Supporting Information

N-Heterocyclic Carbene-Base Tetradentate Platinum(II) Complexes for Phosphorescent OLEDs with High Maximum Brightness

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General Information.

Synthesis and Characterization. Unless noted, all commercial reagents were purchased and used as received without further purification. ^{1}H NMR spectra were recorded at 400 or 500 MHz, and ^{13}C NMR spectra were recorded at 100 or 150 MHz NMR instruments in $CDCl_3$ or DMSO-d_6 solutions and chemical shifts were referenced to tetramethylsilane (TMS) or residual protiated solvent. If $CDCl_3$ was used as solvent, ^{1}H and ^{13}C NMR spectra were recorded with TMS (δ = 0.00 ppm) and $CDCl_3$ (δ = 77.00 ppm) as internal references, respectively. If DMSO-d_6 was used as solvent, ^{1}H and ^{13}C NMR spectra were recorded with TMS (δ = 0.00 ppm) and DMSO-d_6 (δ = 39.52 ppm) as internal references, respectively. The following abbreviations (or combinations thereof) were used to explain ^{1}H NMR ultiplicities: s = singlet, d = doublet, t = triplet, q = quartet, p = quintet, m = multiplet, br = broad. All of the new compounds were analyzed for HRMS on a Waters mass spectrometer using electrospray ionization in positive ion mode of ESI-Q-TOF.

Electrochemistry. Cyclic voltammetry and different pulsed voltammetry were performed using a CH1760E electrochemical analyzeraccording previous report.[1] 0.1 M tetra-*n*-butylammonium hexafluorophosphate was used as the supporting electrolyte, anhydrous *N*,*N*-dimethylformamide, was used as the solvents for the E_{ox} and E_{red} measurements, and the solutions were bubbled with nitrogen for 15 min prior to the test. Silver wire, platinum wire and glassy carbon were used as pseudoreference electrode, counter electrode, and working electrode respectively. Scan rate was 300 mV/s. The redox potentials are based on the values measured from different pulsed voltammetry and are reported relative to an internal reference ferrocenium/ferrocene (Cp_2Fe/Cp_2Fe^+).[2] The reversibility of reduction or oxidation was determined using CV.[3] As defined, if the magnitudes of the peak anodic and the peak cathodic current have an equal magnitude as scan speeds of 100 mV/s or slower, then the process is considered reversible; if the magnitudes of the peak anodic and the peak cathodic currents are not equal, but the return sweeps are nonzero, the process is considered quasi-reversible; otherwise, the process is considered irreversible.[2,3]

DFT Calculations. The theoretical calculations of the Pt(II) complexes were performed using Gaussian 09. The molecular geometries of ground states (S_0) were optimized with the density functional theory (DFT) method. The DFT calculations were performed using a B3LYP function with a basis set of 6-31G(d) for C, H, O and N atoms and a LANL2DZ basis set for Pt atom.[4,5]

Photophysical Measurements. The absorption spectra were measured on an Agilent 8453 UV−VS Spectrometer. Steady state emission experiments and lifetime measurements were performed on a Horiba Jobin Yvon FluoroLog-3 spectrometer. Low temperature (77 K) emission spectra and lifetimes were measured in 2-MeTHF cooled with liquid nitrogen.

Device Fabrication and Characterization. All devices were fabricated by vacuum thermal evaporation, and were tested outside glove box after encapsulation. Prior to deposition, the prepatterned ITO coated glass substrates were cleaned by subsequent sonication in deionized water, acetone, and isopropanol. Organic layers were deposited at rates of 0.5 to 2.0 Å/s, monitored by crystal oscillator, in a custom-made vacuum thermal evaporation chamber built by LN Inc (LN-1082FS). The Al cathode was deposited through a shadow mask without breaking vacuum, defining device areas of 0.09 cm^2. The current-voltage-luminance characteristics were measured using a Keithley 2400 SourceMeter in conjunction with a PMTH-S1-CR131A Photodiode. Electroluminescent spectra were measured with an Ocean Optics USB2000 spectrometer.

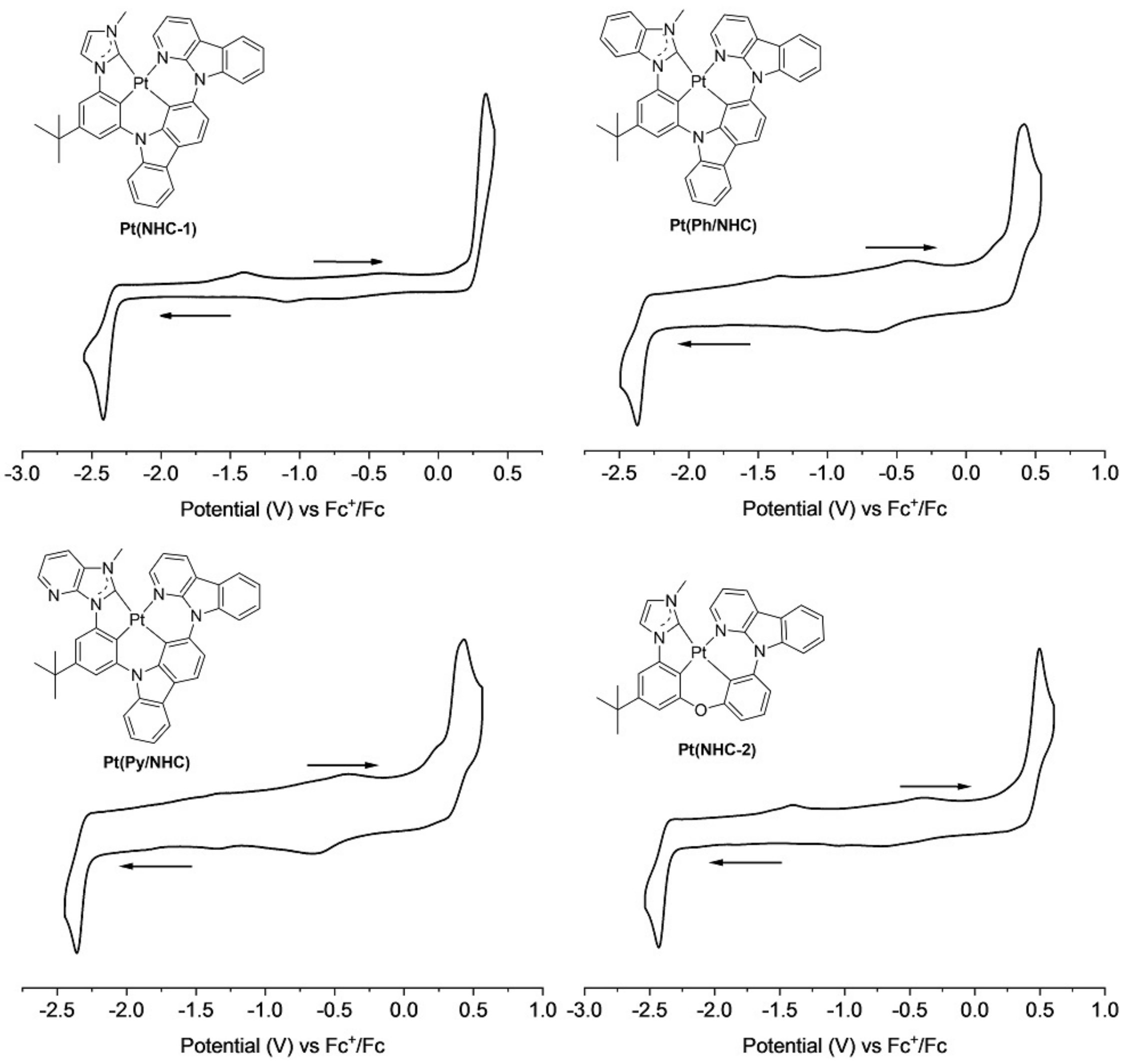


Figure S1. The cyclic voltammetry (CV) of tetradentate Pt(II) complexes measured in *N*,*N*-dimethylformamide under an nitrogen atmosphere.

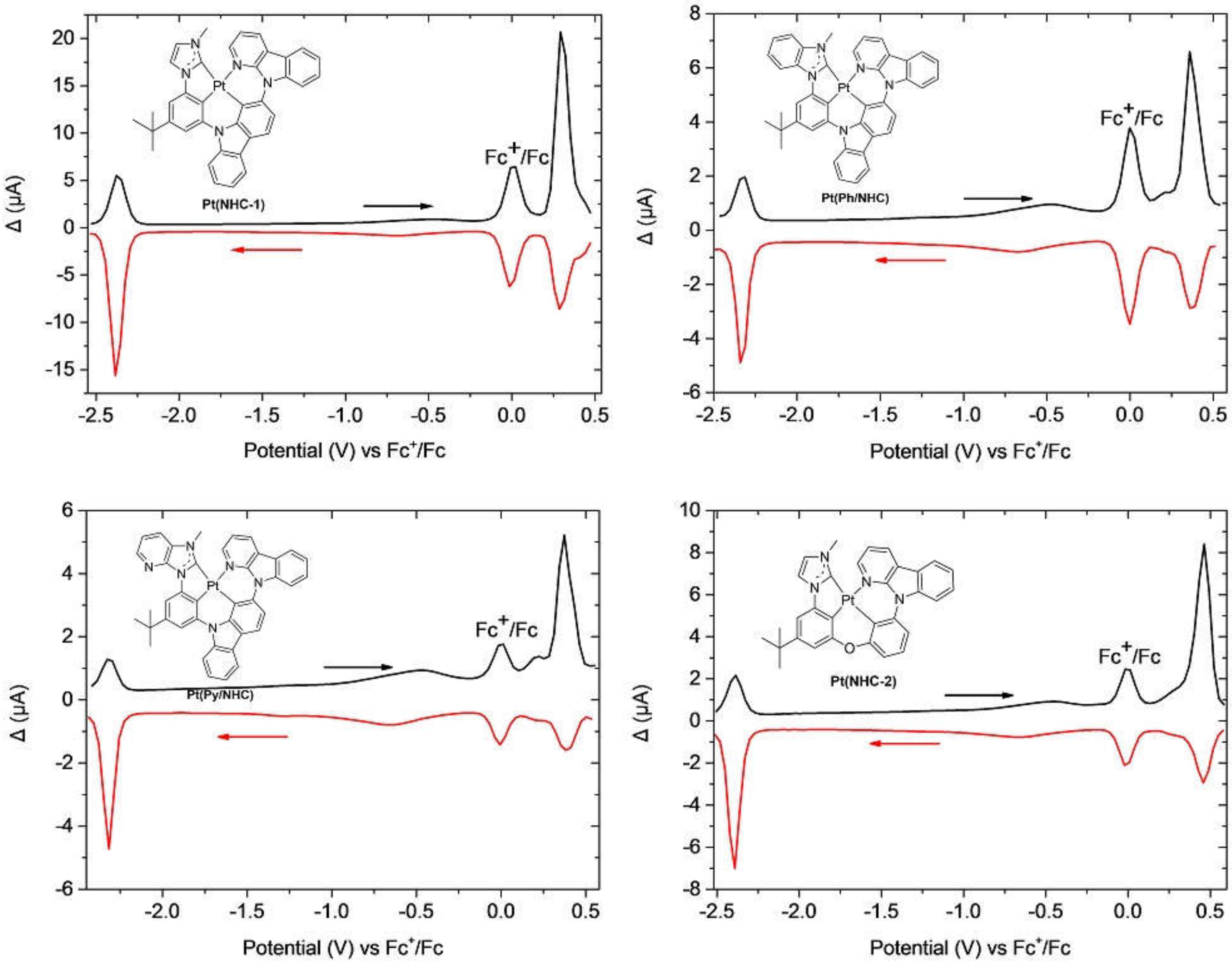
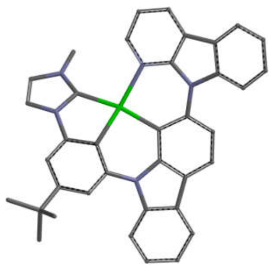
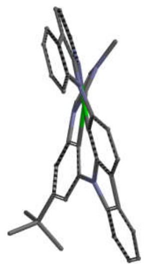
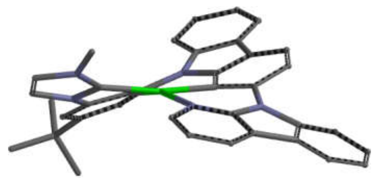
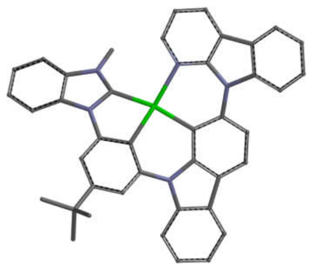
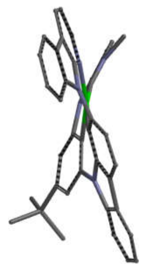
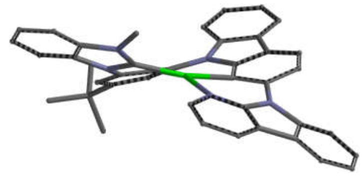
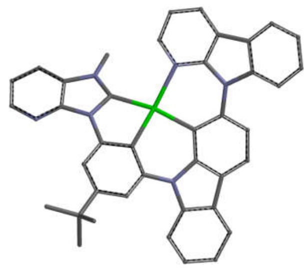
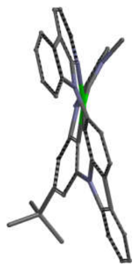
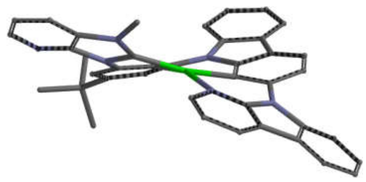
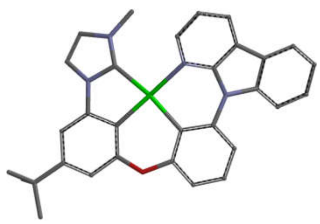
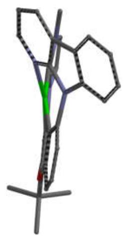
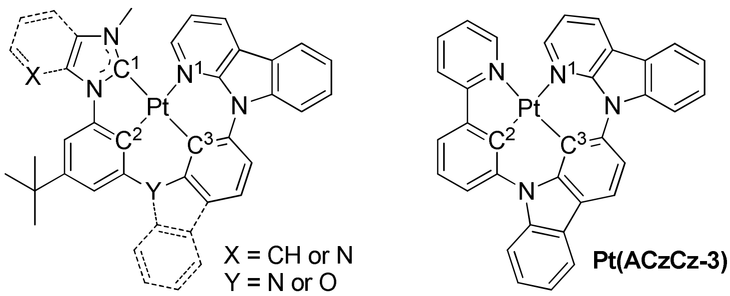


Figure S2. The different pulsed voltammetry (DPV) of tetradentate Pt(II) complexes measured in *N*,*N*-dimethylformamide under an nitrogen atmosphere.

Table S1. DFT Calculations for Pt(II) Complexes[a]			
Pt(II) complexes	Front view	Side view	Top view
Pt(NHC-1)			
Pt(Ph/NHC)			
Pt(Py/NHC)			
Pt(NHC-2)			

[a]Optimized S_0 were calculated using a B3LYP method with a basic set of 6-31G(d) for C, H, O and N atoms and a LANL2DZ basic set for Pt atoms.

Table S2. Selected Bond Lengths (Å), Bond Angles (°) and Dihedral Angles (°) for Tetradentate Pt(II) Complexes Based on the DFT Calculations.



metal compleses	Pt–C^1(N)	Pt–C^2	Pt–C^3	Pt–N^1
Pt(NHC-1)	2.082	1.997	2.047	2.173
Pt(Ph/NHC)	2.056	1.996	2.050	2.176
Pt(Py/NHC)	2.055	1.998	2.050	2.180
Pt(NHC-2)	2.090	1.998	2.046	2.175
Pt(ACzCz-3)[6]	2.200	1.984	2.007	2.200

metal compleses	C^1–Pt–C^2	C^2–Pt–C^3	C^3–Pt–N^1	N^1–Pt–C^1	C^1–Pt–C^3	C^2–Pt–N^1	dihedral angle^a
Pt(NHC-1)	78.77	91.27	90.69	100.88	167.34	165.89	46.72
Pt(Ph/NHC)	78.64	91.64	90.54	101.05	166.96	165.57	48.47
Pt(Py/NHC)	78.84	91.37	90.62	100.90	167.23	165.67	48.15
Pt(NHC-2)	79.25	90.73	89.24	102.19	165.98	170.94	49.19

^{a}Dihedral angle between terminal NHC and ACz planes. Optimized S_0 were calculated using a B3LYP method with a basic set of 6-31G(d) for C, H, O and N atoms and a LANL2DZ basic set for Pt atoms.

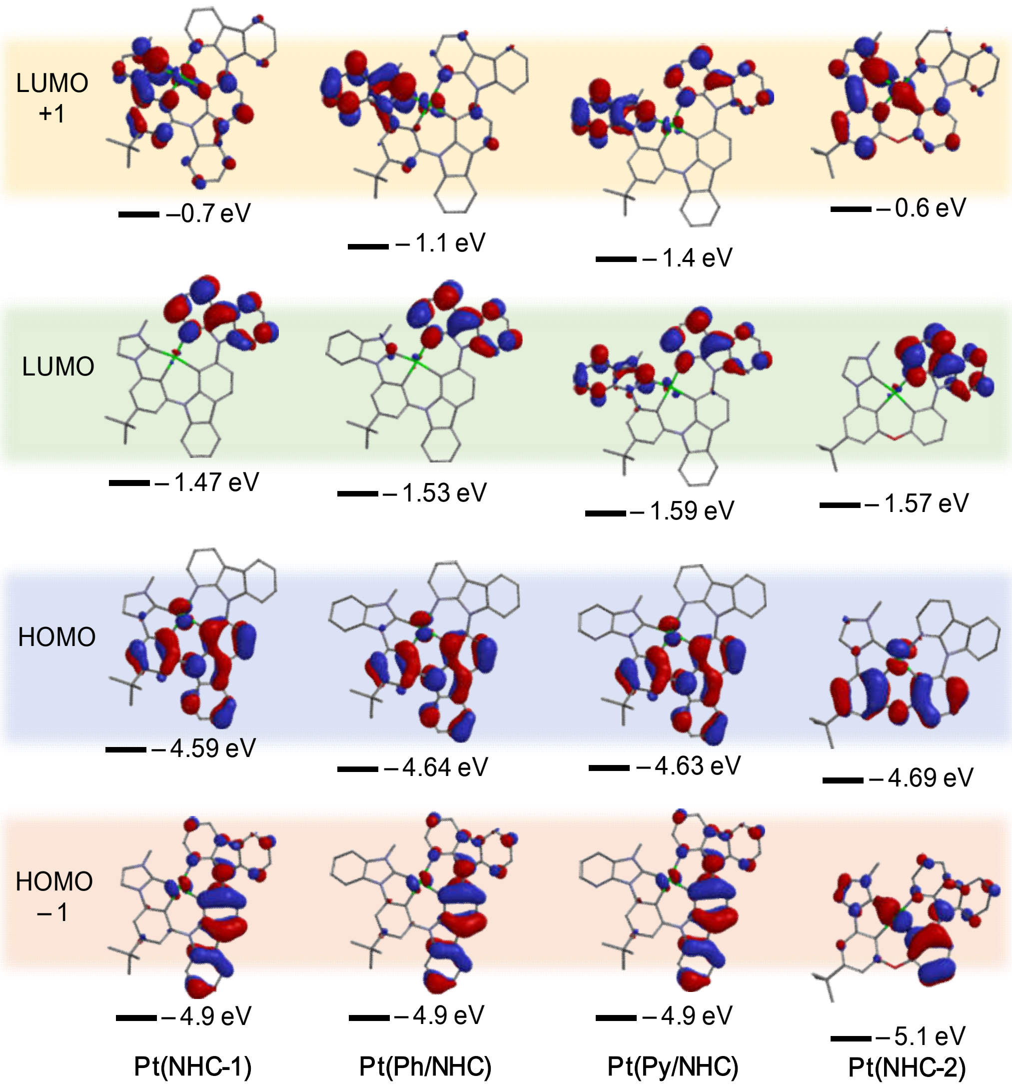


Figure S3. Density functional theory calculations of frontier orbitals for Pt(II) complexes based on optimized S_0 geometries. The H atoms were omitted for clarity.

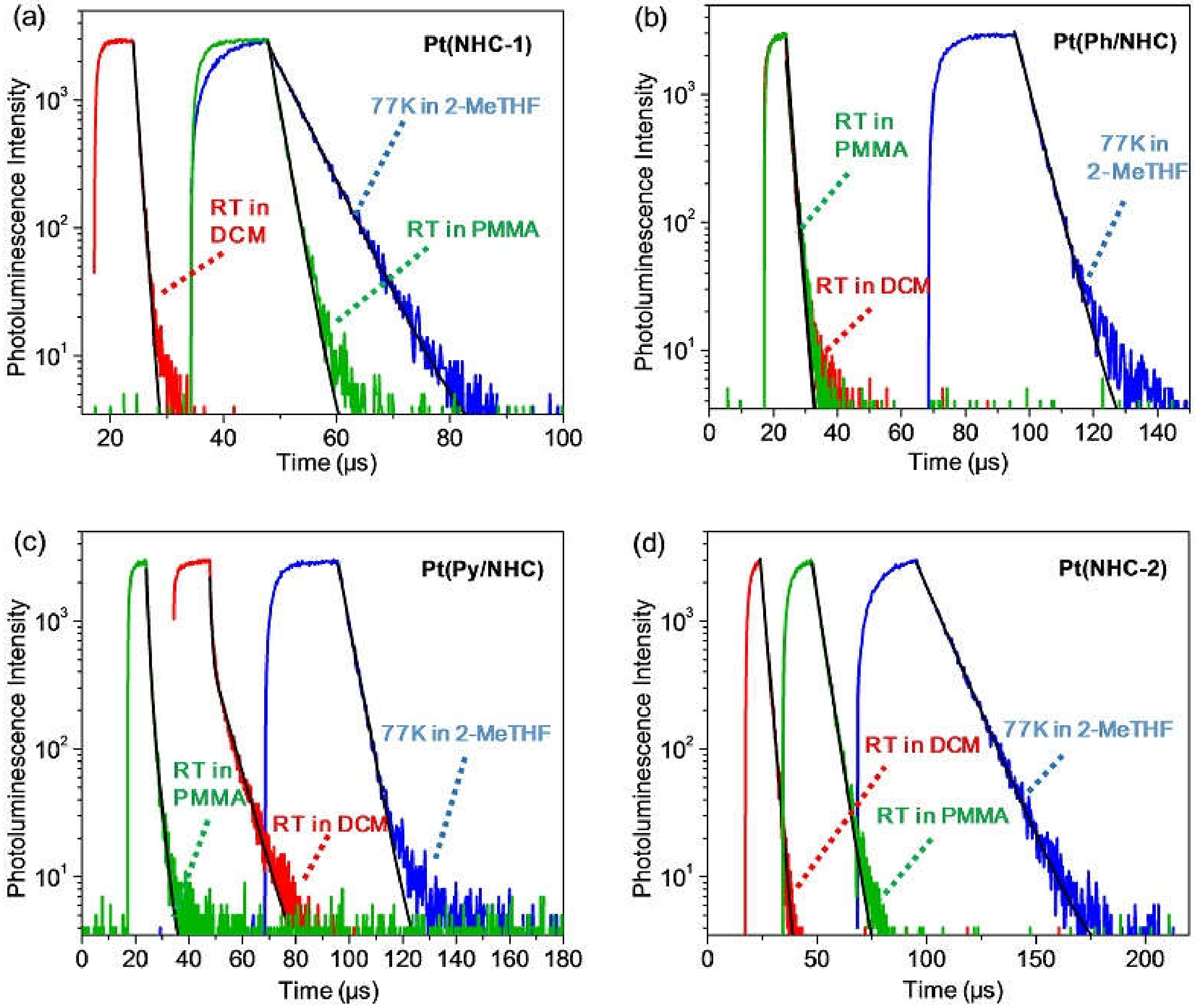


Figure S4. Transient decay spectra of (a) Pt(NHC-1), (b) Pt(Ph/NHC), (c) Pt(Py/NHC) and (d) Pt(NHC-2) in various conditions. The solid black lines represent biexponential fit of the experimental data.

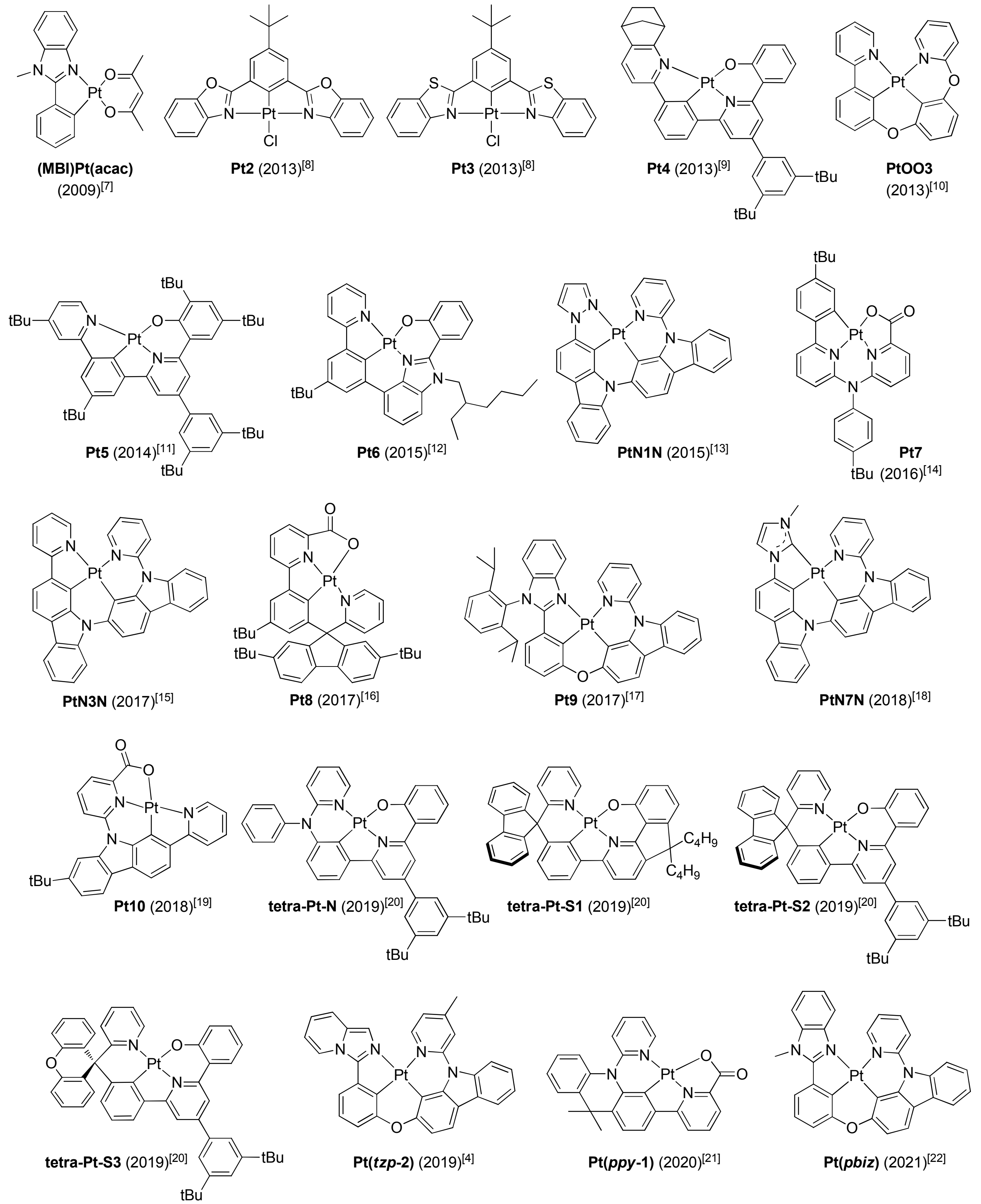


Figure S5. Bidentate, tridentate and tetradentate Pt(II) complexes for green to yellow OLEDs discussed in this study.

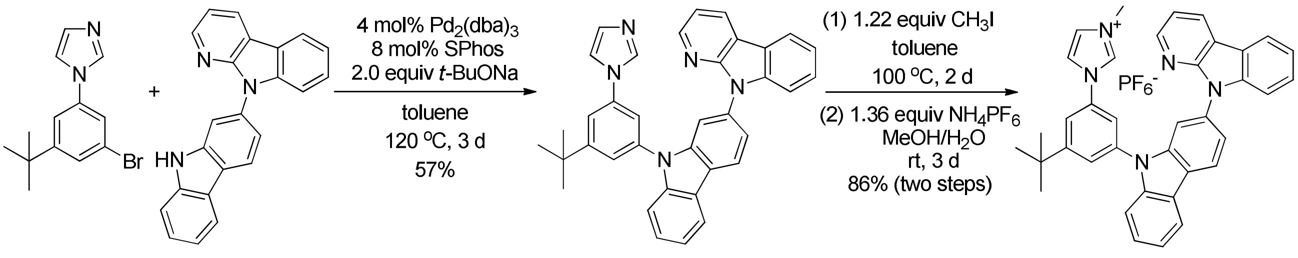
Table S3. Device Performances Comparison for Pt(II) Complexes-Based Green to Orange OLEDs

dopant/host	λ_{EL} (nm)	peak EQE (%)	CIE (x, y)	L_{max} (cd/m^2)	reference
(MBI)Pt(acac)/CBP	534	--	(0.38, 0.55)	13605	[7]
Pt2/CBP	～535	4.6	(0.50, 0.49)	--	[8]
Pt3/CBP	～555	6.9	(0.50, 0.49)	--	[8]
Pt4/mCP	～540	18.2	(0.282, 0.657)	--	[9]
PtNOO3/26mCPy	～505	22.3	--	--	[10]
Pt5/TCTA	～560	27.1	(0.41, 0.57)	2900	[11]
Pt6/TCTA	512	21.4	(0.33, 0.61)	--	[12]
PtN1N/26mCPy	498	26.1	(0.15, 0.56)	--	[13]
Pt7/mCP	540	13.8	(0.36, 0.58)	--	[14]
PtN3N/26mCPy	584	18.2	(0.55, 0.45)	--	[15]
Pt8/mCP	520	22.9	(0.36, 0.60)	--	[16]
Pt9/26mCPy	541	22.3	(0.31, 0.62)	--	[17]
PtN7N/BN-DBC-Ph_2	～520	～22.5	(0.27, 0.67)	--	[18]
Pt10/mCP	552	12.6	(0.49, 0.51)	--	[19]
tetra-Pt-N/o-CzPy^a	～555	16.83	(0.48, 0.51)	18500	[20]
tetra-Pt-S1/o-CzPy^a	～510	16.63	(0.29, 0.64)	49600	[20]
tetra-Pt-S2/o-CzPy^a	～500	3.89	(0.28, 0.58)	5970	[20]
tetra-Pt-S3/m-TPAPy^a	～505	22.9	(0.28, 0.63)	37600	[20]
Pt(*tzp*-2)/mCBP	545	8.7	(0.31, 0.61)	28280	[4]
Pt(*ppy*-1)/26mCPy	516	18.5	(0.298, 0.634)	40979	[21]
Pt(*pbiz*)/mCBP	505	25.5	(0.265, 0.602)	49781	[22]
Pt(*pbiz*)/26mCPy	501	21.6	(0.251, 0.595)	55481	[22]
Pt(NHC-1)/mCBP	512	13.9	(0.288, 0.588)	60275	**This work**
Pt(NHC-1)/26mCPy	509	13.1	(0.261, 0.575)	64416	**This work**

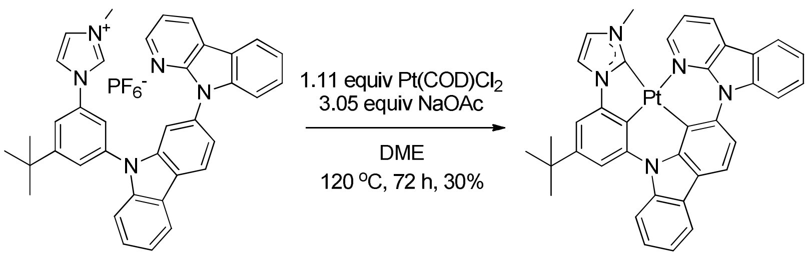
^{a} Solution-processed OLED.

Experimental Procedures

Synthesis of **Pt(NHC-1)**:



1(NHC-1) **2** **3(NHC-1)** **Ligand(NHC-1)**



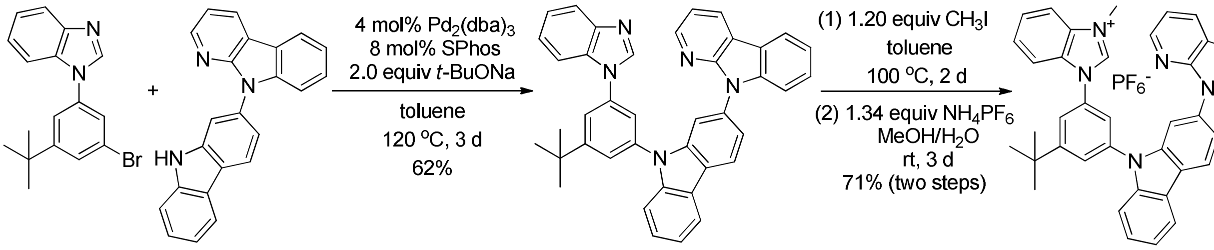
Ligand(NHC-1) **Pt(NHC-1)**

Synthesis of **3(NHC-1)**: A mixture of 1-(3-bromo-5-(*tert*-butyl)phenyl)-1*H*-imidazole **1(NHC-1)** (112 mg, 0.40 mmol, 1.0 equiv, synthesized according our previous report.[23]), 9-(9*H*-carbazol-2-yl)-9*H*-pyrido[2,3-*b*]indole **2** (133 mg, 0.40 mmol, 1.0equiv, synthesized according our previous report.[6]), $Pd_2(dba)_3$ (15 mg, 0.016 mmol, 4 mol%), SPhos (13 mg, 0.032 mmol, 8 mol%) and *t*-BuONa (77 mg, 0.80 mmol, 2.0 equiv) in toluene (5 mL) was stirred in a sealed vessel at a temperature of 120 °C under a nitrogen atmosphere for 3 days, then cooled down to ambient temperature. The reaction was concentrated under reduced pressure, then the residue was purified through column chromatography on silica gel (eluent: petroleum ether/ ethyl acetate = 6:1−2:1) to obtain the desired product as white foamy solid 121 mg in 57% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 1.41 (s, 9H), 7.24−7.26 (m, 2H), 7.32−7.40 (m, 3H), 7.43−7.50 (m, 4H), 7.54−7.57 (m, 2H), 7.59 (dd, J = 8.5, 2.0 Hz, 1H), 7.74 (t, J = 2.0 Hz, 1H), 7.76 (d, J = 1.5 Hz, 1H), 8.06 (s, 1H), 8.13 (d, J = 7.5 Hz, 1H), 8.23 (d, J = 8.0 Hz, 1H), 8.36 (d, J = 8.5 Hz, 1H), 8.39 (dd, J = 7.5, 1.5 Hz, 1H), 8.48 (dd, J = 8.5, 2.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 31.16, 35.30, 109.07, 109.62, 110.37, 116.12, 116.35, 117.03, 117.56, 118.38, 119.59, 120.64, 120.72, 120.74, 120.78, 120.93, 121.29, 122.94, 123.26, 123.29, 126.44, 126.90, 128.28, 130.38, 134.24, 135.60, 138.45, 138.62, 140.32, 141.03, 141.17, 146.44, 152.12, 155.65.

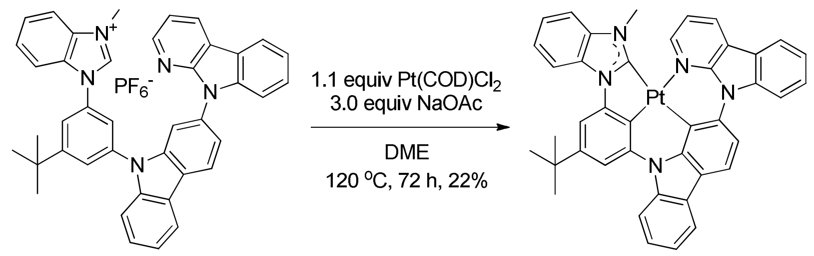
Synthesis of **Ligand(NHC-1)**: A solution of CH_3I (426 mg, 3.00 mmol, 1.22 equiv) and **3(NHC-1)** (1.30 g, 2.45 mmol, 1.00 equiv) in toluene (30 mL) was stirred in a sealed vessel at a temperature of 100 ^{o}C for 2 day, then cooled down to ambient temperature. The precipitate was filtered off and washed with petroleum ether (30 mL), dried under reduced pressure to afford a gray solid which was used directly for the next step. The gray solid was added to a mixture of MeOH/H_2O (30 mL/20 mL), then stirred for a few minutes until the solid was entirely dissolved. Then NH_4PF_6 (544 mg, 3.34 mmol, 1.36 equiv) was added to the solution. The mixture was stirred at room temperature for 3 days, diluted with water, and removed most of the solvent methanol under reduced pressure. The precipitate was collected through filtration, washed with water and petroleum ether. The gray solid was dried under reduced pressure to give the desired product 1.46 g in 86% yield. ^1H NMR (500 MHz, DMSO-d_6): δ (ppm) 1.41 (s, 9H), 3.90 (s, 3H), 7.33−7.38 (m, 2H), 7.42 (t, J = 7.0 Hz, 1H), 7.48−7.51 (m, 1H), 7.53−7.56 (m, 1H), 7.59−7.65 (m, 3H), 7.73 (d, J = 1.5 Hz, 1H), 7.85 (t, J = 1.5 Hz, 1H), 7.89 (t, J = 1.5 Hz, 1H), 7.99−8.01 (m, 2H), 8.30 (d, J = 8.0 Hz, 1H), 8.35 (t, J = 2.0 Hz, 1H), 8.39−8.40 (m, 2H), 8.53 (d, J = 8.5 Hz, 1H), 8.64 (dd, J = 7.5, 1.5 Hz, 1H), 9.77 (s, 1H). ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 30.77, 35.39, 36.12, 108.70, 110.06, 110.39, 115.74, 116.60, 117.41, 118.20, 119.77, 120.41, 120.92, 120.97, 121.00, 121.26, 121.45, 121.53, 122.14, 122.71, 124.19, 124.73, 126.85, 127.24, 129.00, 134.12, 136.11, 136.39, 137.87, 139.57, 140.22, 140.61. HRMS (ESI): calcd for $C_{37}H_{32}N_5$ $[M]^+$ 546.2652, found 546.2650.

Synthesis of **Pt(NHC-1)**: A mixture of **Ligand(NHC-1)** (97 mg, 0.140 mmol, 1.0 equiv), Pt(COD)Cl_2 (58 mg, 0.155 mmol, 1.11 equiv) and NaOAc (35 mg, 0.427 mmol, 3.05 equiv) in DME (3 mL) was stirred in a sealed vessel at a temperature of 120 ^{o}C under a nitrogen atmosphere for 3 days, then cooled down to ambient temperature. The reaction was concentrated under reduced pressure, then the residue was purified through column chromatography on silica gel (eluent: petroleum ether/CH_2Cl_2 = 5:1−1:1) to obtain the desired product as a yellow solid 31 mg in 30% yield. ^1H NMR (500 MHz, DMSO-d_6): δ (ppm) 1.46 (s, 9H), 3.56 (s, 3H), 7.31 (t, J = 7.0 Hz, 1H), 7.40 (d, J = 1.5 Hz, 1H), 7.42 (d, J = 1.0 Hz, 1H), 7.46−7.54 (m, 3H), 7.70−7.73 (m, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.97 (d, J = 8.0 Hz, 2H), 8.20−8.28 (m, 4H), 8.44 (d, J = 7.5 Hz, 1H), 8.98 (d, J = 7.5 Hz, 1H), 9.42 (dd, J = 5.5, 1.0 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 31.47, 34.95, 37.42, 104.57, 109.40, 110.63, 114.06, 115.15, 116.02, 116.36, 117.13, 117.29, 119.43, 120.25, 120.29, 122.17, 122.31, 122.35, 123.24, 124.82, 126.11, 126.32, 127.97, 130.31, 135.86, 136.96, 138.93, 139.22, 141.93, 146.90, 146.96, 149.15, 153.35, 180.47. HRMS (ESI): calcd for $C_{37}H_{30}N_5Pt$ $[M+H]^+$ 739.2143, found 739.2121.

Synthesis of **Pt(Ph/NHC)**:



1(Ph/NHC) **2** **3(Ph/NHC)** **Ligand(Ph/NHC)**



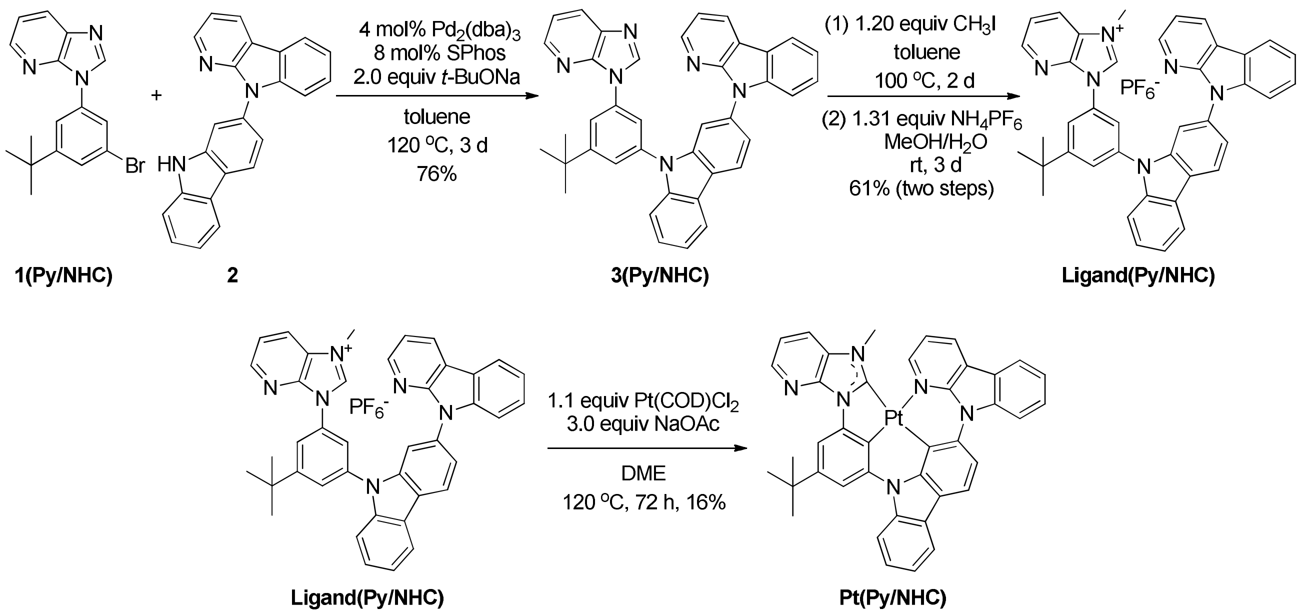
Ligand(Ph/NHC) **Pt(Ph/NHC)**

Synthesis of **3(Ph/NHC)**: A mixture of 1-(3-bromo-5-(*tert*-butyl)phenyl)-1*H*-benzo[*d*]imidazole **1(Ph/NHC)** (99 mg, 0.30 mmol, 1.0 equiv, synthesized according our previous report.[24]), 9-(9*H*-carbazol-2-yl)-9*H*-pyrido[2,3-*b*]indole **2** (100 mg, 0.30 mmol, 1.0 equiv, synthesized according our previous report.[6]), $Pd_2(dba)_3$ (11 mg, 0.012 mmol, 4 mol%), SPhos (10 mg, 0.024 mmol, 8 mol%) and *t*-BuONa (58 mg, 0.60 mmol, 2.0 equiv) in toluene (3 mL) was stirred in a sealed vessel at a temperature of 120 ^{o}C under a nitrogen atmosphere for 3 days, then cooled down to ambient temperature. The reaction was concentrated under reduced pressure, then the residue was purified through column chromatography on silica gel (eluent: petroleum ether/ ethyl acetate = 6:1−4:1) to obtain the desired product as white foamy solid 108 mg in 62% yield. ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 1.41 (s, 9H), 7.20 (t, J = 7.5 Hz, 1H), 7.28 (t, J = 7.5 Hz, 1H), 7.32−7.41 (m, 3H), 7.47 (t, J = 7.5 Hz, 1H), 7.54 (t, J = 7.0 Hz, 1H), 7.61−7.67 (m, 4H), 7.75−7.77 (m, 2H), 7.82 (d, J = 1.5 Hz, 1H), 7.87−7.88 (m, 2H), 8.30 (d, J = 7.5 Hz, 1H), 8.36−8.39 (m, 2H), 8.52 (d, J = 8.5 Hz, 1H), 8.63−8.66 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 31.21, 35.39, 109.13, 109.67, 110.38, 110.42, 116.12, 116.36, 119.19, 119.74, 120.02, 120.68, 120.75, 120.79, 120.94, 121.35, 123.05, 123.08, 123.35, 123.80, 124.02, 126.49, 126.95, 128.29, 133.39, 134.30, 135.78, 137.44, 138.84, 140.41, 141.11, 141.23, 142.03, 143.66, 146.48, 152.18, 155.84.

Synthesis of **Ligand(Ph/NHC)**: A solution of CH_3I (85 mg, 0.60 mmol, 1.2 equiv) and **3(Ph/NHC)** (291 mg, 0.50 mmol, 1.0 equiv) in toluene (7 mL) was stirred in a sealed vessel at a temperature of 100 °C for 2 days, then cooled down to ambient temperature. The precipitate was filtered off and washed with petroleum ether (7 mL), dried under reduced pressure to afford a gray solid which was used directly for the next step. The gray solid was added to a mixture of MeOH/H_2O (7 mL/4 mL), then stirred for a few minutes until the solid was entirely dissolved. Then NH_4PF_6 (109 mg, 0.67 mmol, 1.34 equiv) was added to the solution. The mixture was stirred at room temperature for 3 days, diluted with water, and removed most of the solvent methanol under reduced pressure. The precipitate was collected through filtration, washed with water and petroleum ether. The gray solid was dried under reduced pressure to give the desired product 265 mg in 71% yield. ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 1.44 (s, 9H), 4.14 (s, 3H), 7.34−7.38 (m, 2H), 7.42 (t, J = 7.5 Hz, 1H), 7.47 (t, J = 7.0 Hz, 1H), 7.53−7.59 (m, 2H), 7.62−7.67 (m, 3H), 7.74 (t, J = 7.5 Hz, 1H), 7.81 (d, J = 1.5 Hz, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.92 (t, J = 1.5 Hz, 1H), 8.01 (t, J = 1.5 Hz, 1H), 8.11 (d, J = 8.5 Hz, 1H), 8.15 (t, J = 1.5 Hz, 1H), 8.31 (d, J = 7.5 Hz, 1H), 8.38−8.41(m, 2H), 8.54 (d, J = 8.0 Hz, 1H), 8.66 (dd, J = 7.5, 1.5 Hz, 1H), 10.15 (s, 1H). ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 30.78, 33.44, 35.36, 108.80, 110.05, 110.37, 113.52, 113.83, 115.74, 116.58, 119.83, 120.39, 120.95, 121.04, 121.43, 121.46, 121.53, 122.22, 122.79, 125.51, 126.83, 126.89, 127.26, 127.39, 129.02, 131.00, 131.77, 134.11, 134.47, 137.97, 139.60, 140.22, 140.57, 143.43, 146.31, 151.40, 155.61. HRMS (ESI): calcd for $C_{41}H_{34}N_5$ $[M]^+$ 596.2809, found 596.2805.

Synthesis of **Pt(Ph/NHC)**: A mixture of **Ligand(Ph/NHC)** (237 mg, 0.32 mmol, 1.0 equiv), Pt(COD)Cl_2 (132 mg, 0.35 mmol, 1.1 equiv) and NaOAc (79 mg, 0.96 mmol, 3.0 equiv) in DME (10 mL) was stirred in a sealed vessel at a temperature of 120 °C under a nitrogen atmosphere for 3 days, then cooled down to ambient temperature. The reaction was concentrated under reduced pressure, then the residue was purified through column chromatography on silica gel (eluent: petroleum ether/CH_2Cl_2 = 5:1−1:1) to obtain the desired product as a yellow solid 56 mg in 22% yield. ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 1.56 (s, 9H), 3.63 (s, 3H), 7.34 (t, J = 7.0 Hz, 1H), 7.48 (t, J = 7.5 Hz, 1H), 7.52−7.57 (m, 4H), 7.72−7.77 (m, 3H), 7.93 (d, J = 7.0 Hz, 1H), 8.05 (d, J = 8.5 Hz, 1H), 8.12 (d, J = 1.5 Hz, 1H), 8.27 (dd, J = 7.5, 1.0 Hz, 1H), 8.31−8.34 (m, 3H), 8.48 (d, J = 7.5 Hz, 1H), 9.05 (dd, J = 7.5, 1.5 Hz, 1H), 9.40 (dd, J = 5.5, 1.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 31.76, 34.21, 35.18, 105.71, 110.60, 110.67, 111.01, 111.59, 114.51, 115.35, 115.51, 116.01, 117.15, 118.13, 120.04, 120.12, 120.30, 121.15, 122.07, 122.51, 122.72, 124.16, 124.39, 126.52, 126.84, 127.66, 128.70, 132.12, 136.27, 136.32, 137.69, 139.98, 140.41, 142.58, 147.10, 147.77, 150.57, 152.16, 192.27. HRMS (ESI): calcd for $C_{41}H_{32}N_5Pt$ $[M+H]^+$ 789.2300, found 789.2267.

Synthesis of **Pt(Py/NHC)**:



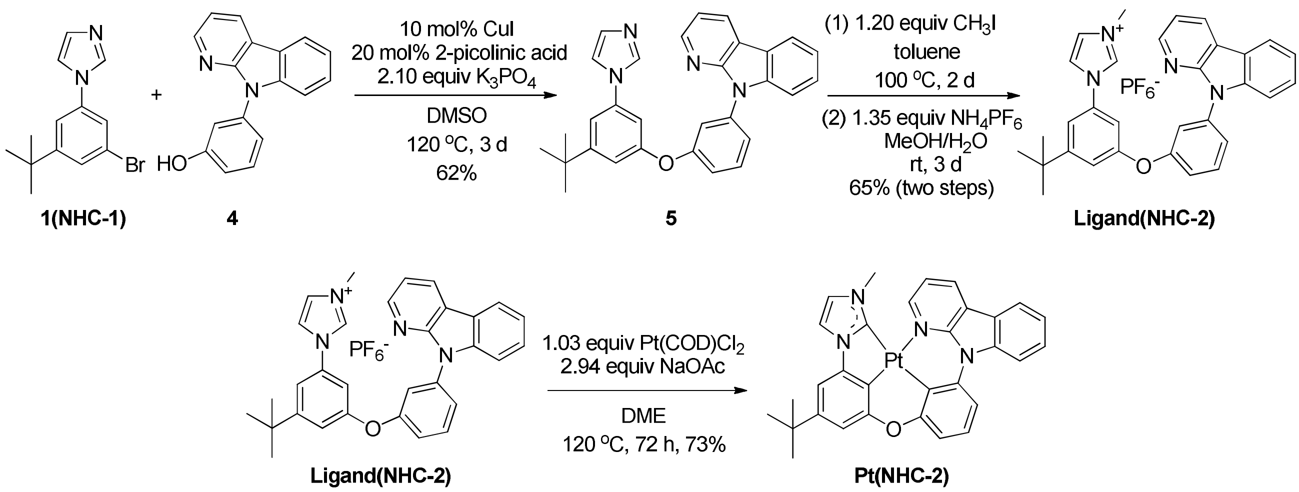
Synthesis of **3(Py/NHC)**: A mixture of 3-(3-bromo-5-(*tert*-butyl)phenyl)-3*H*-imidazo[4,5-*b*]pyridine **1(Ph/NHC)** (50 mg, 0.15 mmol, 1.0 equiv, synthesized according our previous report.[24]), 9-(9*H*-carbazol-2-yl)-9*H*-pyrido[2,3-*b*]indole **2** (50 mg, 0.15 mmol, 1.0 equiv, synthesized according our previous report.[6]), $Pd_2(dba)_3$ (6 mg, 0.0060 mmol, 4 mol%), SPhos (5 mg, 0.012 mmol, 8 mol%) and *t*-BuONa (29 mg, 0.30 mmol, 2.0 equiv) in toluene (2 mL) was stirred in a sealed vessel at a temperature of 120 °C under a nitrogen atmosphere for 3 days, then cooled down to ambient temperature. The reaction was concentrated under reduced pressure, then the residue was purified through column chromatography on silica gel (eluent: petroleum ether/ ethyl acetate = 6:1−3:1) to obtain the desired product as white foamy solid 66 mg in 76% yield. ^1H NMR (500 MHz, DMSO-d_6): δ (ppm) 1.42 (s, 9H), 7.28 (dd, J = 8.0, 4.5 Hz, 1H), 7.32−7.36 (m, 2H), 7.39−7.44 (m, 2H), 7.54−7.57 (m, 1H), 7.60−7.63 (m, 2H), 7.73 (d, J = 8.0 Hz, 1H), 7.86 (t, J = 2.0 Hz, 1H), 7.94 (d, J = 2.0 Hz, 1H), 8.02 (dd, J = 5.0, 1.5 Hz, 1H), 8.04 (t, J = 2.0 Hz, 1H), 8.18 (dd, J = 8.0, 1.5 Hz, 1H), 8.25 (t, J = 2.0 Hz, 1H), 8.31 (d, J = 8.0 Hz, 1H), 8.36 (dd, J = 4.5, 1.5 Hz, 1H), 8.40 (d, J = 7.5 Hz, 1H), 8.53 (d, J = 8.0 Hz, 1H), 8.65 (dd, J = 7.5, 1.5 Hz, 1H), 9.05 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 31.23, 35.37, 109.51, 109.98, 110.50, 116.00, 116.30, 119.01, 119.27, 119.76, 120.57, 120.66, 120.72, 120.87, 121.25, 123.13, 123.20, 123.34, 126.43, 126.92, 128.24, 128.26, 134.22, 135.82, 136.18, 138.35, 140.52, 141.07, 141.18, 142.72, 145.07, 146.47, 152.23, 155.18.

Synthesis of **Ligand(Py/NHC)**: A solution of CH_3I (44 mg, 0.31 mmol, 1.2 equiv) and **3(Py/NHC)** (152 mg, 0.26 mmol, 1.0 equiv) in toluene (4 mL) was stirred in a sealed vessel at a temperature of 100 °C for 2 days, then cooled down to ambient temperature. The precipitate was filtered off and washed with petroleum ether (4 mL), dried under reduced pressure to afford a gray solid which was used directly for the next step. The gray solid was added to a mixture of MeOH/H_2O (40 mL/20 mL), then stirred for a few minutes until the solid was entirely dissolved. Then NH_4PF_6 (56 mg, 0.34 mmol, 1.31 equiv) was added to the solution. The mixture was stirred at room temperature for 3 days, diluted with water, and removed most of the solvent methanol under reduced pressure. The precipitate was collected through filtration, washed with water and petroleum ether. The gray solid was dried under reduced pressure to give the desired product 118 mg in 61% yield. ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 1.44 (s, 9H), 4.17 (s, 3H), 7.34−7.38 (m, 2H), 7.42−7.48 (m, 2H), 7.57−7.61 (m, 2H), 7.64 (dd, J = 8.0, 1.5 Hz, 1H), 7.72 (d, J = 8.5 Hz, 1H), 7.77 (dd, J = 8.0, 4.5 Hz, 1H), 7.90 (d, J = 1.5 Hz, 1H), 8.01 (t, J = 1.5 Hz, 1H), 8.13 (dt, J = 8.5, 2.0 Hz, 2H), 8.33 (d, J = 8.0 Hz, 1H), 8.37 (ddd, J = 8.5, 4.5, 1.5 Hz, 2H), 8.42 (d, J = 8.0 Hz, 1H), 8.56 (d, J = 8.0 Hz, 1H), 8.63 (dd, J = 8.0, 1.0 Hz, 1H), 8.67 (dd, J = 7.5, 1.5 Hz, 1H), 10.45 (s, 1H). ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 30.80, 34.01, 35.33, 108.83, 109.95, 110.33, 115.68, 116.55, 120.01, 120.11, 120.34, 120.87, 120.93, 121.02, 121.10, 121.51, 121.54, 122.34, 122.48, 122.83, 123.79, 124.65, 125.18, 126.92, 127.26, 129.00, 133.46, 134.16, 137.37, 139.65, 140.02, 140.39, 142.77, 144.32, 146.33, 148.45, 151.45, 155.10. HRMS (ESI): calcd for $C_{40}H_{33}N_6$ $[M]^+$ 597.2761, found 597.2758.

Synthesis of **Pt(Py/NHC)**: A mixture of **Ligand(Py/NHC)** (149 mg, 0.20 mmol, 1.0 equiv), Pt(COD)Cl_2 (82 mg, 0.22 mmol, 1.1 equiv) and NaOAc (49 mg, 0.60 mmol, 3.0 equiv) in DME (6 mL) was stirred in a sealed vessel at a temperature of 120 °C under a nitrogen atmosphere for 3 days, then cooled down to ambient temperature. The reaction was concentrated under reduced pressure, then the residue was purified through column chromatography on silica gel (eluent: petroleum ether/CH_2Cl_2 = 5:1−1:1) to obtain the desired product as a yellow solid 26 mg in 16% yield. ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 1.52 (s, 9H), 3.60 (s, 3H), 7.35 (t, J = 7.0 Hz, 1H), 7.42 (t, J = 7.0 Hz, 1H), 7.48 (dd, J = 8.0, 5.0 Hz, 1H), 7.51−7.58 (m, 2H), 7.71−7.74 (m, 1H), 7.88 (d, J = 8.0 Hz, 1H), 8.04 (d, J = 8.0 Hz, 1H), 8.13−8.17 (m, 2H), 8.28 (dd, J = 8.0, 1.5 Hz, 2H), 8.35 (d, J = 8.5

Hz, 1H), 8.45 (d, J = 8.0 Hz, 1H), 8.58 (dd, J = 4.5, 1.0 Hz, 1H), 8.76 (d, J = 1.0 Hz, 1H), 8.99 (d, J = 7.5 Hz, 1H), 9.44 (dd, J = 5.5, 1.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 31.81, 34.11, 35.28, 108.42, 110.67, 110.76, 114.58, 115.11, 115.61, 115.87, 116.49, 117.42, 117.63, 118.15, 120.08, 120.20, 121.10, 122.04, 122.53, 124.48, 126.33, 126.87, 127.56, 128.39, 128.79, 136.46, 137.11, 139.91, 140.22, 142.51, 144.42, 145.83, 147.47, 147.82, 149.32, 152.71, 193.41. HRMS (ESI): calcd for $C_{40}H_{31}N_6Pt$ $[M+H]^+$ 790.2252, found 790.2224.

Synthesis of **Pt(NHC-2)**:

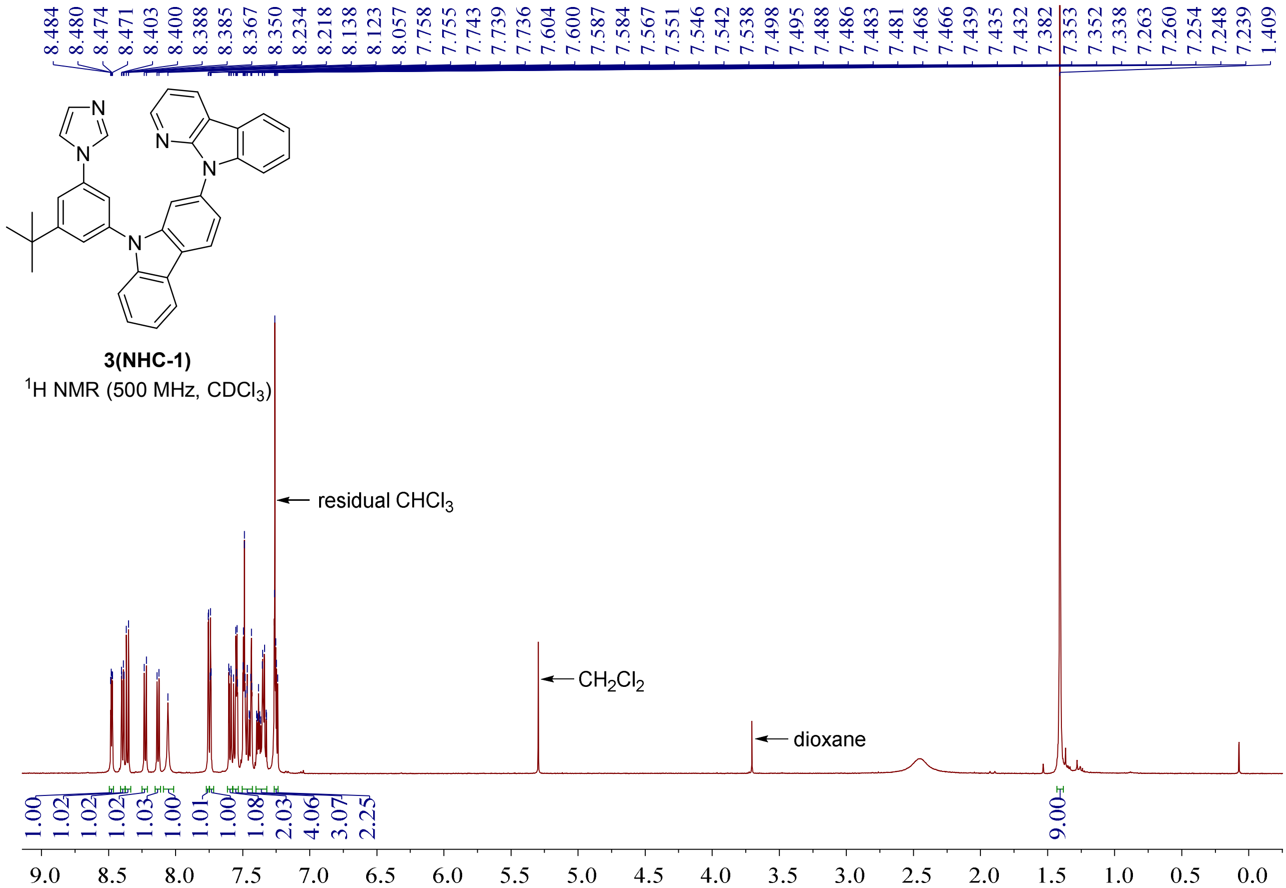


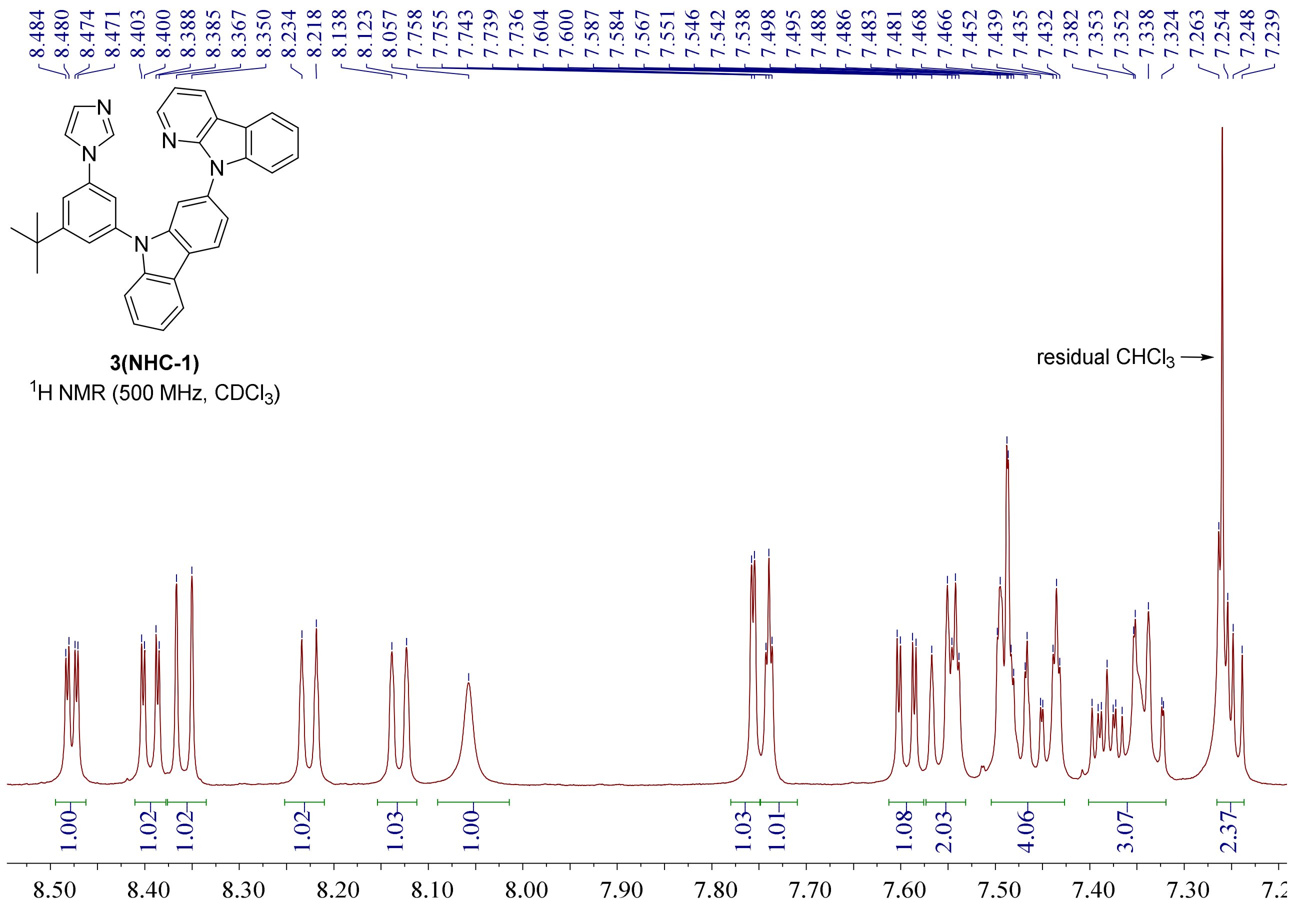
Synthesis of **5**: A mixture of 3-(9*H*-pyrido[2,3-*b*]indol-9-yl)phenol **4** (273 mg, 1.05 mmol, 1.0 equiv, synthesized according our previous report.[5,25,26]), 1-(3-bromo-5-(*tert*-butyl)phenyl)-1*H*-imidazole **1(NHC-1)** (279 mg, 1.00 mmol, 1.00 equiv, synthesized according our previous report.[23]), CuI (19 mg, 0.10 mmol, 10 mol%), 2-picolinic acid (25 mg, 0.20 mmol, 20 mol%) and K_3PO_4 (446 mg, 2.10 mmol, 2.10 equiv) in DMSO (4 mL) was stirred in a sealed vessel at a temperature of 120 °C under a nitrogen atmosphere for 3 days, the reaction was monitored by TLC until the reaction was completed. The resulting mixture was cooled down to room temperature, and diluted with ethyl acetate. The mixture washed with brine two times. The organic layer was separated and the aqueous layer was extracted with ethyl acetate two times. The combined organic layer was dried over anhydrous sodium sulfate, and concentrated under reduced pressure, then the residue was purified through column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 6:1−2:1) to obtain the desired product as a brown solid 284 mg in 62% yield. ^{1}H NMR (500 MHz,$CDCl_3$): δ (ppm) 1.36 (s, 9H), 7.02 (t, J = 2.0 Hz, 1H), 7.15 (t,

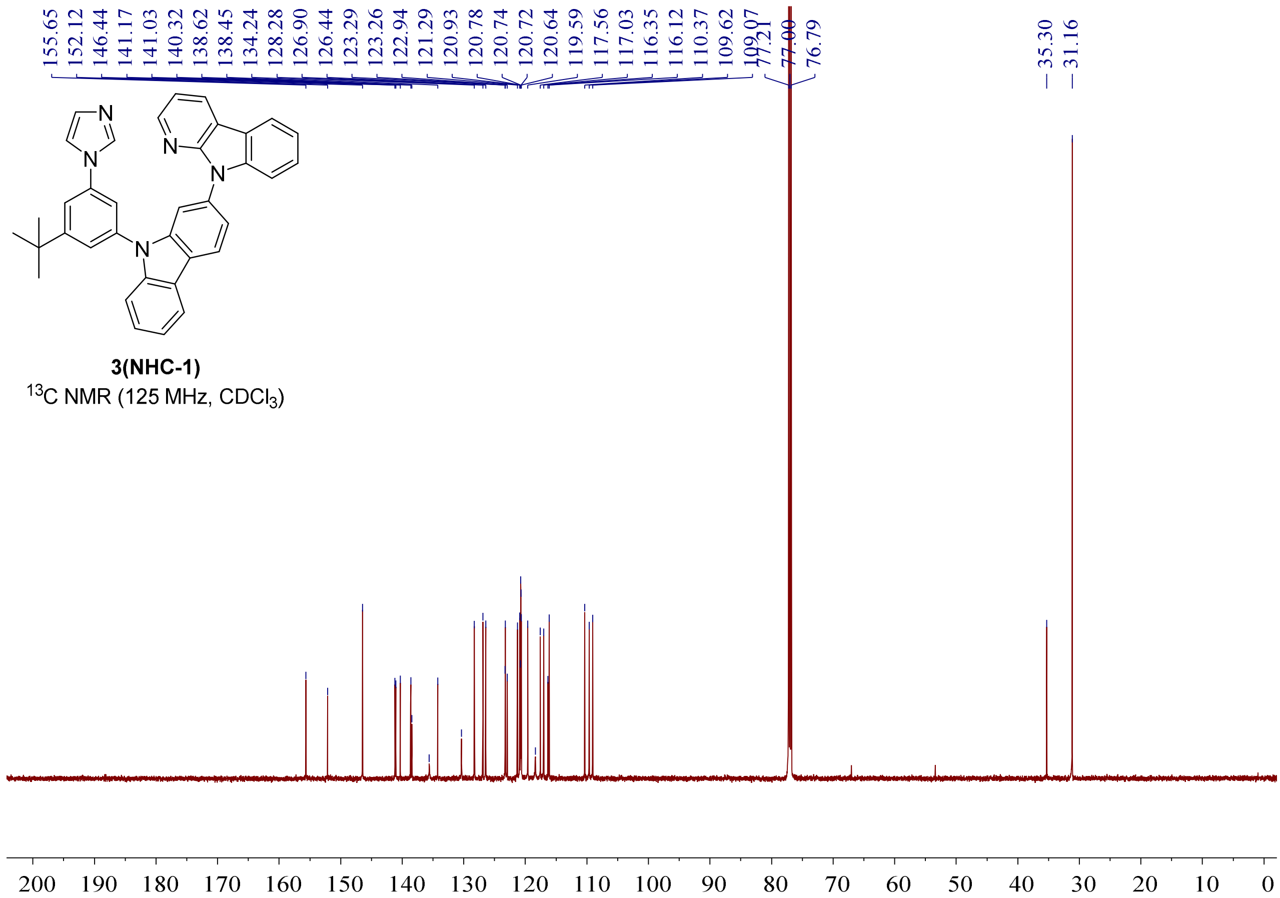
J = 2.0 Hz, 1H), 7.17 (ddd, J = 8.5, 2.0, 0.5 Hz, 1H), 7.24−7.25 (m, 3H), 7.32−7.36 (m, 2H), 7.37 (t, J = 2.0 Hz, 1H), 7.45−7.49 (m, 2H), 7.52 (d, J = 8.0 Hz, 1H), 7.62 (t, J = 8.0 Hz, 1H), 8.05 (s, 1H), 8.16 (d, J = 7.5 Hz, 1H), 8.38 (dd, J = 7.5, 1.5 Hz, 1H), 8.44 (dd, J = 5.0, 2.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 31.14, 35.21, 109.44, 110.28, 113.92, 115.75, 116.36, 116.42, 117.70, 117.74, 120.93, 120.97, 121.00, 122.44, 127.01, 128.32, 130.83, 137.71, 139.73, 146.48, 151.75, 155.67, 157.45, 157.57.

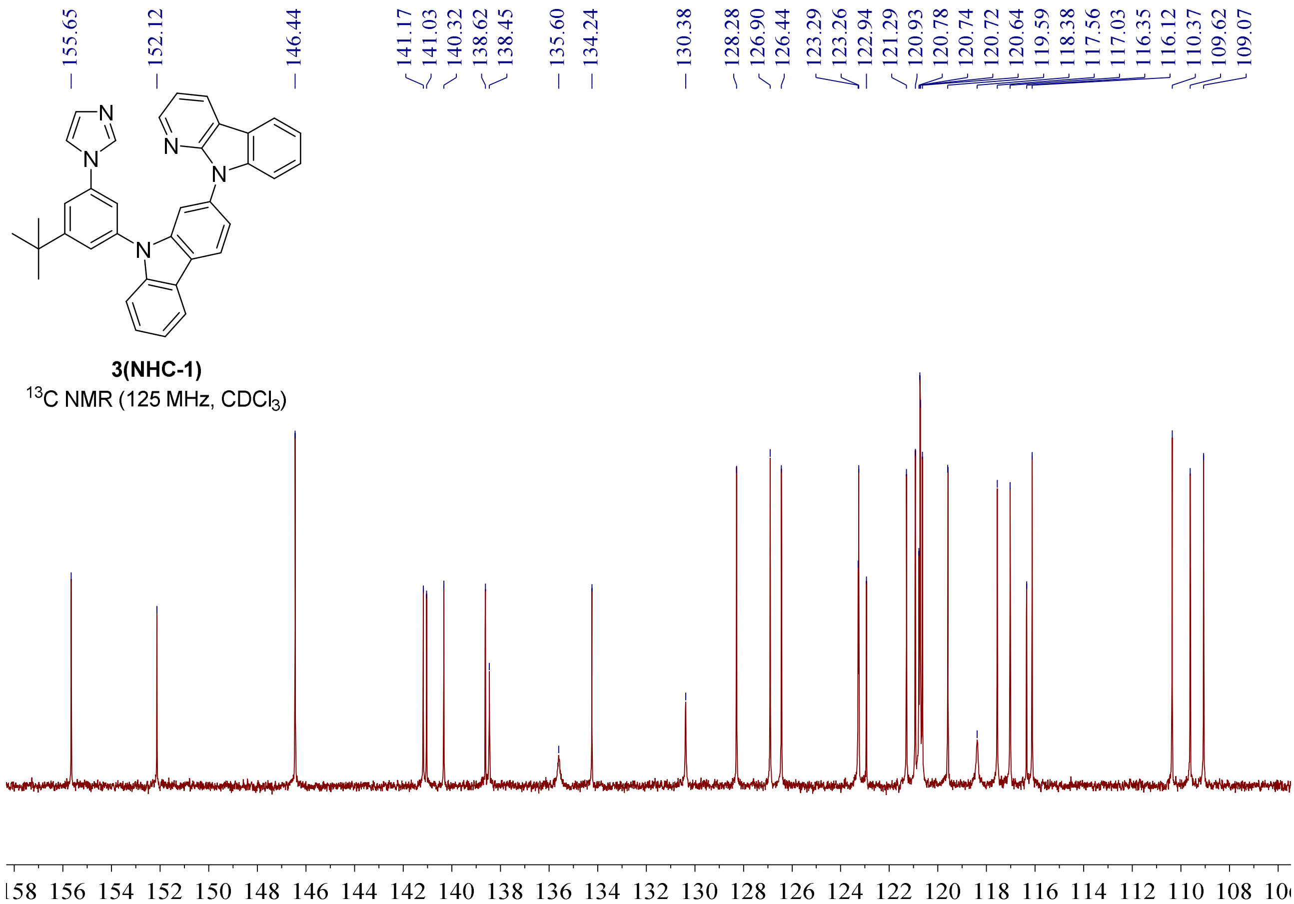
Synthesis of **Ligand(NHC-2)**: A solution of CH_3I (94 mg, 0.66 mmol, 1.20 equiv) and **5** (252 mg, 0.55 mmol, 1.00 equiv) in toluene (6 mL) was stirred in a sealed vessel at a temperature of 100 ^{o}C for 2 days, then cooled down to ambient temperature. The precipitate was filtered off and washed with petroleum ether (6 mL), dried under reduced pressure to afford a gray solid which was used directly for the next step. The gray solid was added to a mixture of MeOH/H_2O (6 mL/4 mL), then stirred for a few minutes until the solid was entirely dissolved. Then NH_4PF_6 (120 mg, 0.74 mmol, 1.35 equiv) was added to the solution. The mixture was stirred at room temperature for 3 days, diluted with water, and removed most of the solvent methanol under reduced pressure. The precipitate was collected through filtration, washed with water and petroleum ether. The gray solid was dried under reduced pressure to give the desired product 222 mg in 65% yield. 1H NMR (500 MHz, DMSO-d_6): δ (ppm) 1.35 (s, 9H), 3.92 (s, 3H), 7.24 (ddd, J = 8.5, 2.5, 1.0 Hz, 1H), 7.35−7.38 (m, 3H), 7.42 (t, J = 1.5 Hz, 1H), 7.47−7.55 (m, 4H), 7.58 (t, J = 2.0 Hz, 1H), 7.70 (t, J = 8.0 Hz, 1H), 7.91 (t, J = 1.5 Hz, 1H), 8.30 (d, J = 7.5 Hz, 1H), 8.32 (t, J = 2.0 Hz, 1H), 8.40 (dd, J = 4.5, 1.5 Hz, 1H), 8.65 (dd, J = 8.0, 2.0 Hz, 1H), 9.76 (s, 1H). ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 30.73, 35.25, 36.11, 110.14, 110.28, 114.65, 115.76, 116.78, 116.89, 117.17, 117.33, 120.48, 121.10, 121.59, 122.36, 124.25, 127.25, 129.05, 131.07, 135.87, 136.24, 137.27, 138.97, 146.30, 151.03, 155.71, 156.70, 156.94. HRMS (ESI): calcd for $C_{31}H_{29}N_4O$ $[M]^+$ 473.2336, found 473.2332.

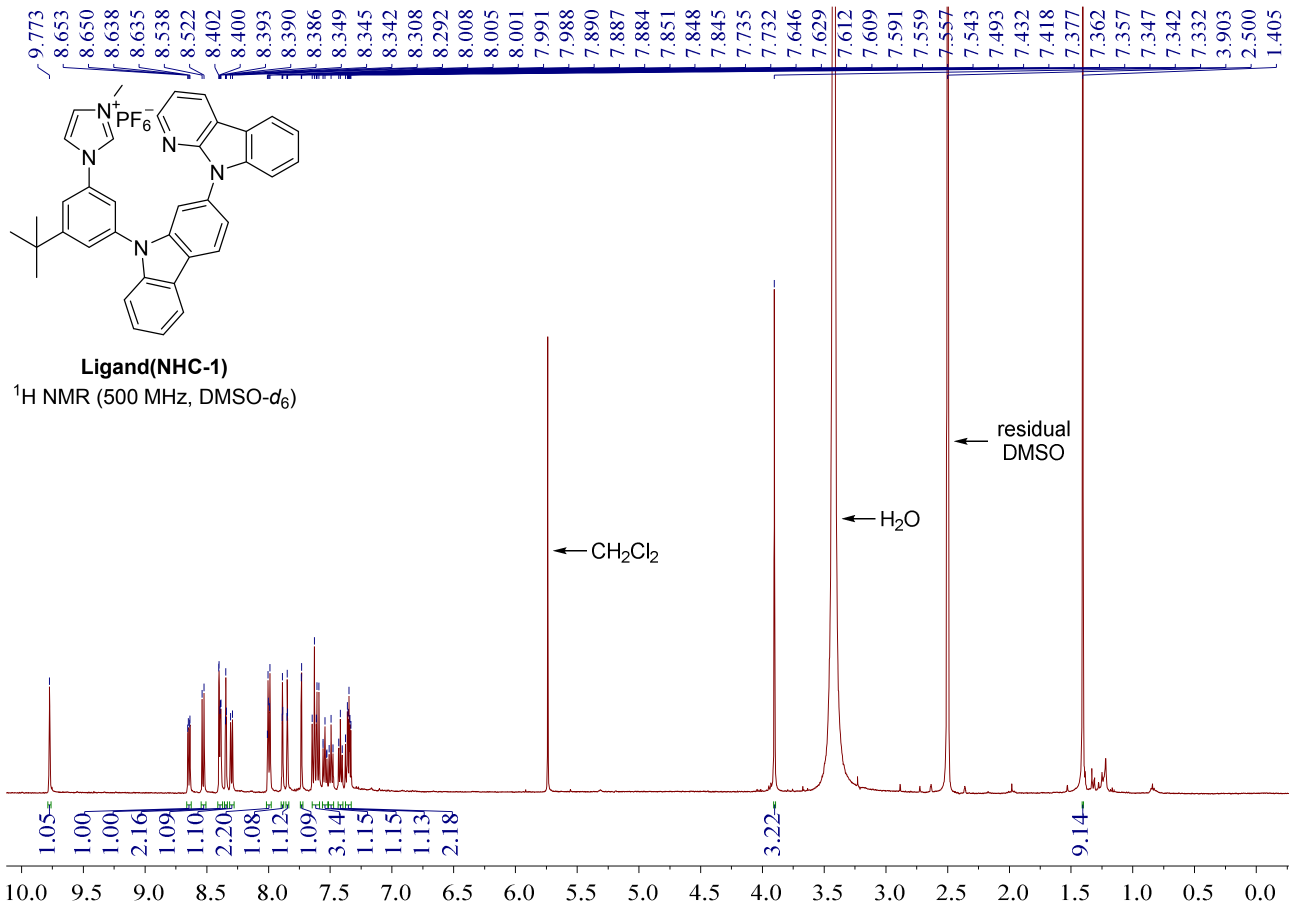
Synthesis of **Pt(NHC-2)**: A mixture of **Ligand(NHC-2)** (202 mg, 0.327 mmol, 1.00 equiv), Pt(COD)Cl_2 (126 mg, 0.337 mmol, 1.03 equiv) and NaOAc (79 mg, 0.963 mmol, 2.94 equiv) in DME (6 mL) was stirred in a sealed vessel at a temperature of 120 ^{o}C under a nitrogen atmosphere for 3 days, then cooled down to ambient temperature. The reaction was concentrated under reduced pressure, then the residue was purified through column chromatography on silica gel (eluent: petroleum ether/CH_2Cl_2 = 5:1−1:1) to obtain the desired product as a yellow solid 160 mg in 73% yield. ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 1.37 (s, 9H), 3.46 (s, 3H), 6.86 (d, J = 2.0 Hz, 1H), 7.06 (dd, J = 8.0, 1.0 Hz, 1H), 7.15 (t, J = 8.0 Hz, 1H), 7.26 (d, J = 1.5 Hz, 1H), 7.35 (d, J = 2.0 Hz, 1H), 7.44−7.50 (m, 3H), 7.64−7.68 (m, 1H), 8.08 (d, J = 2.0 Hz, 1H), 8.12 (d, J = 8.5 Hz, 1H), 8.39 (d, J = 7.0 Hz, 1H), 8.93 (dd, J = 7.5, 1.5 Hz, 1H), 9.24 (dd, J = 5.5, 1.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 31.59, 34.71, 37.30, 103.07, 108.94, 110.37, 110.75, 113.68, 114.85, 115.74, 116.33, 119.88, 121.10, 121.30, 121.99, 122.60, 124.51, 126.56, 127.50, 128.38, 138.71, 140.46, 148.37, 148.58, 149.09, 151.81, 151.88, 156.40, 181.55. HRMS (ESI): calcd for $C_{31}H_{27}N_4OPt$ $[M+H]^+$ 666.1827, found 666.1820.


8.484 8.480 8.474 8.471 8.403 8.400 8.388 8.385 8.367 8.350 8.234 8.218 8.138 8.123 8.057 7.758 7.755 7.743 7.739 7.736 7.604 7.600 7.587 7.584 7.567 7.551 7.546 7.542 7.538 7.498 7.495 7.488 7.486 7.483 7.481 7.468 7.466 7.439 7.435 7.432 7.382 7.353 7.352 7.338 7.263 7.260 7.254 7.248 7.239 1.409
3(NHC-1)
^{1}H NMR (500 MHz, $CDCl_3$)
residual $CHCl_3$
CH_2Cl_2
dioxane
1.00 1.02 1.02 1.02 1.03 1.00 1.01 1.00 1.08 2.03 4.06 3.07 2.25
9.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

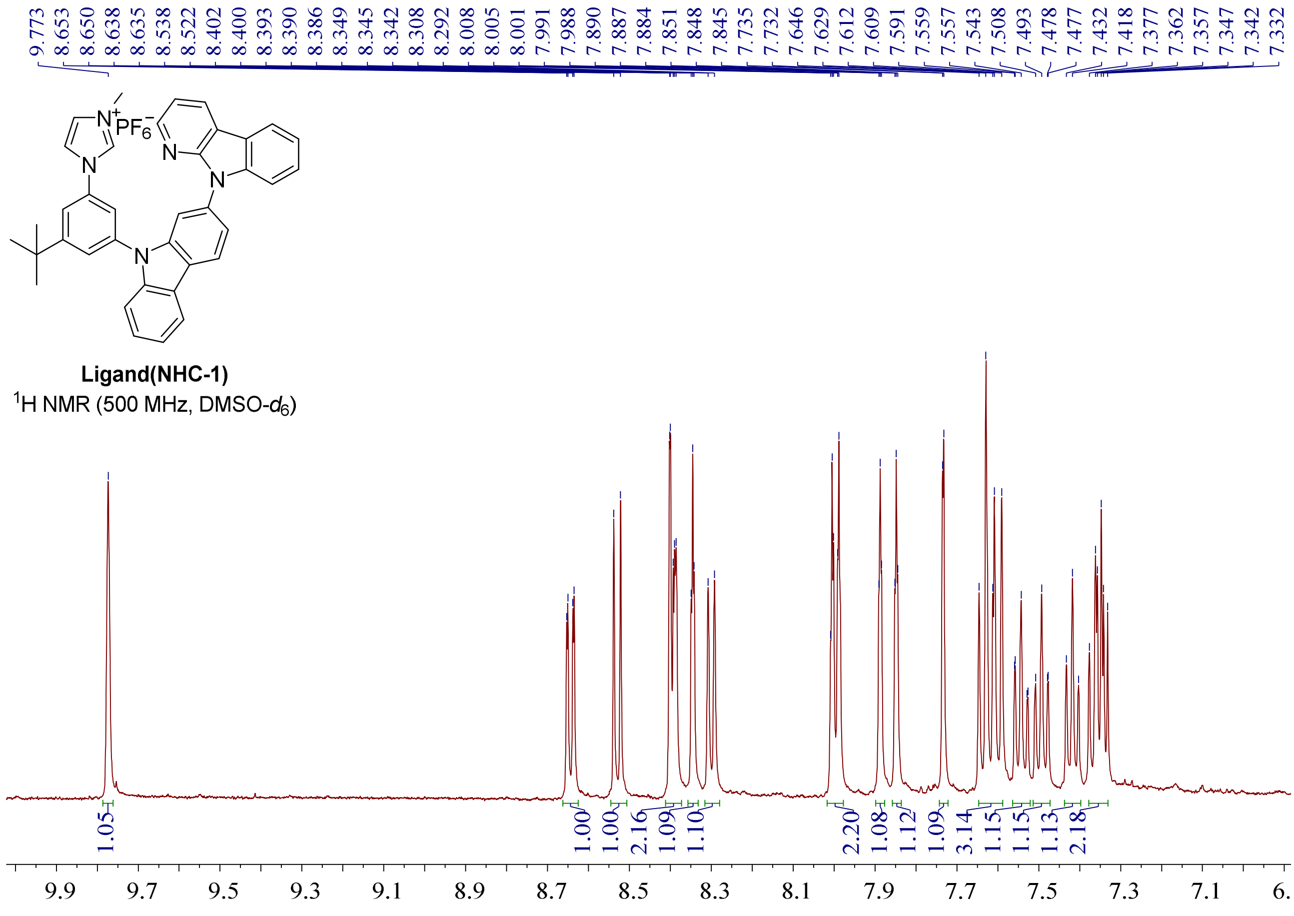

8.484 8.480 8.474 8.471 8.403 8.400 8.388 8.385 8.367 8.350 8.234 8.218 8.138 8.123 8.057 7.758 7.755 7.743 7.739 7.736 7.604 7.600 7.587 7.584 7.567 7.551 7.546 7.542 7.538 7.498 7.495 7.488 7.486 7.483 7.481 7.468 7.466 7.452 7.439 7.435 7.432 7.382 7.353 7.352 7.338 7.324 7.263 7.254 7.248 7.239
3(NHC-1)
^{1}H NMR (500 MHz, $CDCl_3$)
residual $CHCl_3$
1.00 1.02 1.02 1.02 1.03 1.00 1.03 1.01 1.08 2.03 4.06 3.07 2.37
8.50 8.40 8.30 8.20 8.10 8.00 7.90 7.80 7.70 7.60 7.50 7.40 7.30 7.2


155.65
152.12
146.44
141.17
141.03
140.32
138.62
138.45
134.24
128.28
126.90
126.44
123.29
123.26
122.94
121.29
120.93
120.78
120.74
120.72
120.64
119.59
117.56
117.03
116.35
116.12
110.37
109.62
109.07
77.21
77.00
76.79
35.30
31.16
N
N
N
N
N
3(NHC-1)
^{13}C NMR (125 MHz, $CDCl_3$)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

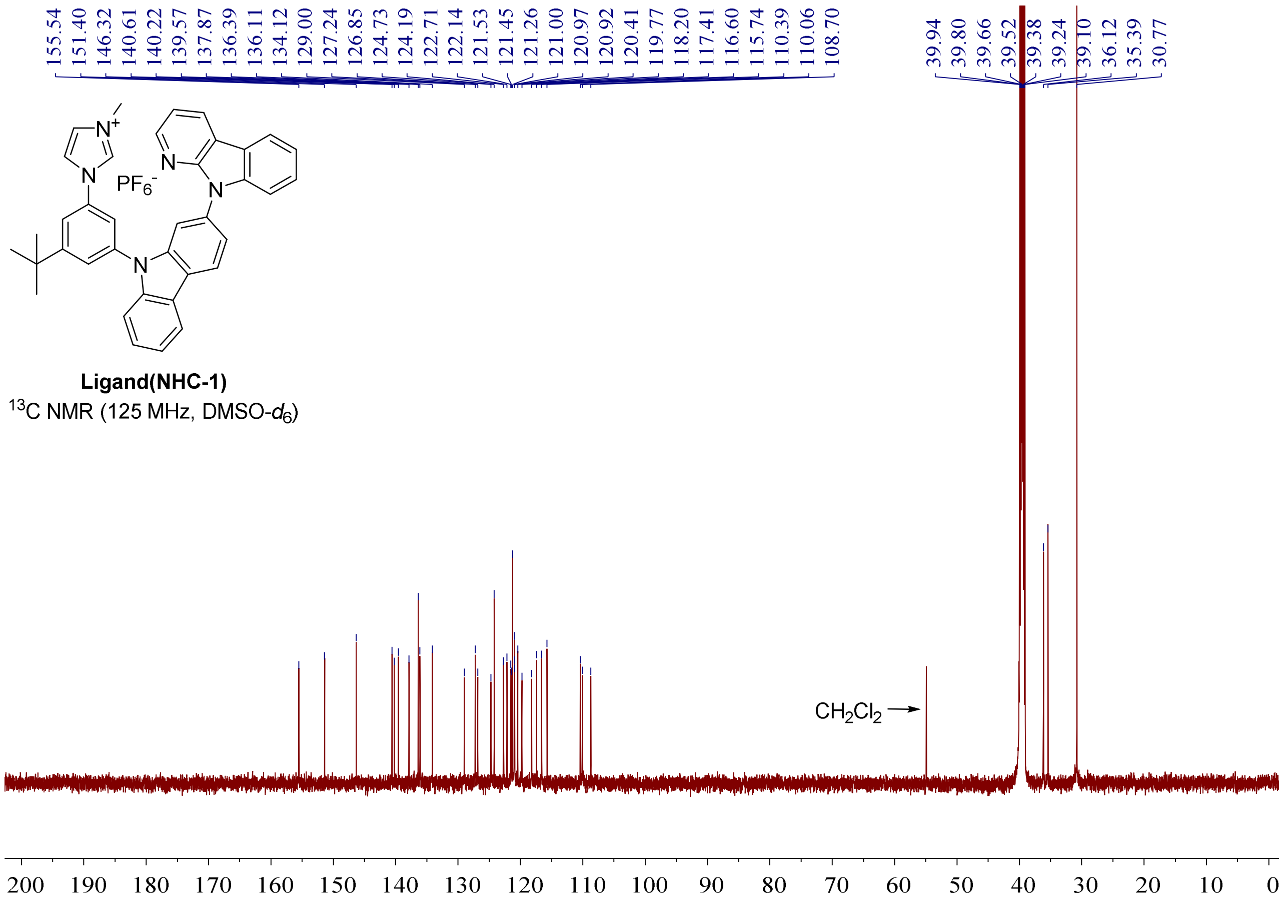

155.65
152.12
146.44
141.17
141.03
140.32
138.62
138.45
135.60
134.24
130.38
128.28
126.90
126.44
123.29
123.26
122.94
121.29
120.93
120.78
120.74
120.72
120.64
119.59
118.38
117.56
117.03
116.35
116.12
110.37
109.62
109.07
N
N
N
N
N
3(NHC-1)
^{13}C NMR (125 MHz, $CDCl_3$)
158 156 154 152 150 148 146 144 142 140 138 136 134 132 130 128 126 124 122 120 118 116 114 112 110 108



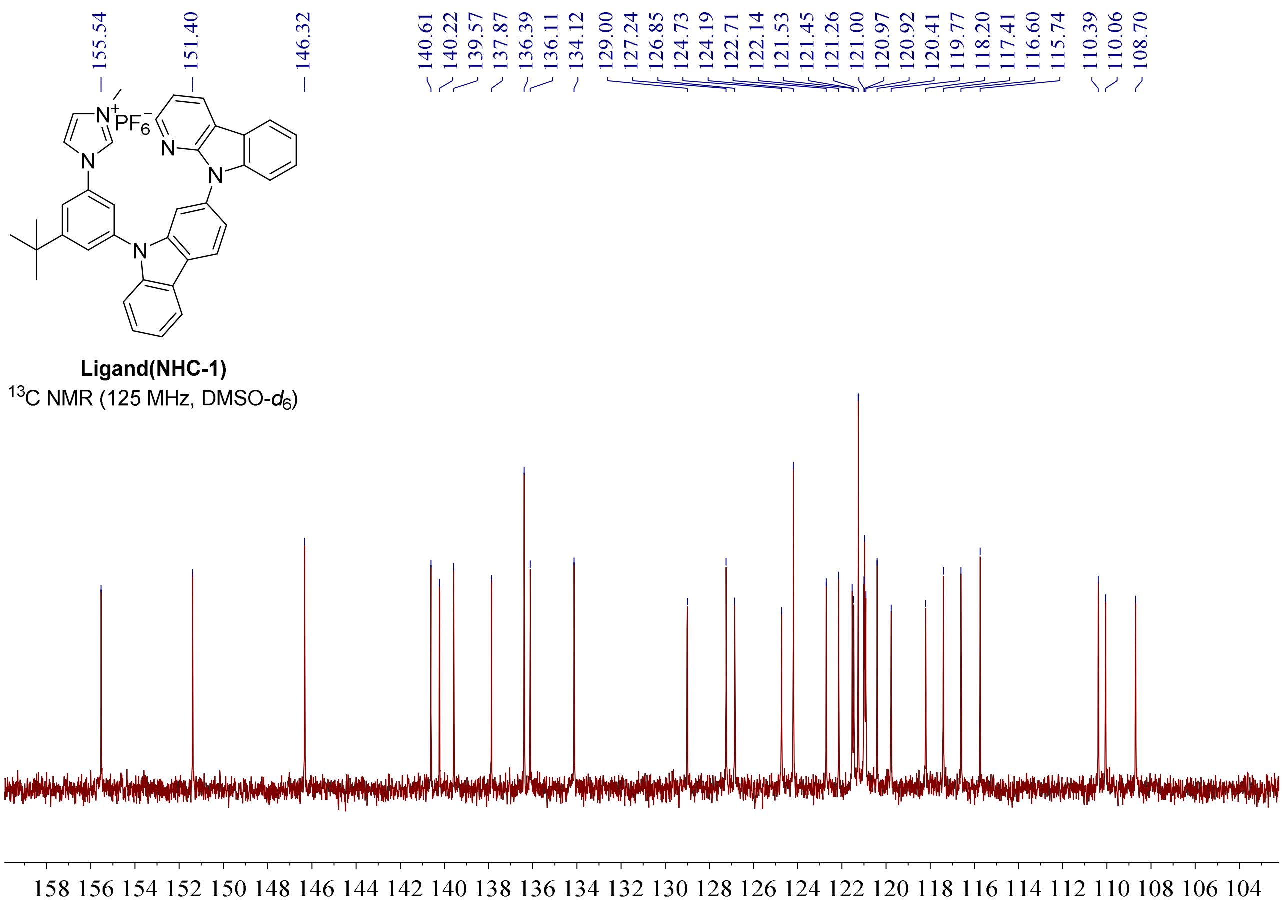
Ligand(NHC-1)
^{1}H NMR (500 MHz, DMSO-d_6)
CH$_2$Cl$_2$
H$_2$O
residual DMSO



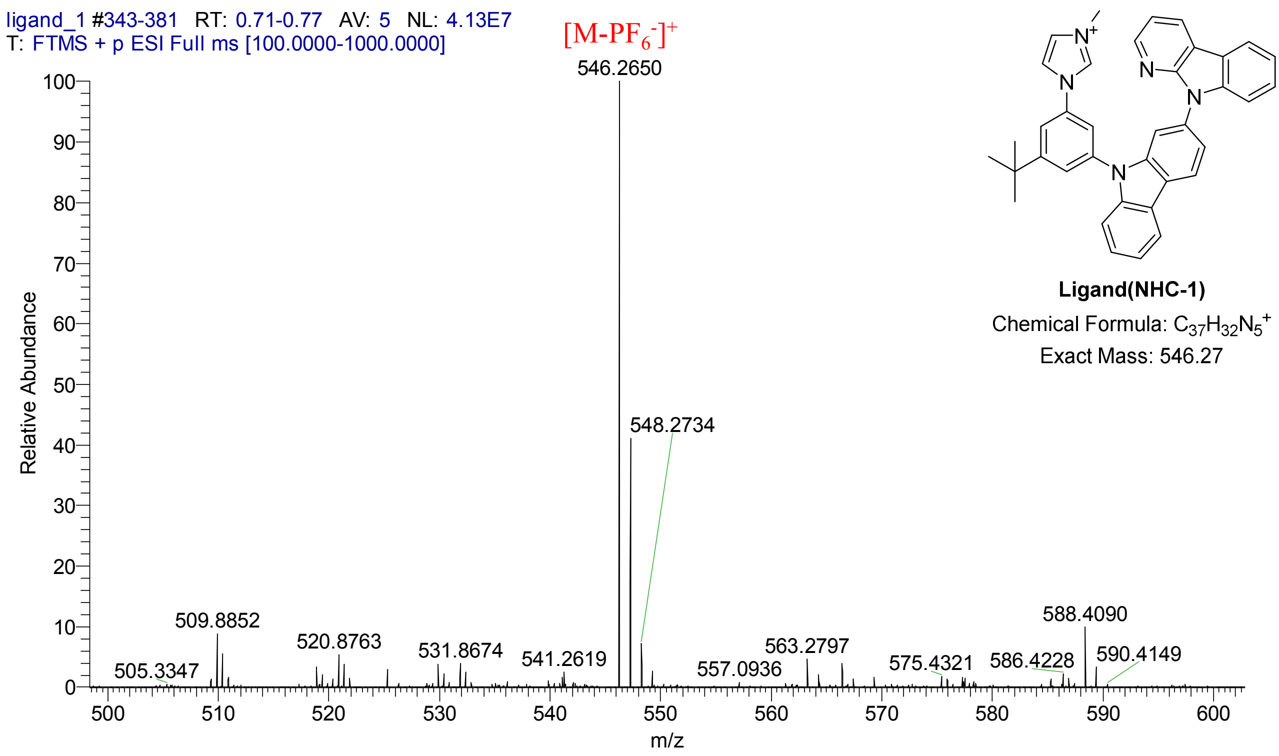
Ligand(NHC-1)
^{1}H NMR (500 MHz, DMSO-d_6)

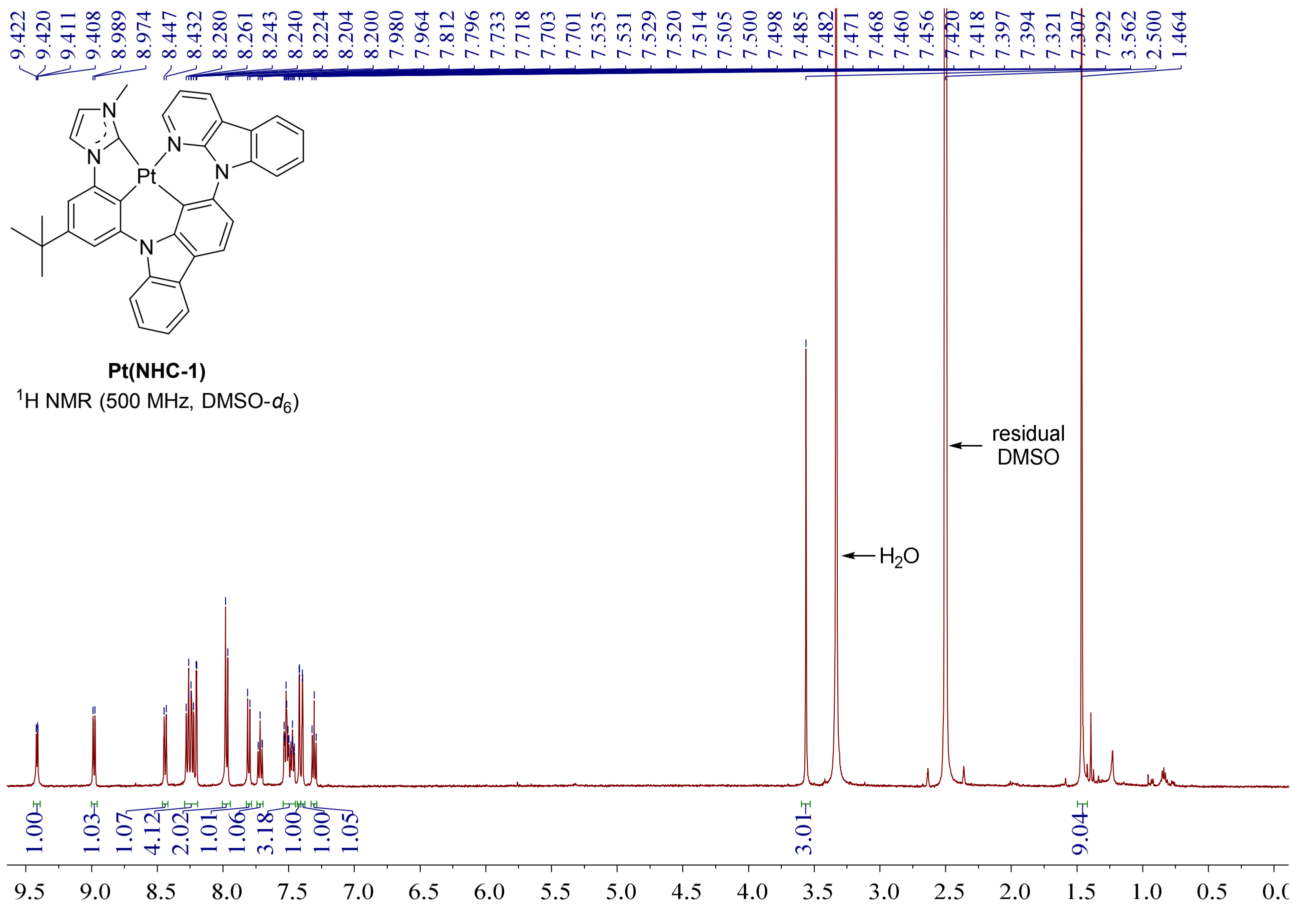


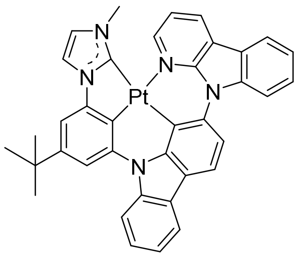
Ligand(NHC-1)
^{13}C NMR (125 MHz, DMSO-d_6)



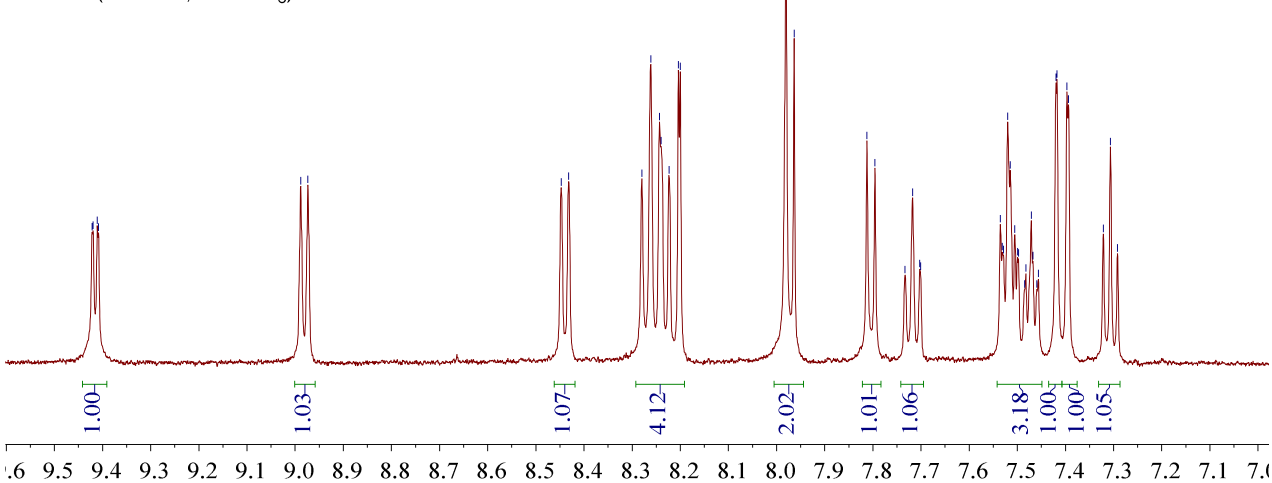
Ligand(NHC-1)
^{13}C NMR (125 MHz, DMSO-d_6)


ligand_1 #343-381 RT: 0.71-0.77 AV: 5 NL: 4.13E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]
[M-PF6-]+
546.2650
548.2734
509.8852
520.8763
531.8674
541.2619
505.3347
557.0936
563.2797
575.4321
586.4228
588.4090
590.4149
Relative Abundance
m/z
Ligand(NHC-1)
Chemical Formula: C37H32N5+
Exact Mass: 546.27

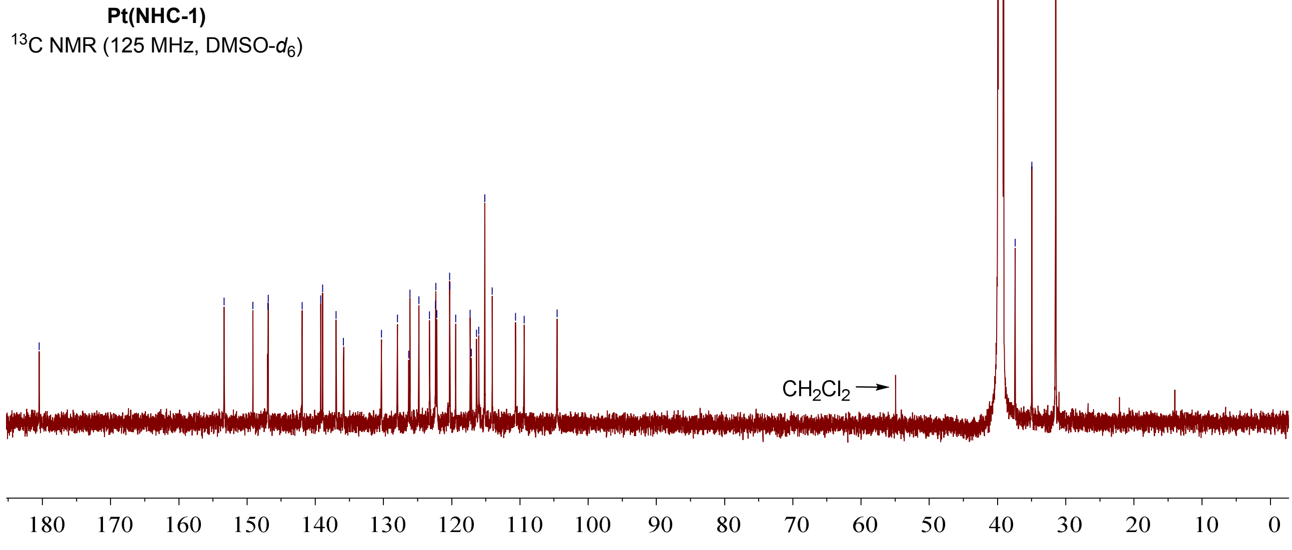

9.422
9.420
9.411
9.408
8.989
8.974
8.447
8.432
8.280
8.261
8.243
8.240
8.224
8.204
8.200
7.980
7.964
7.812
7.796
7.733
7.718
7.703
7.701
7.535
7.531
7.529
7.520
7.514
7.505
7.500
7.498
7.485
7.482
7.471
7.468
7.460
7.456
7.420
7.418
7.397
7.394
7.321
7.307
7.292
3.562
2.500
1.464
Pt(NHC-1)
1H NMR (500 MHz, DMSO-d6)
residual DMSO
H2O
1.00
1.03
1.07
4.12
2.02
1.01
1.06
3.18
1.00
1.00
1.05
3.01
9.04

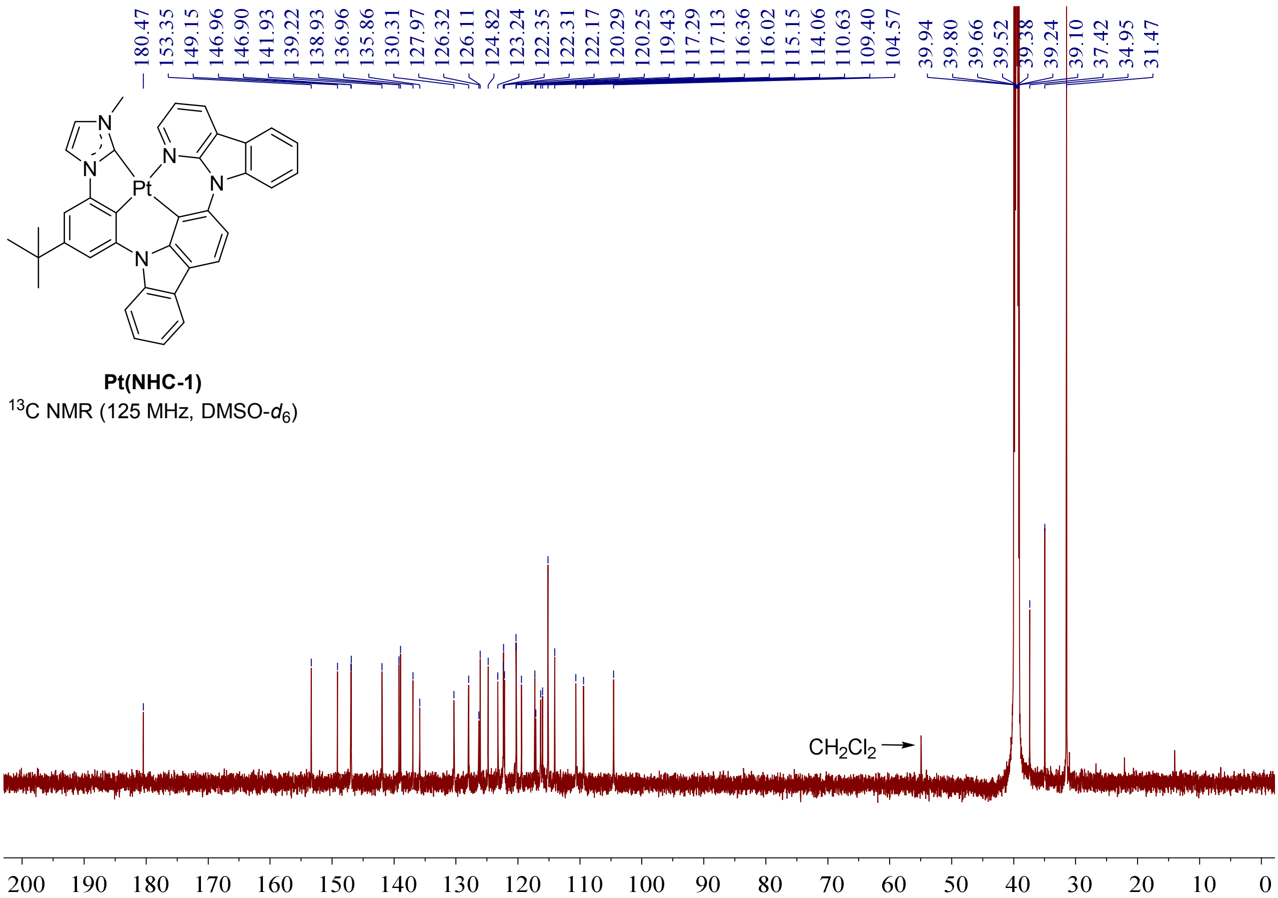


Pt(NHC-1)
^{1}H NMR (500 MHz, DMSO-d_6)

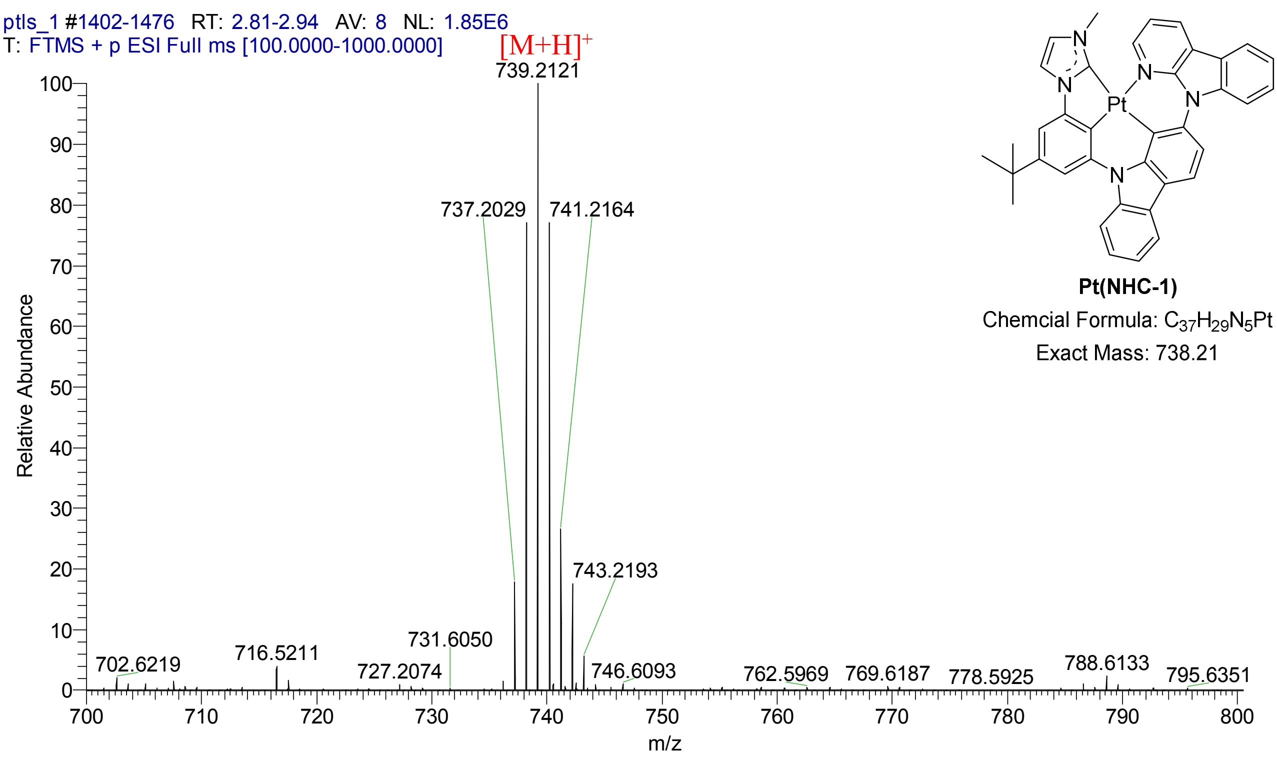


Pt(NHC-1)
^{13}C NMR (125 MHz, DMSO-d_6)





180.47
153.35
149.15
146.96
146.90
141.93
139.22
138.93
136.96
135.86
130.31
127.97
126.32
126.11
124.82
123.24
122.35
122.31
122.17
120.29
120.25
119.43
117.29
117.13
116.36
116.02
115.15
114.06
110.63
109.40
104.57
39.94
39.80
39.66
39.52
39.38
39.24
39.10
37.42
34.95
31.47
Pt(NHC-1)
13C NMR (125 MHz, DMSO-d6)
CH2Cl2
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0



ptls_1 #1402-1476 RT: 2.81-2.94 AV: 8 NL: 1.85E6
T: FTMS + p ESI Full ms [100.0000-1000.0000]
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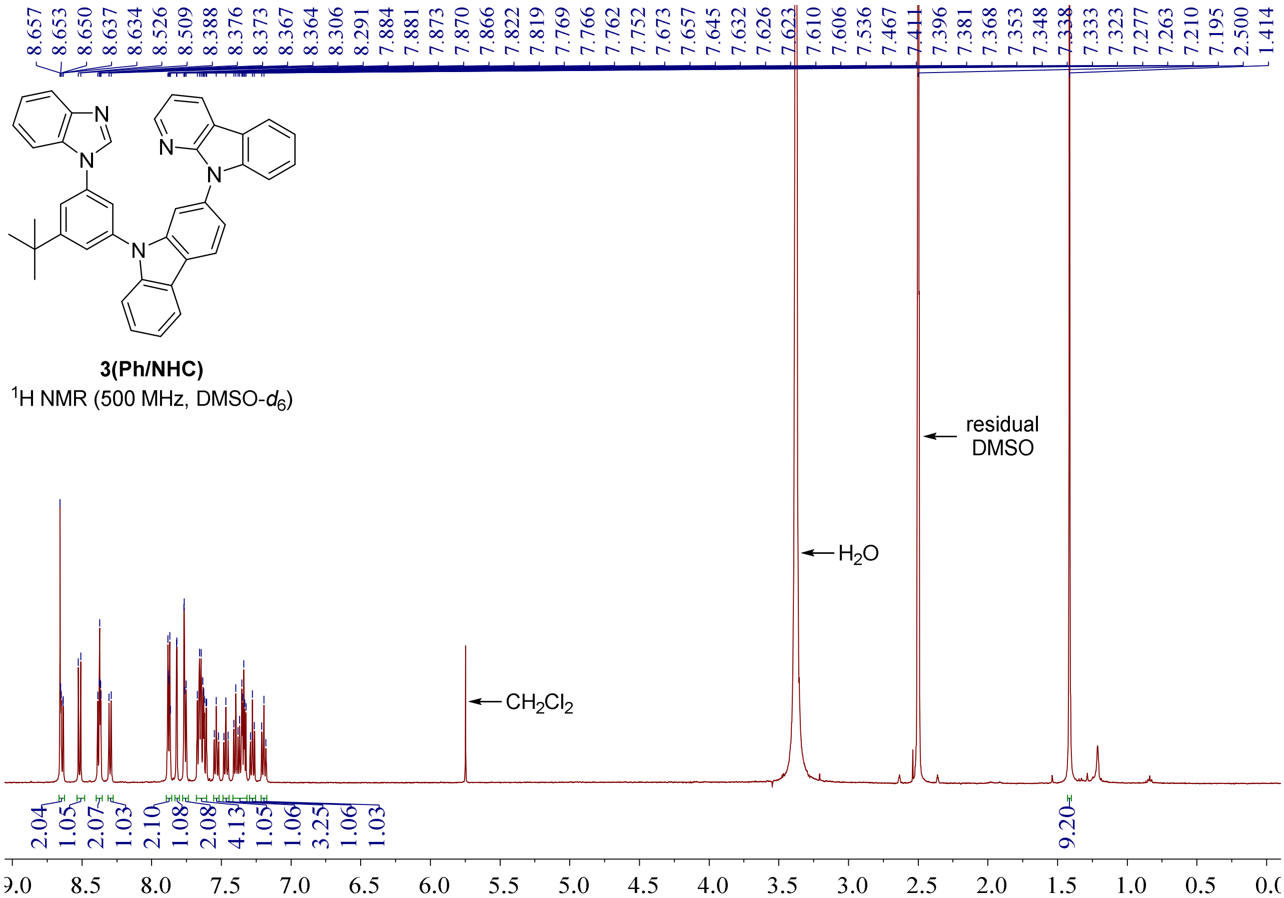
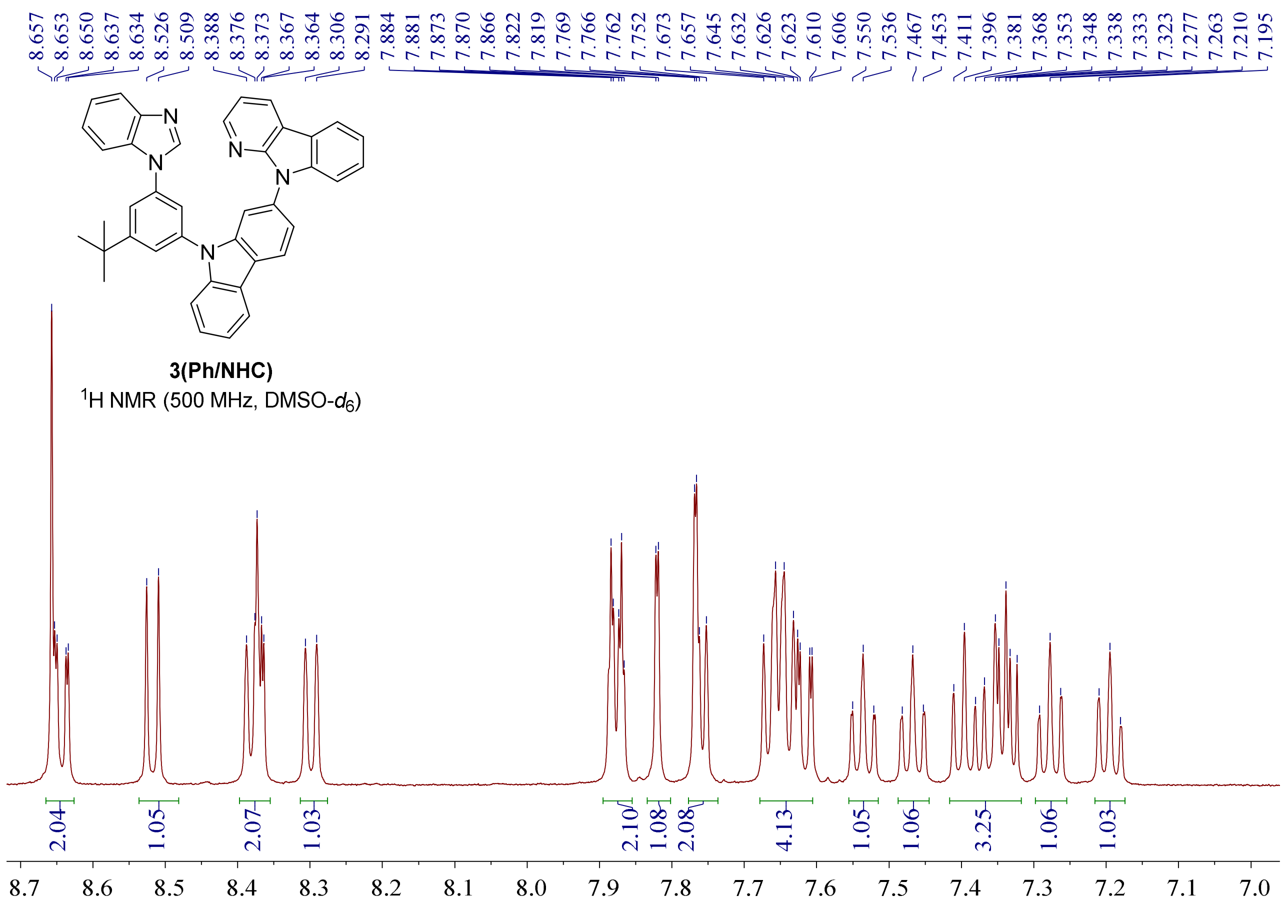
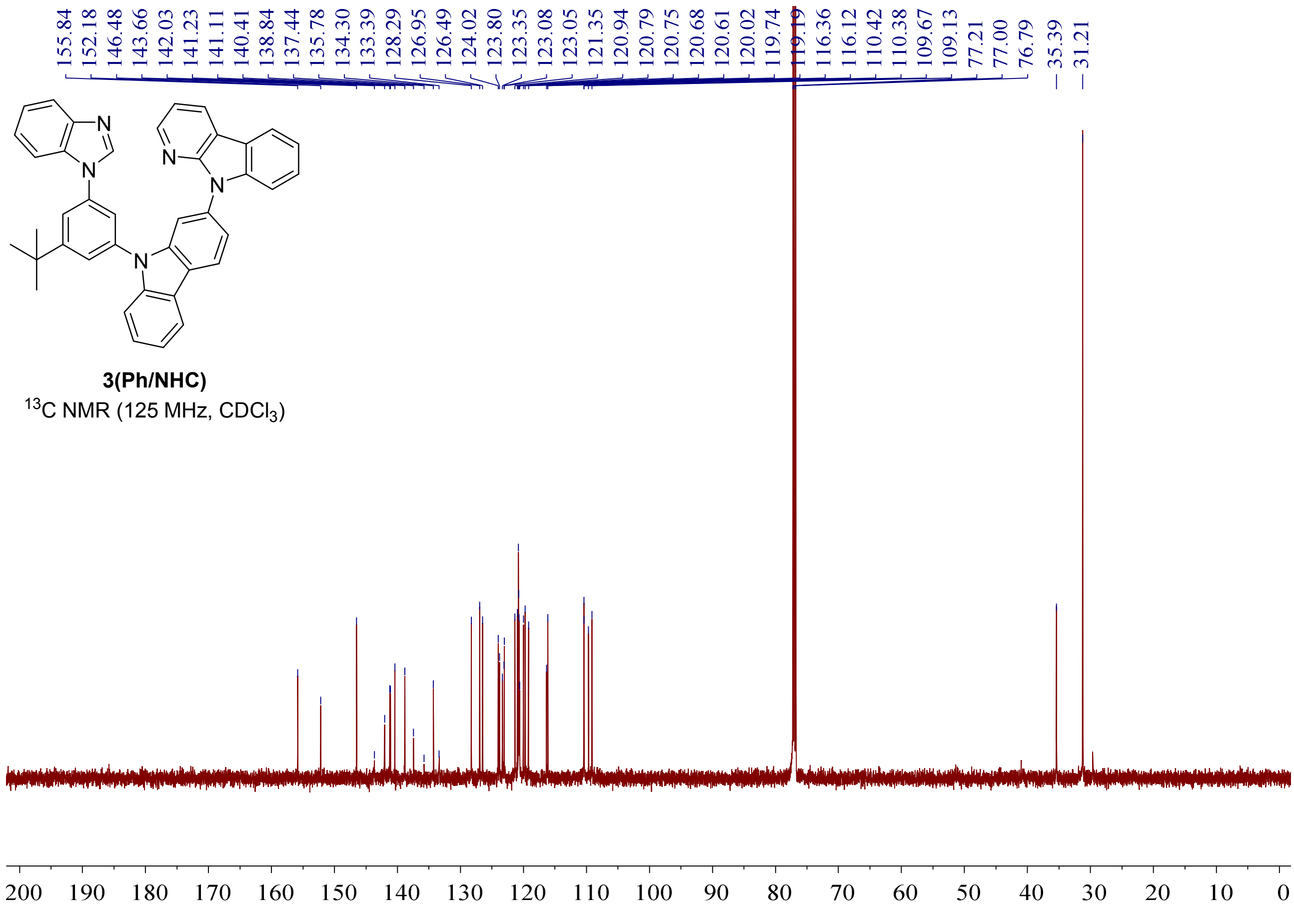
741.2164
743.2193
731.6050
716.5211
702.6219
727.2074
746.6093
762.5969
769.6187
778.5925
788.6133
795.6351
Relative Abundance
m/z
Pt(NHC-1)
Chemcial Formula: C37H29N5Pt
Exact Mass: 738.21

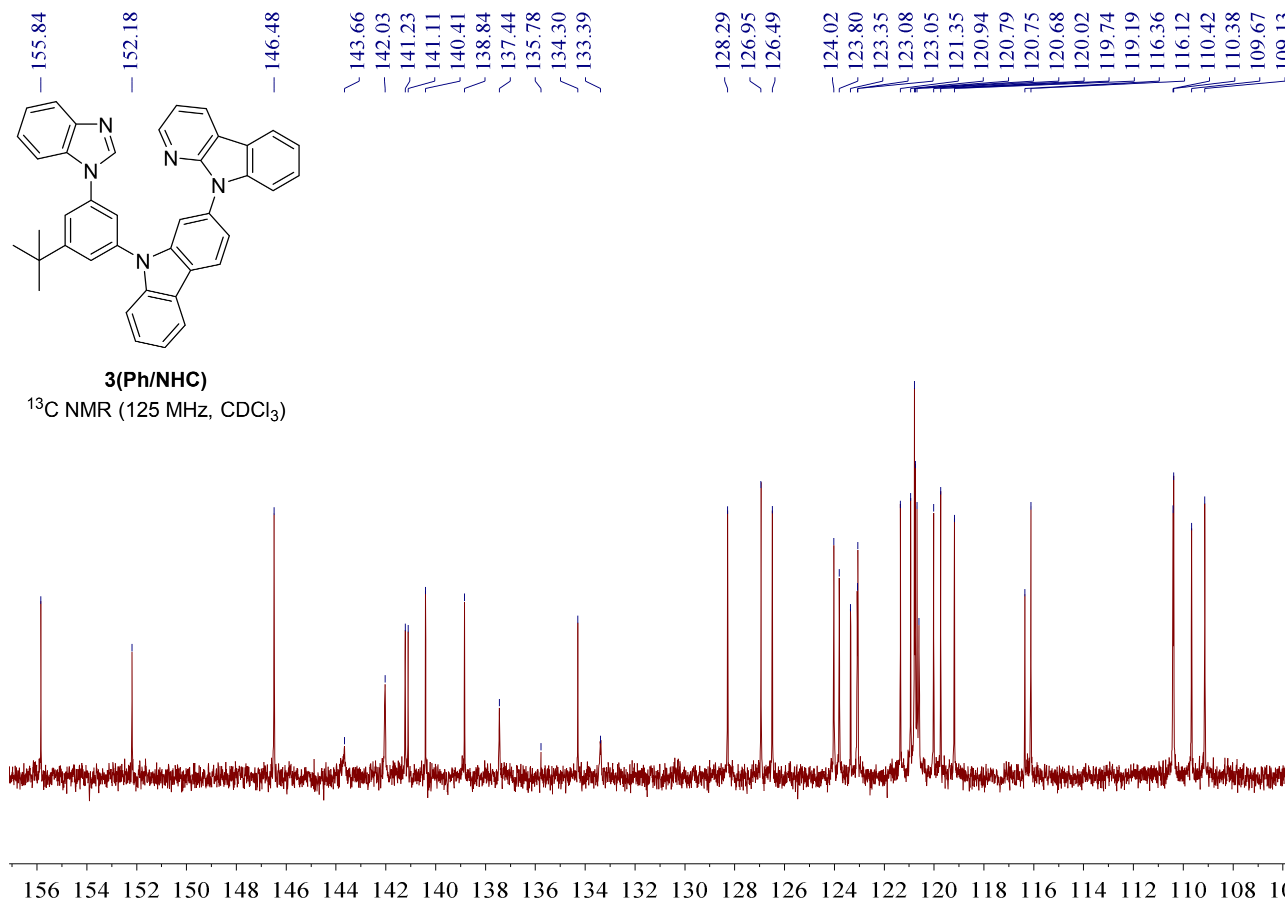

3(Ph/NHC)
^{1}H NMR (500 MHz, DMSO-d_6)
residual DMSO
H_2O
CH_2Cl_2


3(Ph/NHC)
^{1}H NMR (500 MHz, DMSO-d_6)



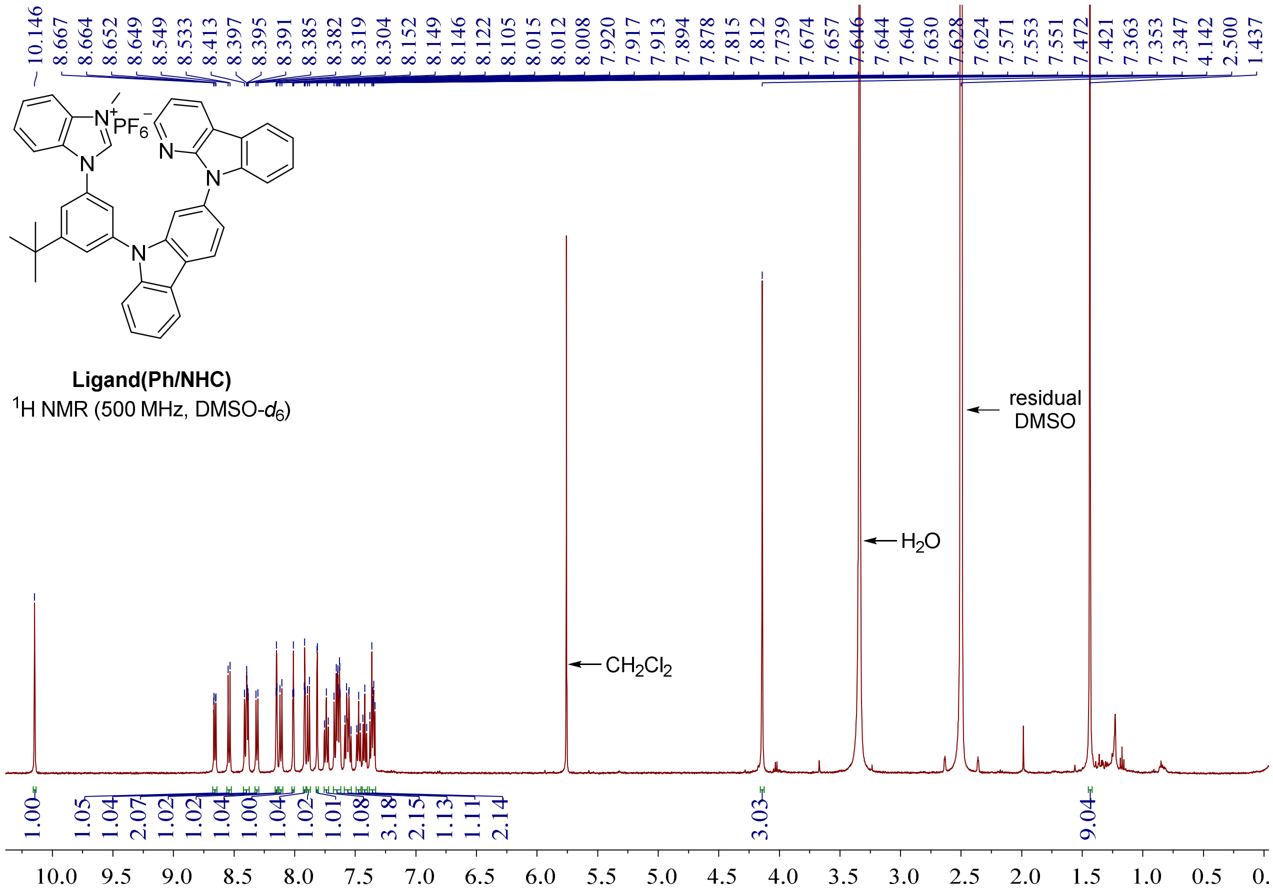
3(Ph/NHC)

^{13}C NMR (125 MHz, $CDCl_3$)

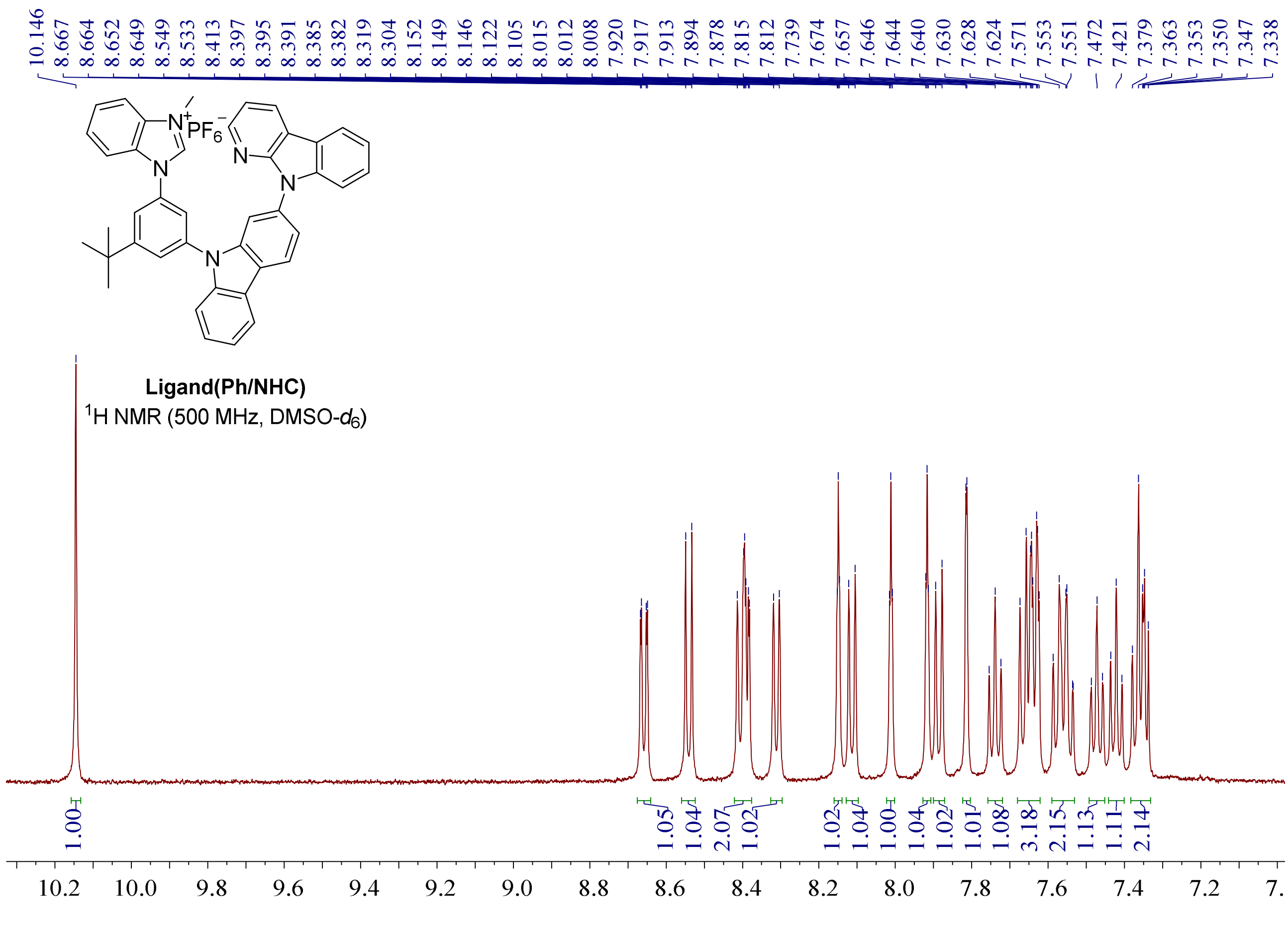


3(Ph/NHC)

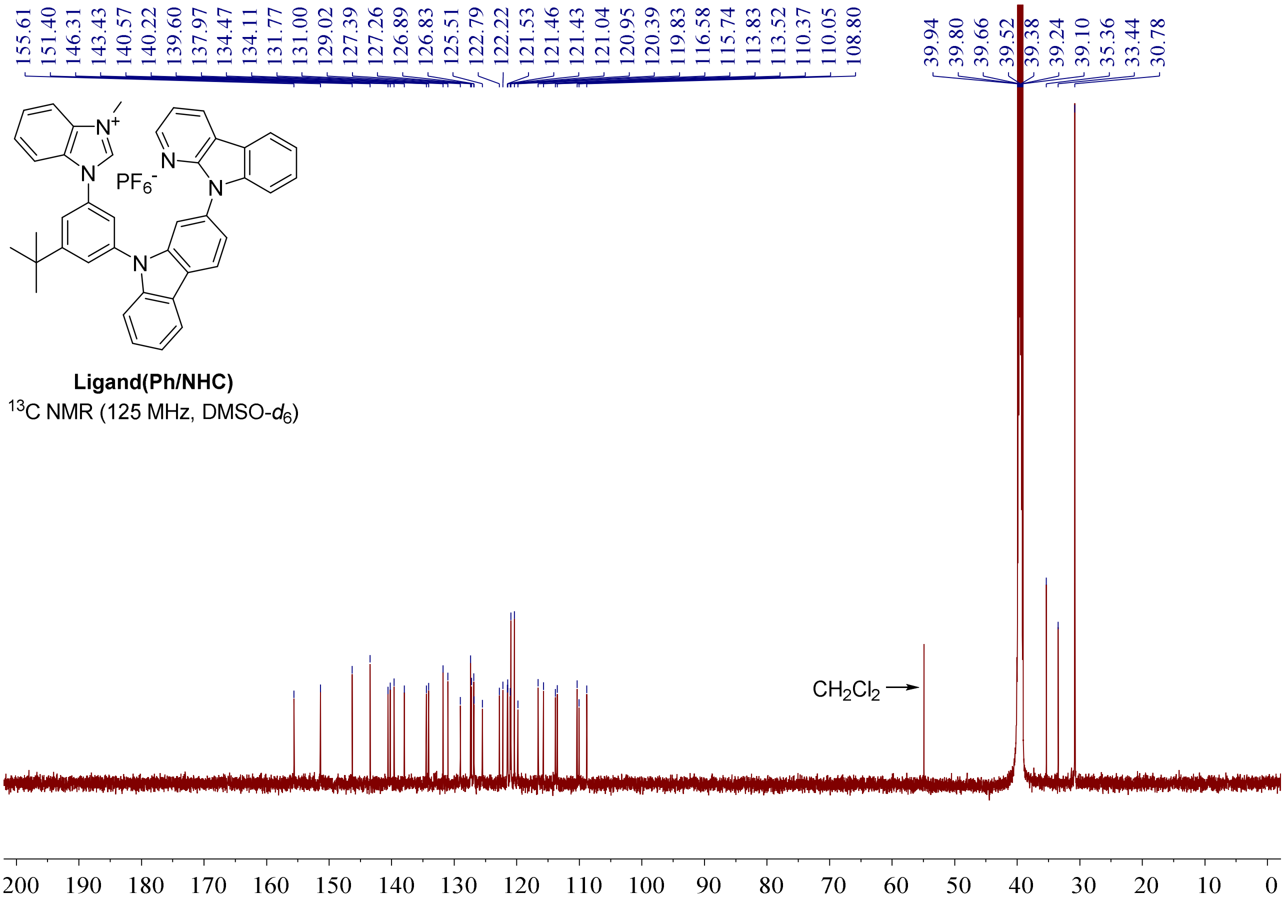
^{13}C NMR (125 MHz, $CDCl_3$)

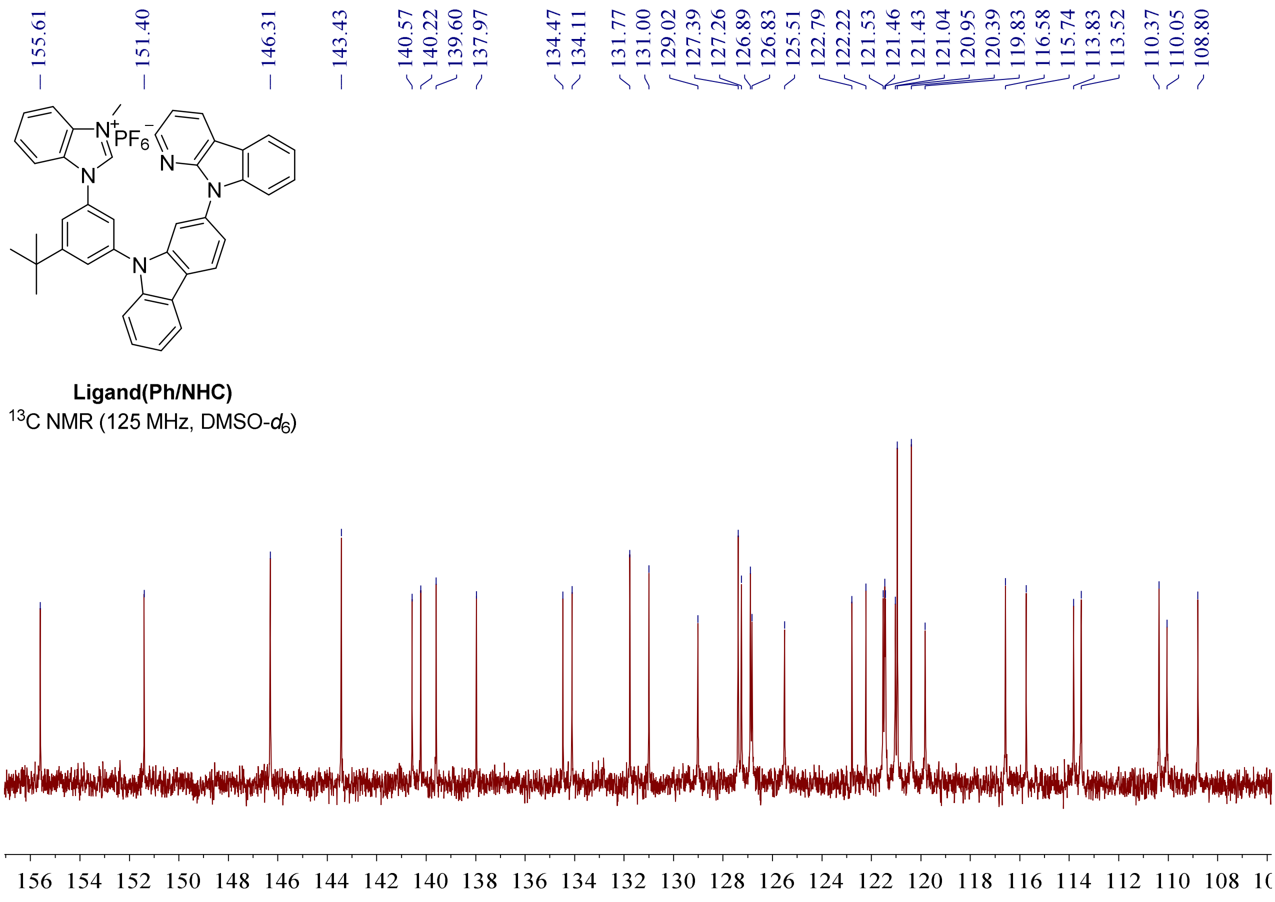


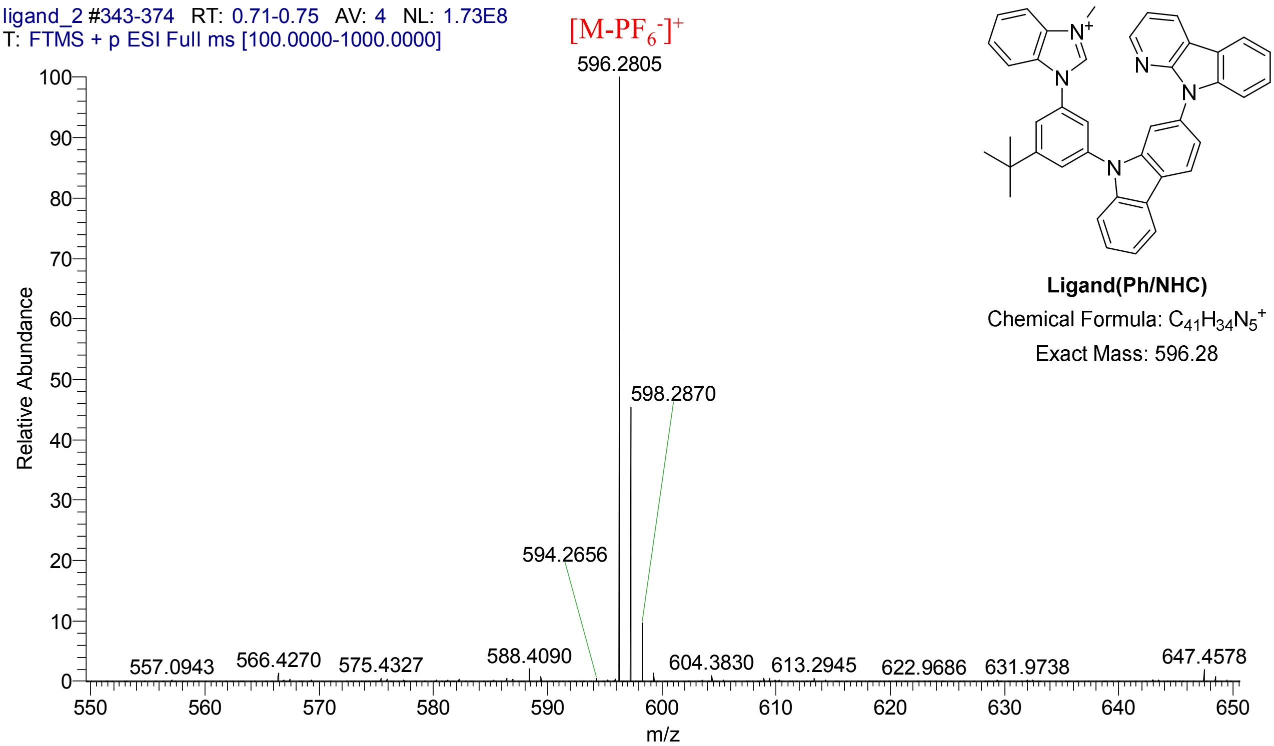
Ligand(Ph/NHC)
^1H NMR (500 MHz, DMSO-d_6)
residual DMSO
H_2O
CH_2Cl_2

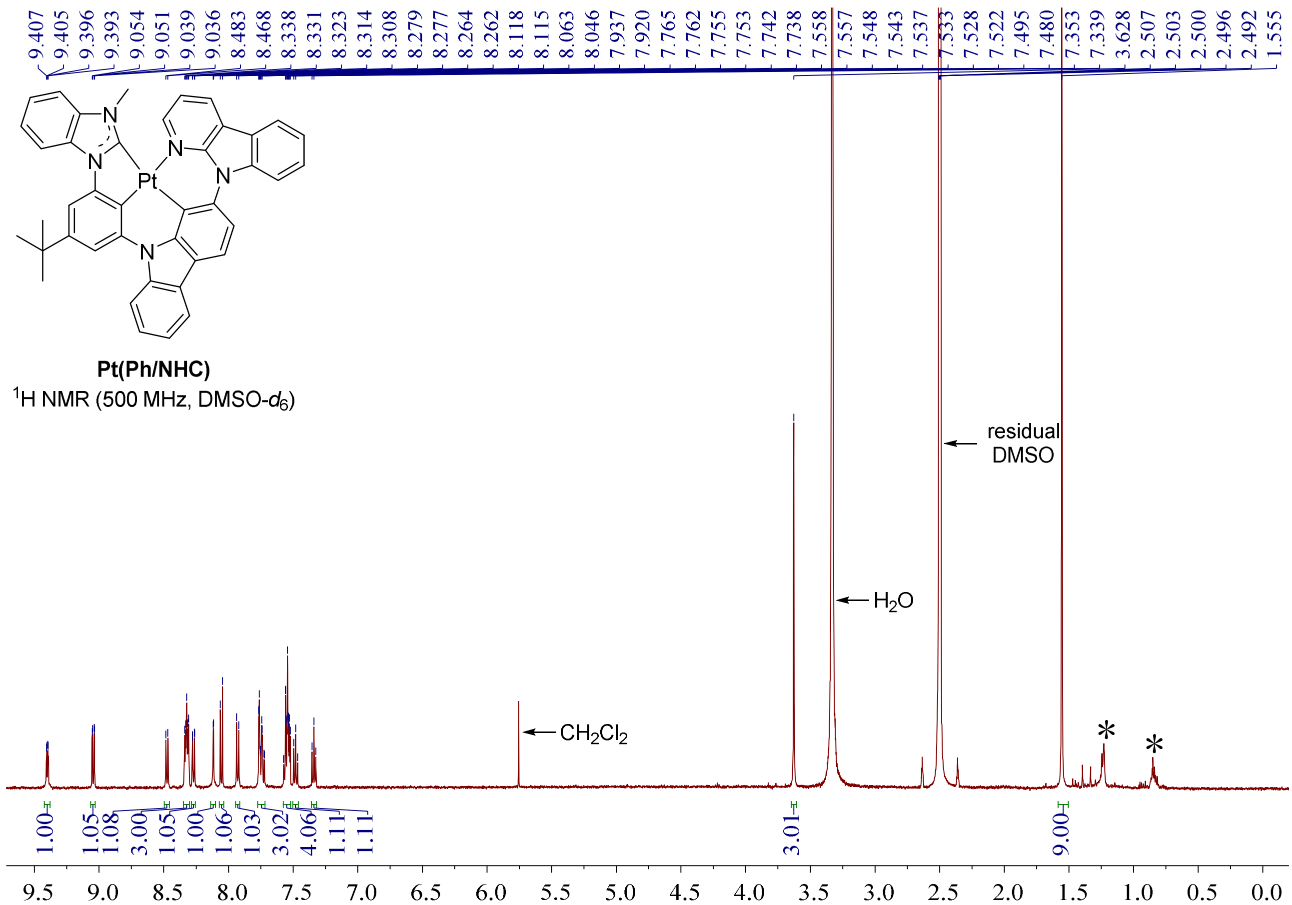


Ligand(Ph/NHC)
^1H NMR (500 MHz, DMSO-d_6)

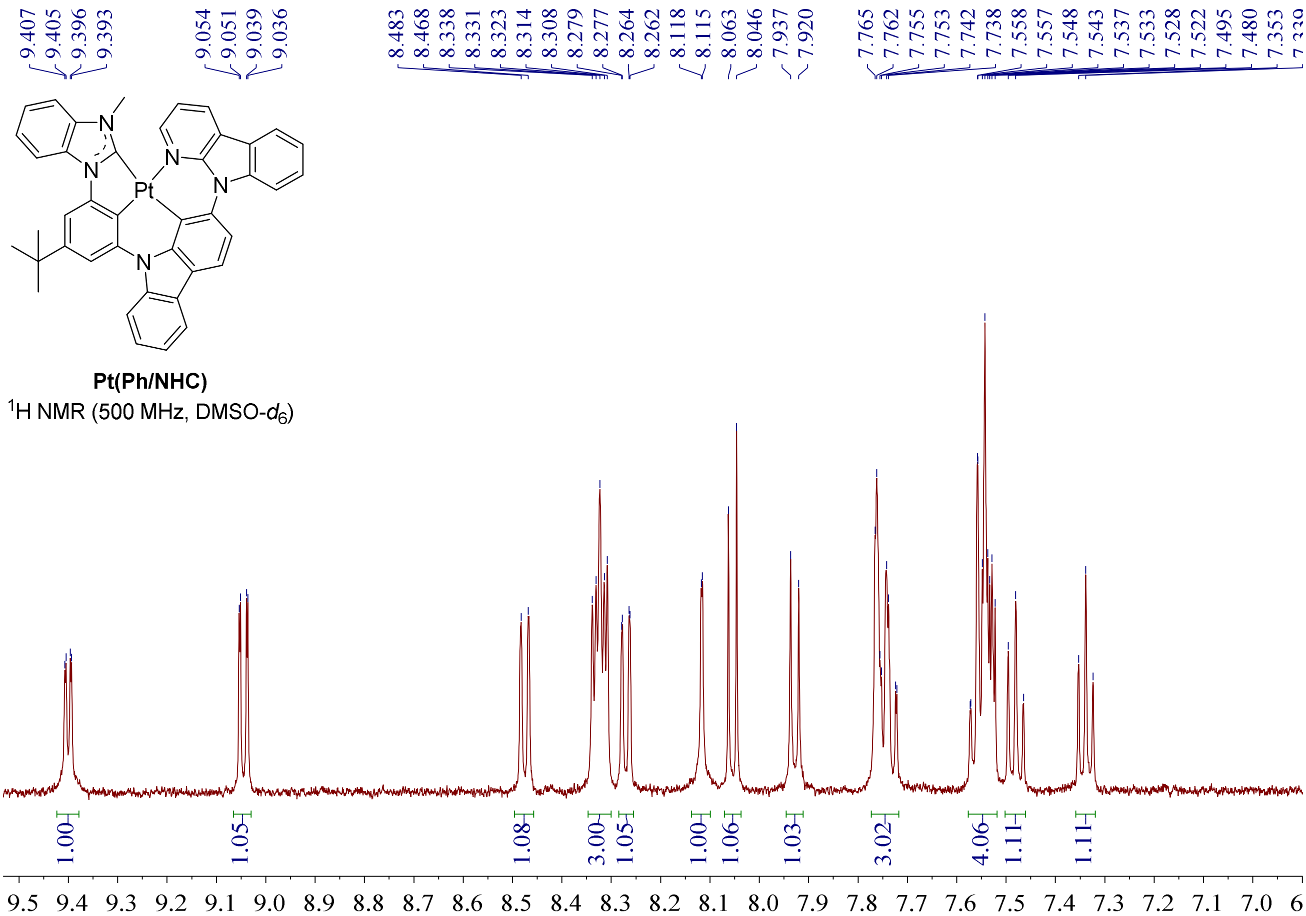

155.61
151.40
146.31
143.43
140.57
140.22
139.60
137.97
134.47
134.11
131.77
131.00
129.02
127.39
127.26
126.89
126.83
125.51
122.79
122.22
121.53
121.46
121.43
121.04
120.95
120.39
119.83
116.58
115.74
113.83
113.52
110.37
110.05
108.80
39.94
39.80
39.66
39.52
39.38
39.24
39.10
35.36
33.44
30.78
PF_6^-
Ligand(Ph/NHC)
^{13}C NMR (125 MHz, DMSO-d_6)
CH_2Cl_2
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


155.61
151.40
146.31
143.43
140.57
140.22
139.60
137.97
134.47
134.11
131.77
131.00
129.02
127.39
127.26
126.89
126.83
125.51
122.79
122.22
121.53
121.46
121.43
121.04
120.95
120.39
119.83
116.58
115.74
113.83
113.52
110.37
110.05
108.80
PF_6^-
Ligand(Ph/NHC)
^{13}C NMR (125 MHz, DMSO-d_6)
156 154 152 150 148 146 144 142 140 138 136 134 132 130 128 126 124 122 120 118 116 114 112 110 108

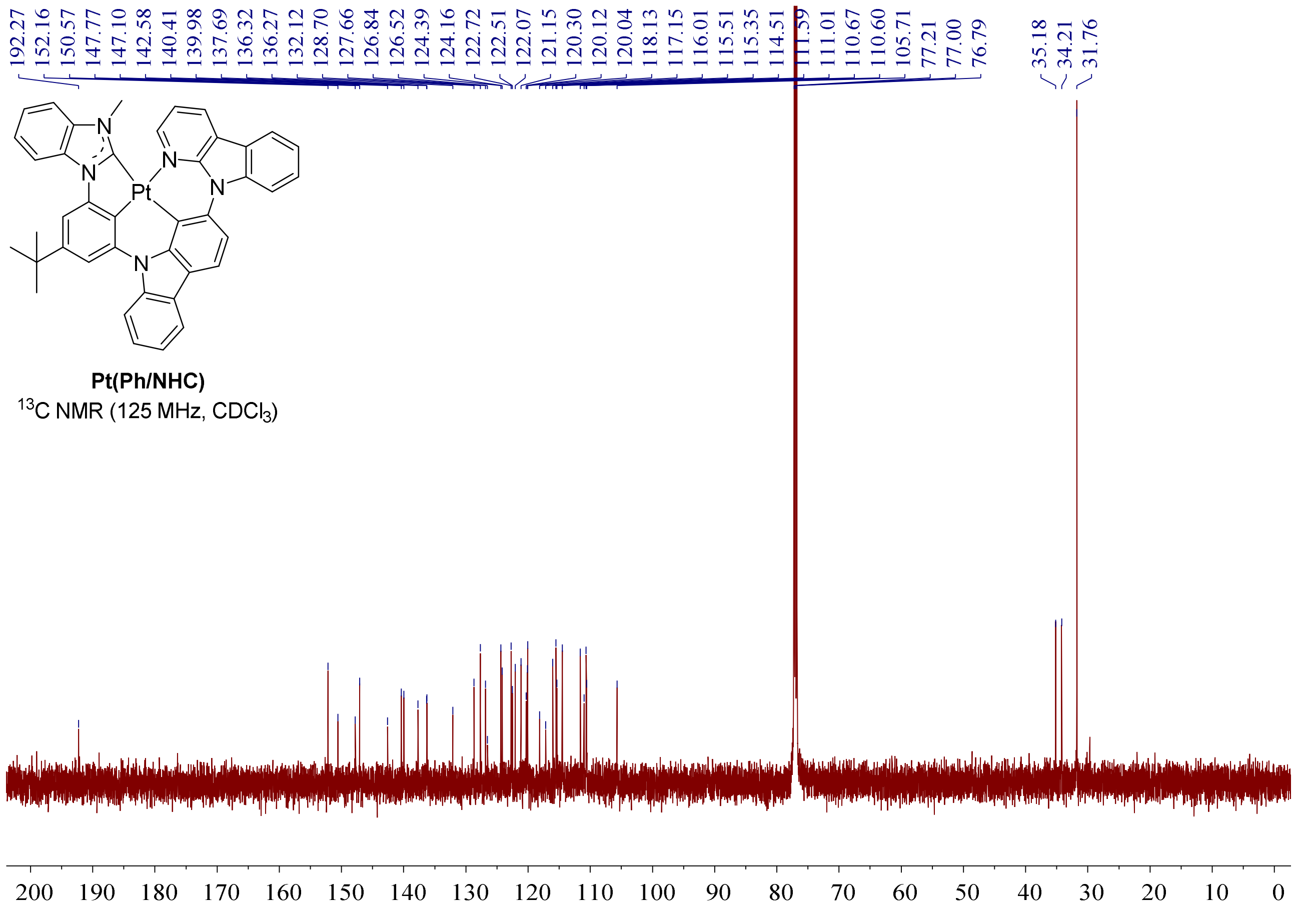

ligand_2 #343-374 RT: 0.71-0.75 AV: 4 NL: 1.73E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]
[M-PF6-]+
596.2805
598.2870
594.2656
588.4090
557.0943
566.4270
575.4327
604.3830
613.2945
622.9686
631.9738
647.4578
Relative Abundance
m/z
Ligand(Ph/NHC)
Chemical Formula: C41H34N5+
Exact Mass: 596.28

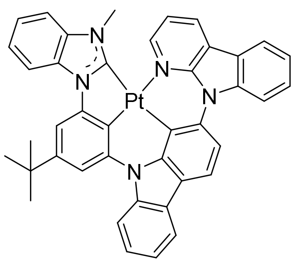

Pt(Ph/NHC)
1H NMR (500 MHz, DMSO-d6)
CH2Cl2
H2O
residual DMSO
*
*

Pt(Ph/NHC)
^{1}H NMR (500 MHz, DMSO-d_6)



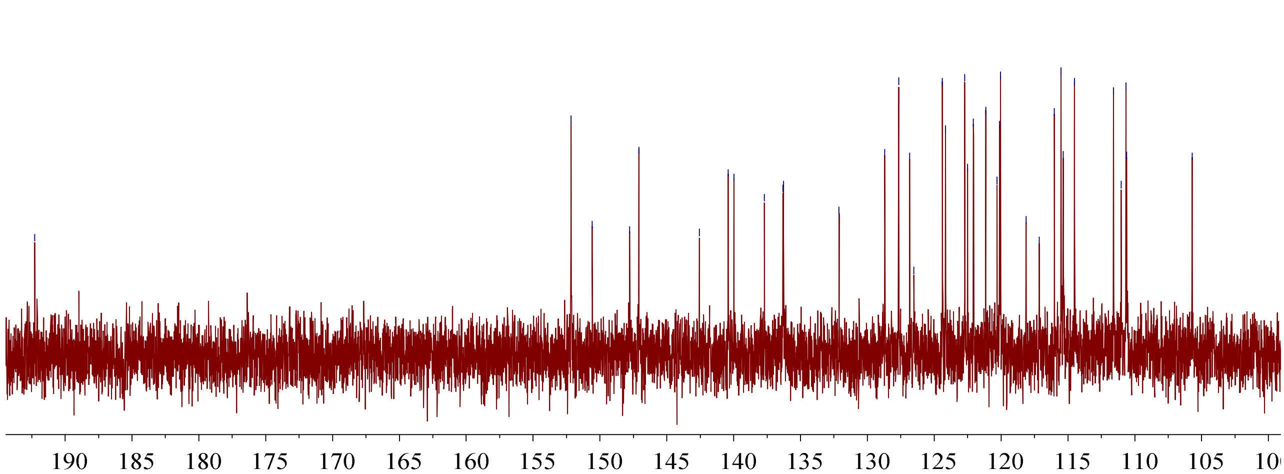
Pt(Ph/NHC)
^{13}C NMR (125 MHz, $CDCl_3$)

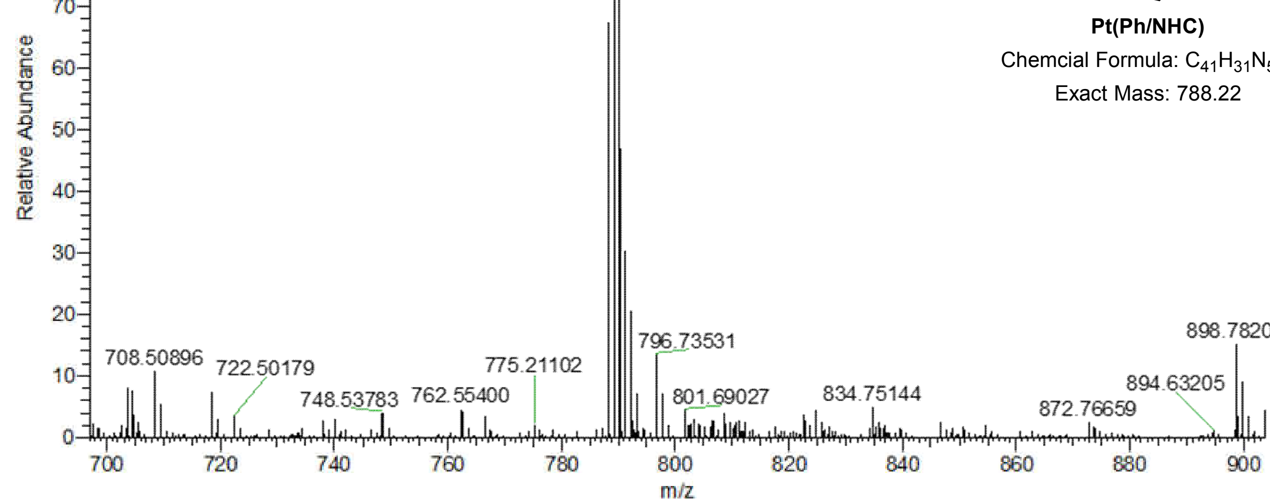


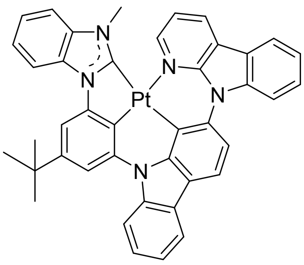


Pt(Ph/NHC)

^{13}C NMR (125 MHz, $CDCl_3$)



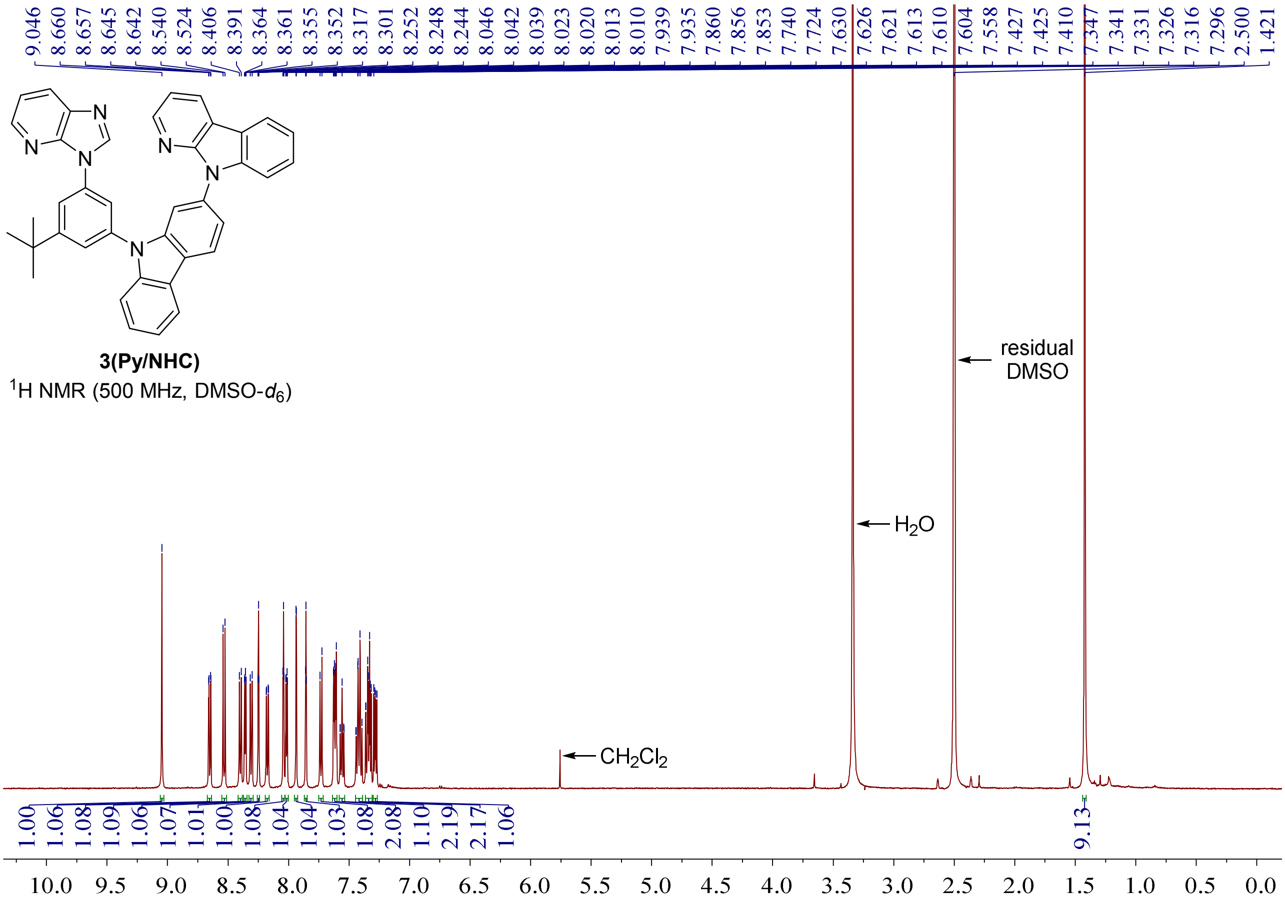




Pt(Ph/NHC)

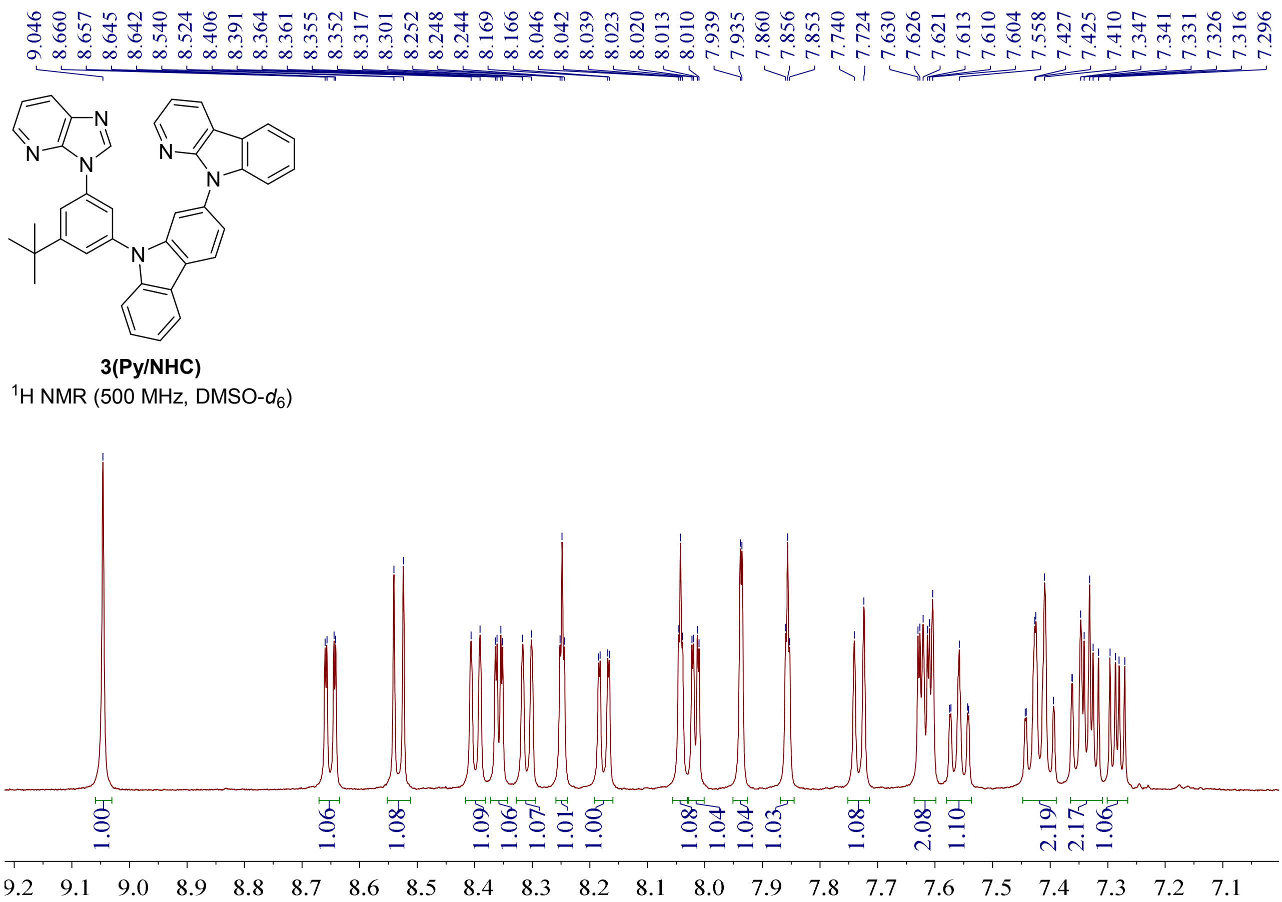
Chemcial Formula: $C_{41}H_{31}N_5Pt$

Exact Mass: 788.22



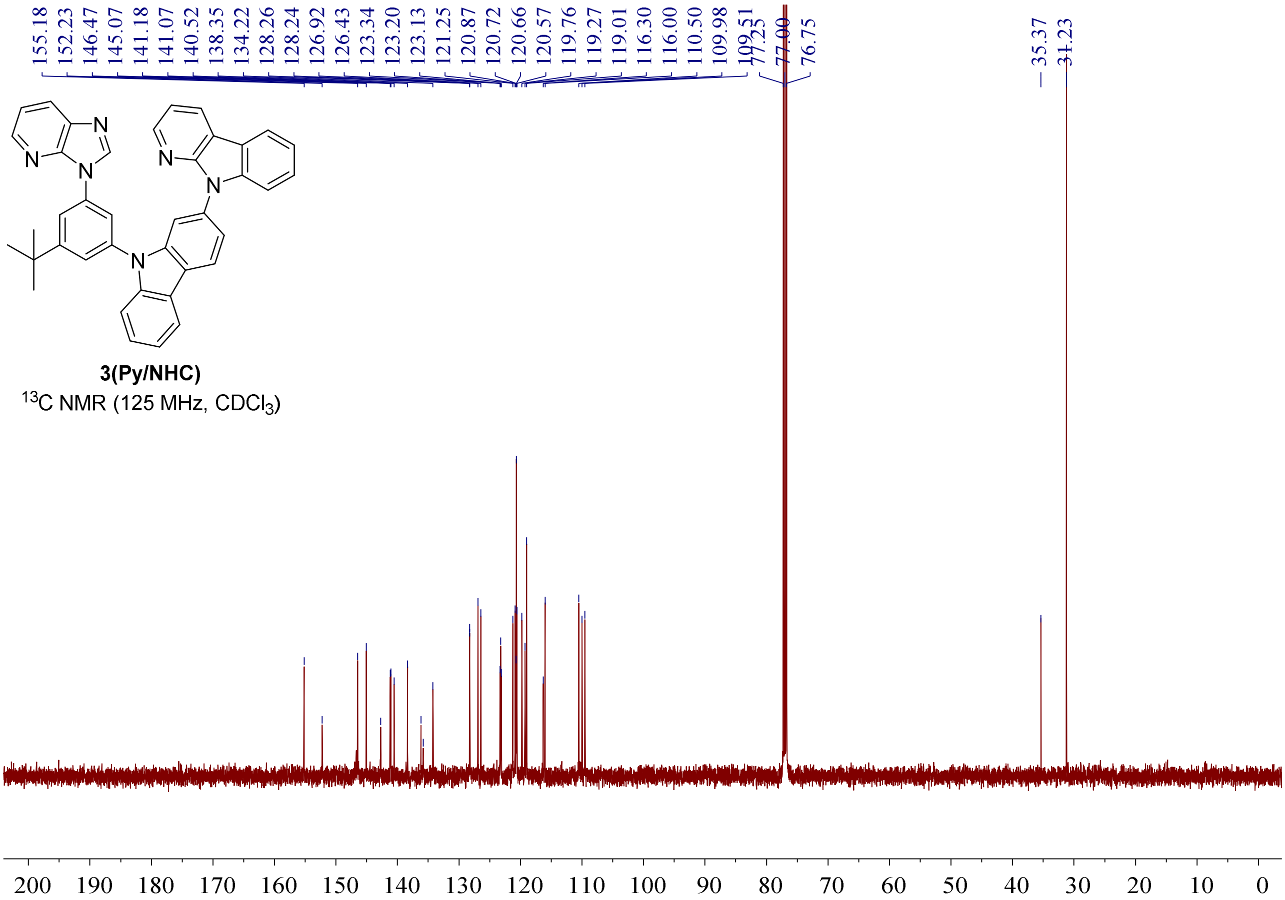
3(Py/NHC)

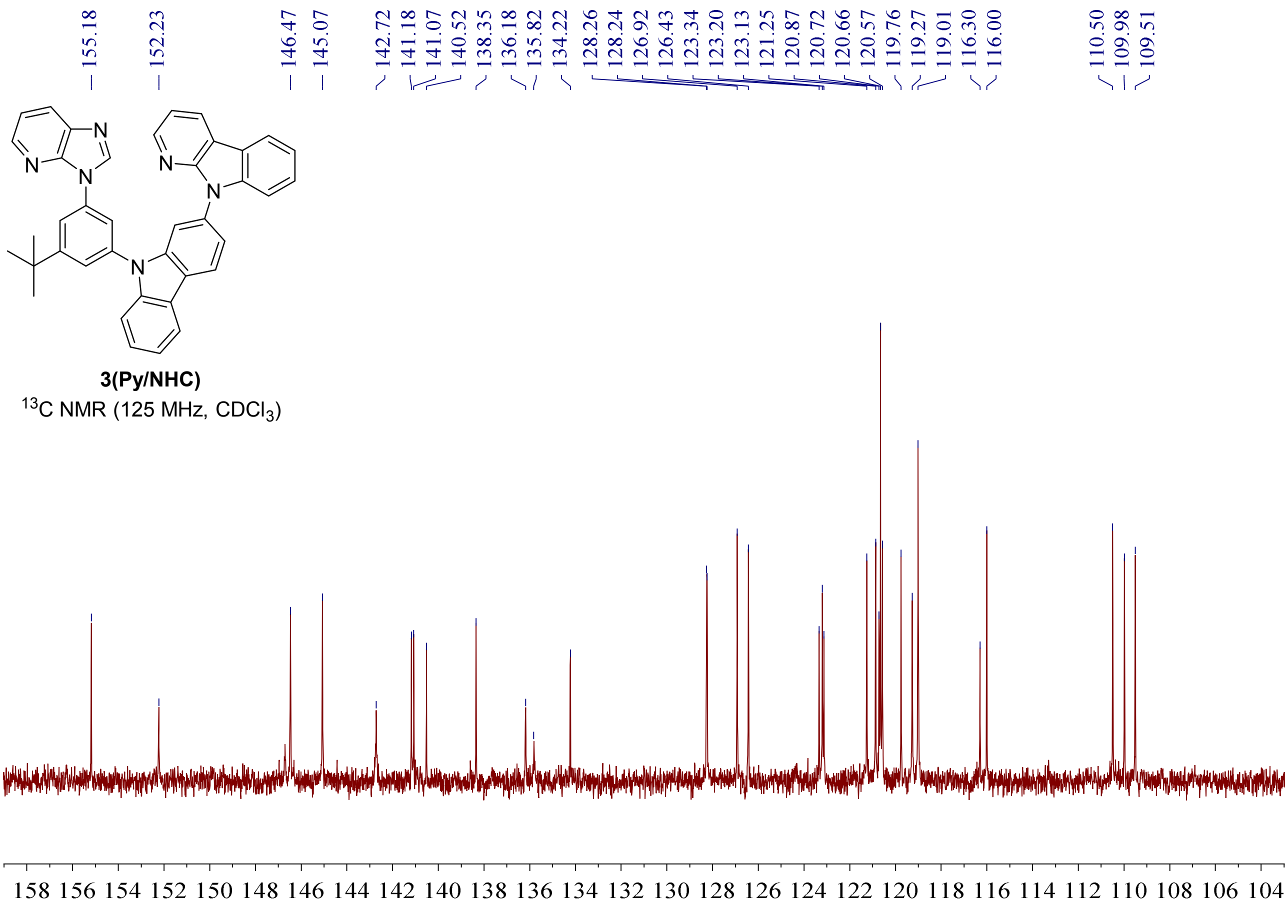
^{1}H NMR (500 MHz, DMSO-d_6)

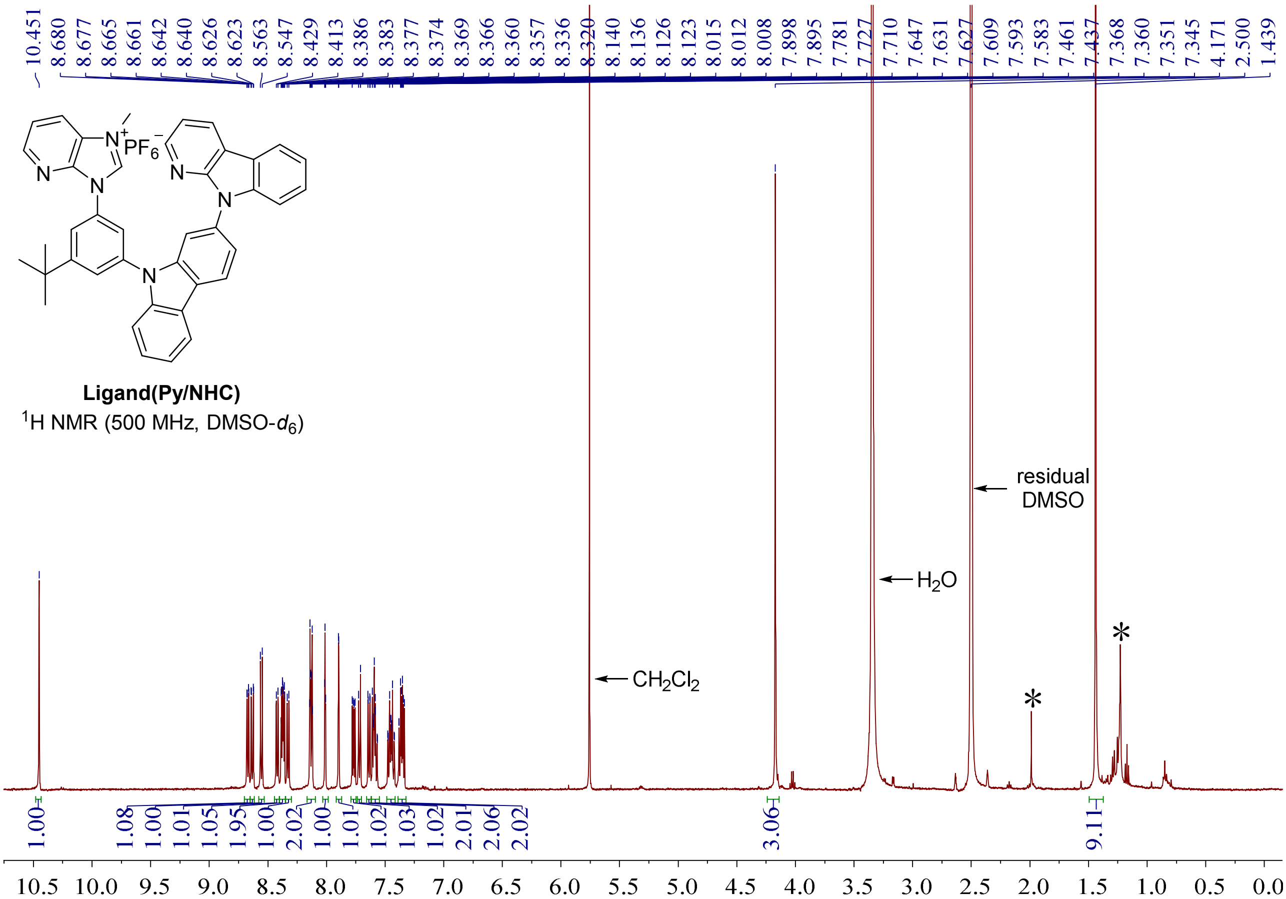


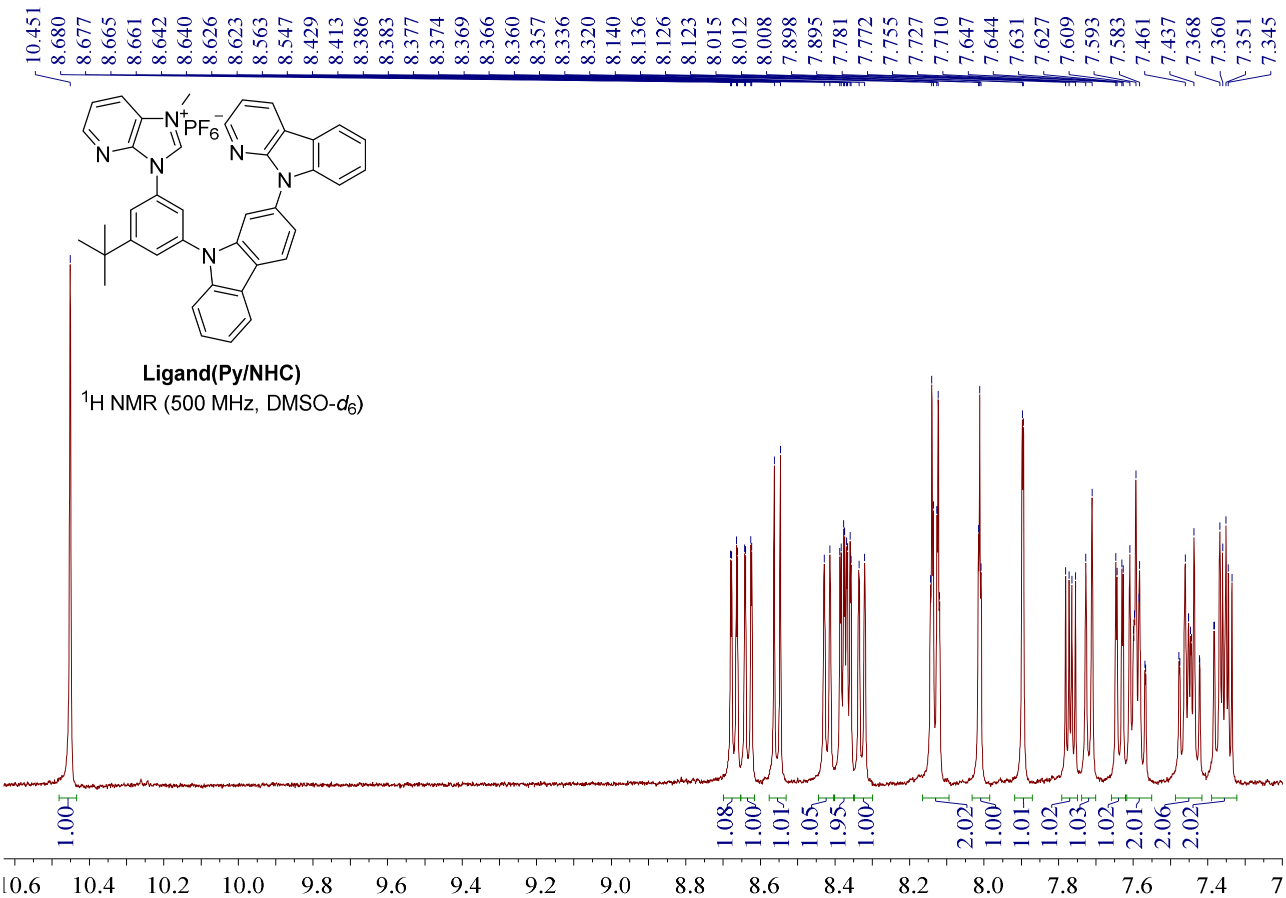
3(Py/NHC)

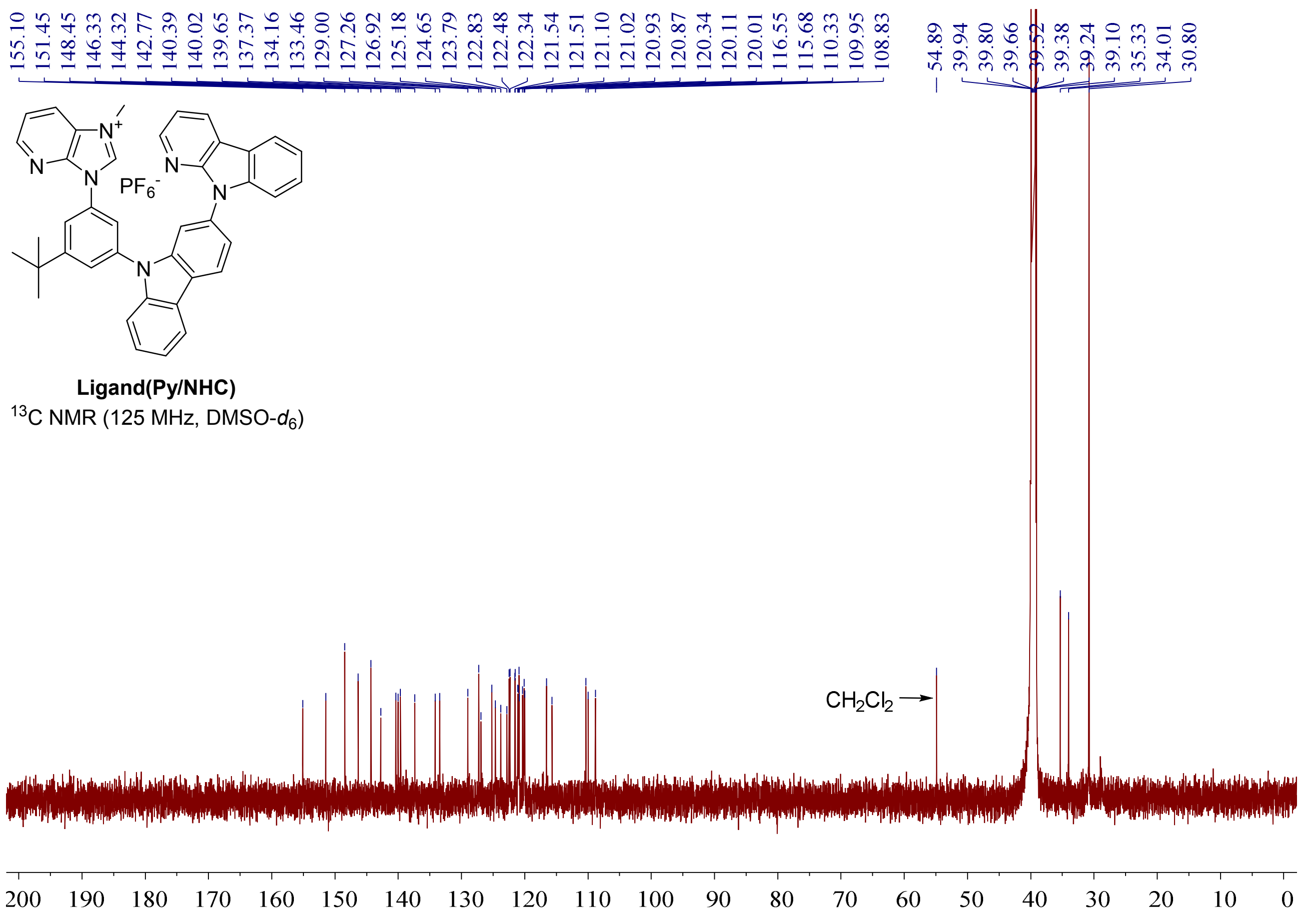
^{1}H NMR (500 MHz, DMSO-d_6)


3(Py/NHC)
^{13}C NMR (125 MHz, CDCl$_3$)

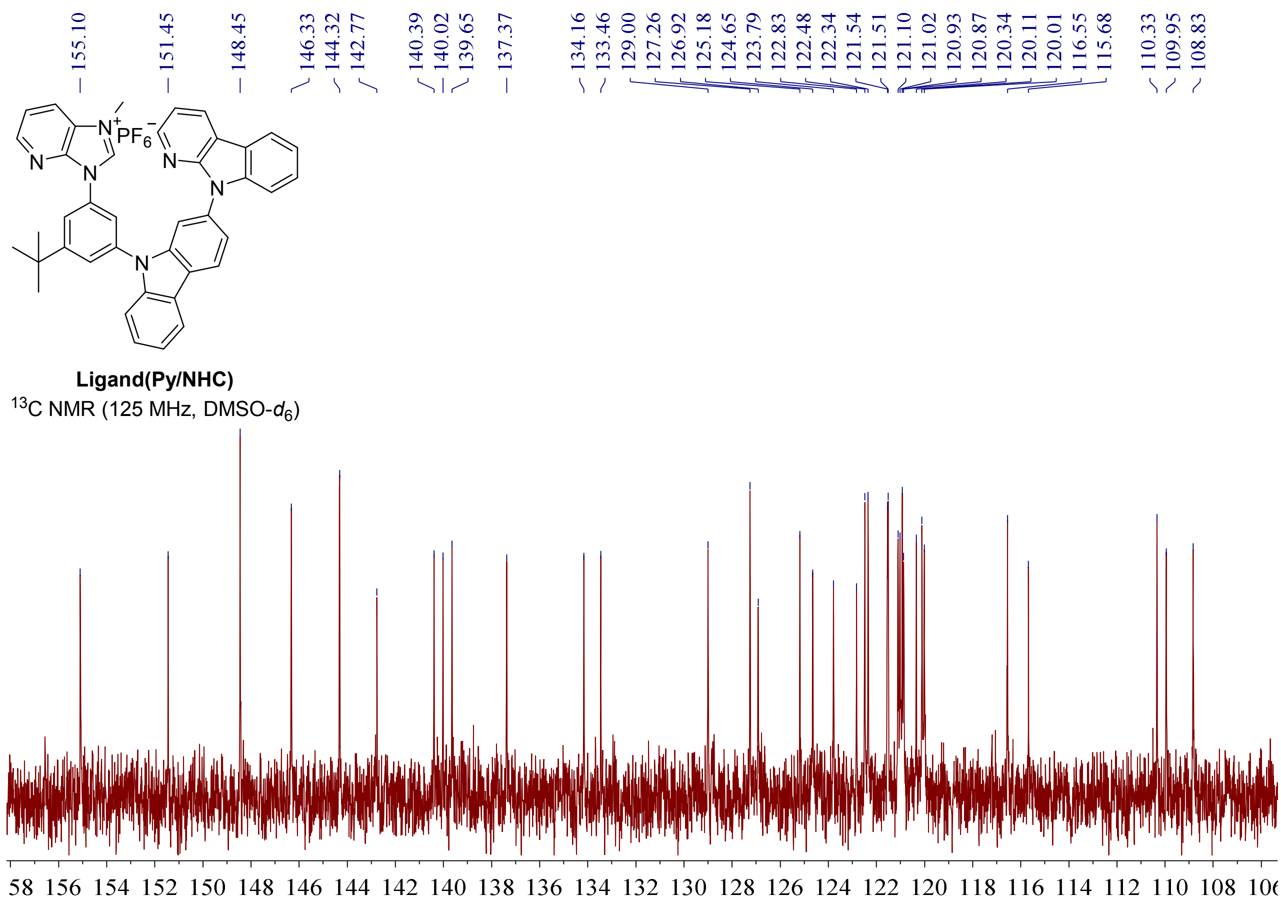

3(Py/NHC)
^{13}C NMR (125 MHz, CDCl$_3$)


Ligand(Py/NHC)
^{1}H NMR (500 MHz, DMSO-d_6)
residual DMSO
H_2O
CH_2Cl_2

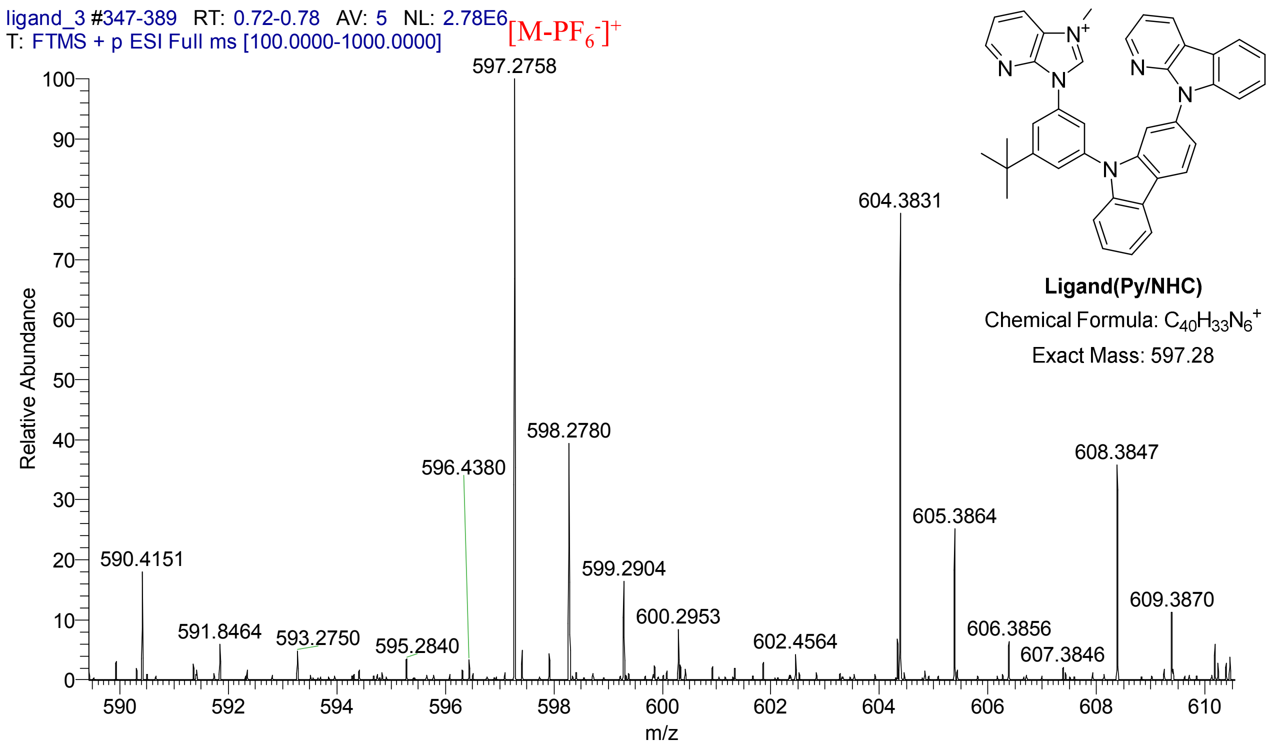

Ligand(Py/NHC)
^{1}H NMR (500 MHz, DMSO-d_6)



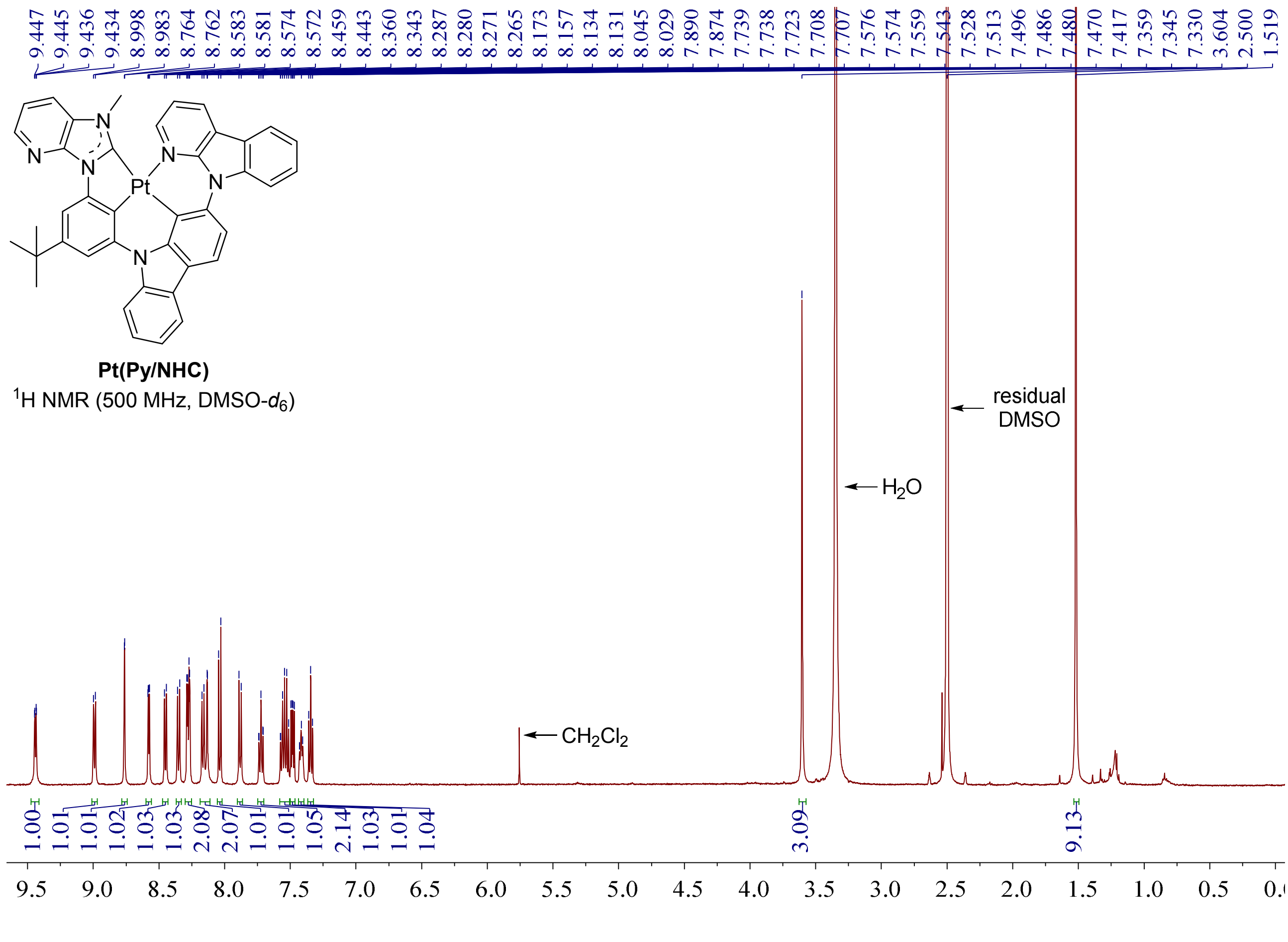
155.10
151.45
148.45
146.33
144.32
142.77
140.39
140.02
139.65
137.37
134.16
133.46
129.00
127.26
126.92
125.18
124.65
123.79
122.83
122.48
122.34
121.54
121.51
121.10
121.02
120.93
120.87
120.34
120.11
120.01
116.55
115.68
110.33
109.95
108.83
54.89
39.94
39.80
39.66
39.52
39.38
39.24
39.10
35.33
34.01
30.80
Ligand(Py/NHC)
13C NMR (125 MHz, DMSO-d6)
CH2Cl2



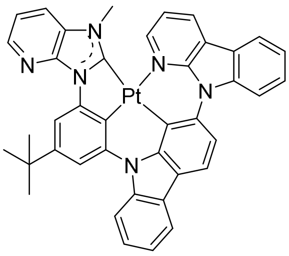
Ligand(Py/NHC)
13C NMR (125 MHz, DMSO-d6)

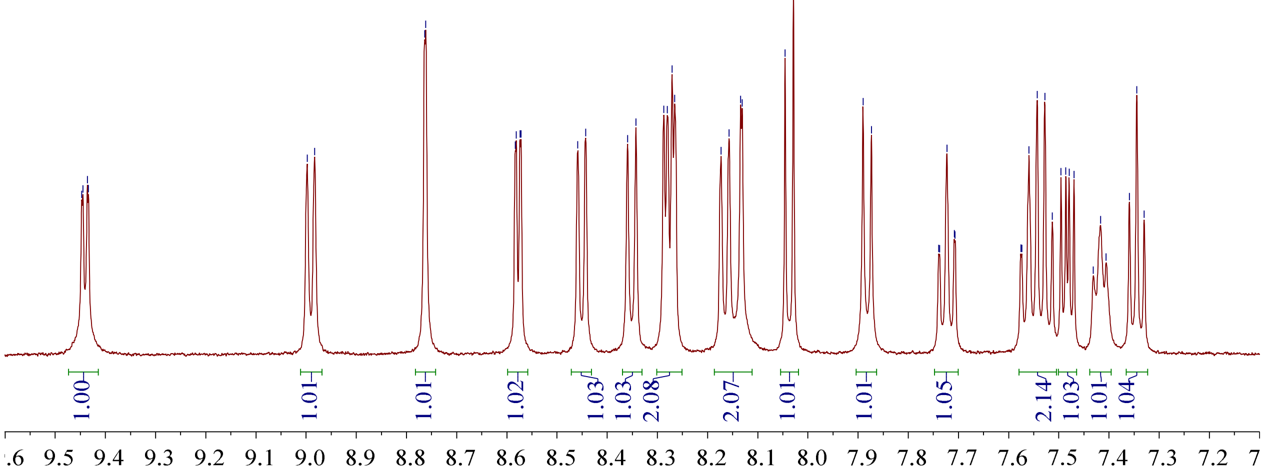


ligand_3 #347-389 RT: 0.72-0.78 AV: 5 NL: 2.78E6
T: FTMS + p ESI Full ms [100.0000-1000.0000]
[M-PF6-]+
597.2758
604.3831
598.2780
596.4380
608.3847
605.3864
599.2904
609.3870
590.4151
600.2953
606.3856
591.8464
593.2750
595.2840
602.4564
607.3846
Relative Abundance
m/z
Ligand(Py/NHC)
Chemical Formula: C40H33N6+
Exact Mass: 597.28

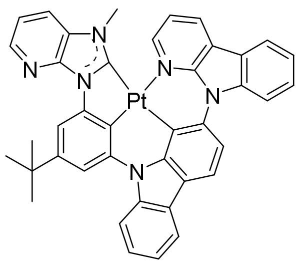


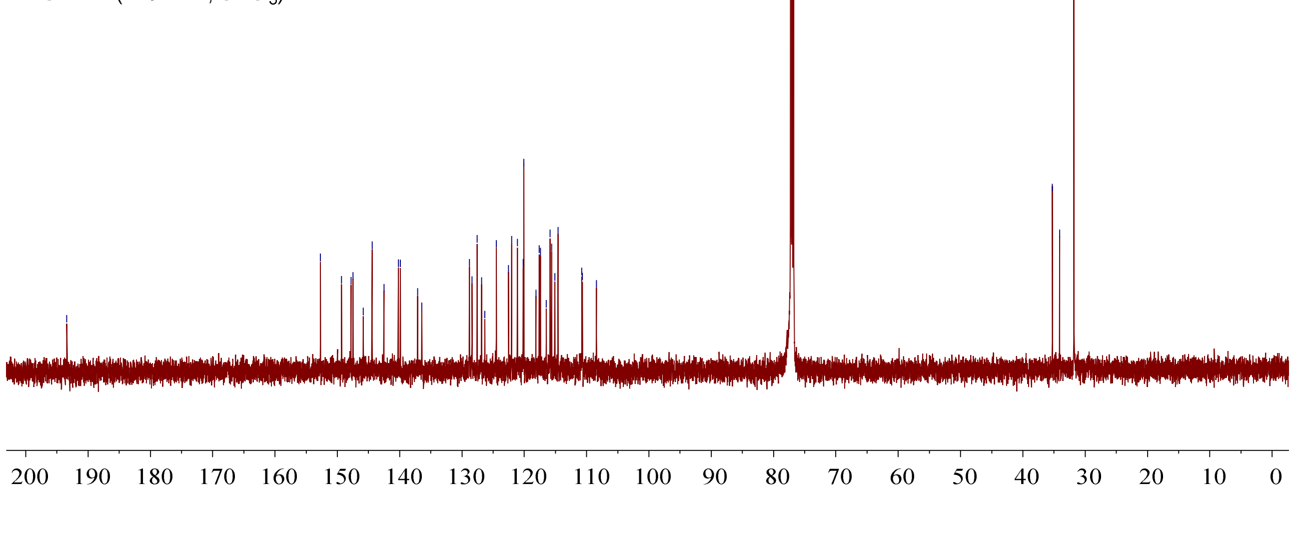
Pt(Py/NHC)
1H NMR (500 MHz, DMSO-d6)
CH2Cl2
H2O
residual DMSO



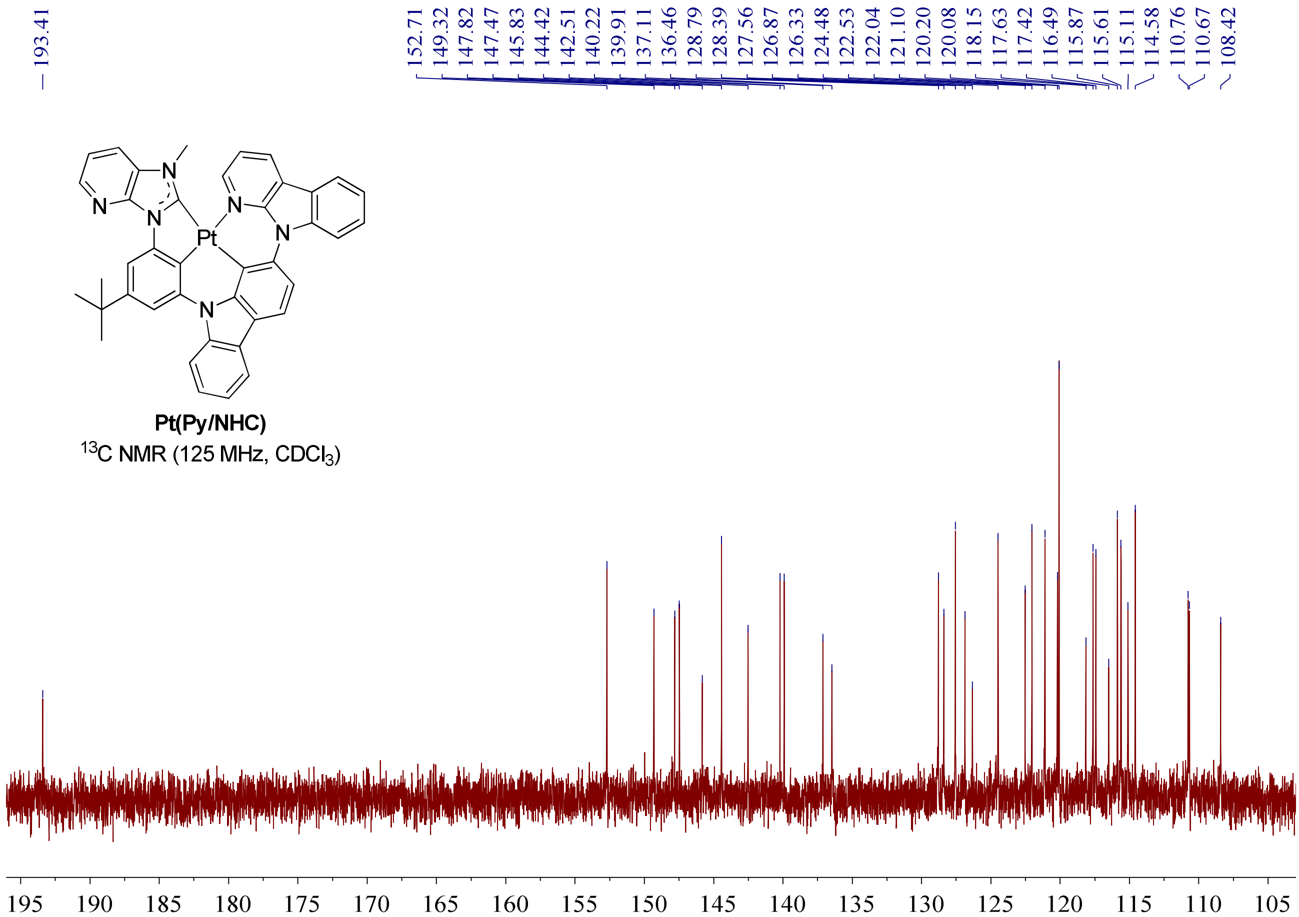


Pt(Py/NHC)
^{1}H NMR (500 MHz, DMSO-d_6)



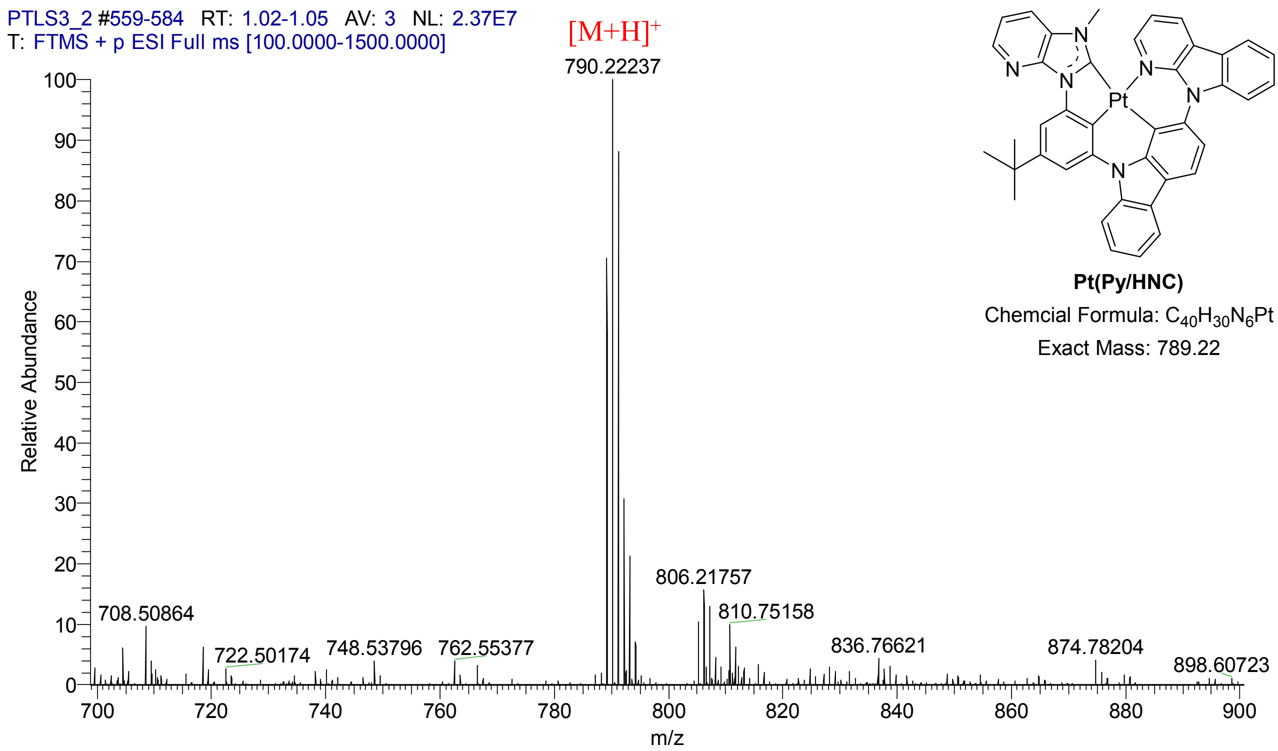


Pt(Py/NHC)
^{13}C NMR (125 MHz, $CDCl_3$)



Pt(Py/NHC)

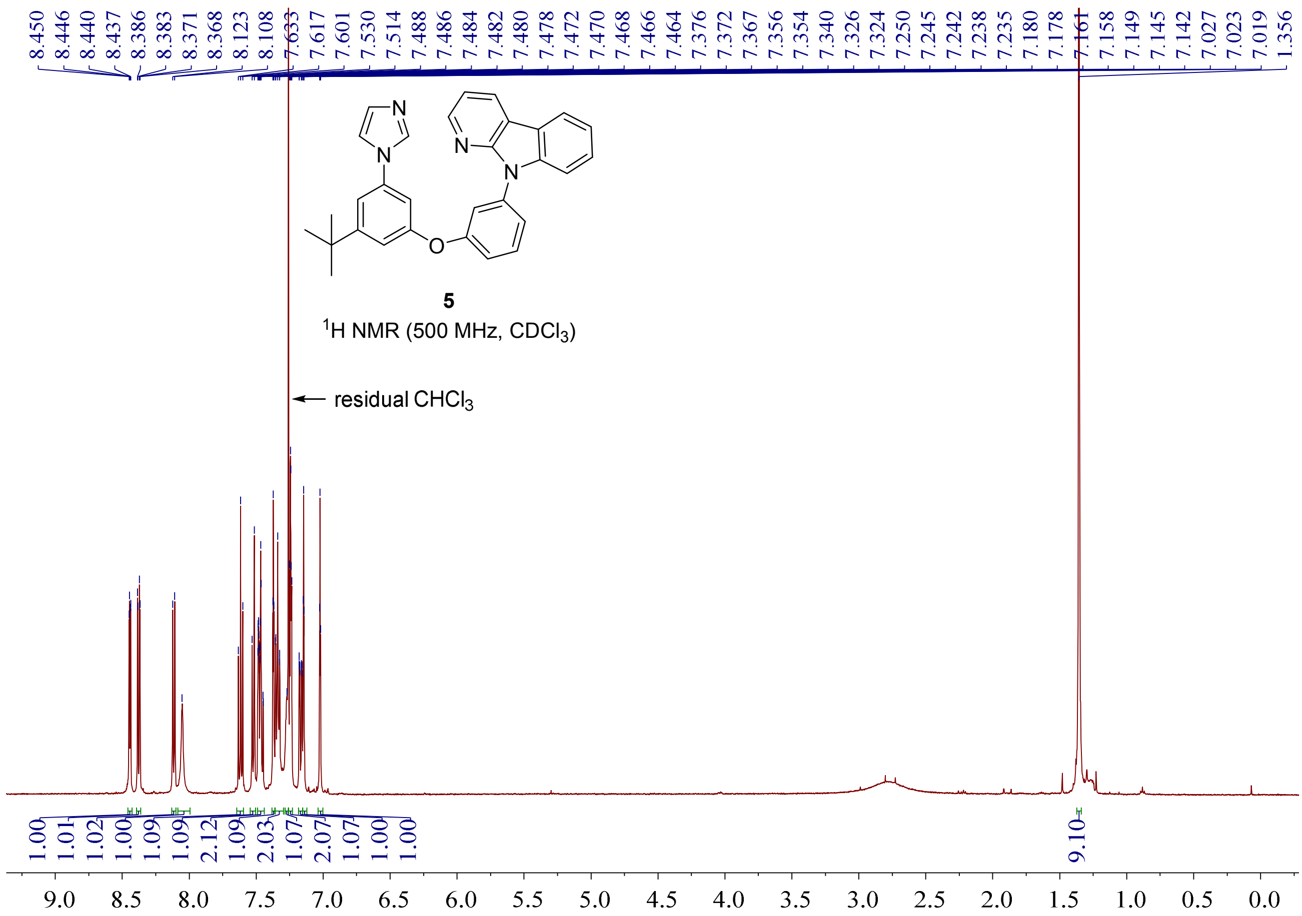
^{13}C NMR (125 MHz, $CDCl_3$)



Pt(Py/HNC)

Chemcial Formula: $C_{40}H_{30}N_6Pt$

Exact Mass: 789.22


8.450
8.446
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7.478
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7.466
7.464
7.376
7.372
7.367
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7.354
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7.245
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7.235
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7.178
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7.158
7.149
7.145
7.142
7.027
7.023
7.019
1.356
5
^{1}H NMR (500 MHz, $CDCl_3$)
residual $CHCl_3$
1.00
1.01
1.02
1.00
1.09
1.09
2.12
1.09
2.03
1.07
2.07
1.07
1.00
1.00
9.10
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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2.0
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1.0
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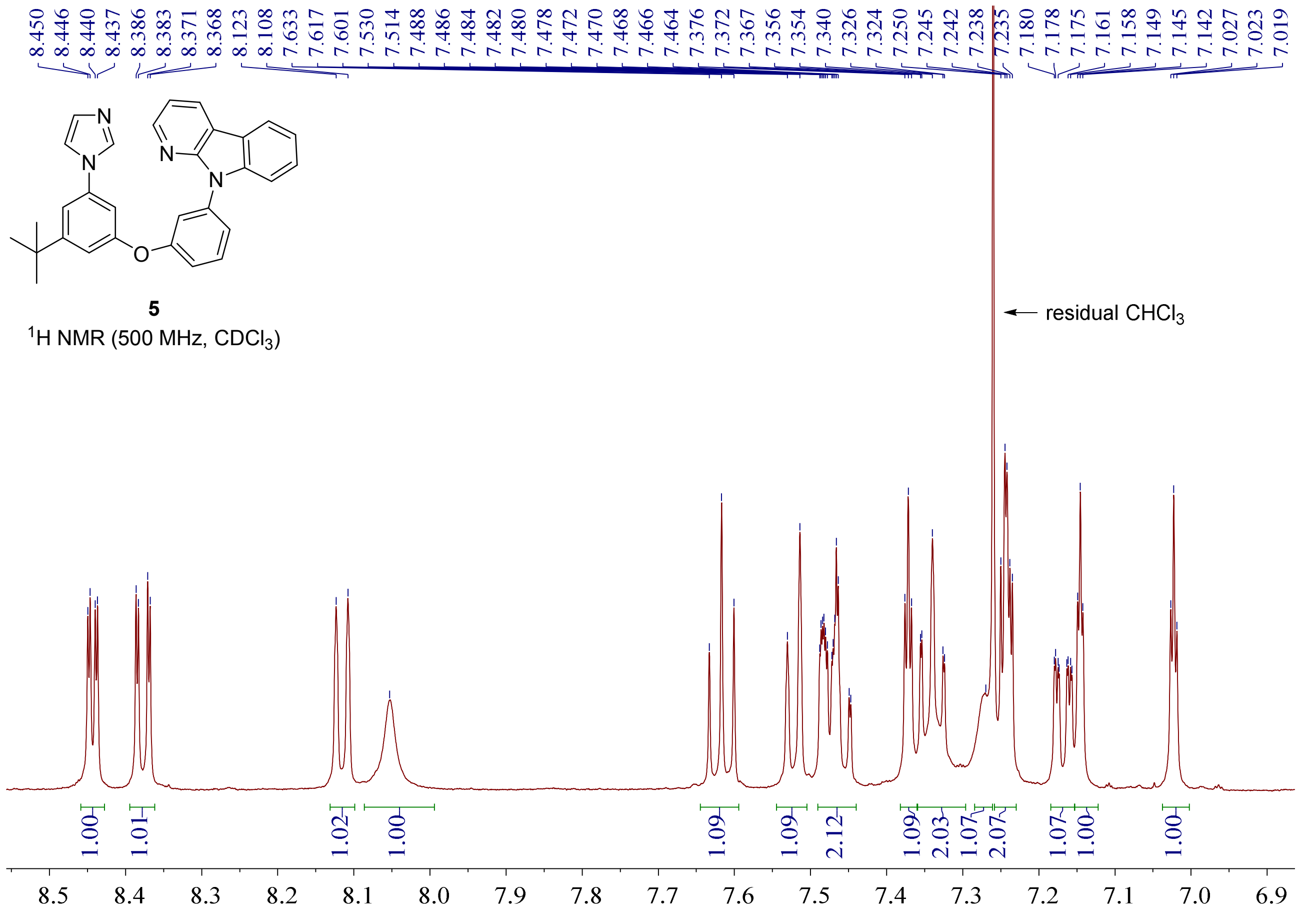
0.0


8.450
8.446
8.440
8.437
8.386
8.383
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8.368
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8.108
7.633
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7.601
7.530
7.514
7.488
7.486
7.484
7.482
7.480
7.478
7.472
7.470
7.468
7.466
7.464
7.376
7.372
7.367
7.356
7.354
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7.324
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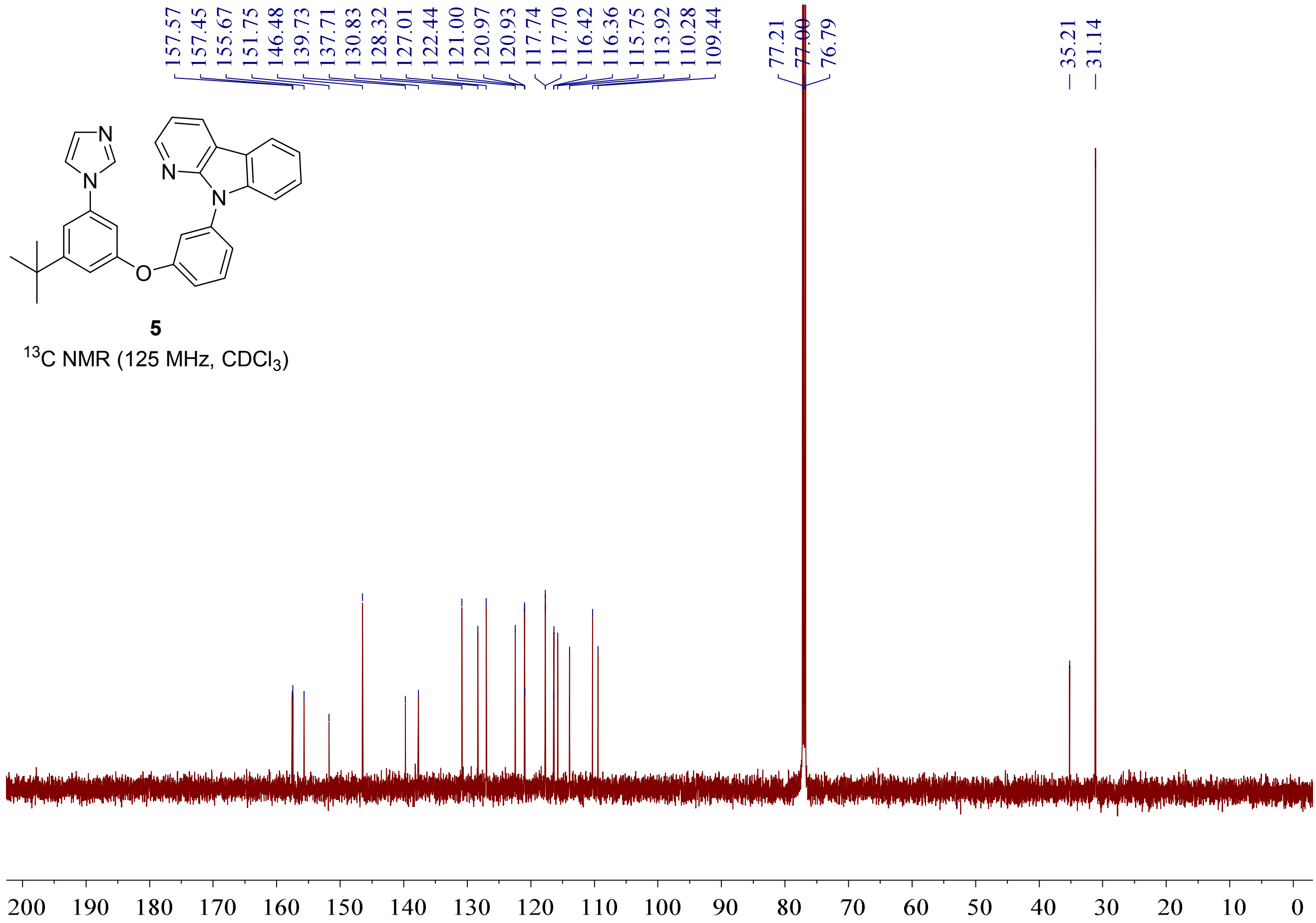
7.235
7.180
7.178
7.175
7.161
7.158
7.149
7.145
7.142
7.027
7.023
7.019
5
^{1}H NMR (500 MHz, $CDCl_3$)
residual $CHCl_3$
1.00
1.01
1.02
1.00
1.09
1.09
2.12
1.09
2.03
1.07
2.07
1.07
1.00
1.00
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9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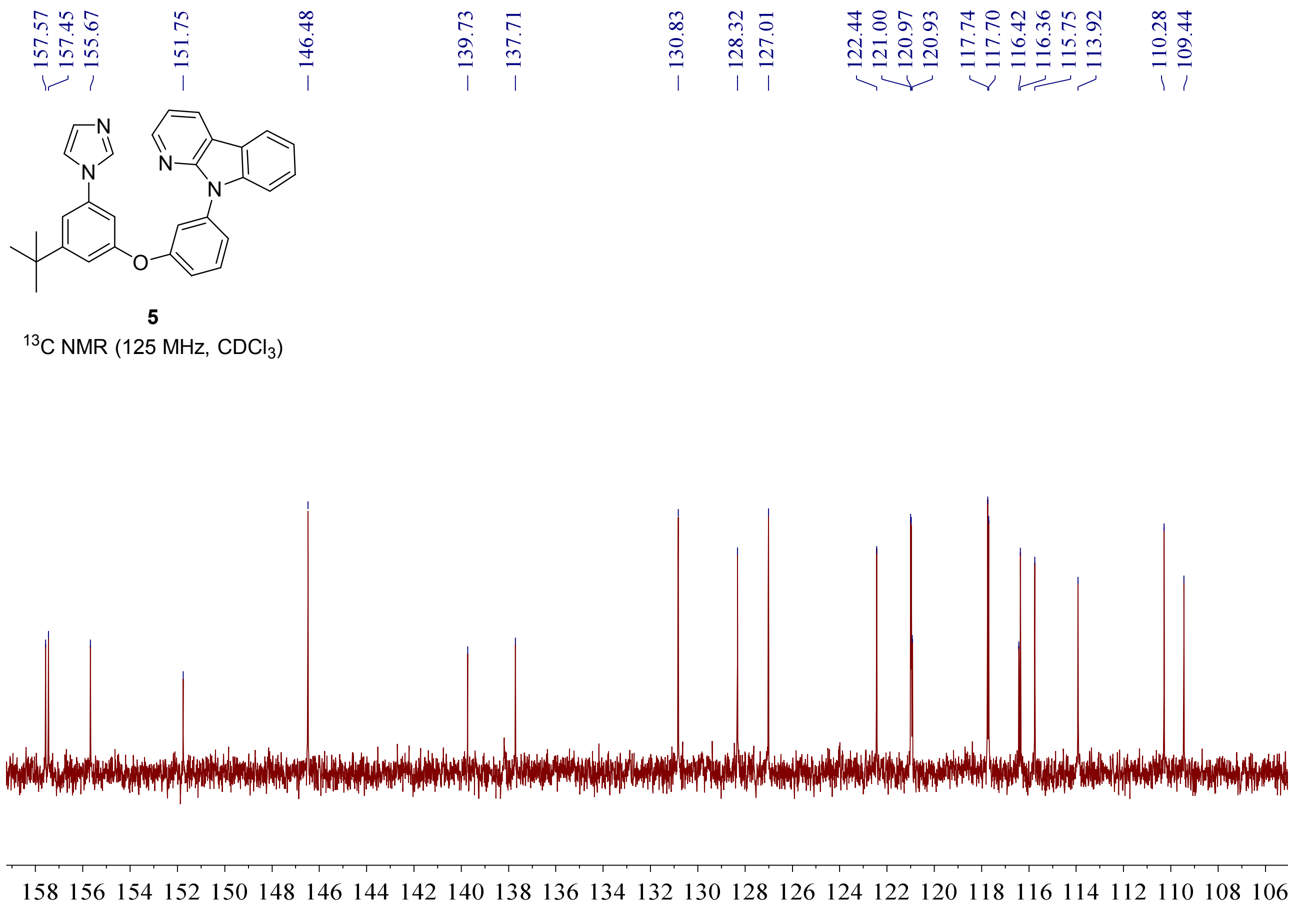
120.93
117.74
117.70
116.42
116.36
115.75
113.92
110.28
109.44
77.21
77.00
76.79
35.21
31.14
N
N
N
N
O
5
^{13}C NMR (125 MHz, $CDCl_3$)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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157.45
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146.48
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130.83
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127.01
122.44
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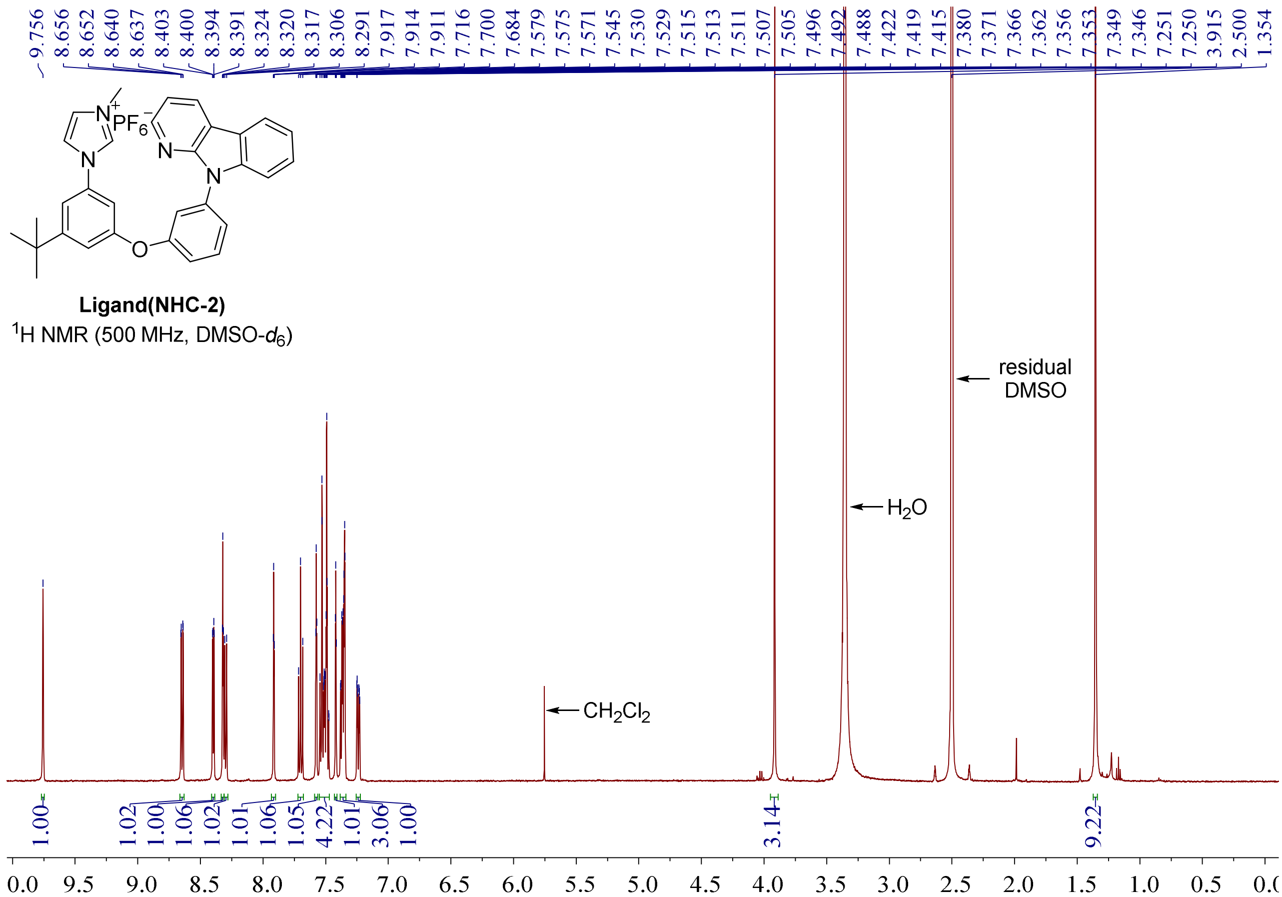
120.93
117.74
117.70
116.42
116.36
115.75
113.92
110.28
109.44
N
N
N
N
O
5
^{13}C NMR (125 MHz, $CDCl_3$)
158 156 154 152 150 148 146 144 142 140 138 136 134 132 130 128 126 124 122 120 118 116 114 112 110 108 106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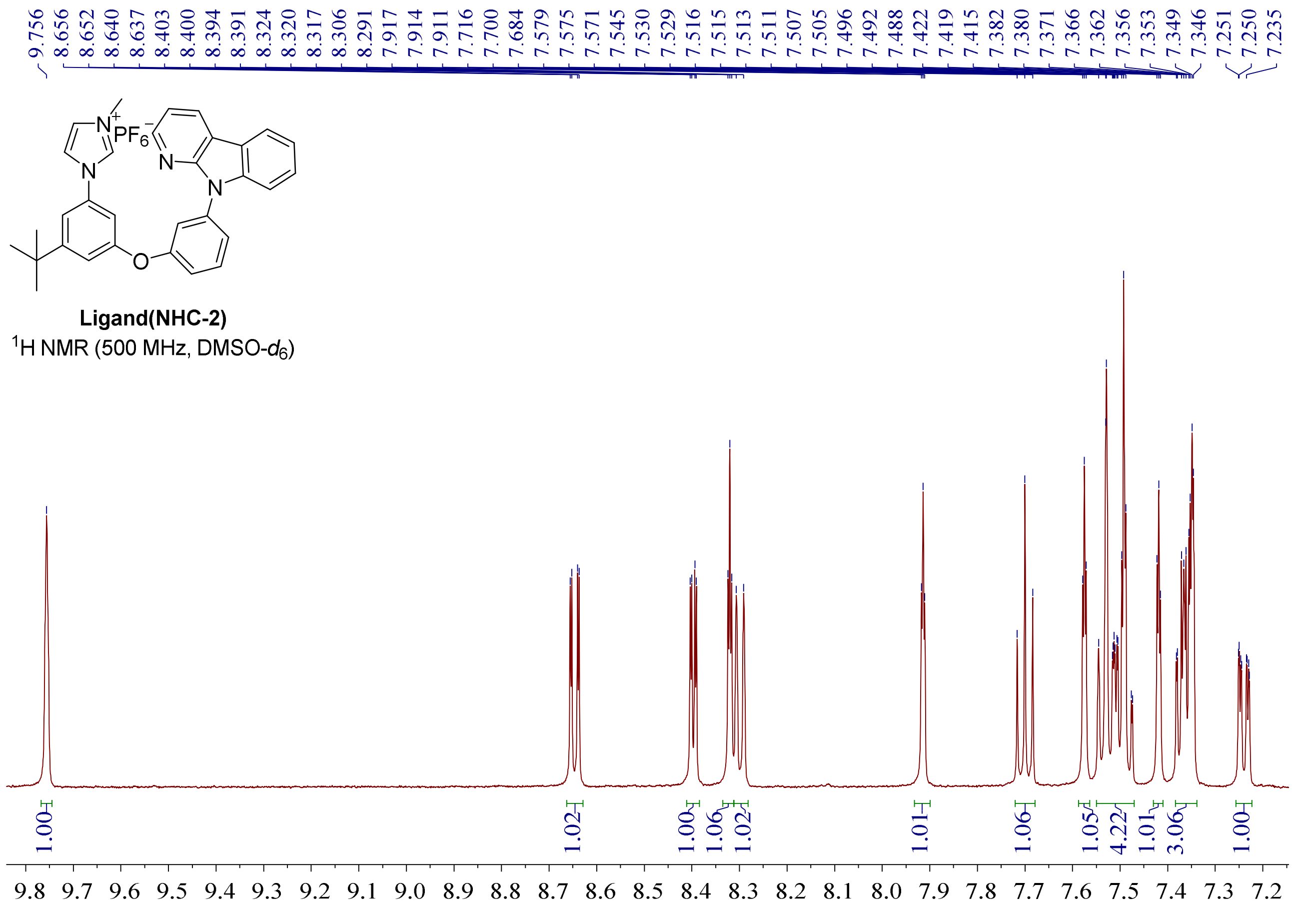
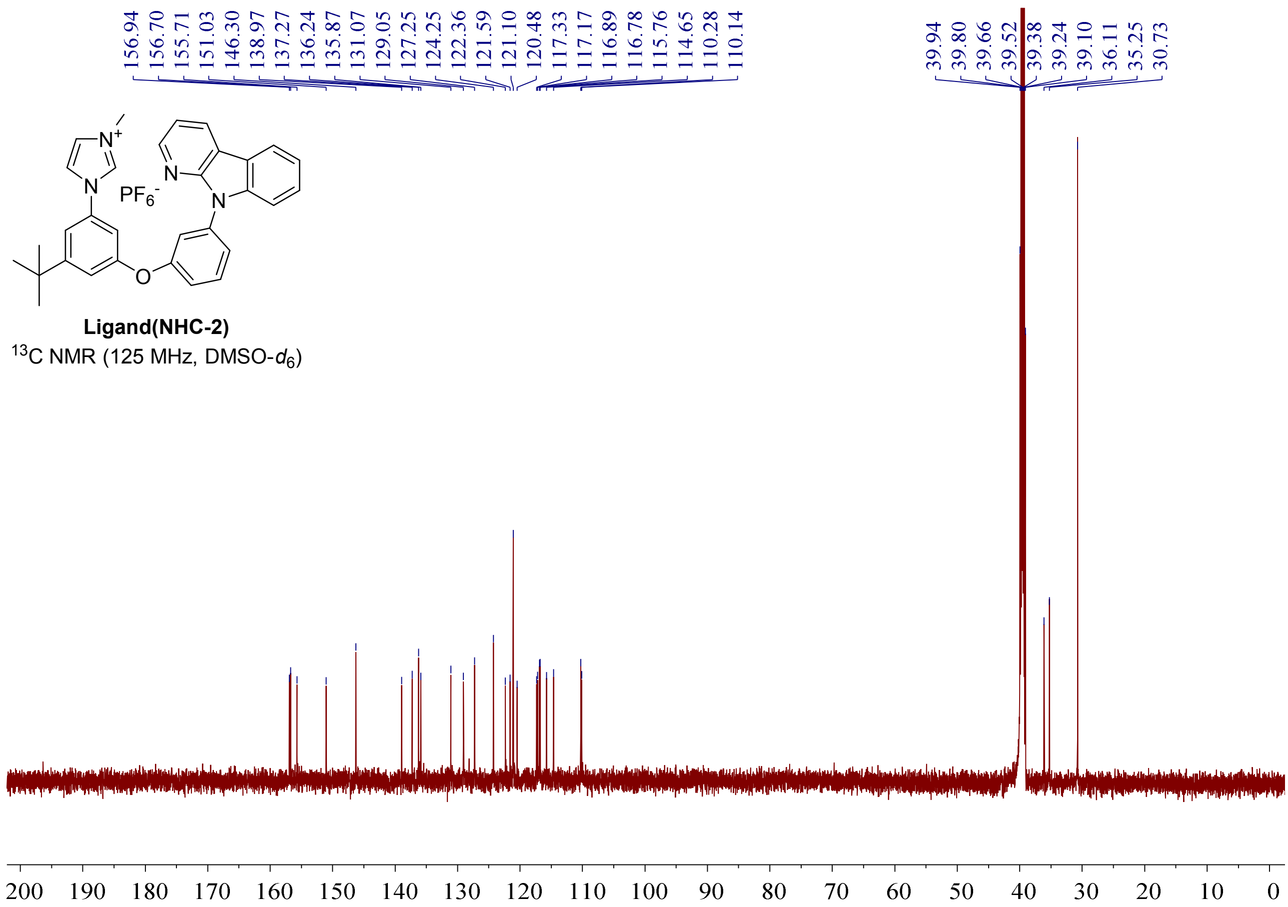
Ligand(NHC-2)
^{1}H NMR (500 MHz, DMSO-d_6)
residual DMSO
H_2O
CH_2Cl_2
1.00 1.02 1.00 1.06 1.02 1.01 1.06 1.05 4.22 1.01 3.06 1.00 3.14 9.22


9.756 8.656 8.652 8.640 8.637 8.403 8.400 8.394 8.391 8.324 8.320 8.317 8.306 8.291 7.917 7.914 7.911 7.716 7.700 7.684 7.579 7.575 7.571 7.545 7.530 7.529 7.516 7.515 7.513 7.511 7.507 7.505 7.496 7.492 7.488 7.422 7.419 7.415 7.382 7.380 7.371 7.366 7.362 7.356 7.353 7.349 7.346 7.251 7.250 7.235
Ligand(NHC-2)
^{1}H NMR (500 MHz, DMSO-d_6)
1.00 1.02 1.00 1.06 1.02 1.01 1.06 1.05 4.22 1.01 3.06 1.00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136.24
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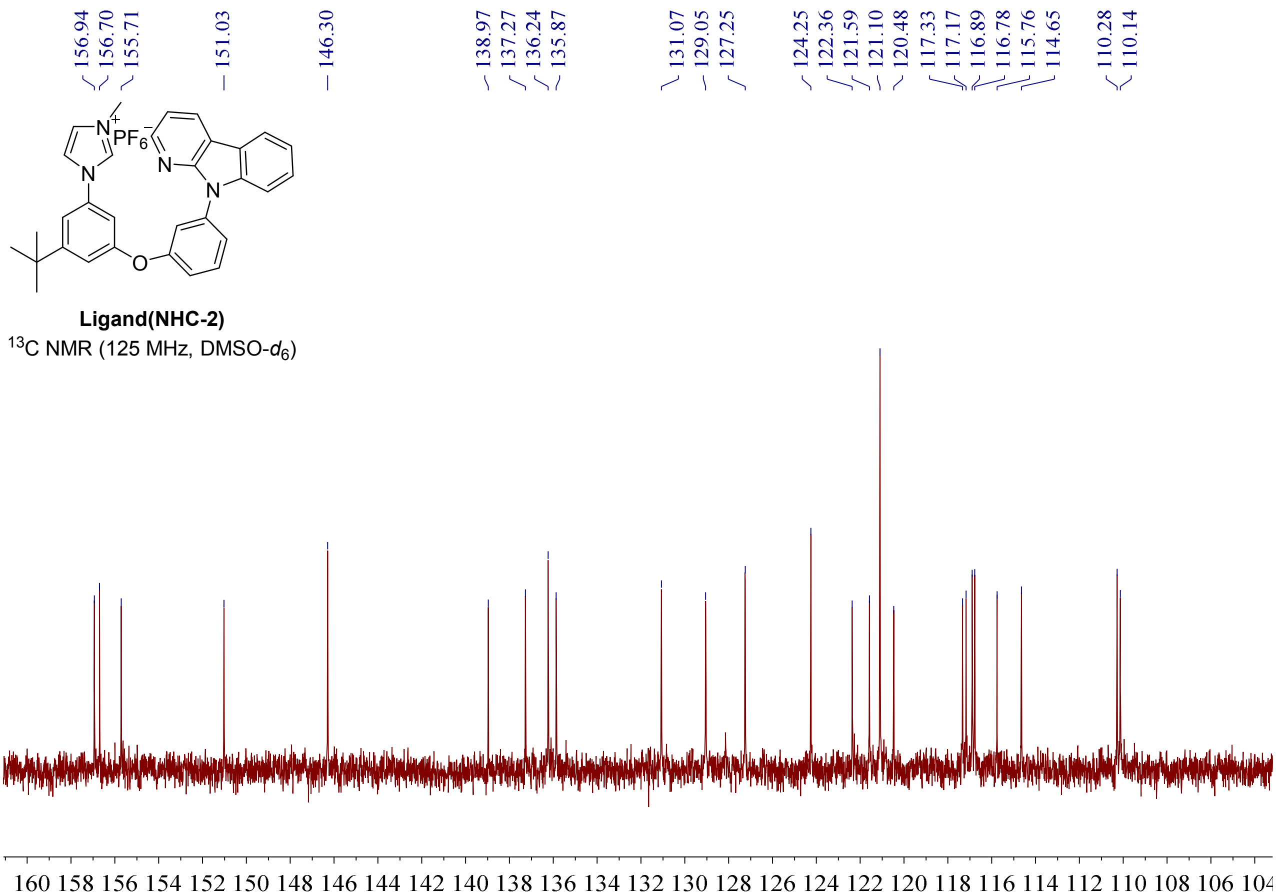
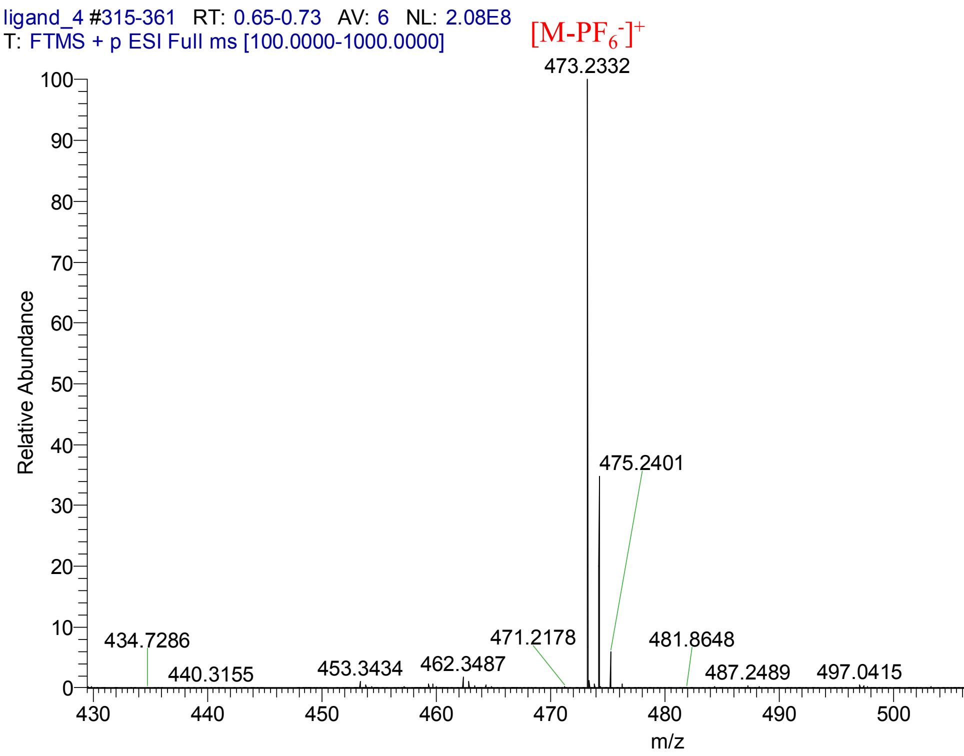
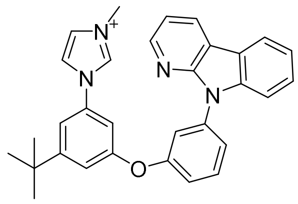
131.07
129.05
127.25
124.25
122.36
121.59
121.10
120.48
117.33
117.17
116.89
116.78
115.76
114.65
110.28
110.14
39.94
39.80
39.66
39.52
39.38
39.24
39.10
36.11
35.25
30.73
Ligand(NHC-2)
13C NMR (125 MHz, DMSO-d6)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


156.94
156.70
155.71
151.03
146.30
138.97
137.27
136.24
135.87
131.07
129.05
127.25
124.25
122.36
121.59
121.10
120.48
117.33
117.17
116.89
116.78
115.76
114.65
110.28
110.14
Ligand(NHC-2)
13C NMR (125 MHz, DMSO-d6)
160 158 156 154 152 150 148 146 144 142 140 138 136 134 132 130 128 126 124 122 120 118 116 114 112 110 108 106 104

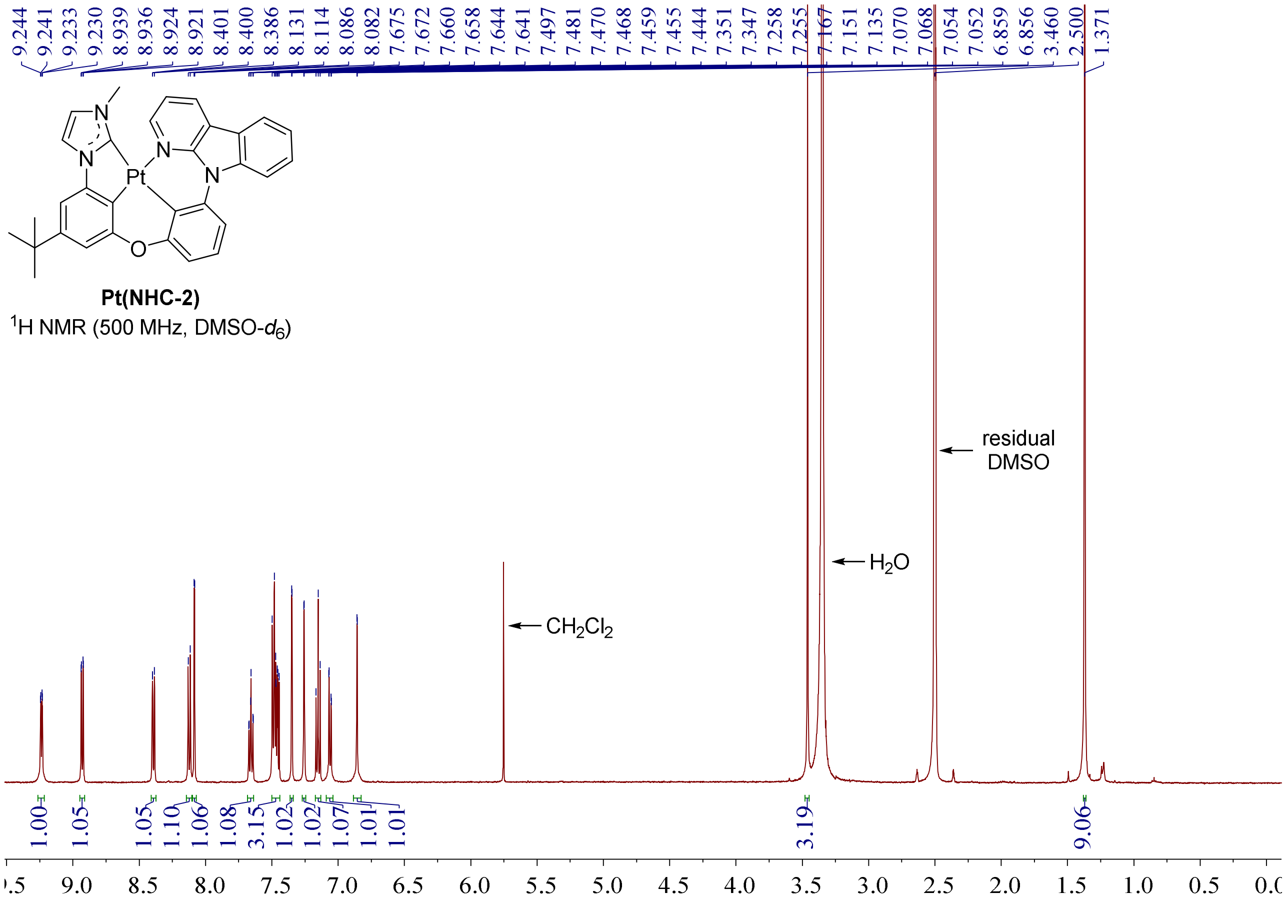


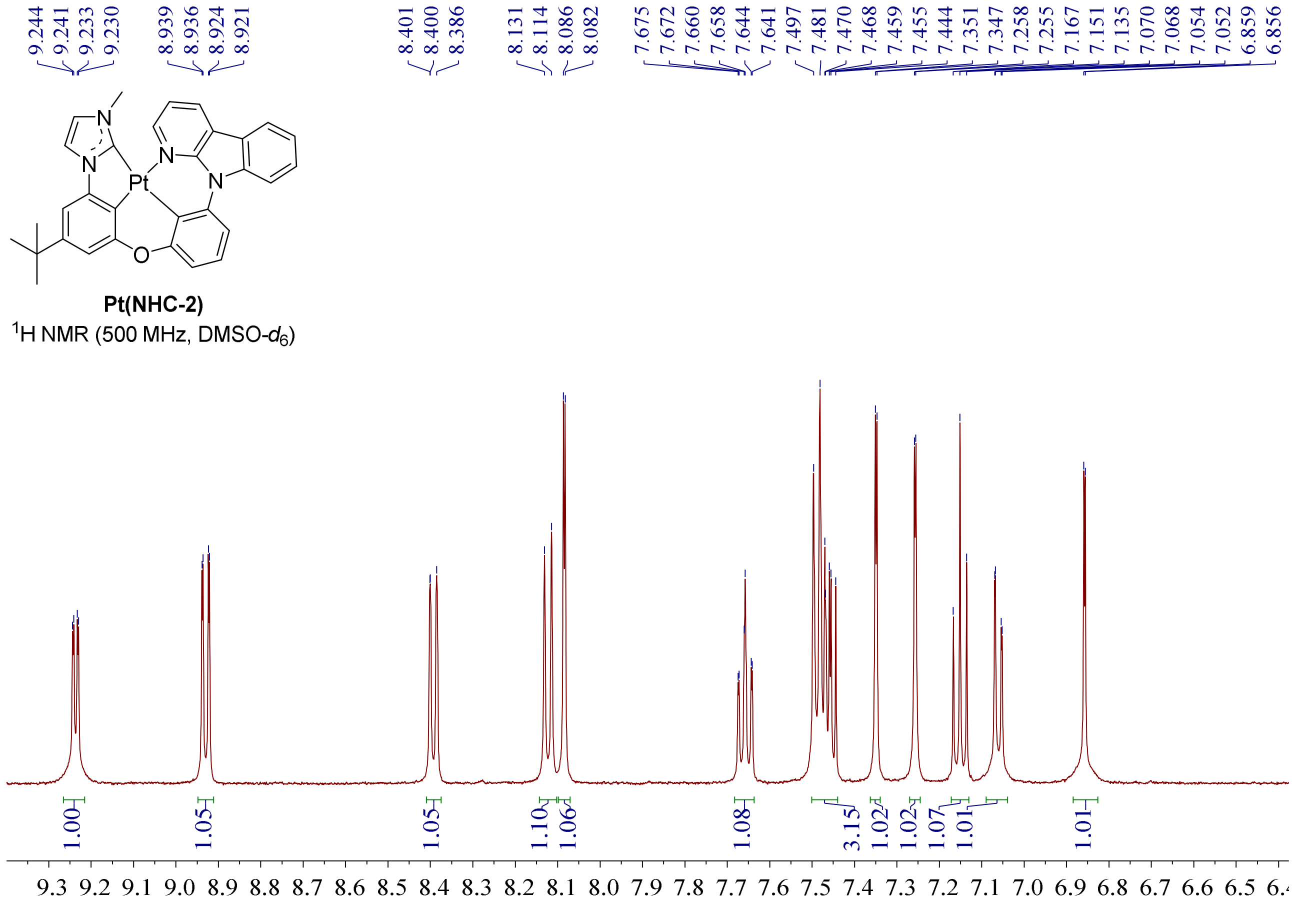


Ligand(NHC-2)

Chemical Formula: $C_{31}H_{29}N_4O^+$

Exact Mass: 473.23

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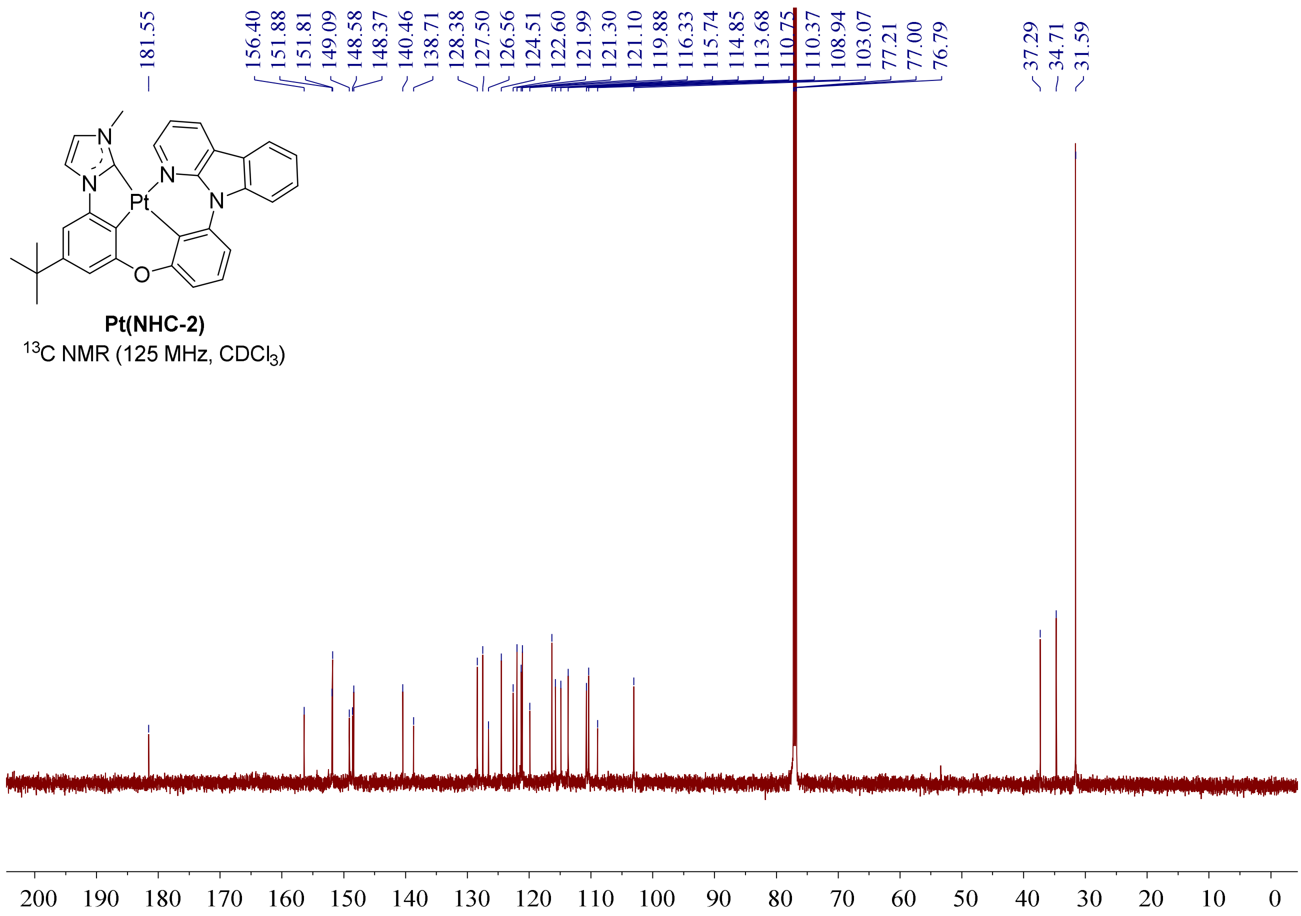
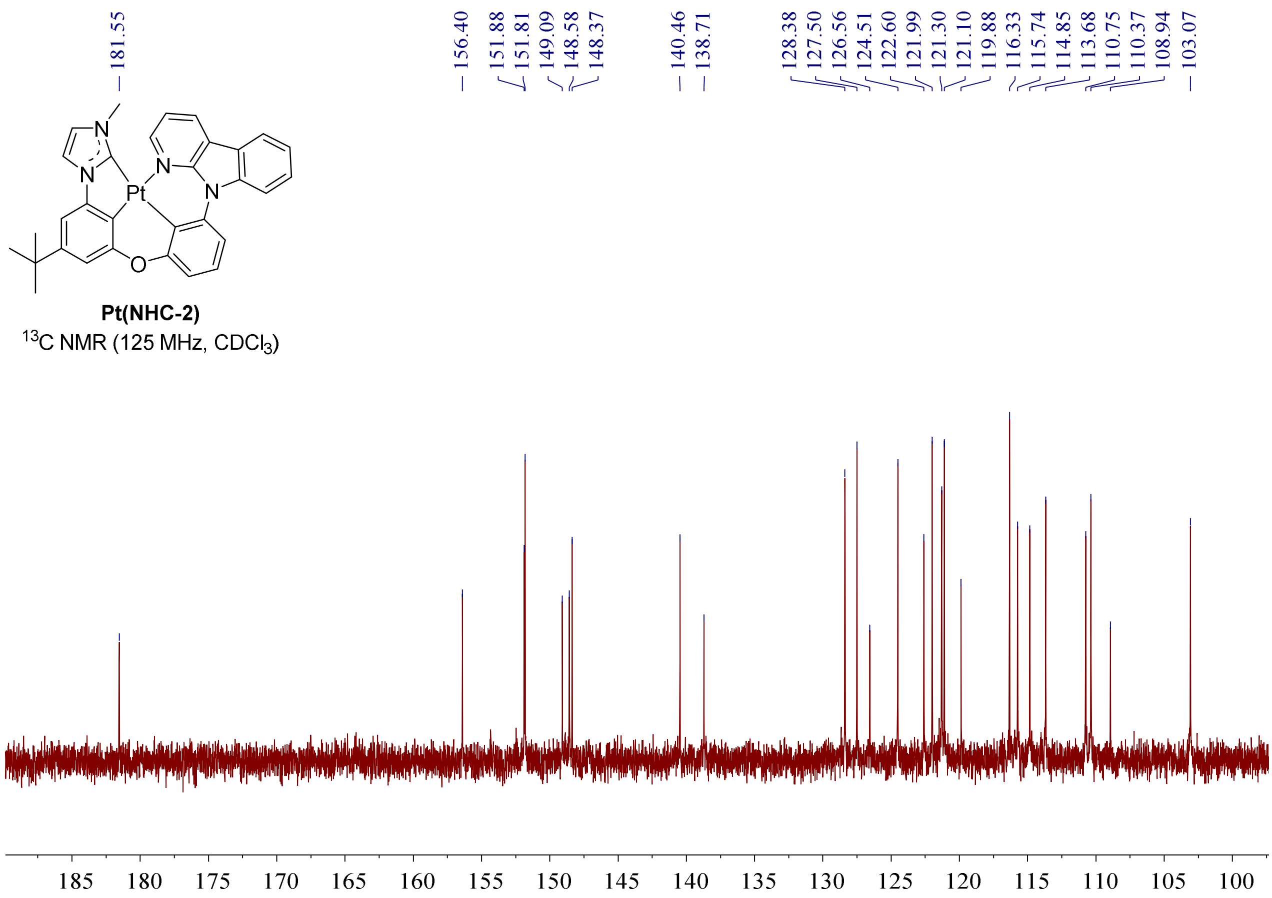
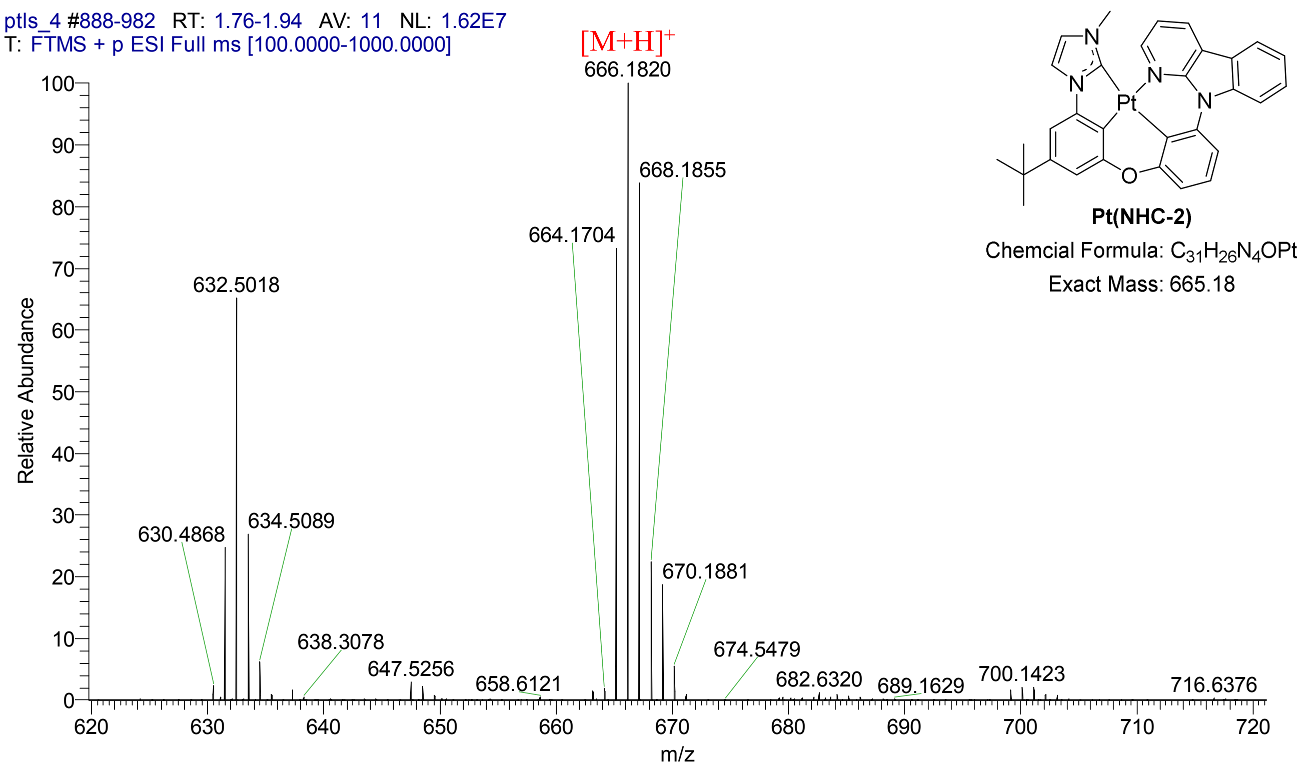
Pt(NHC-2)
^{1}H NMR (500 MHz, DMSO-d_6)
1.00 1.05 1.05 1.10 1.06 1.08 3.15 1.02 1.02 1.07 1.01 1.01


181.55 156.40 151.88 151.81 149.09 148.58 148.37 140.46 138.71 128.38 127.50 126.56 124.51 122.60 121.99 121.30 121.10 119.88 116.33 115.74 114.85 113.68 110.75 110.37 108.94 103.07 77.21 77.00 76.79 37.29 34.71 31.59
Pt(NHC-2)
^{13}C NMR (125 MHz, CDCl$_3$)


181.55
156.40
151.88
151.81
149.09
148.58
148.37
140.46
138.71
128.38
127.50
126.56
124.51
122.60
121.99
121.30
121.10
119.88
116.33
115.74
114.85
113.68
110.75
110.37
108.94
103.07
N
N
Pt
N
N
O
Pt(NHC-2)
^{13}C NMR (125 MHz, $CDCl_3$)
185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100


ptls_4 #888-982 RT: 1.76-1.94 AV: 11 NL: 1.62E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]
[M+H]+
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668.1855
664.1704
632.5018
630.4868
634.5089
670.1881
638.3078
674.5479
647.5256
658.6121
682.6320
689.1629
700.1423
716.6376
Relative Abundance
m/z
Pt(NHC-2)
Chemcial Formula: $C_{31}H_{26}N_4OPt$
Exact Mass: 665.18

Cartesian coordinates of the optimized structures

Pt(NHC-1)_S_0

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C	3.55276950	0.61285530	0.84861230
C	3.67618500	-1.78113970	0.83461440
C	1.62894420	-0.64033550	0.03865610
C	2.28938600	0.58231840	0.23008880
C	4.25792150	-0.55170030	1.17442780
H	4.19493710	-2.71419220	1.02021980
N	1.76726170	-2.98865360	-0.16956690
N	0.28213920	-4.02559280	-1.33982130
C	1.39108720	-4.86601450	-1.24289540
C	2.32611440	-4.20775560	-0.51303770
H	1.41228200	-5.84131300	-1.70421090
H	3.32651690	-4.49465070	-0.23194260
C	-0.83842000	-4.29602420	-2.23276310
H	-1.39586980	-3.37239110	-2.38739400
H	-1.50134050	-5.06573250	-1.82336610
H	-0.45258520	-4.63767550	-3.19755910
H	3.97765580	1.57354710	1.10785530
C	5.62031390	-0.44705250	1.88474900
C	6.24415920	-1.82872600	2.15735560
H	6.42992220	-2.38262100	1.22950330
H	5.60814370	-2.44364820	2.80464540
H	7.20791450	-1.70420310	2.66382700
C	5.43540650	0.27256670	3.24255910
H	5.03134220	1.28206250	3.11429380
H	6.39664200	0.35884300	3.76475050
H	4.74486290	-0.28273830	3.88737160
C	6.60897580	0.36005430	1.01090830
H	6.24370000	1.37341920	0.81388370
H	6.77093470	-0.13225310	0.04498950
H	7.57974980	0.44970680	1.51423820
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C	3.05880990	5.50824100	-1.47661960
C	3.67335700	3.24205730	-0.80300500
C	1.33270410	3.94051760	-0.87991460
C	1.70895020	5.21790860	-1.30768940
C	4.02498750	4.51780150	-1.24156850
H	4.44017140	2.48973400	-0.67242510
H	0.95061700	5.96730970	-1.52055490
H	5.07499930	4.74137730	-1.41173300
H	3.36608160	6.49573780	-1.80973640
C	0.27913900	1.96877500	-0.30296900
C	-2.29534750	2.87276290	-0.63580570
C	0.04968430	3.31107420	-0.69423600
C	-0.73883920	1.01325370	-0.10823440
C	-2.03638020	1.56585510	-0.16404260
C	-1.25763330	3.74856140	-0.90627130
H	-1.46298980	4.74606750	-1.28478280
H	-3.31594820	3.18081900	-0.82562630
N	-3.18466360	0.80845490	0.25128190
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H	-6.07054620	3.93690670	2.18967860
H	-7.78751790	2.16678230	2.45487740
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Pt	-0.31334980	-0.98214450	-0.27781550
C	0.49723880	-2.86090410	-0.66349920

Pt(Ph/NHC)_S_0

C	2.50774190	-0.67319830	0.45197510
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C	1.44432210	0.18337030	0.11142410
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C	3.86494500	1.12708470	1.30129490
H	4.43494920	-0.95528360	1.36108420
N	2.26477980	-2.03624110	0.07300230
N	1.08545920	-3.48971960	-1.06370020
C	0.07351990	-4.02897860	-1.96142350
H	-0.73725310	-3.30617900	-2.04321160
H	-0.31502620	-4.98602940	-1.59690210
H	0.51558160	-4.18051330	-2.95158270
H	2.98152940	3.06717060	1.04550440
C	5.10234770	1.67823530	2.03456860
C	6.11440150	0.57126110	2.38615220
H	6.49261200	0.06654930	1.48931080
H	5.68058970	-0.18525630	3.05019040
H	6.97443230	1.00768980	2.90664570
C	4.65708720	2.36158280	3.34899020
H	3.95803800	3.18238020	3.15967750
H	5.52392960	2.77260040	3.88181030
H	4.15616420	1.64662330	4.01170550
C	5.82399800	2.71320620	1.13941600
H	5.18436770	3.57176680	0.90943770
H	6.13177890	2.26177400	0.18922670
H	6.72115170	3.09573980	1.64187870
N	0.77797200	2.48174830	-0.30931840

C	1.06934590	3.76331840	-0.80656020
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C	-0.14307940	4.38505570	-1.20244150
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H	-7.33134390	2.48593650	1.78724660
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C	-2.17705570	-3.13287380	0.30690010
C	-4.48729080	-3.20963060	0.97064280

H	-1.21709270	-3.61342000	0.19276670
H	-5.35897600	-3.74775920	1.33202490
H	-3.17054510	-4.93124760	0.90368690
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C	2.37764570	-4.01160540	-0.97023550
C	5.05123240	-4.48986280	-0.52677460
C	2.92017120	-5.19403410	-1.46567880
C	3.14528930	-3.07334280	-0.25377580
C	4.50465030	-3.30509530	-0.03117500
C	4.27559570	-5.42357940	-1.22898140
H	2.31549720	-5.90854880	-2.01541610
H	5.12984530	-2.59569240	0.49348810
H	4.73535430	-6.33620780	-1.59611660
H	6.10624270	-4.68898110	-0.36314300

Pt(Py/NHC)_S_0

C	2.47406400	-0.62374780	0.43656070
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C	3.66648830	-0.19622360	1.00797290
C	1.40166980	0.21975940	0.09662310
C	1.64743730	1.59349450	0.21887310
C	3.82918970	1.17190790	1.27107080
H	4.43602260	-0.91943340	1.23609490
N	2.24119300	-1.98708100	0.05724690
N	1.12300040	-3.46586460	-1.11924300
C	0.15612950	-4.02075220	-2.05783250
H	-0.66543640	-3.31416330	-2.16880460
H	-0.22820220	-4.98557170	-1.70985570
H	0.63698430	-4.15958270	-3.03184110
H	2.91472920	3.10354660	1.06224490
C	5.07588060	1.72841230	1.98328850
C	6.09998680	0.62379540	2.30631800
H	6.46260750	0.12703490	1.39941270
H	5.67967810	-0.14221000	2.96761350

H	6.96643430	1.06022460	2.81669970
C	4.65086080	2.39924630	3.31052030
H	3.94768590	3.22107680	3.14097360
H	5.52596850	2.80726680	3.83201210
H	4.16317840	1.67717420	3.97535430
C	5.77276680	2.77500500	1.08228570
H	5.12426320	3.63262640	0.87326930
H	6.06286620	2.33274580	0.12230900
H	6.67863660	3.15810330	1.56865320
N	0.71635040	2.51636580	-0.30544870
C	0.99549550	3.80982610	-0.77911340
C	0.98231400	6.39609460	-1.84600060
C	2.21377070	4.47556270	-0.97236100
C	-0.22103220	4.42200430	-1.17674460
C	-0.22441920	5.72102930	-1.69583360
C	2.18779630	5.76489430	-1.50146700
H	3.16290610	4.00260960	-0.75765190
H	-1.16059500	6.18817900	-1.99133130
H	3.12932890	6.28562530	-1.65563890
H	0.99566100	7.40513800	-2.24863170
C	-0.65917850	2.26815980	-0.46997220
C	-3.36494350	2.31496740	-0.95812140
C	-1.26262810	3.44597470	-0.97853900
C	-1.35004640	1.06307050	-0.23122280
C	-2.74909280	1.18539260	-0.37430560
C	-2.62688090	3.44572110	-1.26673810
H	-3.10324310	4.30358710	-1.73327030
H	-4.41922780	2.28354900	-1.20343790
N	-3.63500750	0.14418870	0.06768490
C	-4.94019840	0.35554890	0.57609750
C	-7.52399000	0.21753180	1.64241080
C	-5.60794480	1.54427370	0.90041900
C	-5.54577150	-0.89339380	0.85558080
C	-6.84474210	-0.96317730	1.37174450
C	-6.89469470	1.45462390	1.42543790

H	-5.13798960	2.51011660	0.77515660
H	-7.30351510	-1.92730120	1.57489120
H	-7.41809520	2.37212180	1.68002770
H	-8.53224500	0.18638960	2.04476030
C	-3.38121310	-1.20853210	0.14816470
C	-3.28348740	-3.90971440	0.52743010
C	-4.55005590	-1.89788930	0.59594480
N	-2.20439110	-1.81771540	-0.08099530
C	-2.18427310	-3.15496130	0.13790100
C	-4.50298790	-3.27226650	0.76478670
H	-1.21772040	-3.62244030	0.02767740
H	-5.37437020	-3.82819620	1.09887480
H	-3.16734410	-4.97814940	0.67447400
Pt	-0.33081710	-0.71545560	-0.24530760
C	1.00703680	-2.25677870	-0.48452730
C	2.40954250	-3.97305870	-0.95796990
C	5.00993750	-4.25416540	-0.26070350
C	3.04523810	-5.13090300	-1.38242650
C	3.13121820	-3.02180380	-0.20752040
N	4.40338980	-3.12946550	0.15093560
C	4.38802800	-5.26055280	-1.01128330
H	2.53805850	-5.89281300	-1.96605810
H	4.95455200	-6.13929970	-1.30153920
H	6.05376300	-4.35805550	0.02562380

Pt(NHC-2)_S$_0$

C	2.71319080	-0.95695960	-0.92146540
C	3.98201690	1.34722220	-0.17853800
C	4.09608070	-0.90313170	-0.99687540
C	1.89817040	0.10763240	-0.49467900
C	2.57984240	1.25359760	-0.10501730
C	4.76148600	0.28258670	-0.62695510
H	4.66451000	-1.76838530	-1.32309290
H	4.42955510	2.28436470	0.13088420
N	1.96417130	-2.12361200	-1.25187920

N	0.15970290	-3.24816480	-1.58676600
C	1.20915410	-3.98490480	-2.13070830
C	2.34417690	-3.27207880	-1.92155590
H	1.05139360	-4.93508310	-2.61746410
H	3.36419260	-3.47738100	-2.20364830
C	-1.23353330	-3.65135290	-1.70087170
H	-1.50708000	-4.36946430	-0.92071100
H	-1.39372970	-4.11256490	-2.67909570
H	-1.86515750	-2.76880860	-1.61910970
C	0.61303370	-2.09172520	-1.02322890
O	1.98047730	2.37012380	0.40713920
C	0.62759690	2.64374660	0.40205830
C	-1.96282610	3.60451900	0.49107930
C	0.39079250	3.97871790	0.75679250
C	-0.39793940	1.72386280	0.10280240
C	-1.69797600	2.28974870	0.08597380
C	-0.90910060	4.45001730	0.82727130
H	1.24196500	4.61347820	0.98159300
H	-1.10930290	5.47161840	1.13802340
Pt	-0.04289100	-0.25643320	-0.26972100
H	-2.98185460	3.96215270	0.56923820
N	-2.84680110	1.50141960	-0.30781700
C	-4.09240380	2.00921760	-0.73722460
C	-6.73107530	2.52004300	-1.49011950
C	-4.39631600	3.22954390	-1.35059860
C	-5.10108370	1.02977270	-0.54395630
C	-6.42530510	1.29377490	-0.91112180
C	-5.71881850	3.46748270	-1.71798000
H	-3.62575700	3.96274660	-1.55439500
H	-7.19765790	0.54405090	-0.75998890
H	-5.96731560	4.40835700	-2.20083840
H	-7.75252030	2.74103890	-1.78534100
C	-3.05493310	0.18308030	0.03339960
C	-3.83918400	-2.28132650	0.85299500
C	-4.44084070	-0.13866260	-0.01280950

N	-2.09191000	-0.70288920	0.30820090
C	-2.50048790	-1.90664620	0.76567290
C	-4.83437520	-1.40068040	0.41395440
H	-1.70349900	-2.59113170	1.03105670
H	-5.88040270	-1.69465580	0.41540400
H	-4.09123040	-3.26854100	1.22544150
C	6.29578160	0.35271150	-0.71822740
C	6.84426280	1.73124370	-0.30598950
H	6.45204540	2.53017990	-0.94533410
H	7.93653880	1.73760250	-0.39708880
H	6.59763010	1.97427960	0.73369520
C	6.91693310	-0.71234150	0.21642380
H	6.59499260	-1.72546940	-0.04853690
H	6.62661310	-0.53292250	1.25804840
H	8.01209790	-0.68342930	0.15654470
C	6.74163050	0.07929470	-2.17429910
H	6.32419540	0.82812430	-2.85710170
H	6.41854040	-0.90696200	-2.52588570
H	7.83515830	0.11790370	-2.25227220

References:

[1] G. Li, A. Wolfe, J. Brooks, Z.-Q. Zhu, J. Li, Modifying Emission Spectral Bandwidth of Phosphorescent Platinum(II) Complexes Through Synthetic Control, *Inorg. Chem.* **2017**, *56*, 8244–8256.

[2] N. G. Connelly, W. E. Geiger, Chemical Redox Agents for Organometallic Chemistry, *Chem. Rev.* **1996**, *96*, 877−910.

[3] D. C. Harris, In Quantitative Chemical Analysis, 6th ed.; W. H. Freeman: New York, **2002**; pp 394−396.

[4] G. Li, Q. Chen, J. Zheng, Q. Wang, F. Zhan, W. Lou, Y.-F. Yang, Y. She, Metal-Assisted Delayed Fluorescent Pd(II) Complexes and Phosphorescent Pt(II) Complex Based on [1,2,4]Triazolo[4,3-*a*]pyridine-containing Ligands: Synthesis, Characterization, Electrochemistry, Photophysical Studies, and Application, *Inorg. Chem.* **2019**, 58, *21*, 14349–14360.

[5] G. Li, F. Zhan, J. Zheng, Y.-F. Yang, Q. Wang, Q. Chen, G. Shen, Y. She, Highly Efficient Phosphorescent Tetradentate Platinum(II) Complexes Containing Fused 6/5/6 Metallocycles, *Inorg. Chem.* **2020**, *59*, 3718–3729.

[6] Y. She, K. Xu, X. Fang, Y.-F. Yang, W. Lou, Y. Hu, Q. Zhang, G. Li, Tetradentate Platinum(II) and Palladium(II) Complexes Containing Fused 6/6/6 or 6/6/5 Metallocycles with Azacarbazolylcarbazole-Based Ligands, *Inorg. Chem.* **2021**, *60*, 12972–12983.

[7] H. Li, J, Ding, Z. Xie, Y. Cheng, L. Wang, Synthesis, Characterization and Electrophosphorescent Properties of Mononuclear Platinum(II) Complexes Based on 2-Phenylbenzoimidazole Derivatives, *J. Organomet. Chem.* **2009**, *694*, 2777–2785.

[8] A. K.-W. Chan, E. S.-H. Lam, A. Y.-Y. Tam, D. P.-K. Tsang, W. H. Lam, M.-Y. Cham, W.-T. Wong, V. W.-W. Yam, Synthesis and Characterization of Luminescent Cyclometalated Platinum(II) Complexes of 1,3-Bis-Hetero-Azolylbenzenes with Tunable Color for Applications in Organic Light-Emitting Devices through Extension of π Conjugation by Variation of the Heteroatom, *Chem. Eur. J.* **2013**, *19*, 13910–13924.

[9] S. C. F. Kui, P. K. Chow, G. Cheng, C.-C. Kwok, C. L. Kwong, K.-H. Low, C.-M. Che, Robust Phosphorescent Platinum(II) Complexes with Tetradentate O^N^C^N Ligands: High Efficiency OLEDs with Excellent Efficiency Stability, *Chem. Commun.* **2013**, *49*, 1497–1499.

[10] E. Turner, N. Bakken, J. Li, Cyclometalated Platinum Complex with Luminescent Quantum Yields Approaching 100%, *Inorg. Chem.* **2013**, *52*, 7344–7351.

[11] G. Cheng, S. C. F. Ang, W.-H. Kui, M.-Y. Ko, P.-K. Chow, C.-L. Kwong, C.-C. Kwok, C. Ma, X. Guan, K.-H. Low, S.-J. Su, C.-M. Che, Structurally Robust Phosphorescent [Pt(O^N^C^N)] Emitters for High Performance Organic Light-Emitting Devices with Power Efficiency up to 126 lm W^{-1} and External Quantum Efficiency over 20%, *Chem. Sci.* **2014**, *5*, 4819–4830.

[12] B. Wang, F. Liang, H. Hu, Y. Liu, Z. Kang, L.-S. Liao. J. Fan, Strongly Phosphorescent Platinum(II) Complexes Supported by Tetradentate Benzazole-Containing Ligands, *J. Mater. Chem. C.* **2015**, *3*, 8212–8218.

[13] G. Li, T. Fleetham, E. Turner, X.-C. Hang, J. Li, Highly Efficient and Stable Narrow-Band Phosphorescent Emitters for OLED Applications, *Adv. Optical Mater.* **2015**, *3*, 390–397.

[14] X.-Q. Zhang, Y.-M. Xie, Y. Zheng, F. Liang, B. Wang, J. Fan, L.-S. Liao, Highly Phosphorescent Platinum(II) Complexes Based on Rigid Unsymmetric Tetradentate Ligands, *Org. Electron.* **2016**, *32*, 120–125.

[15] Z.-Q. Zhu, K. Klimes, S. Holloway, J. Li, Efficient Cyclometalated Platinum(II) Complex with Superior Operational Stability, *Adv. Mater.* **2017**, *29*, 1605002.

[16] G. Liu, Y.-M. Xie, F. Liang, Y. Zhao, H. Hu, J. Fan, L.-S. Liao, Phosphorescent Platinum(II) Complexes Based on Spiro Linkage-Containing Ligands, *J. Mater. Chem. C.* **2017**, *5*, 1944–1951.

[17] J. Li, F. Liang, Y. Zhao, X.-Y. Liu, J. Fan, L.-S. Liao, Highly Phosphorescent Cyclometalated Platinum(II) Complexes Based on 2-Phenylbenzimidazole-Containing Ligands, *J. Mater. Chem. C.* **2017**, *5*, 6202–6209.

[18] H. Fukagawa, T. Oono, Y. Iwasaki, T. Hatakeyama, T. Shimizu, High-Efficiency Ultrapure Green Organic Light-Emitting Diodes, *Mater. Chem. Front.* **2018**, *2*, 704−709.

[19] D. Zhao, C.-C. Huang, X.-Y. Liu, B. Song, L. Ding, M.-K. Fung, J. Fan, Efficient OLEDs with Saturated Yellow and Red Emission Based on Rigid Tetradentate Pt(II) Complexes, *Org. Electron.* **2018**, *62*, 542−547.

[20] G. Cheng, Y. Kwak, W.-P. To, T.-L. Lam, G. S. M. Tong, M.-K. Sit, S. Gong, B. Choi, W. Choi, C. Yang, C.-M. Che, High-Efficiency Solution-Processed Organic Light-Emitting Diodes with Tetradentate Platinum(II) Emitters, *ACS Appl. Mater. Interfaces* **2019**, *11*, 45161–45170.

[21] G. Li, G. Shen, X. Fang, Y.-F. Yang, F. Zhan, J. Zheng, W. Lou, Q. Zhang, Y. She, Phosphorescent Tetradentate Platinum(II) Complexes Containing Fused 6/5/5 or 6/5/6 Metallocycles, *Inorg. Chem.* **2020**, *59*, 18109–18121.

[22] G. Li, H. Guo, X. Fang, Y.-F. Yang, Y. Sun, W. Lou, Q. Zhang, Y. She, Tuning the Excited State of Tetradentate Pd(II) and Pt(II) Complexes Through Benzannulated *N*-Heteroaromatic Ring and Central Metal, *Chin. J. Chem.*, **2022**, *40*, 223–234.

[23] T. Fleetham, G. Li, L.Wen, J. Li, Efficient "Pure" Blue OLEDs Employing Tetradentate Pt Complexes with Narrow Spectral Bandwidth, *Adv. Mater.* **2014**, *26*, 7116–7121.

[24] G. Li, J. Zheng, X. Fang, K. Xu, Y.-F. Yang, J. Wu, J. Li, Y. She, *N*-Heterocyclic Carbene-Based Tetradentate Palladium(II) Complexes for Deep-Blue Phosphorescent Materials, *Organometallics* **2021**, *40*, 472–481.

[25] X. Zhao, Y. She, K. Fang, G. Li, CuCl-Catalyzed Ullmann-Type C-N Cross-Coupling Reaction of Carbazoles and 2-Bromopyridine Derivatives, *J. Org. Chem.* **2017**, *82*, 1024–1033.

[26] G. Li, X. Zhao, K. Fang, J. Li, Y. She, CuCl-Catalyzed Hydroxylation of *N*-Heteroarylcarbazole Bromide: Approach for the Preparation of *N*-Heteroarylcarbazolyl Phenols and Its Application in the Synthesis of Phosphorescent Emitters, *J. Org. Chem.* **2017**, *82*, 8634–8644.