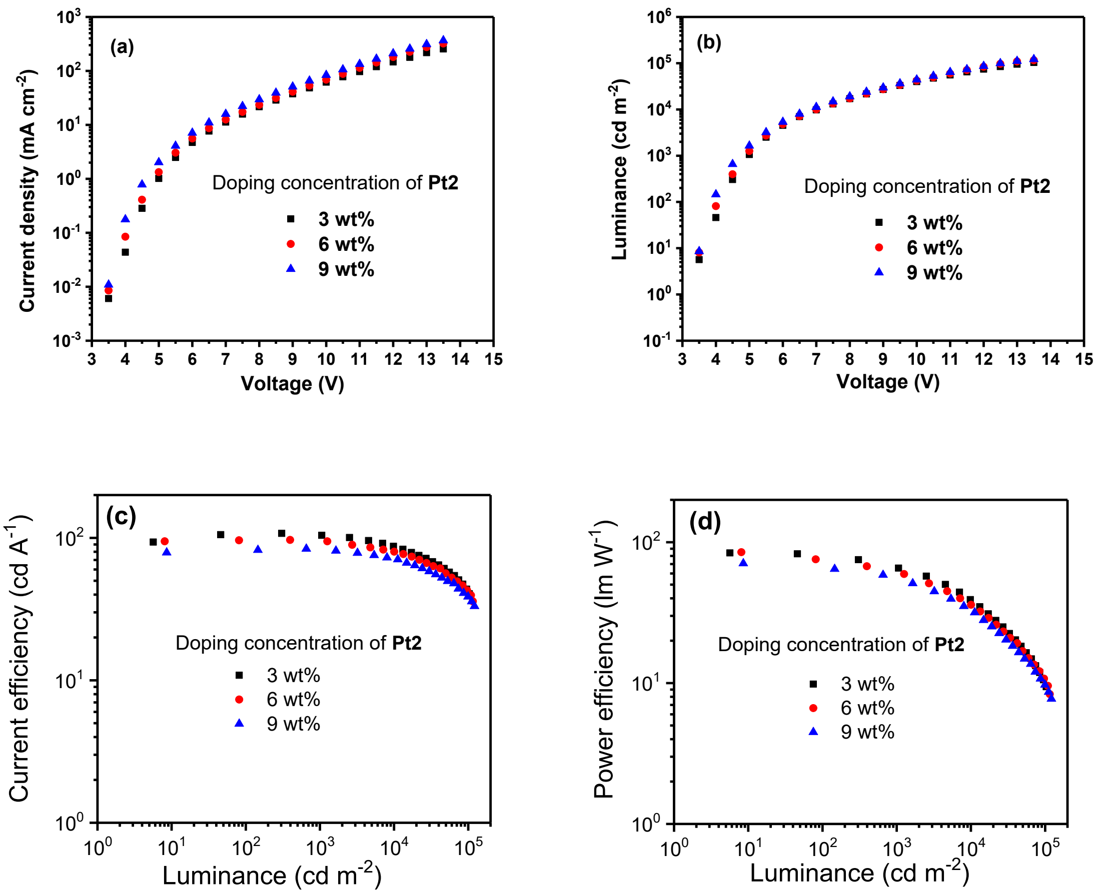


Figure S11. (a) Current density-voltage, (b) luminance-voltage, (c) current efficiency-luminance, and (d) power efficiency-luminance characteristics of the OLEDs based on **Pt2** with different doping concentrations.

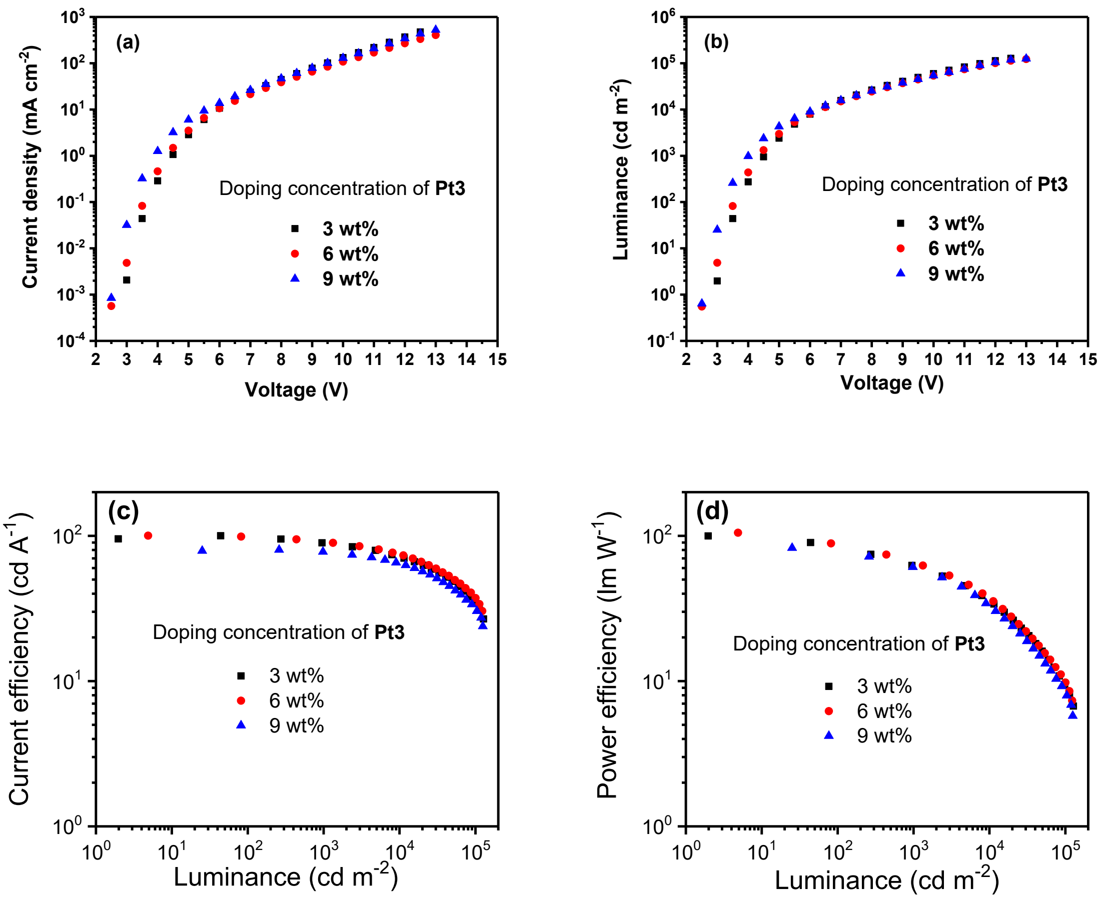


Figure S12. (a) Current density-voltage, (b) luminance-voltage, (c) current efficiency-luminance, and (d) power efficiency-luminance characteristics of the OLEDs based on **Pt3** with different doping concentrations.

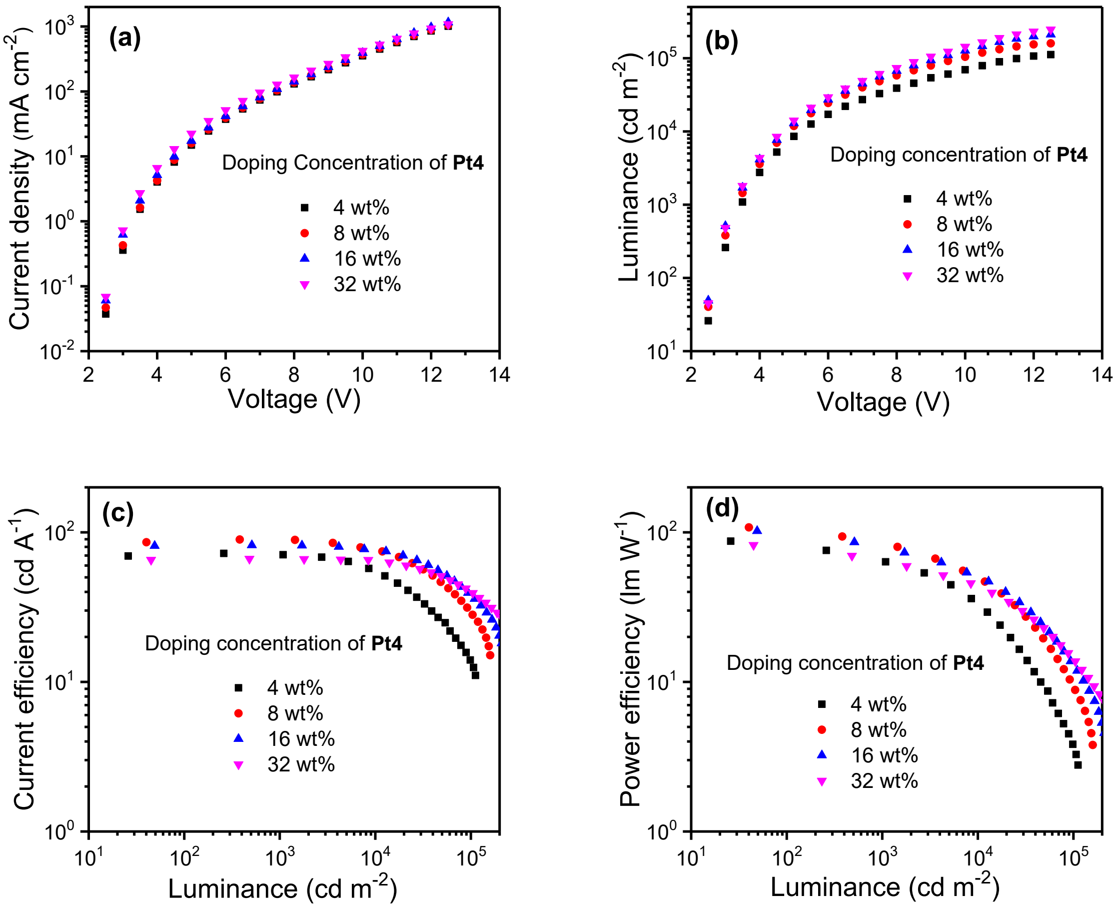


Figure S13. (a) Current density-voltage, (b) luminance-voltage, (c) current efficiency-luminance, and (d) power efficiency-luminance characteristics of the OLEDs based on **Pt4** with different doping concentrations.

Details for the measurement of device stability

Devices with **Pt1–Pt3** for operating lifetime measurement were fabricated in an ALS vacuum deposition system with a base pressure of 1.0 × 10^{-5} Pa, and they were encapsulated in a glovebox (N_2 < 1 ppm, O_2 < 1 ppm). The device structure for OLEDs with **Pt1–Pt3** is given in Figure S14. Prior to deposition, the patterned ITO coated glass substrates were cleaned with detergent, rinsed in deionized water, acetone, and isopropanol, and then dried in an oven for 1 h. Organic layers were deposited in sequence at a rate of 1.0 Å/s. Afterward, Yb (1 nm) and Ag (100 nm) were thermally deposited at rates of 0.1 Å s^{-1} and 1 Å s^{-1}, respectively. Current density-luminance-voltage characteristics, EL spectra, and EQE of EL device were obtained by using a Keithley 2400 source-meter and an absolute external quantum efficiency measurement system (CS2000, KONICA MINOLTA). Devices with **Pt4** for operating lifetime measurement were fabricated in a Kurt J. Lesker SPECTROS vacuum deposition system. Current density-brightness-voltage characteristics, EL spectra, and EQE of EL device were obtained by using a Keithley 2400 source-meter and an absolute external quantum efficiency measurement system (C9920-12, Hamamatsu Photonics). The **Pt4**-devices were encapsulated in a 200-nm-thick Al_2O_3 thin film deposited by atomic layer deposition (ALD) in a Kurt J. Lesker SPECTROS ALD system before measurements. The device structure for **Pt4**-OLEDs is ITO/HAT-CN (10 nm)/BPBPA (80 nm)/NBP-BC (5 nm)/**Pt4**: RH (40 nm)/HB (5 nm)/ZADN: Liq (35 nm)/Yb (1 nm)/Ag (100 nm), which is the same as described in the "OLED fabrication and characterization" section.

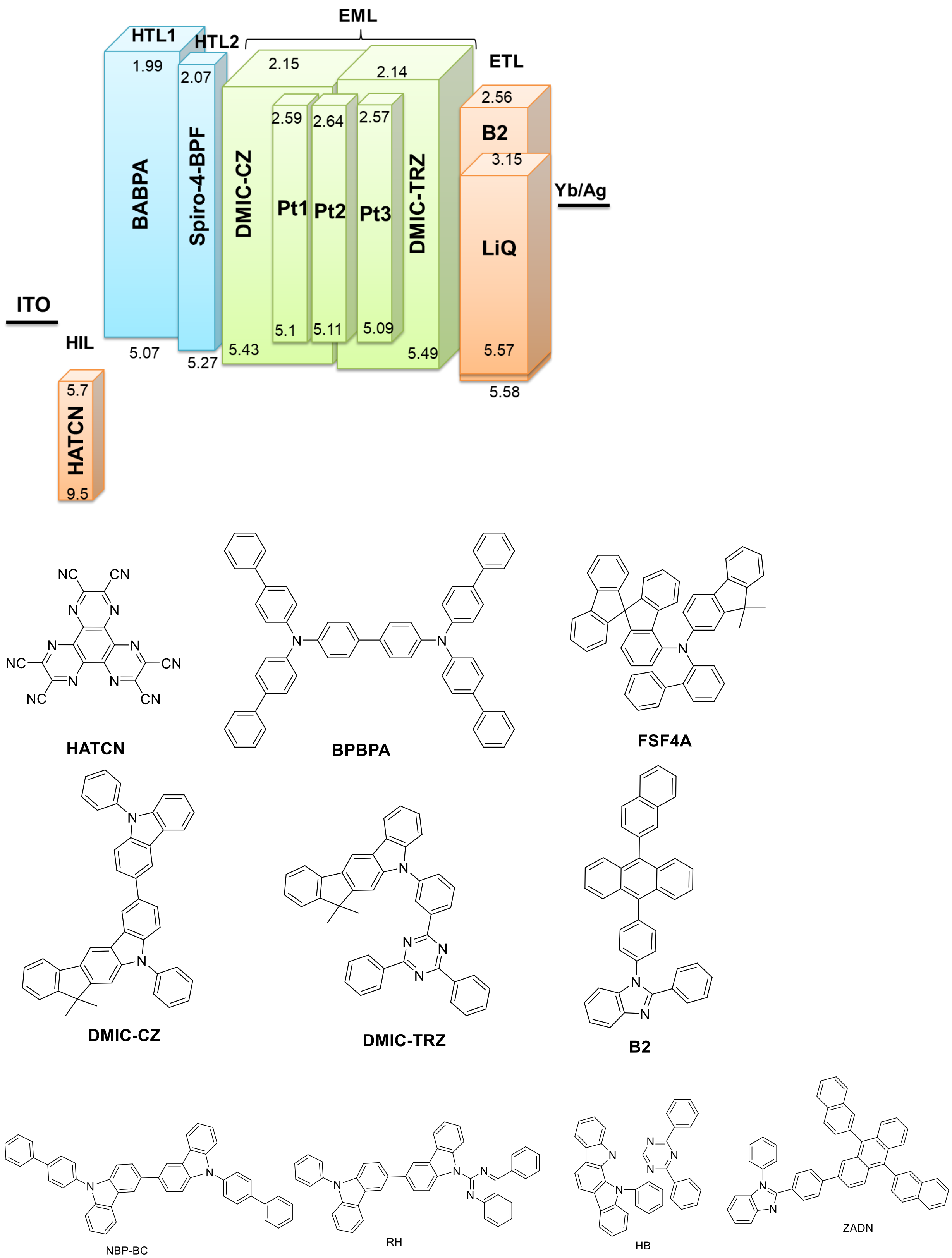


Figure S14. Device structure used in the OLEDs with **Pt1**–**Pt3** for operating lifetime measurement and chemical structures of the organic materials for the devices with **Pt1**–**Pt4**.

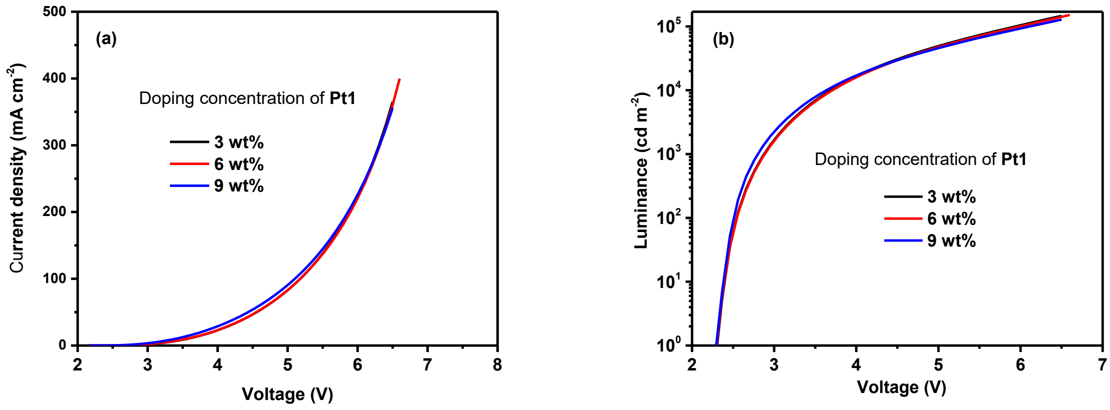


Figure S15. (a) Current density-voltage and (b) luminance-voltage characteristics of the OLEDs based on **Pt1** with different doping concentrations for operating lifetime measurement.

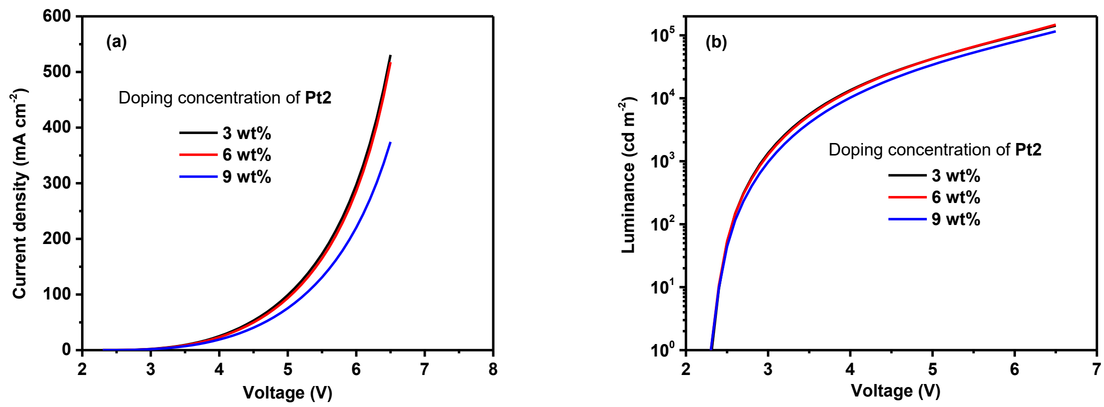


Figure S16. (a) Current density-voltage and (b) luminance-voltage characteristics of the OLEDs based on **Pt2** with different doping concentrations for operating lifetime measurement.

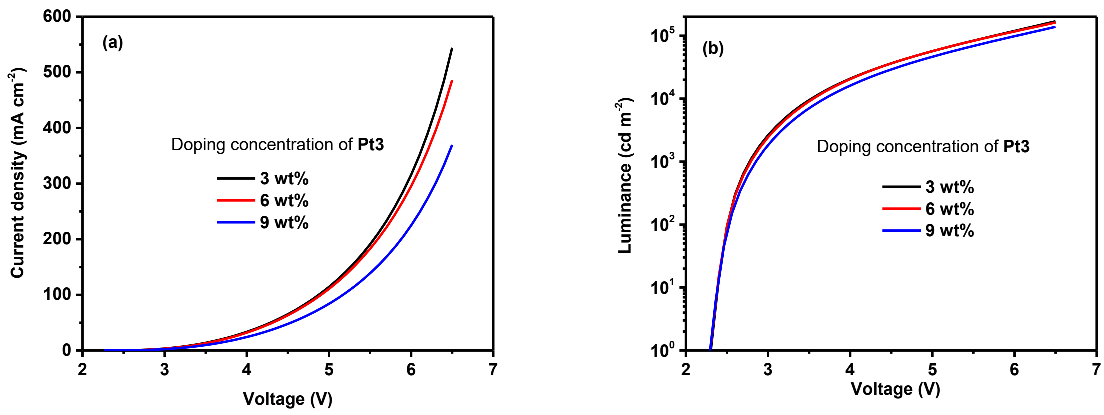


Figure S17. (a) Current density-voltage and (b) luminance-voltage characteristics of the OLEDs based on **Pt3** with different doping concentrations for operating lifetime measurement.

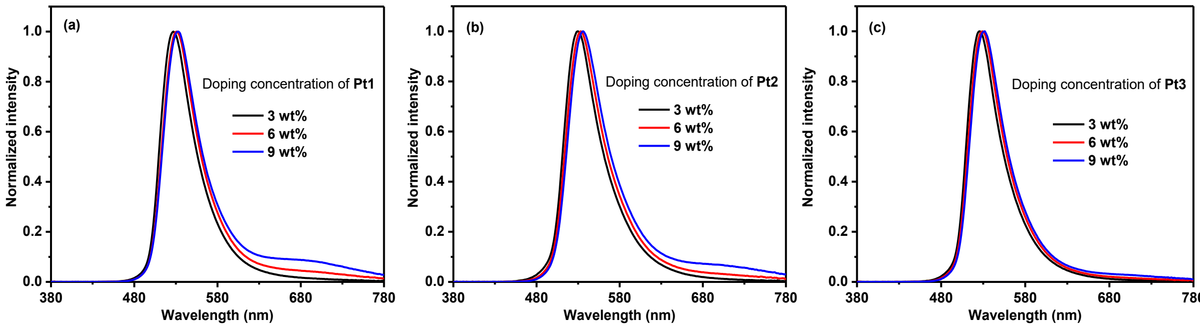


Figure S18. Normalized EL spectra of the OLEDs (at 1000 cd m^{-2}) based on (a) **Pt1**, (b) **Pt2** and (c) **Pt3** with different concentrations for operating lifetime measurement.

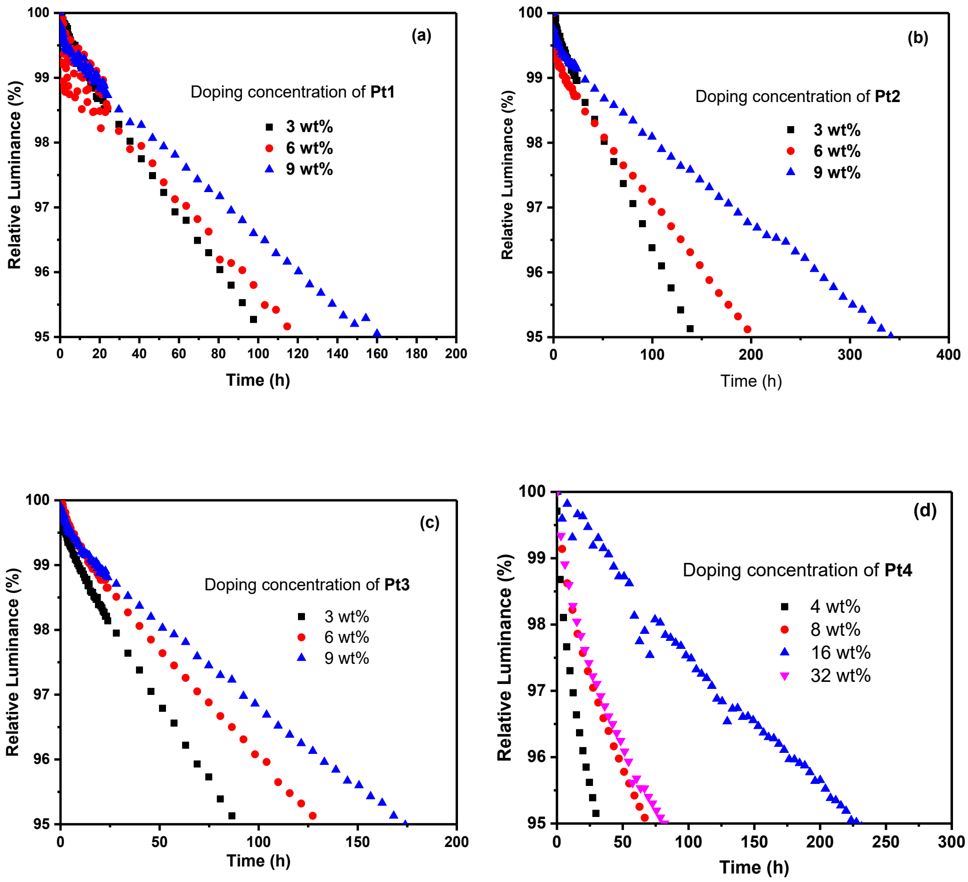


Figure S19. Operational lifetime of the OLEDs based on (a) **Pt1**, (b) **Pt2**, (c) **Pt3** and (d) **Pt4** with different doping concentrations at 10000 cd m^{-2}.

Table S3. Electroluminescence data of OLEDs for operating lifetime measurements (data of **Pt4**-devices are given in the manuscript).

Complex (Conc.)[a]	PE[b] (lm W^{-1})			CE[c] (cd A^{-1})			EQE[d] (%)			CIE (x,y) @1000 cd m^{-2}
	1000 cd m^{-2}	5000 cd m^{-2}	10000 cd m^{-2}	1000 cd m^{-2}	5000 cd m^{-2}	10000 cd m^{-2}	1000 cd m^{-2}	5000 cd m^{-2}	10000 cd m^{-2}	
Pt1 (3 wt%)	93.6	75.6	63.6	85.1	80.6	75.7	22.3	21.1	19.8	(0.29,0.66)
Pt1 (6 wt%)	82.6	68.1	60.3	77.7	74.7	71.8	21.4	20.3	19.5	(0.32,0.65)
Pt1 (9 wt%)	71.0	62.0	53.3	64.5	64.2	61.9	19.4	18.9	18.0	(0.33,0.63)
Pt2 (3 wt%)	70.5	53.1	46.1	65.1	59.1	55.7	17.2	15.6	14.7	(0.31,0.64)
Pt2 (6 wt%)	71.7	55.1	48.1	66.2	61.4	58.2	18.1	16.6	15.7	(0.33,0.63)
Pt2 (9 wt%)	61.6	49.6	42.3	58.8	56.8	53.9	17.2	16.3	15.3	(0.35,0.62)
Pt3 (3 wt%)	87.5	71.6	61.7	78.0	73.0	68.8	20.4	19.1	18.0	(0.29,0.66)
Pt3 (6 wt%)	87.1	72.5	63.0	77.6	73.9	70.2	20.5	19.4	18.4	(0.30,0.66)
Pt3 (9 wt%)	84.0	68.9	60.7	76.4	73.4	70.5	20.5	19.5	18.7	(0.31,0.65)

[a] Doping concentration. [b] Power efficiency. [c] Current efficiency. [d] External quantum efficiency.

Details for the fabrication of phosphorescent sensitized fluorescent (PSF) devices

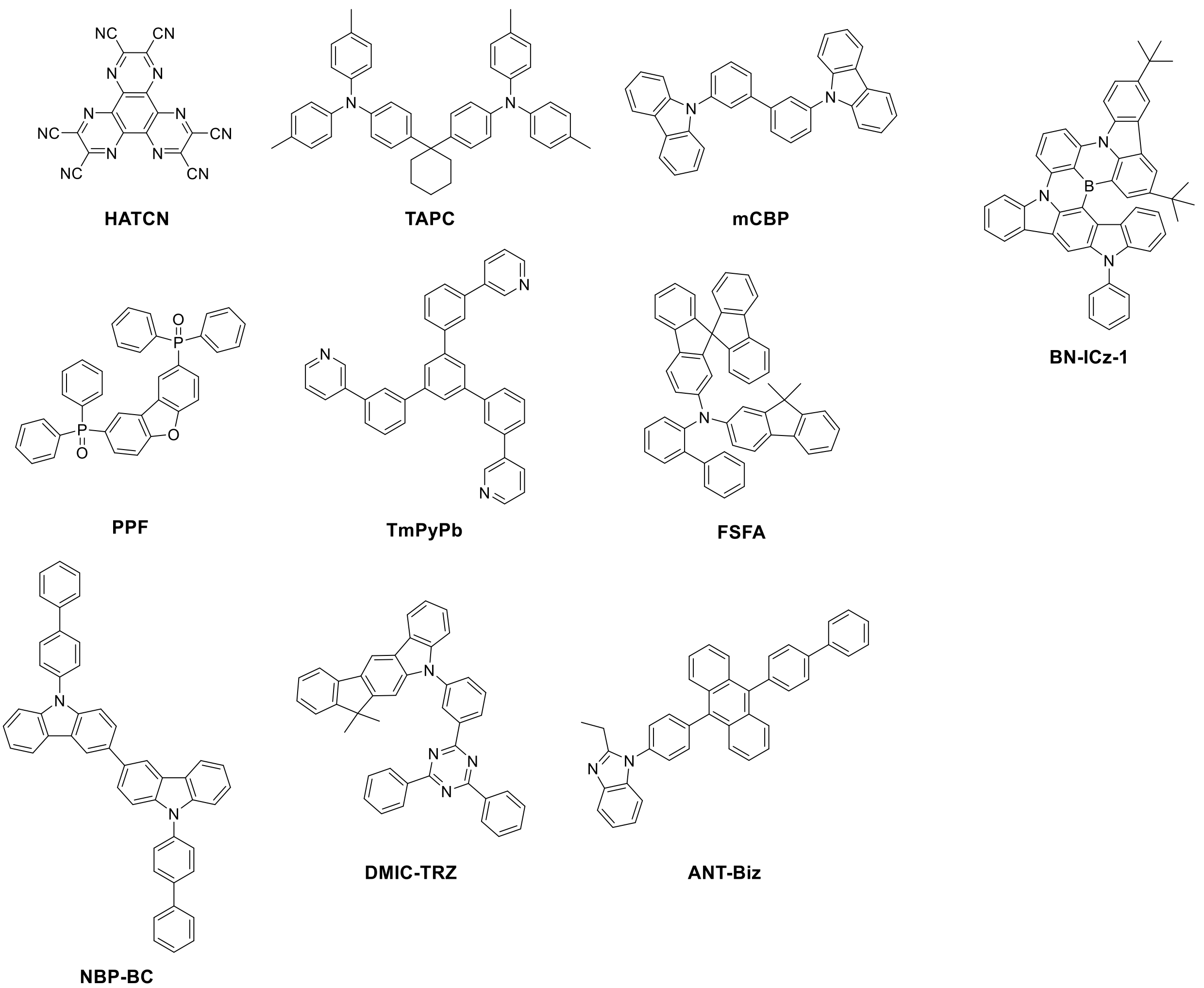


Figure S20. Chemical structures of the organic materials used in the PSF-OLEDs.

Device structure for EQE measurement:
ITO/HAT-CN (5 nm)/TAPC (40 nm)/mCBP(5 nm)/**Pt2**: **BN-ICz-1**: mCBP (25 nm)/PPF (10 nm)/TmPyPb (40 nm)/LiF (1.2 nm)/Al (100 nm)

Table S4. Electroluminescence data of PSF-OLED and fluorescent OLED for EQE measurement

Dopant(s) (Conc.)[a]	PE[b] (lm W^{-1})			CE[c] (cd A^{-1})			EQE[d] (%)			CIE (x,y) @1000 cd m^{-2}	FWHM (nm)
	1000 cd m^{-2}	5000 cd m^{-2}	10000 cd m^{-2}	1000 cd m^{-2}	5000 cd m^{-2}	10000 cd m^{-2}	1000 cd m^{-2}	5000 cd m^{-2}	10000 cd m^{-2}		
Pt2: BN-ICz-1 (10:1 wt%)	92.9	34.1	16.6	104	74.4	54.1	30.3	21.2	15.4	(0.29,0.67)	29
BN-ICz-1 (1 wt%)	27.8	4.34	1.54	34.7	12.4	6.89	9.20	3.45	1.85	(0.24,0.66)	23

[a] Doping concentration. [b] Power efficiency. [c] Current efficiency. [d] External quantum efficiency.

Device structure for operational lifetime measurement:

ITO/HAT-CN (10 nm)/FSFA (60 nm)/NBP-BC (5 nm)/**Pt2**: **BN-ICz-1**: DMIC-TRZ (30 nm)/ANT-Biz (5 nm)/ ANT-Biz: Liq (25 nm)/Liq (2 nm)/Al (100 nm)

Table S5. Electroluminescence data of the PSF-OLED for operating lifetime measurement

Dopants (Conc.)[a]	PE[b] (lm W^{-1})			CE[c] (cd A^{-1})			EQE[d] (%)			CIE (x,y) @1000 cd m^{-2}	FWHM (nm)
	1000 cd m^{-2}	5000 cd m^{-2}	10000 cd m^{-2}	1000 cd m^{-2}	5000 cd m^{-2}	10000 cd m^{-2}	1000 cd m^{-2}	5000 cd m^{-2}	10000 cd m^{-2}		
Pt2: BN-ICz-1 (10:1 wt%)	98.9	76.8	36.9	78.7	74.3	57.2	23.3	22.0	16.4	(0.30,0.66)	29

[a] Doping concentration. [b] Power efficiency. [c] Current efficiency. [d] External quantum efficiency.

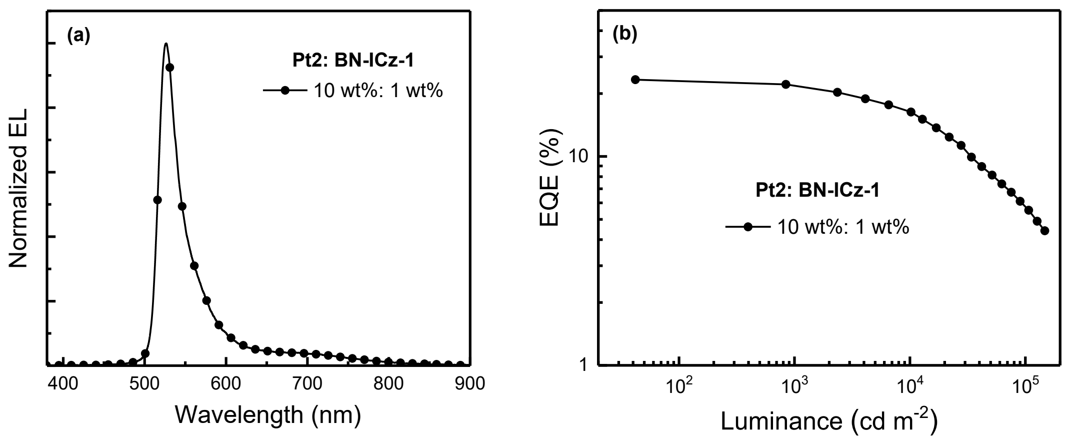


Figure S21. (a) Normalized EL spectra and (b) EQE-luminance characteristics of the PSF-OLED for operating lifetime measurement.

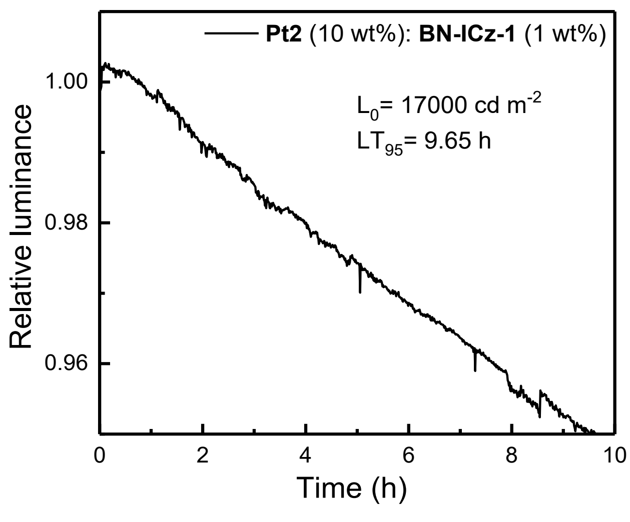


Figure S22. Operational lifetime of the PSF-OLED at an initial luminance of 17000 cd m^{-2}.

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Cartesian Coordinates of Optimized Ground-State Structures

Pt1

Pt	-0.344751	-1.295095	-0.328526
N	1.556950	-0.780972	-0.017567
N	-2.340574	-1.230544	-0.733559
O	-0.039602	-3.303638	-0.040087
C	1.063107	-3.760305	0.482136
C	1.037439	-5.131283	0.858337
H	0.114939	-5.662592	0.643565
C	2.090799	-5.755178	1.482620
H	2.010634	-6.802043	1.764781
C	3.252546	-5.027638	1.775565
H	4.079075	-5.484967	2.309955
C	3.324201	-3.707482	1.388148
C	2.284008	-3.030726	0.704075
C	2.555279	-1.640734	0.298878
C	3.877471	-1.159028	0.246075
C	4.166586	0.174645	-0.007339
C	3.094609	1.049663	-0.228378
H	3.270500	2.097547	-0.443612
C	1.806600	0.557749	-0.256625
C	0.610298	1.351676	-0.567400
C	0.485495	2.722885	-0.806008
C	-0.774405	3.255501	-1.104292
H	-0.865708	4.323242	-1.278844
C	-1.918045	2.454570	-1.190094
C	-1.799289	1.080012	-0.965966
C	-0.542033	0.563106	-0.641281
C	-2.819873	0.031058	-0.997418
C	-4.174696	0.225978	-1.219552
H	-4.536521	1.229818	-1.412846
C	-5.067567	-0.842844	-1.144626
C	-4.548438	-2.117320	-0.902382
H	-5.201791	-2.978732	-0.820266
C	-3.186009	-2.266147	-0.703711
H	-2.736007	-3.229636	-0.488139
H	4.697577	-1.843275	0.411632
H	4.214981	-3.153589	1.662261

H	1.345655	3.386582	-0.762893
H	-2.876643	2.911734	-1.425206
C	-6.520897	-0.613576	-1.270965
C	-7.283610	-1.357557	-2.175695
C	-7.159472	0.360702	-0.478397
C	-8.641372	-1.108593	-2.339373
C	-8.523408	0.606332	-0.648643
C	-9.257972	-0.114122	-1.582561
H	-9.214406	-1.683076	-3.060705
H	-8.998785	1.359577	-0.027671
C	5.562226	0.656164	-0.047406
C	5.882285	1.926379	0.451835
C	6.572302	-0.144793	-0.576077
C	7.191897	2.394364	0.432469
H	5.092114	2.530167	0.884044
C	7.900645	0.292971	-0.612726
H	6.311705	-1.114421	-0.990504
C	8.183024	1.559337	-0.104628
H	9.206297	1.917783	-0.122271
C	8.975364	-0.618100	-1.207539
C	8.640810	-0.899008	-2.679672
H	7.669531	-1.391063	-2.789396
H	8.613083	0.029515	-3.259593
H	9.398387	-1.555046	-3.123137
C	10.369166	0.007332	-1.140291
H	10.675112	0.212403	-0.108740
H	11.101752	-0.683629	-1.569945
H	10.425820	0.941677	-1.709042
C	9.002696	-1.942307	-0.430025
H	9.234067	-1.772320	0.626808
H	8.043284	-2.466166	-0.483182
H	9.767702	-2.609466	-0.842901
C	7.583880	3.767312	0.980216
C	8.587046	3.586685	2.128901
H	9.495532	3.073496	1.798833
H	8.882851	4.561652	2.532574
H	8.148501	3.000294	2.943142
C	6.378727	4.544539	1.511634
H	5.632813	4.724388	0.729839

H	5.889376	4.023310	2.341281
H	6.706790	5.520346	1.884347
C	8.233702	4.592931	-0.139812
H	8.523139	5.580841	0.235966
H	9.133974	4.110792	-0.532879
H	7.539396	4.736559	-0.974432
H	-10.318431	0.086546	-1.703435
C	-5.773483	0.307999	1.515866
C	-6.360352	2.462915	0.467711
C	-6.377154	-0.847120	2.021789
C	-6.449365	3.128990	-0.764088
C	-5.696895	-1.650850	2.930974
H	-7.374882	-1.116918	1.689330
C	-3.821446	-0.148388	2.866338
C	-6.366414	4.516032	-0.820602
H	-6.593276	2.556398	-1.675210
C	-6.101214	4.605536	1.562915
C	-4.416638	-1.309791	3.357205
H	-6.177160	-2.548515	3.310329
H	-2.816667	0.123789	3.176490
C	-6.184515	5.265555	0.338209
H	-6.438185	5.010876	-1.785240
H	-5.972324	5.173909	2.479870
H	-3.884470	-1.941715	4.061543
H	-6.113131	6.347679	0.289588
N	-6.436167	1.062920	0.520125
H	-6.789568	-2.112512	-2.781096
C	-4.488522	0.655808	1.951141
H	-4.005238	1.541329	1.551937
C	-6.196279	3.221939	1.635426
H	-6.142556	2.721432	2.596417

Pt2

Pt	-0.479360	1.449144	-0.578381
N	1.455259	0.966821	-0.591391
N	-2.513217	1.349973	-0.631732
O	-0.169982	3.434131	-0.157833
C	1.010689	3.977131	-0.250543
C	1.036627	5.396827	-0.177168

H	0.076474	5.879229	-0.019469
C	2.188133	6.132256	-0.325102
H	2.147809	7.217683	-0.278297
C	3.403784	5.476354	-0.562943
H	4.318126	6.036400	-0.730915
C	3.418995	4.099149	-0.598673
C	2.268154	3.294678	-0.408378
C	2.475810	1.836238	-0.395586
C	3.761746	1.302752	-0.186466
C	4.019562	-0.057975	-0.278958
C	2.949661	-0.910962	-0.580384
H	3.098346	-1.982662	-0.647801
C	1.677687	-0.392982	-0.706834
C	0.462813	-1.190704	-0.919724
C	0.319512	-2.569898	-1.093819
C	-0.963225	-3.115371	-1.224816
H	-1.068432	-4.188064	-1.356322
C	-2.115597	-2.324633	-1.174516
C	-1.980500	-0.944077	-1.004005
C	-0.695135	-0.407204	-0.892163
C	-3.008139	0.087438	-0.858683
C	-4.378811	-0.125824	-0.892287
H	-4.744511	-1.127543	-1.085792
C	-5.267207	0.921448	-0.648367
C	-4.733954	2.198488	-0.442876
H	-5.377855	3.046982	-0.239016
C	-3.360138	2.368431	-0.448108
H	-2.897607	3.335183	-0.278002
H	4.578209	1.968963	0.053081
H	4.362611	3.615464	-0.825037
H	1.183023	-3.230300	-1.122134
H	-3.091796	-2.796621	-1.251855
C	-6.724255	0.687115	-0.565956
C	-7.615498	1.536731	-1.229349
C	-7.253107	-0.378561	0.189089
C	-8.987213	1.315571	-1.183725
C	-8.628710	-0.592571	0.239926
C	-9.495582	0.244096	-0.454796
H	-9.658109	1.978058	-1.722081

H	-9.005396	-1.412533	0.843634
C	5.378186	-0.592152	-0.055508
C	5.838419	-1.682168	-0.807197
C	6.213988	-0.020421	0.901602
C	7.117171	-2.194766	-0.615814
H	5.187826	-2.103698	-1.565424
C	7.505412	-0.510639	1.123140
H	5.838248	0.802621	1.502397
C	7.931409	-1.592057	0.354647
H	8.929290	-1.987541	0.508416
C	8.383973	0.142061	2.191350
C	7.699820	0.005985	3.559454
H	6.719205	0.491415	3.574210
H	7.555935	-1.047156	3.822922
H	8.313425	0.471340	4.339166
C	9.767876	-0.502739	2.277943
H	10.317252	-0.418657	1.334048
H	10.359292	0.001294	3.049259
H	9.708725	-1.562189	2.549379
C	8.565208	1.630415	1.858770
H	9.044870	1.759234	0.882743
H	7.609280	2.162822	1.835657
H	9.195027	2.114107	2.613883
C	7.661406	-3.374410	-1.422641
C	8.914660	-2.929280	-2.190473
H	9.702712	-2.579904	-1.516203
H	9.320574	-3.764371	-2.772595
H	8.680776	-2.113932	-2.883049
C	6.642222	-3.904931	-2.431753
H	5.731242	-4.264180	-1.940910
H	6.360313	-3.143165	-3.166375
H	7.074032	-4.747918	-2.980985
C	8.029750	-4.515832	-0.463313
H	8.424534	-5.370713	-1.023917
H	8.793253	-4.211133	0.259094
H	7.152939	-4.853619	0.099180
H	-10.565973	0.067239	-0.413140
H	-7.217175	2.359619	-1.816094
C	-6.097134	-2.550303	0.542257

C	-5.508089	-0.850415	1.909130
C	-6.669196	-3.332028	-0.459744
C	-5.007528	-3.009962	1.320258
C	-5.409571	0.375739	2.562532
C	-4.630987	-1.921569	2.193185
C	-6.142603	-4.603484	-0.660083
H	-7.491903	-2.960467	-1.062403
C	-4.499291	-4.291590	1.098636
C	-4.396497	0.520357	3.501908
H	-6.090478	1.189987	2.337336
C	-3.623055	-1.751286	3.144954
C	-5.072599	-5.082198	0.110168
H	-6.569318	-5.236247	-1.432932
H	-3.658799	-4.656921	1.681727
C	-3.509508	-0.527707	3.790524
H	-4.287484	1.468465	4.020361
H	-2.932918	-2.560251	3.366351
H	-4.685962	-6.080072	-0.073694
H	-2.724432	-0.375847	4.524774
N	-6.396690	-1.243657	0.913248

Pt3

Pt	-0.470134	1.337315	-0.597806
N	1.481079	0.926748	-0.611436
N	-2.498897	1.163215	-0.662007
O	-0.235925	3.317938	-0.110665
C	0.924031	3.906606	-0.182377
C	0.897904	5.323509	-0.066728
H	-0.079562	5.765598	0.102354
C	2.021868	6.104736	-0.190242
H	1.941493	7.186117	-0.111852
C	3.261257	5.501308	-0.444001
H	4.154552	6.099303	-0.593378
C	3.327198	4.127125	-0.519096
C	2.206337	3.276039	-0.355438
C	2.467761	1.826608	-0.383045
C	3.771208	1.335076	-0.179525
C	4.079597	-0.012154	-0.309117
C	3.043469	-0.894520	-0.642366

H	3.231359	-1.957717	-0.739459
C	1.754089	-0.420105	-0.763310
C	0.570807	-1.255393	-1.006801
C	0.478755	-2.634918	-1.211394
C	-0.782401	-3.223941	-1.360813
H	-0.847897	-4.297280	-1.511367
C	-1.963207	-2.476701	-1.301115
C	-1.878913	-1.095892	-1.103823
C	-0.614890	-0.515159	-0.969947
C	-2.944601	-0.108082	-0.934074
C	-4.307018	-0.370940	-0.976017
H	-4.638604	-1.378884	-1.197064
C	-5.233439	0.627722	-0.680206
C	-4.749535	1.914575	-0.423678
H	-5.422347	2.727920	-0.177707
C	-3.383634	2.139661	-0.433813
H	-2.958002	3.116254	-0.227695
H	4.560552	2.024139	0.085262
H	4.288179	3.684706	-0.756756
H	1.365902	-3.262855	-1.246377
H	-2.921664	-2.982329	-1.387278
C	-6.673129	0.295226	-0.554184
C	-7.661283	0.941555	-1.319226
C	-7.055537	-0.706729	0.360133
C	-8.993768	0.550615	-1.160374
C	-8.389324	-1.072933	0.508572
C	-9.360070	-0.444257	-0.261761
H	-9.755670	1.036357	-1.764287
H	-8.647113	-1.839592	1.232270
C	5.455194	-0.503459	-0.090686
C	5.958376	-1.556305	-0.867529
C	6.264164	0.070760	0.887731
C	7.252674	-2.029601	-0.679747
H	5.328512	-1.979250	-1.642182
C	7.570371	-0.380230	1.106037
H	5.856085	0.863845	1.507464
C	8.039092	-1.425160	0.312368
H	9.049259	-1.789526	0.462995
C	8.417599	0.272939	2.199012

C	7.728615	0.074536	3.557086
H	6.731244	0.524376	3.577229
H	7.620267	-0.990008	3.790000
H	8.319580	0.539174	4.354507
C	9.822723	-0.325071	2.279502
H	10.375557	-0.195893	1.342783
H	10.390347	0.178036	3.069078
H	9.798970	-1.393003	2.521491
C	8.548376	1.775417	1.909006
H	9.032500	1.947828	0.941949
H	7.574123	2.273592	1.889824
H	9.153045	2.260451	2.683561
C	7.842504	-3.168511	-1.512639
C	9.081856	-2.659155	-2.262854
H	9.853343	-2.297952	-1.575791
H	9.520812	-3.464119	-2.863160
H	8.821255	-1.835933	-2.936308
C	6.847389	-3.710781	-2.539435
H	5.947476	-4.113292	-2.061926
H	6.542003	-2.942437	-3.257624
H	7.311349	-4.524809	-3.105864
C	8.248061	-4.319256	-0.579869
H	8.676735	-5.144741	-1.159319
H	8.996380	-4.005056	0.154211
H	7.381589	-4.702984	-0.030982
H	-10.403394	-0.726268	-0.157282
C	-5.574621	-2.635295	0.875574
C	-5.241821	-0.751940	2.075271
C	-6.035278	-3.582736	-0.036742
C	-4.413015	-2.849066	1.655912
C	-5.334266	0.524699	2.624143
C	-4.200636	-1.642819	2.423316
C	-5.318521	-4.770139	-0.144885
H	-6.918993	-3.398516	-0.639630
C	-3.713329	-4.050397	1.527483
C	-4.346708	0.907812	3.523136
H	-6.142814	1.195369	2.351816
C	-3.221531	-1.233676	3.331334
C	-4.172609	-5.005764	0.628998

H	-5.655568	-5.528833	-0.845425
H	-2.813888	-4.227073	2.110150
C	-3.298784	0.042921	3.872066
H	-4.386103	1.900847	3.961354
H	-2.407536	-1.900344	3.601017
H	-3.635810	-5.943082	0.517892
H	-2.539456	0.378973	4.571379
N	-6.070942	-1.364576	1.142137
C	-7.316040	2.008653	-2.319548
H	-7.195611	2.986998	-1.840480
H	-6.382355	1.790178	-2.844712
H	-8.111158	2.107829	-3.063034

Pt4

Pt	0.343174	-0.921328	-0.102441
N	2.319384	-0.811858	0.141712
N	-1.643366	-0.473488	-0.142214
O	0.372226	-2.771357	-0.989702
C	1.434168	-3.525211	-0.964617
C	1.238404	-4.868687	-1.387299
H	0.234118	-5.118235	-1.716715
C	2.234984	-5.814445	-1.357447
H	2.025132	-6.833005	-1.674446
C	3.509743	-5.464113	-0.891524
H	4.299683	-6.204242	-0.813244
C	3.743207	-4.159806	-0.514042
C	2.762567	-3.138280	-0.567049
C	3.202051	-1.780051	-0.203941
C	4.571568	-1.452710	-0.196797
C	5.033107	-0.221611	0.248146
C	4.088601	0.715391	0.687540
H	4.397344	1.696964	1.028899
C	2.744139	0.419755	0.604484
C	1.658325	1.351139	0.936533
C	1.722334	2.656171	1.432306
C	0.537530	3.379355	1.615365
H	0.594108	4.395422	1.994158
C	-0.716457	2.841558	1.307528
C	-0.788638	1.534938	0.817129

C	0.398350	0.816347	0.651194
C	-1.948476	0.764041	0.370030
C	-3.267256	1.194276	0.402758
H	-3.489781	2.164456	0.831902
C	-4.283010	0.403226	-0.128612
C	-3.944523	-0.850881	-0.645119
H	-4.694078	-1.507424	-1.071620
C	-2.620398	-1.252151	-0.620301
H	-2.304452	-2.216639	-1.003445
H	5.291643	-2.178972	-0.546276
H	4.724405	-3.922083	-0.118665
H	2.673919	3.126122	1.669564
H	-1.606701	3.452643	1.434418
C	-5.674319	0.905807	-0.172341
C	-6.741142	0.158397	0.354585
C	-5.966568	2.153089	-0.756502
C	-8.049130	0.637873	0.295265
C	-7.274708	2.625994	-0.818805
C	-8.315398	1.867930	-0.293336
H	-8.844495	0.040913	0.730058
H	-7.460786	3.583561	-1.294673
C	6.475799	0.094880	0.247361
C	7.029553	0.859709	1.283336
C	7.298614	-0.362367	-0.779822
C	8.386994	1.162671	1.302917
H	6.383664	1.188269	2.090014
C	8.667836	-0.075204	-0.794726
H	6.855875	-0.928071	-1.594593
C	9.185021	0.684127	0.252947
H	10.244013	0.917138	0.261450
C	9.530309	-0.588729	-1.948639
C	9.018097	0.010584	-3.266589
H	7.976983	-0.264287	-3.461627
H	9.077636	1.103938	-3.249304
H	9.620993	-0.349955	-4.107754
C	11.002804	-0.209218	-1.786833
H	11.433511	-0.626248	-0.870091
H	11.577948	-0.604446	-2.630486
H	11.145866	0.876582	-1.771709

C	9.431165	-2.119933	-2.012882
H	9.785711	-2.575677	-1.082339
H	8.403007	-2.455463	-2.180089
H	10.043439	-2.505883	-2.835659
C	9.030955	1.983635	2.421141
C	10.109665	1.139049	3.114979
H	10.896896	0.831238	2.419838
H	10.582605	1.713129	3.919826
H	9.676789	0.233341	3.552542
C	8.014139	2.424129	3.475026
H	7.227714	3.053555	3.044656
H	7.539594	1.568938	3.967851
H	8.518740	3.011373	4.249162
C	9.675866	3.240828	1.819265
H	10.145212	3.840941	2.607043
H	10.449346	2.992190	1.086175
H	8.927519	3.863540	1.317748
H	-9.334492	2.238210	-0.339778
C	-4.366895	4.049193	-0.672806
C	-4.092394	2.561631	-2.352085
C	-4.804124	4.722120	0.466227
C	-3.170305	4.402841	-1.340615
C	-4.228566	1.494157	-3.235652
C	-2.996489	3.451711	-2.415136
C	-4.026281	5.781474	0.922333
H	-5.715474	4.428953	0.978184
C	-2.410210	5.471828	-0.862401
C	-3.230721	1.320637	-4.186723
H	-5.075119	0.817797	-3.175587
C	-2.009394	3.257616	-3.383788
C	-2.844793	6.156536	0.266163
H	-4.342096	6.326823	1.807003
H	-1.484757	5.751854	-1.357210
C	-2.131711	2.189122	-4.261771
H	-3.302746	0.490740	-4.883580
H	-1.154829	3.925636	-3.440229
H	-2.261188	6.987836	0.649945
H	-1.367046	2.018649	-5.013251
N	-4.922272	2.939445	-1.300730

N	-6.491724	-1.088044	0.970095
C	-5.707178	-1.299266	2.099036
C	-6.898561	-2.319473	0.469867
C	-5.092751	-0.365832	2.930363
C	-5.604218	-2.690162	2.329601
C	-7.661901	-2.599327	-0.661800
C	-6.366148	-3.343221	1.288888
C	-4.346752	-0.851869	3.996704
H	-5.188389	0.699682	2.749418
C	-4.852380	-3.151796	3.412411
C	-7.904554	-3.936637	-0.954949
H	-8.052977	-1.803884	-1.288503
C	-6.626823	-4.677519	0.970814
C	-4.223471	-2.228351	4.236449
H	-3.847224	-0.148448	4.656349
H	-4.758220	-4.217144	3.602612
C	-7.397378	-4.965562	-0.148578
H	-8.498433	-4.186926	-1.829286
H	-6.226335	-5.477572	1.586946
H	-3.628182	-2.572653	5.076513
H	-7.606391	-5.999196	-0.407082

Cartesian Coordinates of Optimized T_1 State Structures

Pt1

Pt	-0.31287200	-1.33875200	-0.32851600
N	1.57390200	-0.82644100	-0.00571400
N	-2.31918100	-1.29262500	-0.68585000
O	0.10515300	-3.36983500	-0.14799400
C	1.20463600	-3.84462700	0.31887600
C	1.19253300	-5.25354600	0.56919400
H	0.28478800	-5.77436000	0.28227700
C	2.24255900	-5.90005500	1.17620600
H	2.20282800	-6.96622200	1.37269900
C	3.34973900	-5.13776800	1.56732200
H	4.17726800	-5.60693600	2.09052900
C	3.40708700	-3.76927700	1.30476700
C	2.40332800	-3.07259100	0.62121700
C	2.63594100	-1.66357600	0.26201500
C	3.92889400	-1.16379500	0.21914400

C	4.21351700	0.19902300	0.01284600
C	3.09197800	1.04942700	-0.13065800
H	3.22727400	2.11361800	-0.29277100
C	1.81684700	0.54693300	-0.15435100
C	0.59919200	1.32987900	-0.38781300
C	0.43304100	2.71091000	-0.52039600
C	-0.84375900	3.23517800	-0.76031900
H	-0.95761400	4.31144400	-0.85148500
C	-1.97634800	2.42344000	-0.88984400
C	-1.82250200	1.03930100	-0.76919600
C	-0.54847400	0.53460500	-0.50856500
C	-2.82710700	-0.02301000	-0.86335700
C	-4.17943900	0.16870800	-1.07448000
H	-4.54804400	1.17861600	-1.21263800
C	-5.06692100	-0.91360800	-1.08001300
C	-4.52221400	-2.19309700	-0.91983700
H	-5.15938400	-3.07050700	-0.89931200
C	-3.15999000	-2.33764300	-0.72981500
H	-2.70697000	-3.31211800	-0.58303900
H	4.75500500	-1.84613900	0.37291900
H	4.27370400	-3.22528400	1.65969100
H	1.27730100	3.39058600	-0.43510900
H	-2.94621200	2.87724300	-1.07889200
C	-6.51758200	-0.70548800	-1.22616900
C	-7.25879900	-1.50460500	-2.10539700
C	-7.19152900	0.29378800	-0.49254600
C	-8.61780000	-1.29300100	-2.29967500
C	-8.55733100	0.50230500	-0.69461400
C	-9.26630500	-0.27603400	-1.60099900
H	-9.16710900	-1.91226900	-3.00231900
H	-9.05541300	1.27540100	-0.11727800
C	5.58501000	0.70013800	-0.03827900
C	5.87720000	2.03825600	0.29399700
C	6.64930100	-0.13145200	-0.41241700
C	7.17462500	2.53151300	0.25886700
H	5.06665500	2.68189100	0.61544900
C	7.96757800	0.32917400	-0.45030800
H	6.43608400	-1.15242100	-0.71522600
C	8.21137200	1.66016800	-0.11362400

H	9.22674200	2.03872100	-0.13961000
C	9.08440100	-0.62957200	-0.87070500
C	8.81758600	-1.12721100	-2.29869300
H	7.86310900	-1.65712100	-2.37358700
H	8.79028000	-0.29087400	-3.00509700
H	9.60821600	-1.81660900	-2.61716400
C	10.46214000	0.03414500	-0.84511400
H	10.72387500	0.39204200	0.15644600
H	11.22543600	-0.69100300	-1.14661700
H	10.51976100	0.88030800	-1.53808900
C	9.11187800	-1.82807900	0.08904400
H	9.30089700	-1.50164600	1.11725500
H	8.16436600	-2.37571500	0.08165200
H	9.90440000	-2.52937900	-0.19688500
C	7.51282600	3.97906700	0.62192100
C	8.48248300	3.99269300	1.81270100
H	9.41478400	3.46715700	1.58422500
H	8.73871500	5.02313700	2.08517000
H	8.03344900	3.51104900	2.68778100
C	6.27349900	4.78929500	1.00469800
H	5.54958900	4.83742400	0.18410200
H	5.76967600	4.37348500	1.88376800
H	6.56574900	5.81642600	1.24748700
C	8.17788100	4.66029500	-0.58330500
H	8.43277300	5.69889700	-0.34241000
H	9.09994500	4.15159600	-0.88086000
H	7.50644100	4.66655800	-1.44847300
H	-10.32835700	-0.10185600	-1.74603100
C	-5.84997700	0.39431500	1.53543100
C	-6.48561300	2.46563600	0.35885100
C	-6.40725500	-0.77294600	2.06671700
C	-6.53071300	3.06081900	-0.91098300
C	-5.72702600	-1.49044200	3.04504300
H	-7.36887300	-1.11952300	1.70103400
C	-3.94470600	0.12085900	2.99860500
C	-6.50201200	4.44523200	-1.03930500
H	-6.59624300	2.43414000	-1.79517700
C	-6.37855300	4.67181300	1.34737000
C	-4.49373300	-1.05078500	3.51740800

H	-6.17187500	-2.39804700	3.44358800
H	-2.97608000	0.47052600	3.34418400
C	-6.41875100	5.26167600	0.08516600
H	-6.53712300	4.88499000	-2.03220300
H	-6.32681600	5.29330100	2.23707300
H	-3.96345900	-1.61401600	4.27918900
H	-6.38967400	6.34184600	-0.01898700
N	-6.50772200	1.06704600	0.48146100
H	-6.74242900	-2.27391600	-2.67286200
C	-4.61022200	0.83855200	2.01306600
H	-4.15814000	1.73134700	1.59392800
C	-6.41994300	3.29099000	1.49057600
H	-6.40029000	2.84410100	2.47895300

Pt2

Pt	-0.41226800	1.51623200	-0.47911700
N	1.51994500	1.00492500	-0.51005700
N	-2.42977300	1.48125800	-0.50727900
O	-0.01413400	3.49382700	-0.13635400
C	1.16403200	4.02466700	-0.23800400
C	1.18420500	5.44730300	-0.18426200
H	0.22786300	5.92844800	-0.00767400
C	2.33575700	6.17448400	-0.38663900
H	2.31513900	7.25925700	-0.35891400
C	3.52122700	5.48868800	-0.65733200
H	4.43817000	6.03166400	-0.86254200
C	3.53691400	4.09598800	-0.67230100
C	2.40612700	3.30945300	-0.42059700
C	2.58341300	1.83934600	-0.36337000
C	3.85550900	1.29395700	-0.17812200
C	4.08874200	-0.08072100	-0.24046700
C	2.98231600	-0.90541200	-0.49652000
H	3.09680300	-1.98245300	-0.54426500
C	1.72052800	-0.36335000	-0.60592300
C	0.48278300	-1.13581000	-0.77903600
C	0.31709300	-2.51142700	-0.92998200
C	-0.98522400	-3.02689100	-1.03963300
H	-1.11299000	-4.09903400	-1.15825500
C	-2.12686200	-2.22047700	-0.98776900

C	-1.97724700	-0.83965000	-0.83271400
C	-0.66788200	-0.33873000	-0.74626000
C	-2.97909100	0.21007100	-0.69231800
C	-4.34093300	0.02014100	-0.69850700
H	-4.70869400	-0.98255200	-0.88034900
C	-5.23970100	1.08744100	-0.49788300
C	-4.65099600	2.37067000	-0.34048800
H	-5.26834300	3.24547900	-0.16665100
C	-3.28696300	2.51932200	-0.34592100
H	-2.82265500	3.48917100	-0.20313700
H	4.69252300	1.95274700	0.00770200
H	4.47478000	3.61065100	-0.91373800
H	1.16448500	-3.19101600	-0.95990000
H	-3.10864200	-2.68196200	-1.05267800
C	-6.68567600	0.89862300	-0.44839200
C	-7.54935200	1.88961800	-0.95635100
C	-7.29807400	-0.24993900	0.11494600
C	-8.92701000	1.73457400	-0.95414600
C	-8.68184400	-0.40060300	0.11651200
C	-9.50555800	0.57915800	-0.42800800
H	-9.55422400	2.51403000	-1.37751100
H	-9.10225400	-1.29106000	0.57500300
C	5.43620100	-0.63907500	-0.04570100
C	5.82631600	-1.80058300	-0.73105300
C	6.34424200	-0.02576400	0.81876500
C	7.09536200	-2.34256300	-0.56348800
H	5.12806200	-2.25559800	-1.42445400
C	7.63019500	-0.54111500	1.00956000
H	6.02915400	0.85066200	1.37797700
C	7.98121700	-1.69508900	0.31136100
H	8.97282000	-2.11255200	0.44532600
C	8.58705000	0.16460200	1.97205800
C	7.97138200	0.17891400	3.37878800
H	7.01223900	0.70541100	3.39887300
H	7.80087200	-0.83993600	3.74202700
H	8.64298000	0.68329700	4.08277000
C	9.94851500	-0.52749900	2.04991500
H	10.45251200	-0.54790400	1.07764100
H	10.59657700	0.01565200	2.74546900

H	9.86294200	-1.55642200	2.41526300
C	8.80724700	1.60837600	1.49697400
H	9.24559900	1.62839300	0.49355900
H	7.87039800	2.17336400	1.46458300
H	9.48829200	2.13315300	2.17646000
C	7.55610200	-3.60190100	-1.29888700
C	8.77864100	-3.26624600	-2.16552700
H	9.61443800	-2.89449700	-1.56478000
H	9.12339700	-4.15938400	-2.69887900
H	8.53356600	-2.50005700	-2.90857700
C	6.46674900	-4.17509300	-2.20625500
H	5.57242300	-4.45828600	-1.64070700
H	6.17065300	-3.46701800	-2.98758200
H	6.84007400	-5.07614400	-2.70372800
C	7.93965300	-4.67537700	-0.26971800
H	8.27715600	-5.58559800	-0.77821000
H	8.74954800	-4.34107200	0.38588800
H	7.08401500	-4.93613200	0.36208200
H	-10.58323100	0.44996900	-0.42461500
H	-7.11281300	2.77734900	-1.40459500
C	-6.29740800	-2.53145900	0.21468300
C	-5.68190100	-1.07772800	1.82458700
C	-6.85605100	-3.13030200	-0.91392400
C	-5.31386700	-3.18440300	0.99839500
C	-5.53569800	0.04564100	2.63611600
C	-4.92040100	-2.25177500	2.02900600
C	-6.42660400	-4.41133900	-1.23990600
H	-7.59460000	-2.61008600	-1.51541500
C	-4.90213300	-4.47255900	0.64805100
C	-4.60064600	-0.02287200	3.65999900
H	-6.12083500	0.94230300	2.46210800
C	-3.98852300	-2.29525500	3.06916800
C	-5.46341200	-5.07956900	-0.46874700
H	-6.84495000	-4.90254200	-2.11380100
H	-4.14633700	-4.98608600	1.23597800
C	-3.83274900	-1.17785400	3.87709800
H	-4.45749500	0.84040500	4.30353800
H	-3.39040100	-3.18673200	3.23574100
H	-5.15182400	-6.08039000	-0.75268900

H	-3.10670500	-1.19253800	4.68435700
N	-6.51513700	-1.26142400	0.72908900

Pt3

Pt	-0.47739700	1.37020900	-0.55365800
N	1.46088500	0.95959700	-0.59355200
N	-2.50863100	1.22738600	-0.62275900
O	-0.14688100	3.36288400	-0.05077500
C	0.99579400	3.94747300	-0.13342700
C	0.95699200	5.36978300	0.01374500
H	-0.01636500	5.79344300	0.23885600
C	2.07046300	6.15679700	-0.16393100
H	2.01213700	7.23559300	-0.06544100
C	3.27284700	5.53084100	-0.51178900
H	4.16078500	6.12459200	-0.70602900
C	3.35160900	4.14275200	-0.62621500
C	2.27083900	3.28740600	-0.38081200
C	2.50382500	1.83381600	-0.37714500
C	3.78509900	1.33704900	-0.18491700
C	4.09688900	-0.02884500	-0.30266800
C	3.02191300	-0.88242700	-0.64760600
H	3.18204700	-1.94995500	-0.75518200
C	1.74413100	-0.40148100	-0.76874500
C	0.54931700	-1.21442800	-1.02203500
C	0.43389600	-2.58657600	-1.25791000
C	-0.83570500	-3.15660900	-1.42112200
H	-0.91075700	-4.22576400	-1.59718300
C	-2.01204000	-2.40297900	-1.34639100
C	-1.91030100	-1.02899100	-1.11525900
C	-0.63880000	-0.47380400	-0.96656800
C	-2.97015300	-0.03878800	-0.91811600
C	-4.32779800	-0.29995800	-0.95220400
H	-4.65873100	-1.30294400	-1.19605900
C	-5.25979500	0.69181000	-0.62912300
C	-4.76542500	1.97318600	-0.35290800
H	-5.43226600	2.78469700	-0.08452400
C	-3.40124200	2.19783800	-0.36820500
H	-2.98370200	3.17347000	-0.14413800
H	4.58308000	2.03197000	0.04373400

H	4.29968100	3.71596900	-0.93033100
H	1.31223200	-3.22535300	-1.30908400
H	-2.97478900	-2.89683600	-1.44552700
C	-6.69272100	0.35135900	-0.48956200
C	-7.70170400	1.03586800	-1.19505100
C	-7.05837400	-0.70139800	0.37606600
C	-9.02980100	0.63423500	-1.02958800
C	-8.38818900	-1.07888200	0.53087800
C	-9.37680400	-0.41100200	-0.18160400
H	-9.80465600	1.15066400	-1.59020500
H	-8.62958900	-1.88442700	1.21718400
C	5.45252600	-0.53117200	-0.08844400
C	5.88846900	-1.71617700	-0.71398200
C	6.35781500	0.14873200	0.73710700
C	7.17406500	-2.20718200	-0.52920300
H	5.20681800	-2.23194100	-1.38029800
C	7.66126200	-0.31193000	0.93831400
H	6.02290100	1.03879700	1.26187900
C	8.05089400	-1.48897300	0.30022900
H	9.05690200	-1.86560700	0.44561700
C	8.60015900	0.47481700	1.85624300
C	8.00129900	0.52883100	3.26919000
H	7.02062000	1.01428800	3.27669800
H	7.87708100	-0.47881600	3.67960700
H	8.65847000	1.09221100	3.94188900
C	9.98972100	-0.15750900	1.94857100
H	10.48119400	-0.20586200	0.97090500
H	10.62439300	0.44389800	2.60802100
H	9.95014300	-1.17032400	2.36348400
C	8.75858000	1.90368100	1.31623800
H	9.18359100	1.89571100	0.30687700
H	7.79947300	2.42880600	1.27046900
H	9.42632700	2.48510200	1.96254000
C	7.66797900	-3.48921500	-1.20292900
C	8.87451100	-3.16419000	-2.09561700
H	9.70134800	-2.73462400	-1.52166900
H	9.24442100	-4.07313200	-2.58415800
H	8.60099900	-2.44598300	-2.87583700
C	6.59244400	-4.14320500	-2.07152000

H	5.71025700	-4.42248100	-1.48542000
H	6.26999300	-3.48577300	-2.88592800
H	6.99067400	-5.05751500	-2.52406500
C	8.09052500	-4.49654800	-0.12328200
H	8.45201700	-5.42254200	-0.58538100
H	8.89348200	-4.10389300	0.50803400
H	7.24690700	-4.74812500	0.52821300
H	-10.41721100	-0.70141400	-0.07137700
C	-5.58412700	-2.66255900	0.78373800
C	-5.21205100	-0.83285100	2.05194800
C	-6.06736300	-3.56696200	-0.16015400
C	-4.41482800	-2.92116600	1.53875200
C	-5.28088000	0.42202800	2.65200100
C	-4.17695300	-1.74879200	2.34970100
C	-5.36640800	-4.75726000	-0.32531900
H	-6.95588400	-3.34790000	-0.74397900
C	-3.73143900	-4.12426300	1.35313600
C	-4.27651700	0.75731500	3.55141500
H	-6.08428000	1.11252600	2.41670700
C	-3.18001800	-1.38762300	3.25858600
C	-4.21380700	-5.03747200	0.42337000
H	-5.72120200	-5.48282700	-1.05173900
H	-2.82620400	-4.33380900	1.91559800
C	-3.23427300	-0.13282600	3.85079400
H	-4.29832500	1.73221800	4.02993200
H	-2.37017700	-2.07374500	3.48906900
H	-3.68991800	-5.97577700	0.26765800
H	-2.46125600	0.16571300	4.55221000
N	-6.06091500	-1.39779700	1.10704900
C	-7.38190000	2.15300100	-2.14814400
H	-7.26807600	3.11038200	-1.62665000
H	-6.45153600	1.97010600	-2.69248200
H	-8.18708000	2.27608500	-2.87728100

Pt4

Pt	0.37392900	-0.92938800	-0.06931500
N	2.36102900	-0.81722100	0.14031700
N	-1.60082300	-0.51321800	-0.11052400
O	0.42999400	-2.82848600	-0.81791700

C	1.48274500	-3.58571100	-0.79680400
C	1.24762600	-4.94158800	-1.16009200
H	0.23443700	-5.18092800	-1.46585500
C	2.23042800	-5.90345000	-1.08810700
H	2.01413100	-6.93340100	-1.35342800
C	3.49908900	-5.53200100	-0.64020000
H	4.28562200	-6.27205300	-0.53352100
C	3.76625400	-4.20332400	-0.31952400
C	2.81731500	-3.17874100	-0.42334000
C	3.26267900	-1.79197800	-0.14584400
C	4.62388500	-1.47611300	-0.15597000
C	5.09397000	-0.21612400	0.21556600
C	4.13838000	0.73689200	0.59873300
H	4.43922000	1.73894300	0.88326900
C	2.79518500	0.43645500	0.53717400
C	1.70747500	1.38166900	0.82493300
C	1.78369900	2.70463400	1.25490800
C	0.59048500	3.43012900	1.41910700
H	0.65043000	4.46257300	1.75135800
C	-0.67081100	2.88636800	1.15726900
C	-0.76336100	1.55997800	0.72428700
C	0.43801700	0.84372400	0.58205900
C	-1.92262200	0.77264800	0.33041900
C	-3.22700100	1.20878300	0.34052000
H	-3.42697900	2.20238100	0.72532200
C	-4.28089200	0.39565200	-0.11305500
C	-3.92570400	-0.90832300	-0.54934300
H	-4.67403500	-1.59521600	-0.92674500
C	-2.61379900	-1.30930000	-0.53031700
H	-2.32200100	-2.29790100	-0.86741200
H	5.34120700	-2.23074200	-0.44756500
H	4.75826900	-3.97033300	0.04774700
H	2.73574800	3.18761400	1.45741900
H	-1.55400700	3.50842900	1.27553500
C	-5.65376000	0.89286700	-0.14680100
C	-6.75007700	0.11127100	0.29086600
C	-5.96234200	2.19022900	-0.63100100
C	-8.05499900	0.59356800	0.25007400
C	-7.26831600	2.66500100	-0.67217100

C	-8.32278300	1.87053700	-0.23153600
H	-8.85310600	-0.04025500	0.62469000
H	-7.44569900	3.65632800	-1.07806600
C	6.53208000	0.09787400	0.20497000
C	7.07261200	0.97200800	1.16107200
C	7.37635600	-0.46896400	-0.75039100
C	8.42970600	1.27407100	1.17228600
H	6.41628800	1.38725700	1.91780900
C	8.74633800	-0.18897600	-0.76867800
H	6.94957500	-1.11459000	-1.51263500
C	9.24738300	0.68041700	0.19840800
H	10.30688000	0.91026900	0.20213000
C	9.62960000	-0.82760800	-1.84180200
C	9.14879100	-0.37361300	-3.22785000
H	8.11111500	-0.66605900	-3.41571600
H	9.21204100	0.71508400	-3.32697500
H	9.76882900	-0.82339800	-4.01163200
C	11.10059300	-0.43782000	-1.69097800
H	11.50885000	-0.75204100	-0.72435800
H	11.69115800	-0.92622200	-2.47294500
H	11.24984400	0.64236400	-1.79327000
C	9.52390100	-2.35636000	-1.74094600
H	9.86015500	-2.70901700	-0.76014300
H	8.49662600	-2.70408700	-1.88817700
H	10.14789500	-2.83210000	-2.50586400
C	9.05577800	2.21244800	2.20524100
C	10.11379600	1.44572500	3.01216600
H	10.91216600	1.05799200	2.37197400
H	10.57472400	2.10418500	3.75713200
H	9.66534600	0.59724100	3.53958500
C	8.02084900	2.77370100	3.18120800
H	7.24707500	3.35350700	2.66646400
H	7.53125600	1.98179300	3.75799200
H	8.51345900	3.44275200	3.89423100
C	9.72274700	3.39056200	1.47989600
H	10.17709300	4.07480100	2.20536200
H	10.51195900	3.05705200	0.79911200
H	8.99063400	3.95492600	0.89272300
H	-9.34131600	2.24293800	-0.26249400

C	-4.41498100	4.13754200	-0.49353100
C	-4.11471200	2.71693000	-2.22014900
C	-4.85363700	4.75822200	0.67514900
C	-3.25612700	4.57256200	-1.18246000
C	-4.22281800	1.66859500	-3.13099800
C	-3.06574600	3.66223600	-2.28825100
C	-4.11884800	5.84356100	1.14017900
H	-5.73373800	4.40279800	1.20186900
C	-2.53916500	5.66679500	-0.69444700
C	-3.24920400	1.57567800	-4.11670200
H	-5.02826800	0.94522100	-3.06102900
C	-2.10218800	3.54906000	-3.29335400
C	-2.97644100	6.29765100	0.46433200
H	-4.43769300	6.34765900	2.04805400
H	-1.64456400	6.00943900	-1.20683900
C	-2.19868400	2.50264000	-4.20006500
H	-3.30055100	0.76252600	-4.83500800
H	-1.28583100	4.26302700	-3.35648900
H	-2.42705900	7.14888600	0.85531100
H	-1.45231600	2.39511300	-4.98131100
N	-4.92934100	3.02033200	-1.13614900
N	-6.52751900	-1.17683800	0.83400800
C	-5.78839400	-1.46062300	1.97471900
C	-6.95830200	-2.37042100	0.27282200
C	-5.16595100	-0.58252300	2.85965300
C	-5.73891000	-2.86270000	2.15327300
C	-7.69668000	-2.57907600	-0.89115100
C	-6.48867200	-3.44665200	1.06461800
C	-4.47180000	-1.13561100	3.92757500
H	-5.21319600	0.49087500	2.71176000
C	-5.03880200	-3.39227300	3.24005000
C	-7.97723100	-3.89356400	-1.24567100
H	-8.03895300	-1.74505600	-1.49556300
C	-6.78701300	-4.75681400	0.68484400
C	-4.40534400	-2.52427600	4.11870900
H	-3.96737600	-0.47619700	4.62794800
H	-4.98939900	-4.46697000	3.39192700
C	-7.53254800	-4.97235200	-0.46745100
H	-8.55254000	-4.08673600	-2.14667100

H	-6.43564500	-5.59494700	1.28035900
H	-3.85081700	-2.92119800	4.96371700
H	-7.77136500	-5.98656400	-0.77335500