Supporting Information

Strongly phosphorescent platinum(II) complexes supported by tetradentate benzazole-containing ligands

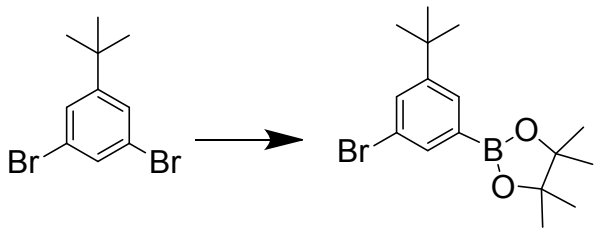
Bin Wang,† Feng Liang,† Hailiang Hu, Yuan Liu, Zhenhui Kang, Liang-Sheng Liao, and Jian Fan*

Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Institute of Functional Nano & Soft Materials (FUNSOM), and Collaborative Innovation Center of Suzhou Nano Science and Technology, Soochow University, Suzhou, Jiangsu 215123, China

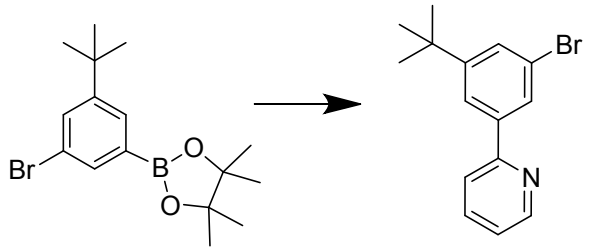
E-mail: jianfan@suda.edu.cn

Table of contents

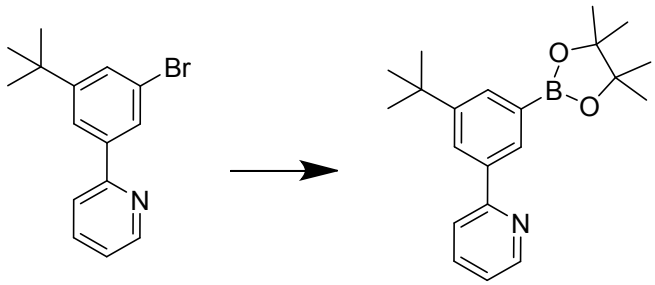
Synthesis



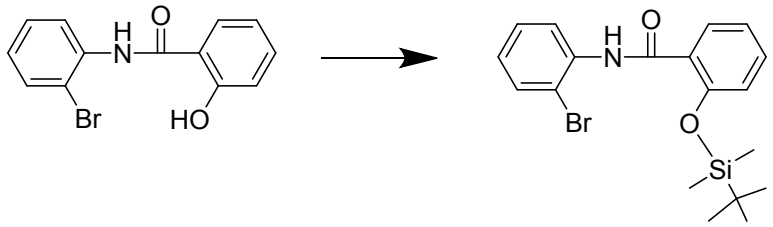
To a solution of 1,3-dibromo-5-(tert-butyl)benzene (1g, 3.4 mmol) in dry THF (50 mL) at -78 ºC under N_2, *n*-BuLi (2.6 mL, 1.6 M in hexane, 4.1mmol) was added slowly. The mixture was stirred for 2 hours before the addition of 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxoborolane (0.7 mL, 3.4 mmol). The resulting solution was stirred at room temperature overnight and then quenched with water (10 mL). The product was extracted with chloroform. The organic phase was washed with water and dried over $MgSO_4$. After removal of the solvent, the residue was used directly for the next step without any additional purification.



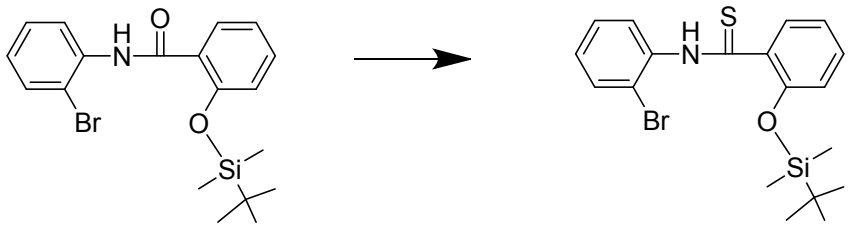
A solution of K_2CO_3 (3.3 g, 24 mmol) in 20 mL of degassed water was added to a solution of 2-(3-bromo-5-tert-butyl-phenyl)-4,4,5,5-tetramethyl-[1,3,2]dioxaborolane (2 g, 6 mmol), 2-bromopyridine (0.9 g, 5.7 mmol), and $Pd(PPh_3)_4$ (346 mg, 0.3 mmol) in 100 mL of toluene. The reaction mixture was heated to reflux overnight before cooling to room temperature. The water phase was extracted with DCM (3×100 mL), and the combined organic phase was washed with water and dried over $MgSO_4$. The crude product was purified by column chromatography (SiO_2, DCM:PE, 8:1) to afford a white solid (0.7 g, 40%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (m, 1H), 7.93 (m, 2H), 7.74 (m, 1H), 7.68 (dt, *J* = 8.0, 1.1 Hz, 1H), 7.56 (t, *J* = 1.8 Hz, 1H), 7.27 (m, 1H), 1.37 (s, 9H). GC-MS: m/z calcd 289.074, found 289.10.



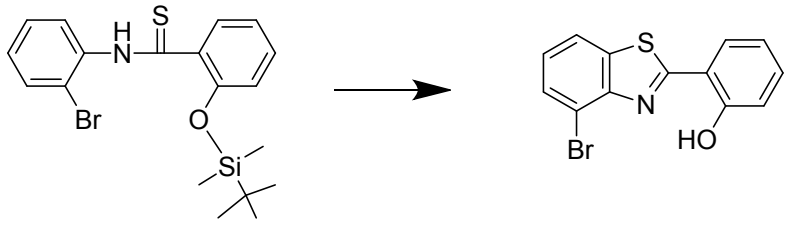
To a solution of 2-(3-bromo-5-(tert-butyl)phenyl)pyridine (2g, 6.9 mmol) in dry THF (50 mL) at -78 ºC under N_2, *n*-BuLi (5 mL, 1.6 M in hexane, 8 mmol) was added slowly. The mixture was stirred for 2 hours before the addition of 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxoborolane (1.54 g, 8.3 mmol). The resulting solution was stirred at room temperature overnight before quenched with water (10 mL). The product was extracted with chloroform. The organic phase was washed with water and dried over $MgSO_4$. After removal of the solvent, the residue was used directly for the next step without any additional purification.



N-(2-bromophenyl)-2-hydroxybenzamide (5 g, 17.2 mmol), tertbutyldimethylsilyl chloride (3.89 g, 25.8 mmol), and imidazole(1.75 g, 25.8 mmol) were dissolved in dry DCM (100 mL). The reaction mixture was stirred at room temperature overnight. The organic phase was washed with water and dried over $MgSO_4$. After removal of solvent, the residue was used directly for the next step without any additional purification.

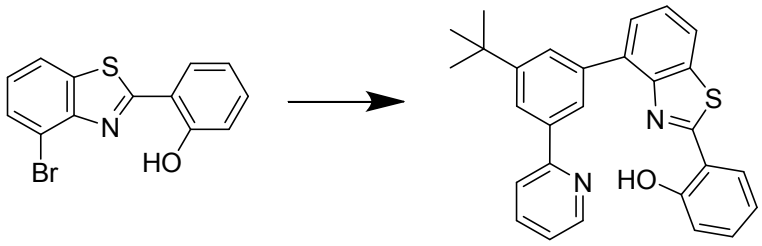


N-(2-bromophenyl)-2-((tert-butyldimethylsilyl)oxy)benzamide(5 g, 12.3 mmol) and Lawesson's reagent (7.49 g, 18.5 mmol) were suspended in 100 mL of dry toluene。The reaction mixture was heated to reflux for 10 hours. After evaporation of solvent under reduced pressure, the residue was purified by column chromatography (SiO_2, DCM:PE, 4:5) to afford a yellow solid (3.6 g, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.17 (s, 1H), 8.26 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.80 (m, 2H), 7.64 (dd, *J* = 8.7, 6.6 Hz, 2H), 7.37 (m, 1H), 7.14 (m, 1H), 6.91 (m, 1H), 1.04 (s, 9H), 0.23 (s, 6H). GC-MS: m/z calcd 421.053, found 421.075.

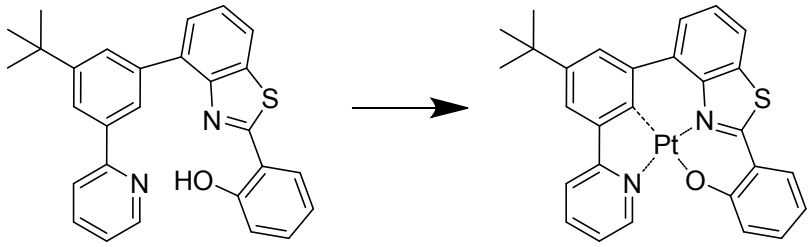


To a suspension of N-(2-bromophenyl)-2-((tert-butyldimethylsilyl)oxy)benzothioamide (1 g, 2.4 mmol) in a small amount of ethanol was added 30% aqueous sodium hydroxide (19 mmol, 760 mg). The mixture was stirred for 10 min, and then was diluted with water to give a solution of 10% NaOH. The diluted sample was added dropwise to an aqueous solution of potassium ferricyanide (20 wt%) at 80-90ºC. The reaction mixture was stirred for 1.5 hours before cooling down to room temperature. The solution was poured into ice-water mixture and neutralized with dilute aqueous HCl. The product was extracted with chloroform (3×100 mL). The organic phase was washed with water and dried over $MgSO_4$. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM:PE, 3:1) to afford a white solid (250 mg, 35%). ^{1}H

NMR (400 MHz, $CDCl_3$) δ 12.42 (s, 1H), 7.84 (dd, *J* = 8.0, 0.9 Hz, 1H), 7.76 (m, 2H), 7.48 (m, 1H), 7.28 (t, *J* = 5.6 Hz, 1H), 7.13 (dd, *J* = 8.3, 0.9 Hz, 1H), 7.02 (m, 1H). GC-MS: m/z calcd 304.95, found 304.75.

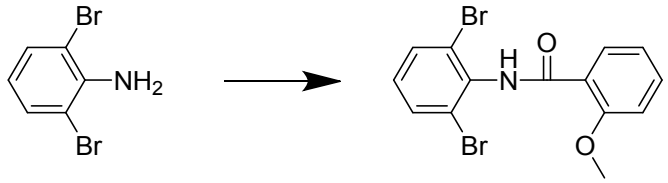


A solution of K_2CO_3 (0.27 g, 1.96 mmol) in 20 mL of degassed water was added to a solution of 2-(3-(tert-butyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)pyridine (165 mg, 0.49 mmol), 2-(7-bromobenzo[d]thiazol-2-yl)phenol (150 mg, 0.49 mmol), and $Pd(PPh_3)_4$ (28 mg, 0.025 mmol) in toluene (100 mL) under N_2. The reaction mixture was heated to reflux overnight before cooling to room temperature. The water phase was extracted with DCM (3×100 mL), and the combined organic phase was washed with water and dried over $MgSO_4$. The crude product was purified by column chromatography (SiO_2, DCM:PE, 3:2) to afford a white solid (165 mg, 77%). ^{1}H NMR (400 MHz, DMSO-d_6) δ11.74 (s, 1H), 8.72 (d, J = 5.5 Hz, 1H), 8.33 (s, 1H), 8.23 – 8.17 (m, 2H), 8.12 (dd, J = 14.9, 8.0 Hz, 2H), 8.06 (s, 1H), 7.98 – 7.86 (m, 1H), 7.78 (d, J = 7.4 Hz, 1H), 7.59 (t, J = 7.8 Hz, 1H), 7.40 (dd, J = 14.2, 8.7 Hz, 2H), 7.07 (d, J = 8.2 Hz, 1H), 7.00 (t, J = 7.5 Hz, 1H), 1.46 (s, 9H). ^{13}C NMR (600 MHz, $CDCl_3$) δ 169.06, 158.20, 158.11, 152.15, 149.80, 139.85, 139.08, 136.88, 136.31, 133.62, 132.86, 128.49, 127.39, 127.22, 125.94, 125.23, 124.11, 122.18, 121.13, 120.65, 119.49, 118.12, 116.99, 35.30, 31.66. GC-MS: m/z calcd 436.16, found 436.08.



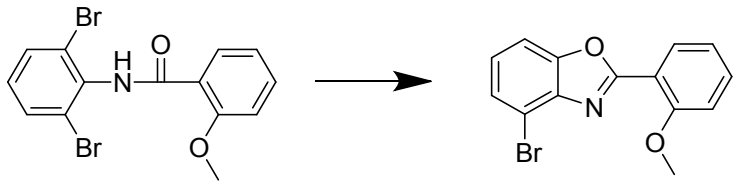
L1

L1 (50 mg, 0.11 mmol) and K_2PtCl_4 (57 mg, 0.138 mmol) were added into a mixture of $CHCl_3$/AcOH (20 mL, v/v= 1:9) under N_2. The reaction solution was heated to reflux for 24 hours. After cooling to room temperature, the precipitate was collected by filtration. The crude product was purified by column chromatography (SiO_2, DCM) to afford a yellow solid (36 mg, 50%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.58 (d, J = 5.5 Hz, 1H), 8.50 (d, J = 8.0 Hz, 1H), 8.34 (s, 1H), 8.01 – 7.80 (m, 4H), 7.74 (s, 1H), 7.59 (t, J = 7.8 Hz, 1H), 7.52 (t, J = 7.6 Hz, 1H), 7.36 (t, J = 5.6 Hz, 1H), 7.31 (d, J = 8.5 Hz, 1H), 6.72 (t, J = 7.4 Hz, 1H), 1.51 (s, 9H). ^{13}C NMR (600 MHz, $CDCl_3$) δ 167.24, 163.95, 163.19, 147.17, 146.04, 145.90, 142.02, 138.76, 138.70, 133.65, 132.92, 130.99, 130.81, 130.48, 125.09, 125.04, 123.30, 122.76, 121.62, 121.11, 119.65, 118.60, 117.41, 115.83, 35.08, 31.74. MALDI-TOF (m/z): calculated for: 629.110, found: 629.186. Anal. calcd for $C_{28}H_{22}N_2OPtS$: C, 53.41; H, 3.52; N, 4.45; S, 5.09; found: C, 53.66; H, 3.49; N, 4.56; S, 5.53%.

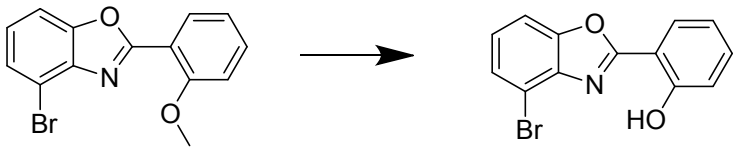


To a solution of 2,6-dibromo-phenylamine (4 g, 15.9 mmol) in THF (30 mL) was added 2-methoxy-benzoyl chloride (2.7 g, 15.9 mmol). The reaction solution was stirred at room temperature overnight. After removal of solvent, the residue was extracted with ethyl acetate. The organic phase was neutralized with aqueous solution of $NaHCO_3$ and dried over $MgSO_4$. After removal of solvent, the remaining oily residue was solidified with the addition of diisopropyl ether (4.48 g, 73%). ^{1}H NMR

(400 MHz, $CDCl_3$) δ 9.62 (d, *J* = 39.3 Hz, 1H), 8.39 (m, 1H), 7.65 (d, *J* = 8.1 Hz, 2H), 7.60 (m, 1H), 7.23 (m, 1H), 7.06 (dt, *J* = 11.8, 6.6 Hz, 2H), 4.10 (s, 3H). GC-MS: m/z calcd 384.91，found 384.75.

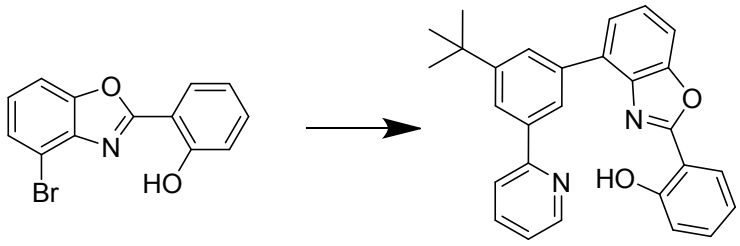


N-(2,6-dibromophenyl)-2-methoxybenzamide (4 g, 10.4 mmol), CuI (197 mg, 1.03 mmol), Cs_2CO_3(374 mg, 1.1 mmol), and 1,10-phenanthroline (5 g, 27.7 mmol) were added into 10 mL of DME. The reaction mixture were heated at 90 ºC overnight, and the solution changed color from yellow to black. After cooling down to room temperature, a large amount of water was added the reaction system. The water phase was extracted with DCM (3×100 mL), and the organic phase was washed with water and dried over $MgSO_4$. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM:PE, 5:4) to afford a white solid (2.77 g, 87.6%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (m, 1H), 7.52 (m, 3H), 7.21 (dd, *J* = 15.2, 7.1 Hz, 1H), 7.13 (m, 2H), 4.00 (s, *J* = 4.1 Hz, 3H). GC-MS: m/z calcd 304.98，found 304.95.

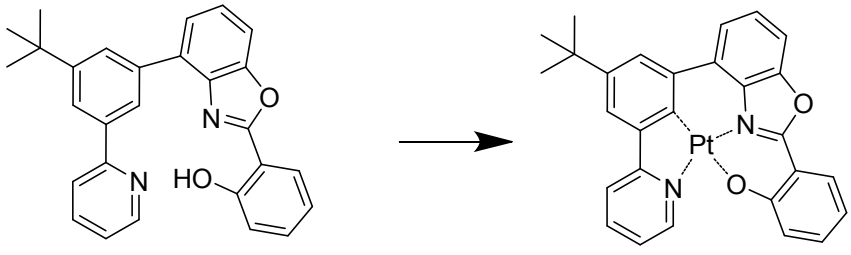


To a solution of BBr_3 (17.3 mL, 1M in DCM, 17.3 mmol) in DCM were added 4-bromo-2-(2-methoxyphenyl)benzo[d]oxazole (1.32 g, 4.3 mmol) and KI (2.88 g, 17.4 mmol). The reaction mixture was stirred overnight at room temperature, and the color turned into reddish brown. The reaction was quenched with the addition of ethanol, and then the solvent was removed by evaporation. The residue was purified by column chromatography (SiO_2, DCM) to afford a white solid (1.15 g, 92%). ^{1}H NMR

(400 MHz, $CDCl_3$) δ 11.28 (s, 1H), 8.02 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.60 (m, 2H), 7.51 (m, 1H), 7.32 (m, 1H), 7.15 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.07 (m, 1H). GC-MS: m/z calcd 288.97, found 288.75.

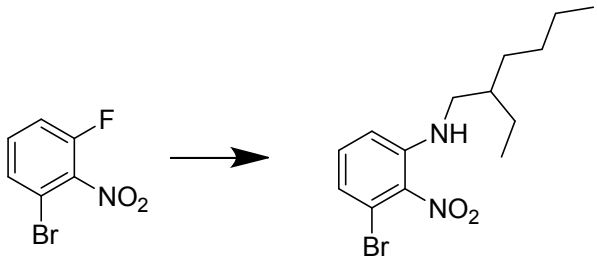


A solution of K_2CO_3 (2.28 g, 16 mmol) in degassed water (20 mL) was added to a solution of 2-(3-(tert-butyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)pyridine (1.54 g, 4.56 mmol), 2-(4-bromobenzo[d]oxazol-2-yl)phenol (1.2 g, 4.1 mmol), and $Pd(PPh_3)_4$ (236 mg, 0.25 mmol) in toluene (100 mL). The reaction mixture was heated to reflux overnight. The water phase was extracted with DCM (3×100 mL), and the combined organic phase was washed with water and dried over $MgSO_4$. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM:PE,1:1) to afford a white solid (900 mg, 51.7%). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 11.37 (s, 1H), 8.77 (m, 1H), 8.39 (t, *J* = 1.6 Hz, 1H), 8.20 (t, *J* = 1.7 Hz, 1H), 8.18 (m, 3H), 8.00 (m, 2H), 7.83 (dd, *J* = 7.7, 0.8 Hz, 1H), 7.61 (t, *J* = 8.0 Hz, 1H), 7.58 (m, 1H), 7.40 (m, 1H), 7.14 (m, 2H), 1.45 (s, 9H). ^{13}C NMR (600 MHz, $CDCl_3$) δ 163.06, 159.01, 158.04, 152.29, 149.87, 149.82, 139.99, 137.95, 137.19, 136.92, 133.75, 133.04, 127.27, 127.09, 125.72, 124.64, 124.40, 123.95, 122.26, 121.01, 119.69, 117.64, 110.73, 109.61, 35.30, 31.68. GC-MS: m/z calcd 420.18, found 420.19.

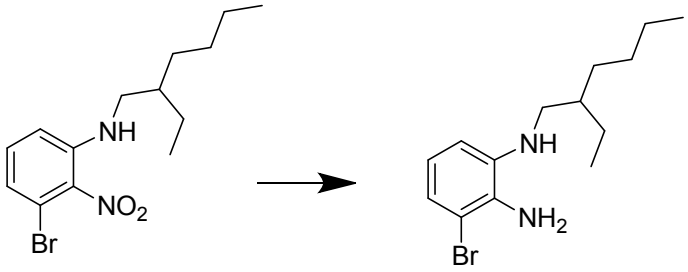


L2

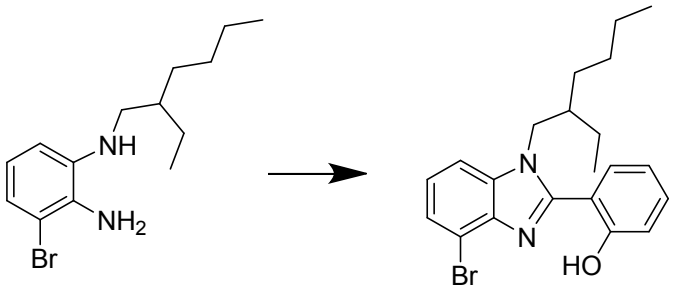
L2 (1 g, 2.38 mmol) and K_2PtCl_4 (1.18 g, 2.86 mmol)) were added into a mixture of $CHCl_3$/AcOH (80 mL, v/v= 1:9) under N_2. The reaction solution was heated to reflux for 24 hours. After cooling to room temperature, the precipitate was collected by filtration. The crude product was purified by column chromatography (SiO_2, DCM) to afford a yellow solid (800 mg, 54.8%).1H NMR (400 MHz, $CDCl_3$) δ 9.25 (d, J = 5.1 Hz, 1H), 8.16 (s, 1H), 8.06 (d, J = 7.7 Hz, 2H), 7.83 (t, J = 7.6 Hz, 1H), 7.70 (d, J = 8.0 Hz, 1H), 7.62 (s, 1H), 7.55 – 7.40 (m, 3H), 7.30 (t, J = 6.4 Hz, 1H), 7.13 (d, J = 8.6 Hz, 1H), 6.75 (t, J = 7.4 Hz, 1H), 1.51 (s, 9H). ^{13}C NMR (600 MHz, CDCl3) δ 167.19, 167.07, 156.88, 149.43, 147.12, 146.13, 145.71, 138.43, 137.66, 133.34, 130.60, 129.56, 128.77, 127.51, 125.23, 124.98, 122.00, 121.71, 121.13, 119.67, 118.67, 115.16, 109.43, 107.98, 35.00, 31.73. MALDI-TOF (m/z): calculated for: 613.133, found: 613.237. Anal. calcd for $C_{28}H_{22}N_2O_2Pt$: C, 54.81; H, 3.61; N, 4.57; found: C, 54.80; H, 3.52; N, 4.61%.



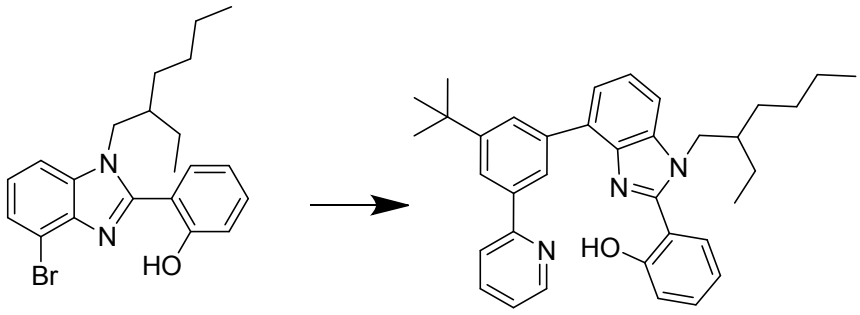
1-bromo-3-fluoro-2-nitro-benzene (1 g, 9 mmol) and 2-ethylhexylamine (5.805 g, 45 mmol) were added into 30 mL of ethanol. The reaction mixture was stirred at room temperature overnight. After the removal of solvent, the residue was extracted with DCM (3×100 mL), and the organic phase was washed with water and dried over $MgSO_4$. A yellow oil was obtained after the removal of solvent, which was used directly for the next step without any additional purification (1.2 g, 80%) GC-MS: m/z calcd 328.08, found 328.02.



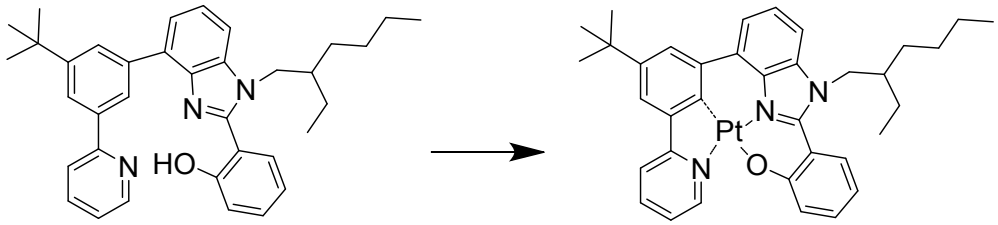
To a solution of 3-bromo-N-(2-ethylhexyl)-2-nitroaniline (5 g, 15.2 mmol) in 150 mL of AcOH was added iron powder (15 g, 268 mmol). The reaction mixture was heated at 60 ^{o}C for 1h, and the solution changed color from orange to dark brown. After the removal of solvent, the residue was extracted with DCM (3×100 mL). The crude product was purified by column chromatography (SiO_2, DCM:PE, 1:1) to afford a brown solid (3.2 g, 70%).^{1}H NMR (400 MHz, DMSO-*d6*) δ 6.72 (m, 1H), 6.44 (dd, *J* = 10.1, 5.6 Hz, 1H), 6.38 (dd, *J* = 7.9, 1.4 Hz, 1H), 4.72 (s, 3H), 2.96 (d, *J* =6.8 Hz, 2H), 1.70 (m, 9H), 0.88 (m, 6H). GC-MS: m/z calcd 298.10, found 298.26.



3-bromo-N1-(2-ethylhexyl)benzene-1,2-diamine (0.45 g, 1.5 mmol) and 2-hydroxy-benzaldehyde (0.183 g, 1.5 mmol) were dissolved in 30 mL of 1,4-dioxane. The reaction mixture was heated to reflux for 5 hours. After the removal of solvent, the residue was dissolved in 30 mL of toluene before the addition of activated MnO_2 (0.533 g, 6.19 mmol). The suspension was heated to reflux overnight. The crude product was purified by column chromatography (SiO_2, DCM:PE, 3:2) to afford a white solid (0.31g, 51%). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 10.30 (s, 1H), 7.62 (d, *J* = 7.6 Hz, 1H), 7.51 (m, 3H), 7.21 (t, *J* = 7.9 Hz, 1H), 7.08 (m, 2H), 4.11 (d, *J* = 7.4 Hz, 2H), 1.35 (m, 9H), 0.88 (m, 6H). GC-MS: m/z calcd 401.34, found 401.12.



A solution of K_2CO_3 (500 mg, 3.6 mmol) in degassed water (20 mL) was added to a solution of 2-(3-(tert-butyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)pyridine (120 mg, 0.36 mmol), 2-[4-bromo-1-(2-ethylhexyl)-1*H*-benzoimidazol-2-yl]phenol (142 mg, 0.36 mmol), and $Pd(PPh_3)_4$ (20 mg, 0.018 mmol) in toluene (100 mL). The reaction mixture was heated to reflux overnight. The water phase was extracted with DCM (3×100 mL), and the combined organic phase was washed with water and dried over $MgSO_4$. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM:EtOAc, 9:1) to afford a white solid (120 mg, 63%). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 10.84 (s, 1H), 8.69 (d, J = 3.9 Hz, 1H), 8.44 (s, 1H), 8.18 (s, 1H), 8.10 (d, J = 1.7 Hz, 1H), 8.02 (d, J = 8.0 Hz, 1H), 7.89 (td, J = 7.8, 1.8 Hz, 1H), 7.63 (d, J = 8.0 Hz, 1H), 7.58 – 7.51 (m, 2H), 7.46 – 7.31 (m, 3H), 7.03 (d, J = 7.7 Hz, 1H), 6.97 (t, J = 7.5 Hz, 1H), 4.26 (d, J = 7.5 Hz, 2H), 1.42 (s,9H), 1.23 (m, 9H), 0.72 (m, 6H). ^{13}C NMR (600 MHz, CDCl3) δ 159.42, 158.37, 152.04, 151.63, 149.74, 139.71, 138.30, 138.22, 136.85, 136.46, 132.37, 131.51, 127.31, 126.77, 125.07, 123.58, 122.63, 122.04, 121.17, 118.52, 118.47, 113.73, 109.66, 49.87, 39.47, 35.26, 31.71, 30.60, 28.47, 25.06, 23.98, 23.05, 14.09.GC-MS: m/z calcd 531.32, found 531.27.



L3

L3 (1 g, 1.8 mmol) and K_2PtCl_4 (780 mg, 1.8 mmol)) were added into a mixture of $CHCl_3$/AcOH (80 mL, v/v= 1:9) under N_2. The reaction solution was heated to reflux for 24 hours. After cooling to room temperature, the precipitate was collected by filtration. The crude product was purified by column chromatography (SiO_2, DCM) to afford a yellow solid (800 mg, 58%).^{1}H NMR (400 MHz, CDCl3) δ 9.47 (d, J = 5.5 Hz, 1H), 8.36 (s, 1H), 8.23 (d, J = 7.8 Hz, 1H), 7.96 – 7.81 (m, 3H), 7.73 (s, 1H), 7.53 (t, J = 7.9 Hz, 1H), 7.49 – 7.37 (m, 3H), 7.32 (t, J = 5.8 Hz, 1H), 6.78 – 6.64 (m, 1H), 4.71 – 4.46 (m, 2H), 1.50 (s, 9H), 1.23 – 0.98 (m, 9H), 0.74 (m, 6H). ^{13}C NMR (600 MHz, $CDCl_3$) δ 167.37, 166.91, 147.43, 147.30, 145.98, 145.75, 139.22, 138.21, 136.50, 131.71, 131.15, 130.85, 130.29, 128.41, 125.21, 123.51, 122.22, 121.68, 120.88, 118.82, 118.66, 114.14, 112.37, 109.06, 52.05, 38.41, 35.03, 31.73, 30.37, 28.38, 23.63, 22.98, 14.09, 10.41.MALDI-TOF (m/z): calculated for:724.274, found: 724.310. Anal. calcd for $C_{36}H_{39}N_3OPt$: C, 59.66; H, 5.42; N, 5.80; found: C, 59.68; H, 5.56; N, 5.92%.

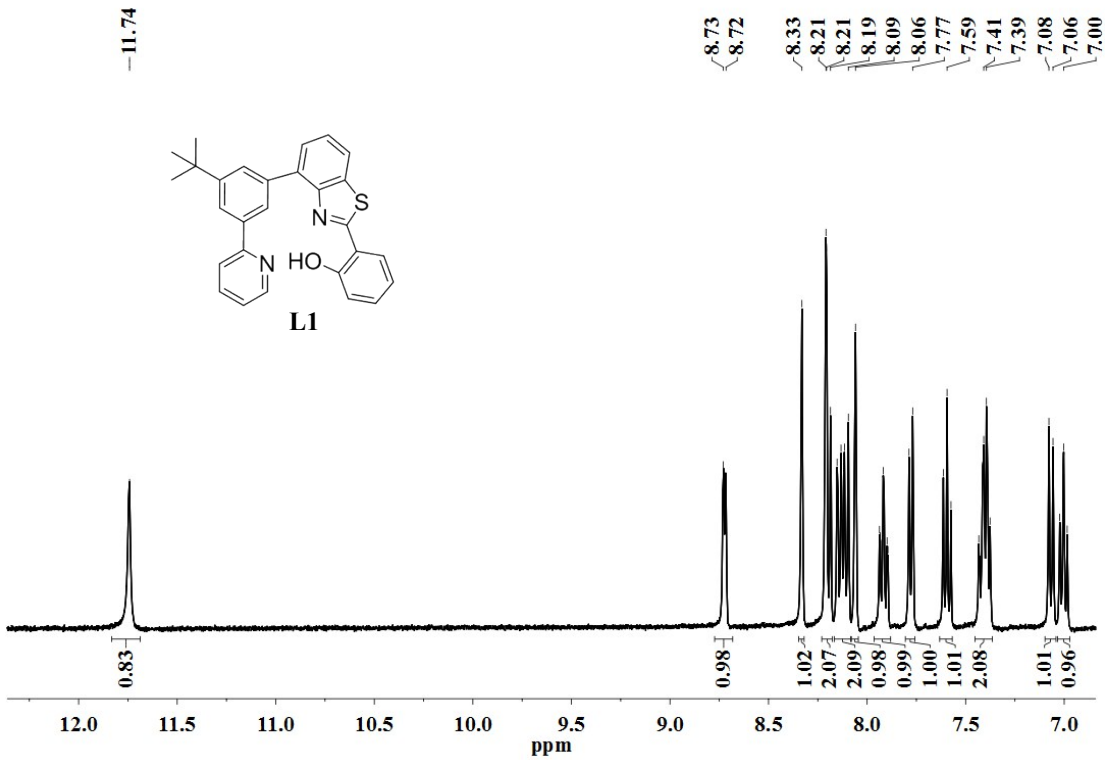


Figure S1. ^{1}H NMR spectrum of ligand of **L1** (DMSO-*d6*)

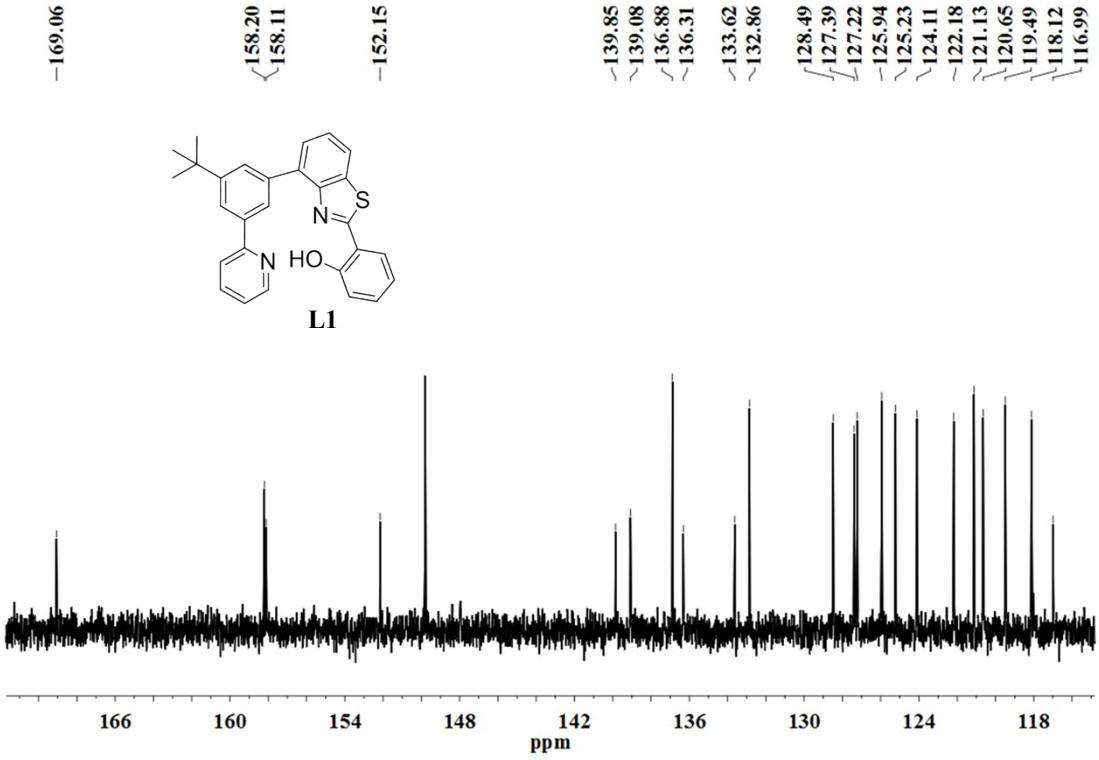


Figure S2. ^{13}C NMR spectrum of ligand of **L1** ($CDCl_3$)

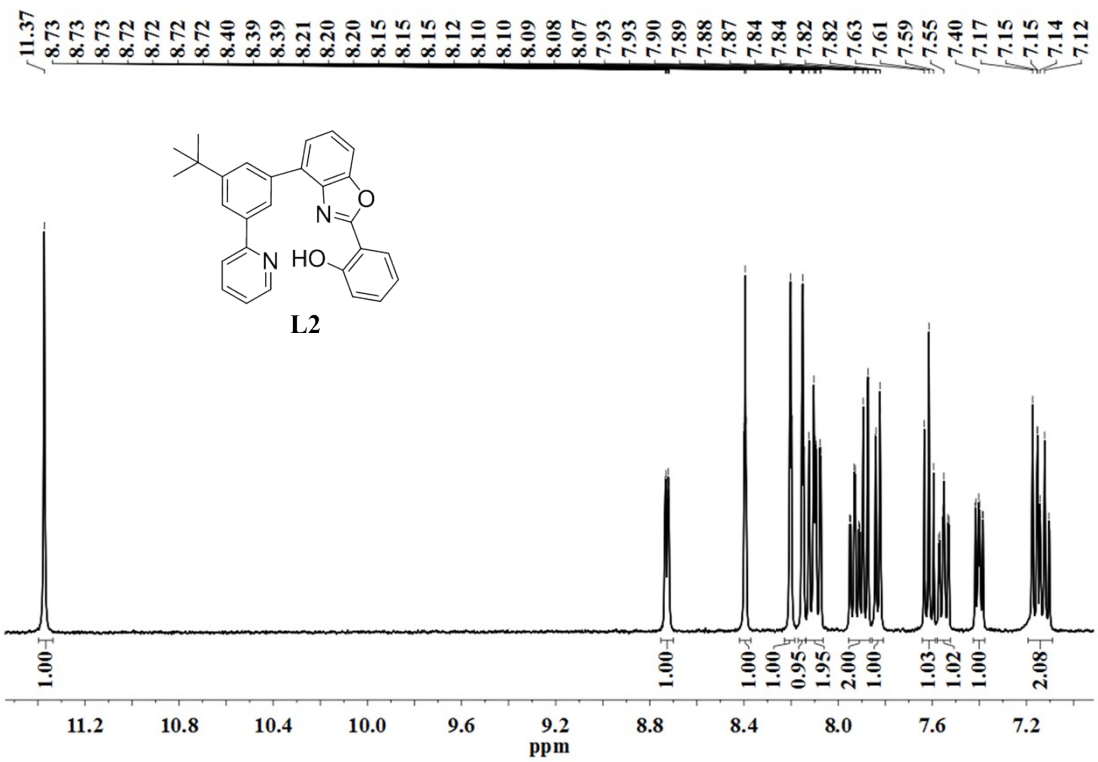


Figure S3. ^{1}H NMR spectrum of ligand of **L2** (DMSO-*d6*)

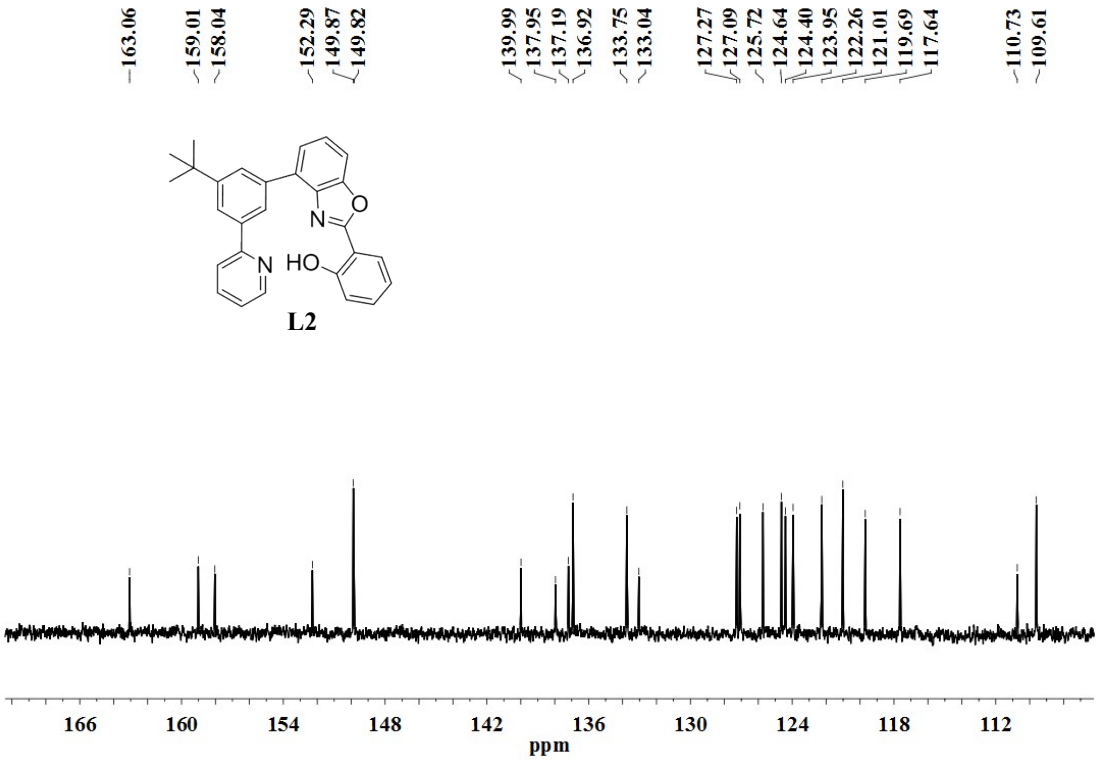


Figure S4. ^{13}C NMR spectrum of ligand of **L2** ($CDCl_3$)

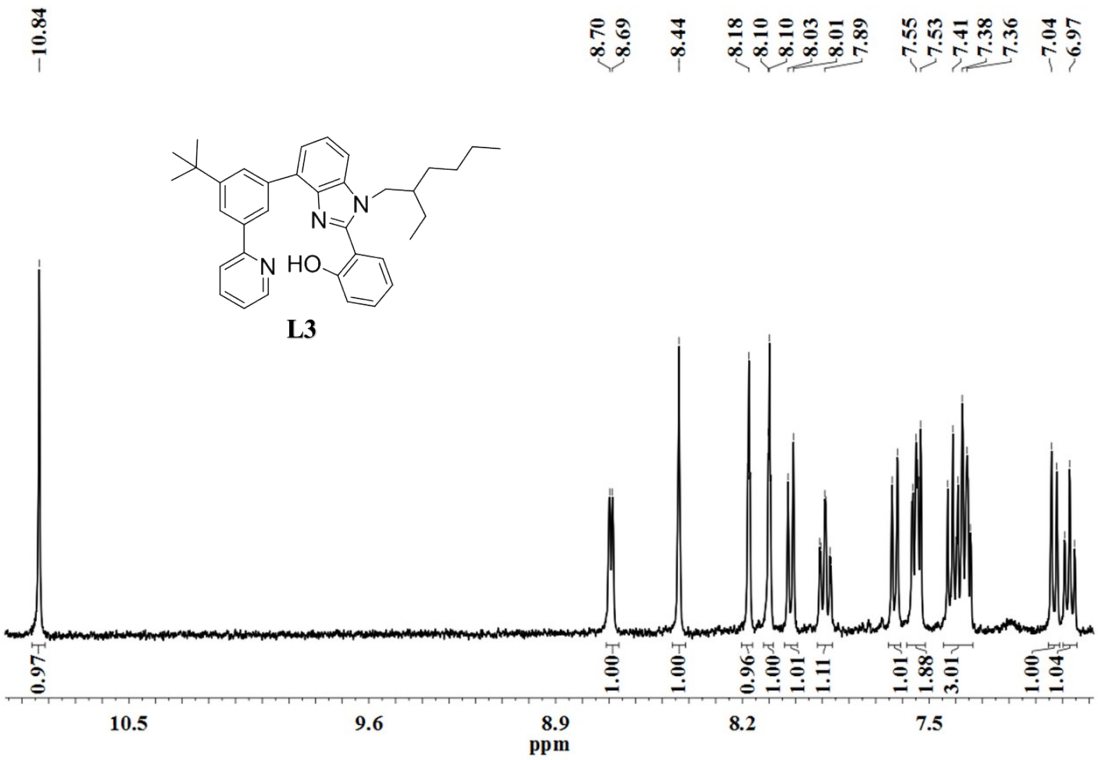


Figure S5. ^{1}H NMR spectrum of ligand of **L3** (DMSO-*d6*)

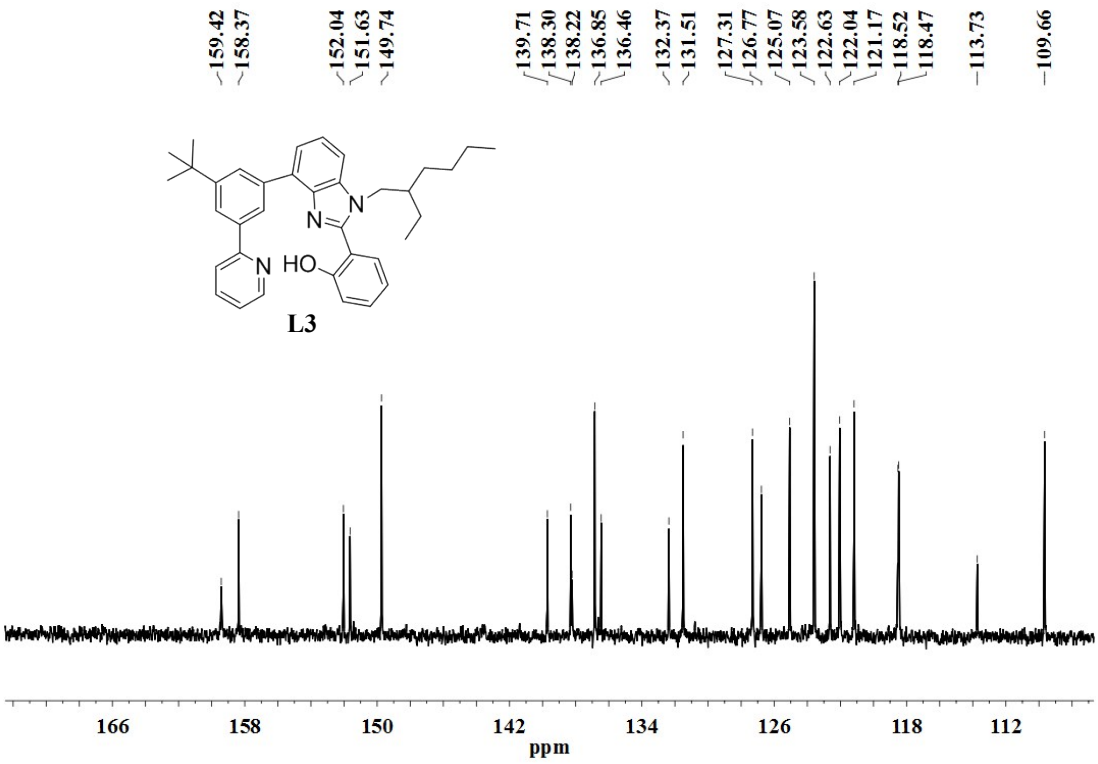


Figure S6. ^{13}C NMR spectrum of ligand of **L3** ($CDCl_3$)

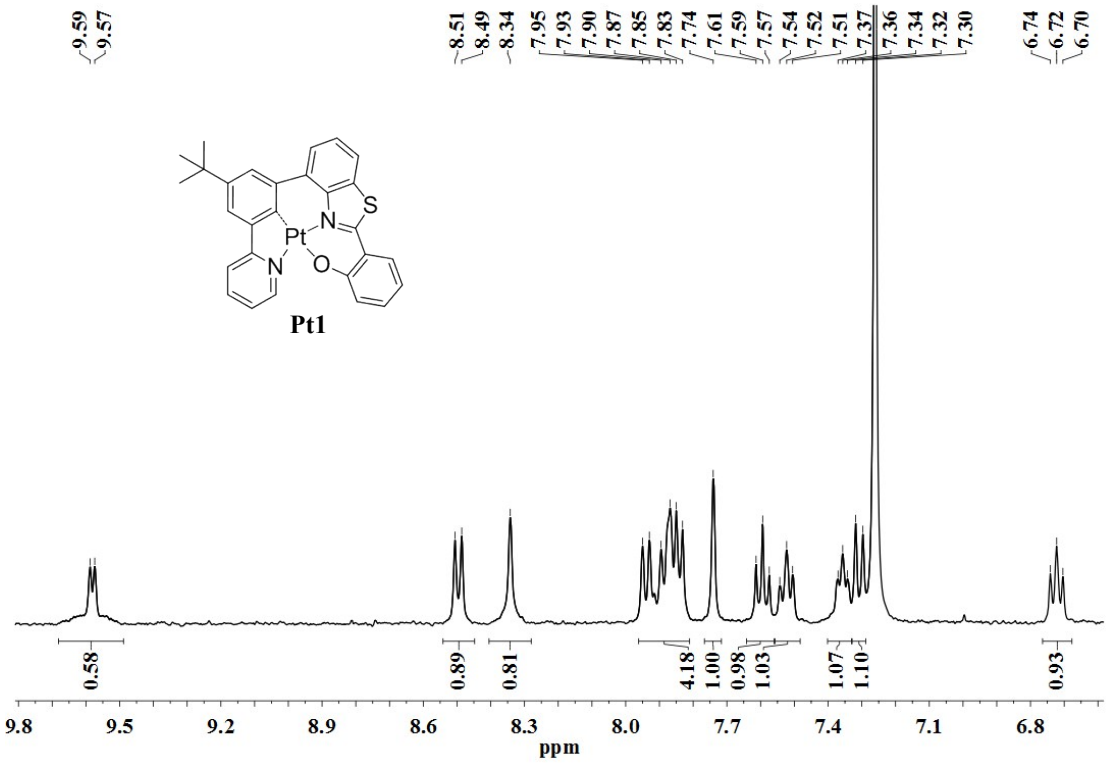


Figure S7. ^{1}H NMR spectrum of complex of **Pt1** ($CDCl_3$)

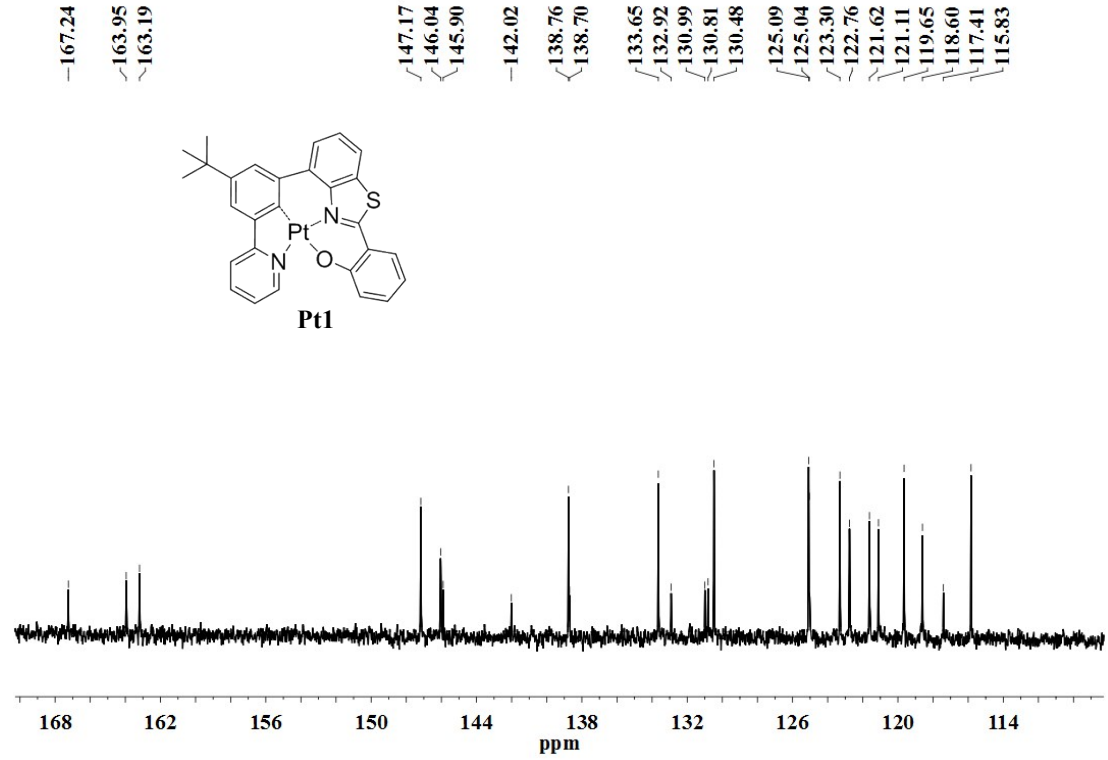


Figure S8. ^{13}C NMR spectrum of complex of **Pt1** ($CDCl_3$)

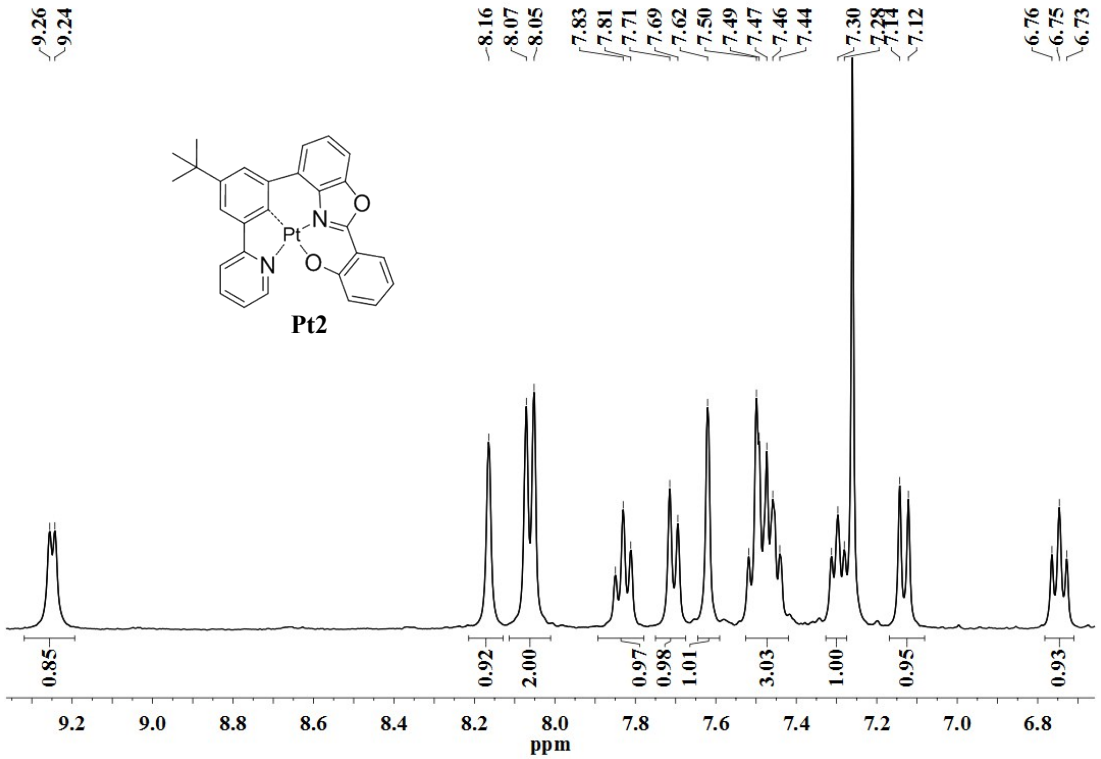


Figure S9. ^{1}H NMR spectrum of complex of **Pt2** ($CDCl_3$)

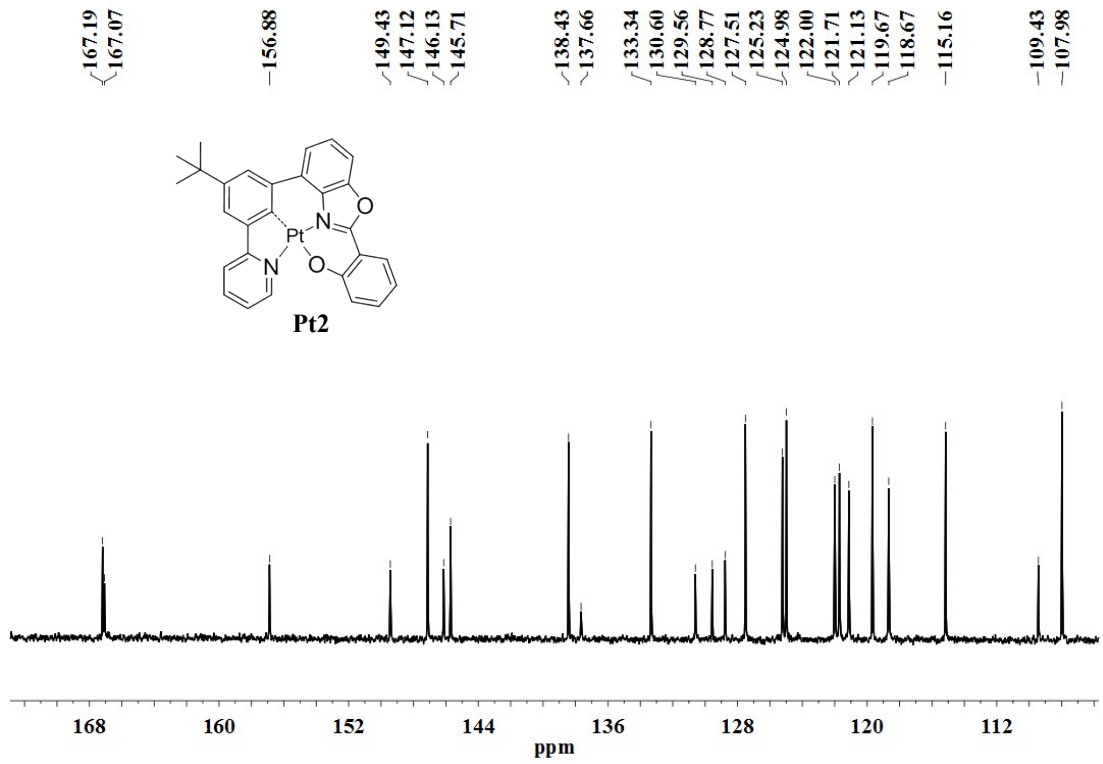


Figure S10. ^{13}C NMR spectrum of complex of **Pt2** ($CDCl_3$)

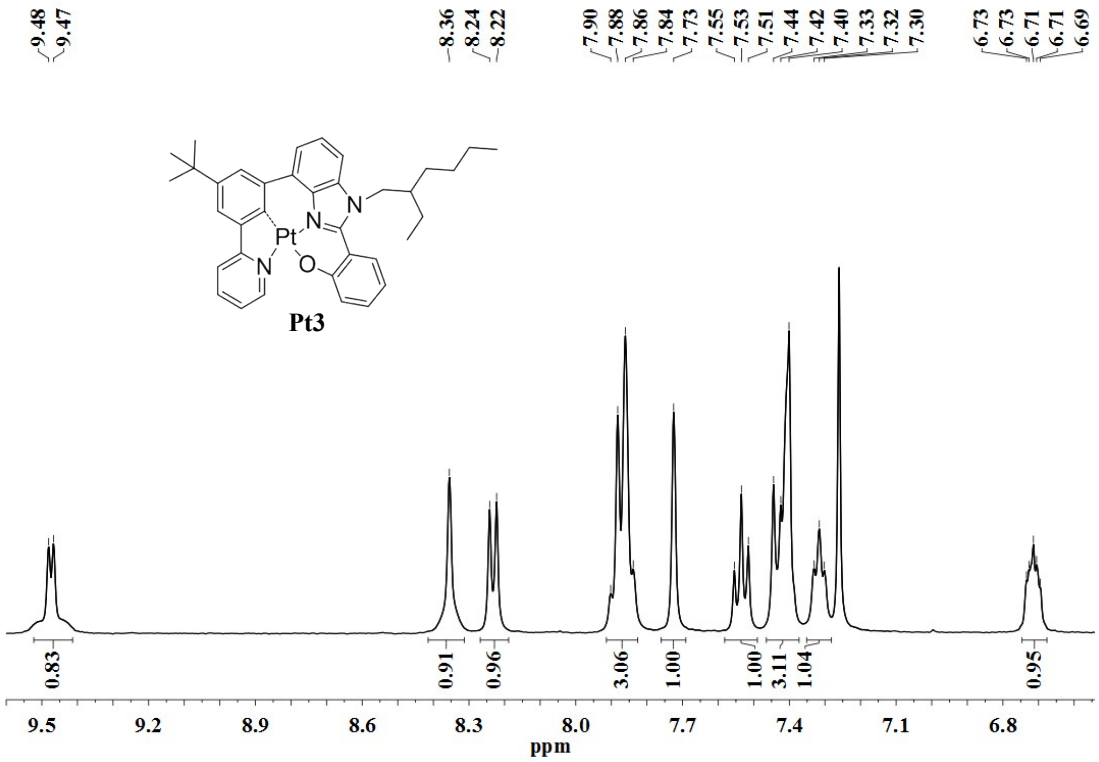


Figure S11. ^{1}H NMR spectrum of complex of **Pt3** ($CDCl_3$)

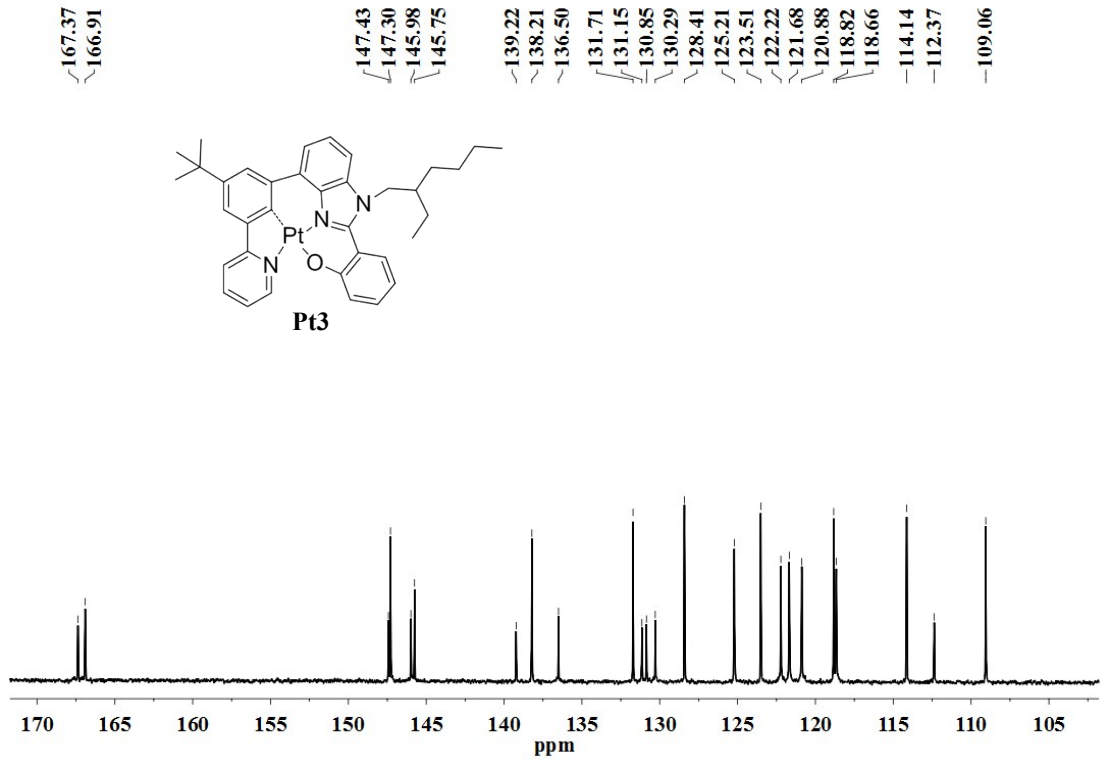


Figure S12. ^{13}C NMR spectrum of complex of **Pt3** ($CDCl_3$)

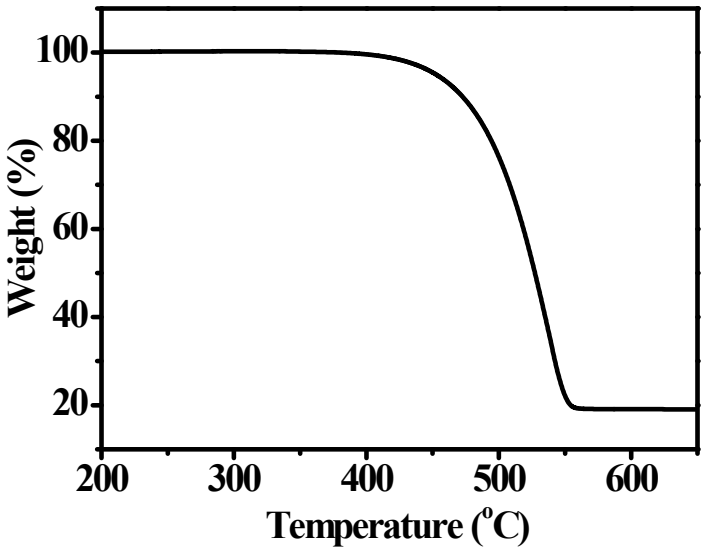


Figure S13. TGA curve of **Pt1**.

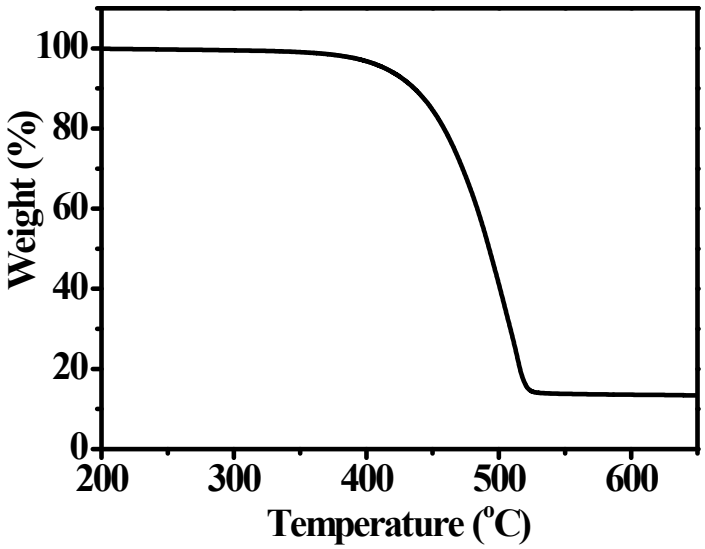


Figure S14. TGA curve of **Pt2**.

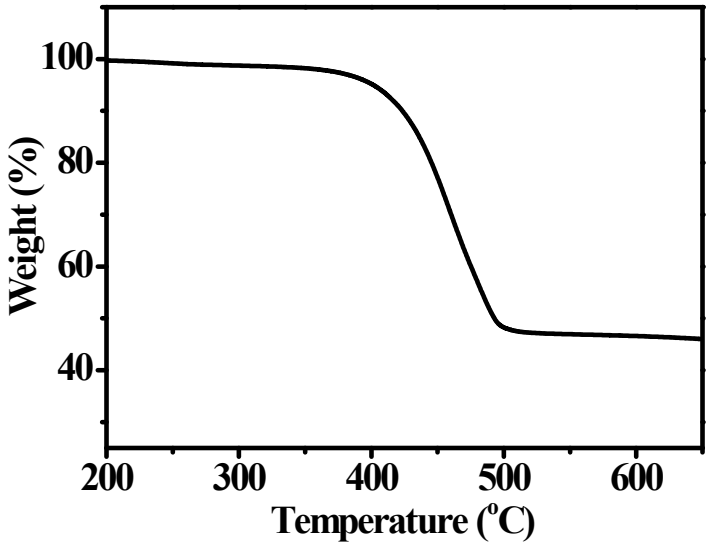


Figure S15. TGA curve of **Pt3**.

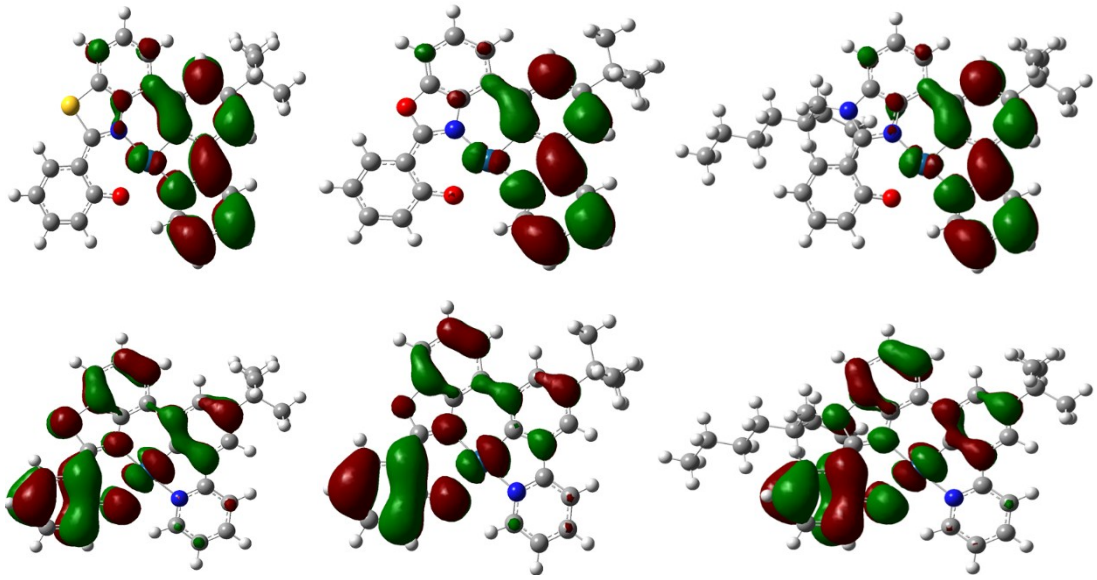


Figure S16. Density functional theory calculation of orbit density for the HOMOs (bottom) and LUMOs (top) of **Pt1**, **Pt2** and **Pt3**.

Table S1. Crystal data and structure refinements for compound **Pt3**.

Compound	**Pt3**
Empirical formula	$C_{36}H_{39}N_3OPt$
Formula weight	724.79
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	6.9855(8)
b (Å)	14.6481(17)
c (Å)	29.888(3)
α (deg)	90.00
β (deg)	94.743(2)
γ (deg)	90.00
V (Å^3)	3047.8(6)
Z	4
D_c (g/cm^3)	1.580
μ (mm^{-1})	4.637
F (000)	1448.0
Collcd reflns	15830
Unique reflns	5354
parameters	370
R_{int}	0.0742
GOF	1.012
R_1[a] [I>2σ (I)]	0.0521
wR_2[b] (all data)	0.1067

[a] $R_1 = \sum||F_o|-|F_c||/\sum|F_o|$; [b] $wR_2 = \sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]^{1/2}$.

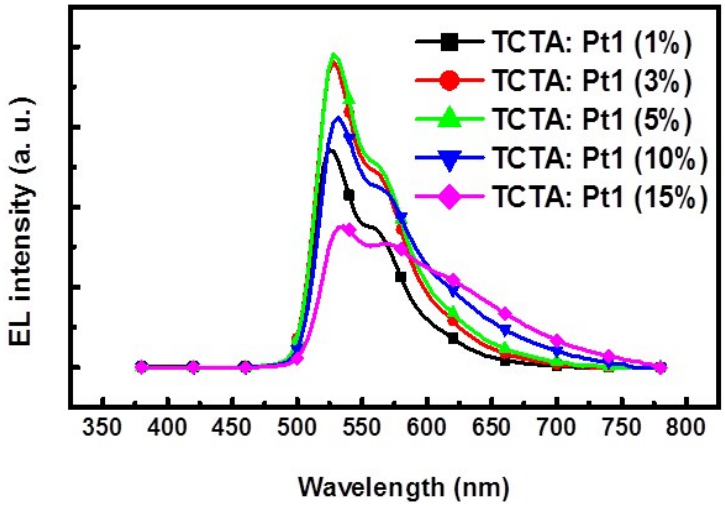


Figure S17. The EL spectra of complex **Pt1** with different doping ratios at 5 mA/cm^2.

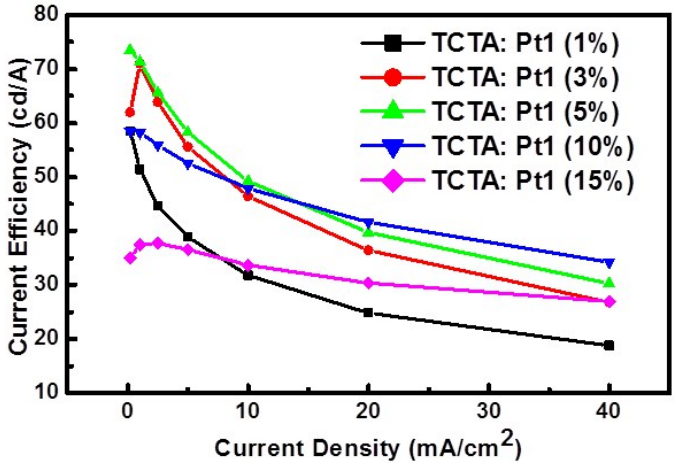


Figure S18. The current efficiency–current density curves for **Pt1** at different doping ratios.

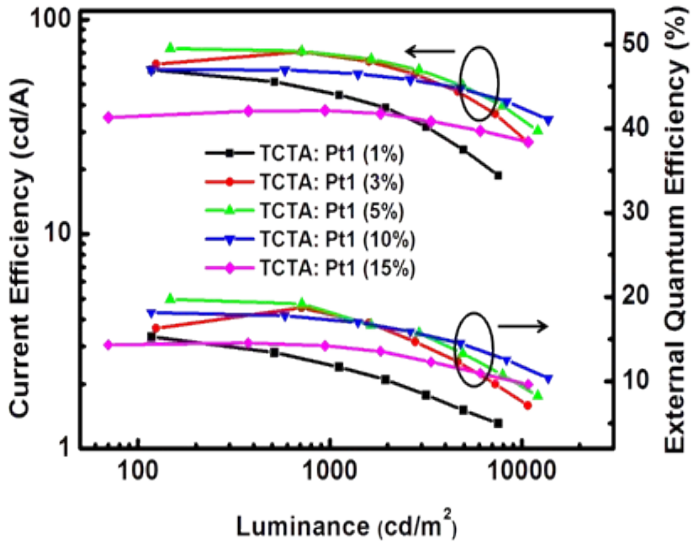


Figure S19. The EQE-luminance-current efficiency curves for **Pt1** at different doping ratios.

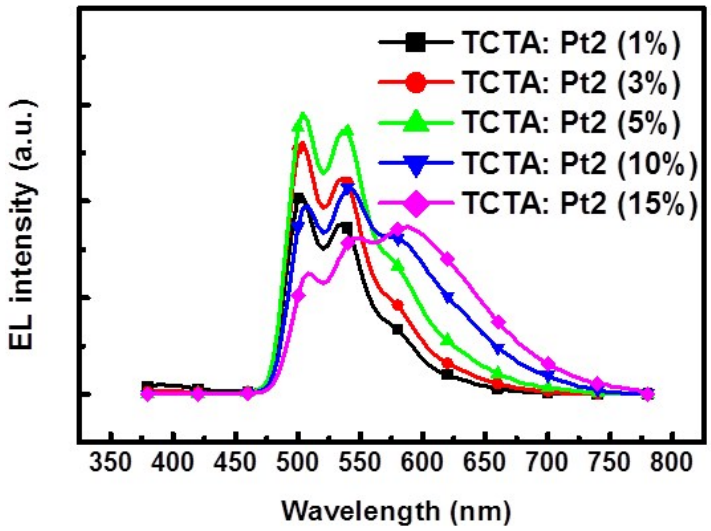


Figure S20. The EL spectra of complex **Pt2** with different doping ratios at 5 mA/cm^2.

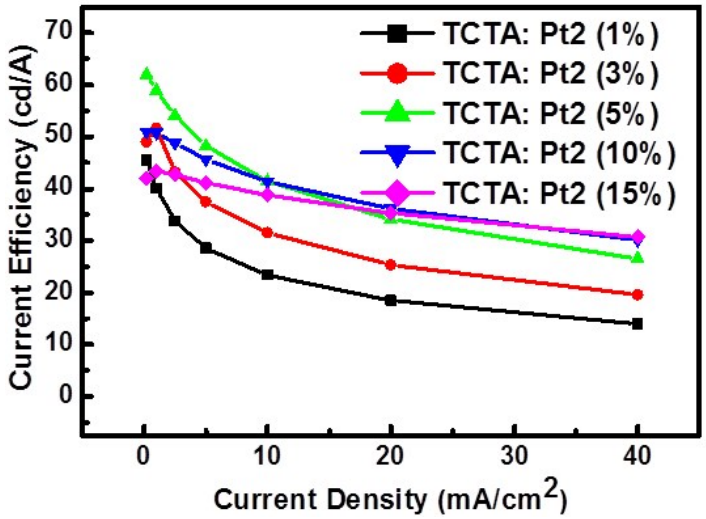


Figure S21. The current efficiency–current density curves for **Pt2** at different doping ratios.

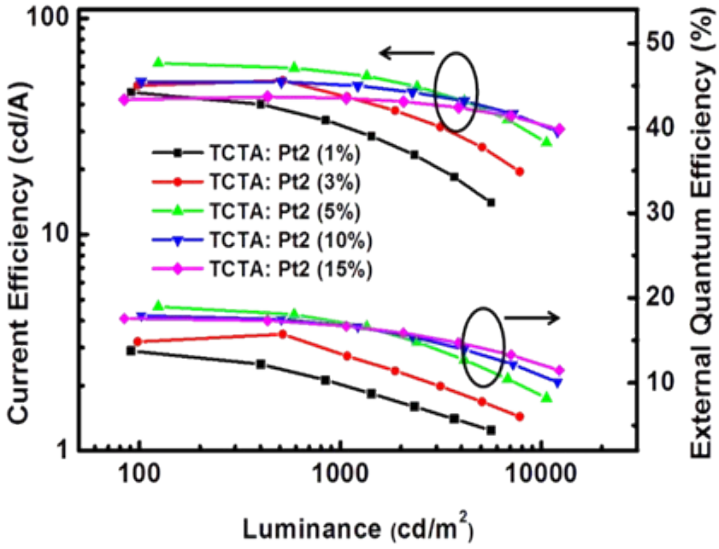


Figure S22. The EQE-luminance-current efficiency curves for **Pt2** at different doping ratios.