Supporting Information

Phosphorescent Tetradentate Platinum(II) Complexes Containing Fused 6/5/5 or 6/5/6 Metallocycles

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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 mass spectrometer using electrospray ionization in positive ion mode on ESI-QTOF mass spectrometer from Applied Biosystems.

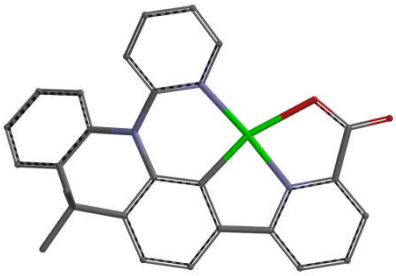
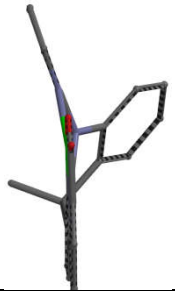
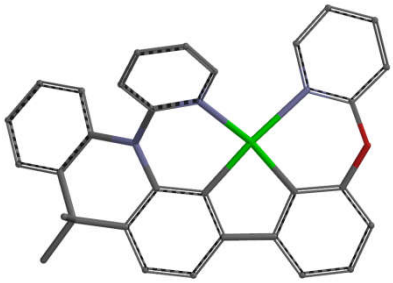
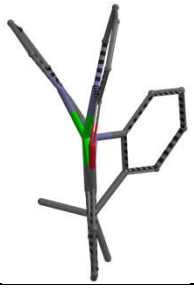
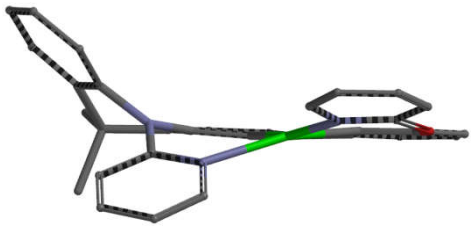
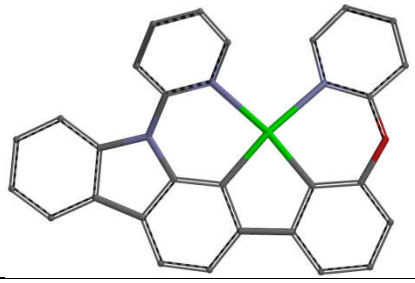
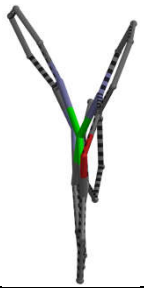
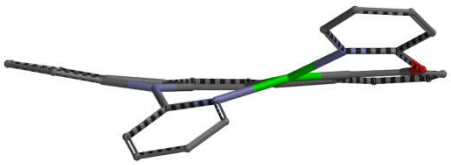
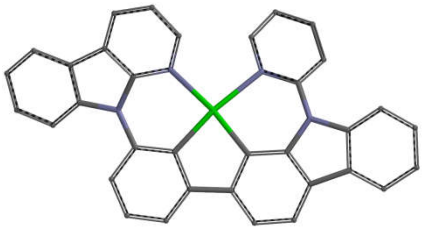
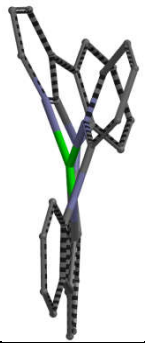
Electrochemistry. Cyclic voltammetry and different pulsed voltammetry were performed using a CH1760E electrochemical analyzeraccording previous report.[1] 0.1 M tetra-*n*-butylammonium hexafluorophosphate was used as the supporting electrolyte, anhydrous *N*,*N*-dimethylformamide, was used as the solvents 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] The energies of the singlet and triplet excited states of the complexes were calculated using TD-B3LYP method with a basis set of SV for H, SVP for C, O and N atoms, and a def2-TZVP basis set for Pt atom base on the optimized S_0 geometry.[4]

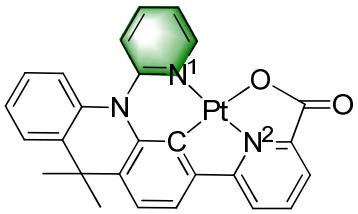
Photophysical Measurements. The absorption spectra were measured on an Agilent 8453 UV−VS Spectrometer. Steady state emission experiments and lifetime measurements were performed on a Horiba Jobin Yvon FluoroLog-3 spectrometer. Low temperature (77 K) emission spectra and lifetimes were measured in 2-MeTHF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

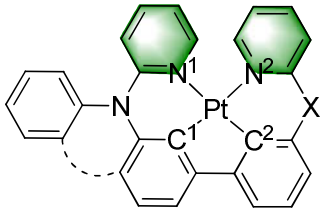
Table S1. DFT Calculations for Pt(II) Complexes[a]			
complexes	Front view	Side view	Top view
Pt(*ppy*-1)			
Pt(*bp*-6)			
Pt(*bp*-7)			
Pt(*bp*-8)			

[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 atom.

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



Pt(ppy-1)



Pt(II) complexes

Pt(*ppy*-1)	Pt-N^1	Pt-C	Pt-N^2	Pt-O
Pt(*ppy*-1)_S_0	2.047	1.952	1.973	2.186
Pt(*ppy*-1)_T_1	2.055	1.921	1.948	2.132
complexes	Pt-N^1	Pt-C^1	Pt-C^2	Pt-N^2
Pt(*bp*-6)_X-ray	2.115(2)	1.981(3)	1.968(3)	2.121(3)
Pt(*bp*-6)_S_0	2.187	1.984	1.980	2.195
Pt(*bp*-6)_T_1	2.176	1.956	1.954	2.166
Pt(*bp*-7)_X-ray	2.1460(19)	1.953(2)	2.126(2)	1.973(2)
Pt(*bp*-7)_S_0	2.232	1.970	1.981	2.196
Pt(*bp*-7)_T_1	2.209	1.942	1.961	2.195
Pt(*bp*-8)_S_0	2.237	1.970	1.993	2.184
Pt(*bp*-8)_T_1	2.214	1.942	1.972	2.174

Pt(*ppy*-1)	N^1-Pt-C	C-Pt-N^2	N^2-Pt-O	O-Pt-N^1	N^1-Pt-N^2	C-Pt-O	dihedral angle[a]
Pt(*ppy*-1)_S_0	93.14	82.43	79.33	104.99	173.27	161.75	16.6
Pt(*ppy*-1)_T_1	93.12	83.65	79.84	103.36	174.76	163.49	16.5
complexes	N^1-Pt-C^1	C^1-Pt-C^2	C^2-Pt-N^2	N^2-Pt-N^1	N^1-Pt-C^2	C^1-Pt-N^2	dihedral angle[a]
Pt(*bp*-6)_X-ray	90.24(10)	82.17(12)	89.65(12)	99.86(9)	164.93(10)	167.23(10)	55.2
Pt(*bp*-6)_S_0	89.04	82.25	89.69	100.63	164.85	168.12	48.9
Pt(*bp*-6)_T_1	89.22	82.93	89.61	99.80	165.86	168.50	46.9
Pt(*bp*-7)_X-ray	88.56(9)	81.43(10)	89.96(9)	101.46(7)	165.37(9)	167.62(9)	51.2
Pt(*bp*-7)_S_0	88.67	81.44	89.48	102.09	165.12	166.27	52.4
Pt(*bp*-7)_T_1	88.79	82.15	89.40	101.28	166.29	166.47	50.8
Pt(*bp*-8)_S_0	88.65	81.95	90.15	100.95	165.65	166.89	52.6
Pt(*bp*-8)_T_1	88.61	82.60	90.22	100.21	166.41	167.37	50.0

[a]Dihedral angle between terminal pyridine and carboxyl planes for Pt(*ppy*-1), between two terminal pyridine planes for Pt(*bp*-6) and Pt(*bp*-7), between terminal pyridine and aza carbazole planes for Pt(*bp*-8). 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 atom.

Table S3. Crystal data and structure refinement for Pt(*bp*-6) (CCDC 2036928).

Identification code	201013_BP_6_0m_sq
Empirical formula	$C_{31}H_{23}N_3OPt$
Formula weight	648.61
Temperature/K	170.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	15.274(6)
b/Å	11.865(3)
c/Å	16.488(5)
α/°	90
β/°	117.245(14)
γ/°	90
Volume/Å^3	2656.5(15)
Z	4
ρ_{calc}g/cm^3	1.622
μ/mm^{-1}	5.310
F(000)	1264.0
Crystal size/mm^3	0.35 × 0.16 × 0.03
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.416 to 58.182
Index ranges	$-18 \leq h \leq 20$, $-16 \leq k \leq 16$, $-22 \leq l \leq 22$
Reflections collected	35564
Independent reflections	7107 [R_{int} = 0.0397, R_{sigma} = 0.0336]
Data/restraints/parameters	7107/0/327
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0238, wR_2 = 0.0534
Final R indexes [all data]	R_1 = 0.0388, wR_2 = 0.0598
Largest diff. peak/hole / e Å^{-3}	0.64/-0.86

Table S4. Crystal data and structure refinement for Pt(*bp*-7) (CCDC 2036927).

Identification code	200930_0929_1_0m
Empirical formula	$C_{29}H_{19}Cl_2N_3OPt$
Formula weight	691.46
Temperature/K	170.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.0827(3)
b/Å	11.0133(4)
c/Å	25.8648(10)
α/°	90
β/°	98.4000(10)
γ/°	90
Volume/Å^3	2277.71(15)
Z	4
ρ_{calc}g/cm^3	2.016
μ/mm^{-1}	6.426
F(000)	1336.0
Crystal size/mm^3	0.26 × 0.16 × 0.09
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.88 to 61.034
Index ranges	$-7 \leq h \leq 11$, $-15 \leq k \leq 15$, $-36 \leq l \leq 36$
Reflections collected	26825
Independent reflections	6942 [R_{int} = 0.0374, R_{sigma} = 0.0331]
Data/restraints/parameters	6942/0/325
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0219, wR_2 = 0.0505
Final R indexes [all data]	R_1 = 0.0245, wR_2 = 0.0519
Largest diff. peak/hole / e Å^{-3}	0.76/-1.54

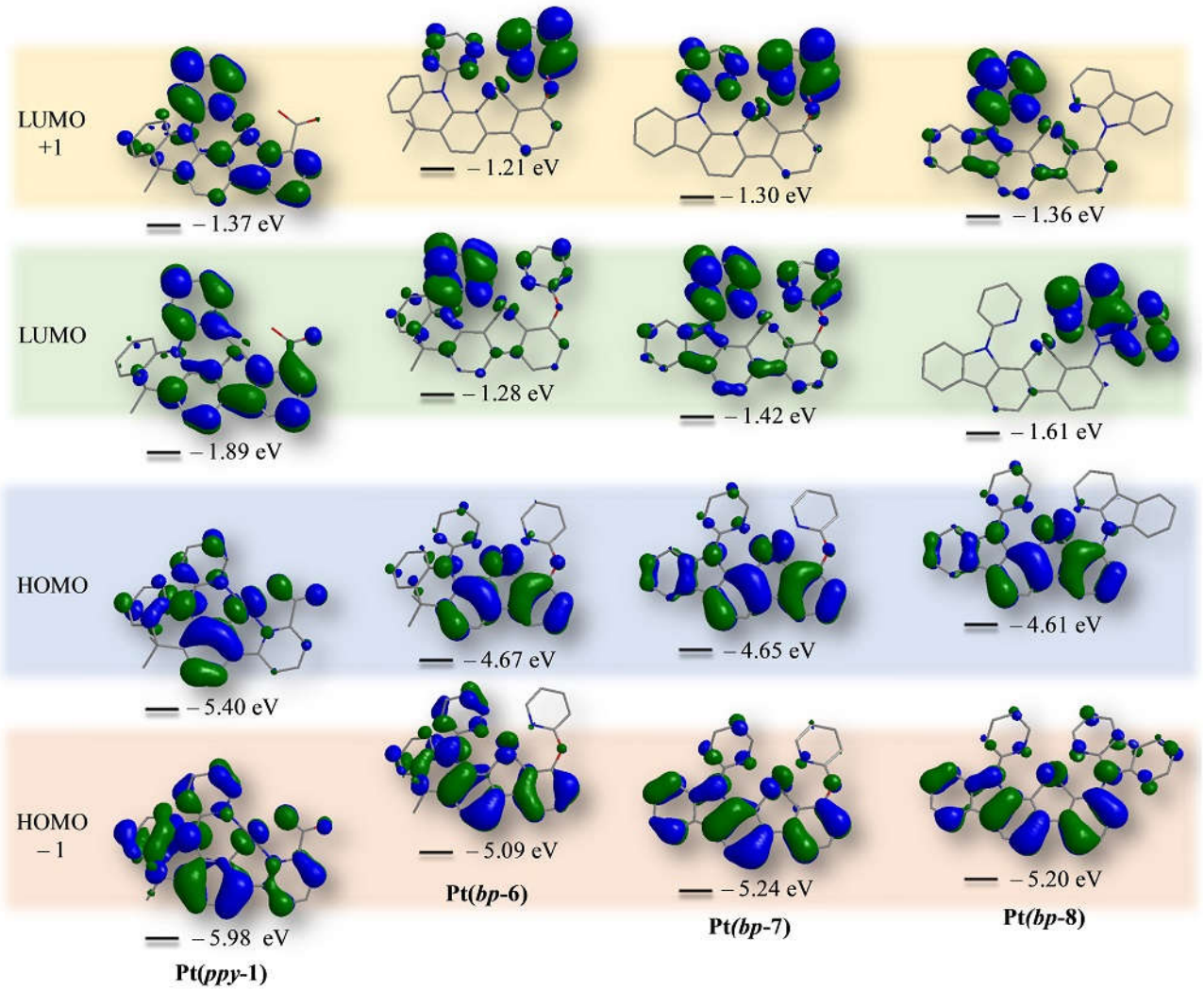


Figure S1. Density functional theory calculations of frontier orbitals and spin densities of T_1 states for Pt(II) complexes based on optimized S_0 and T_1 geometries. The H atoms were omitted for clarity.

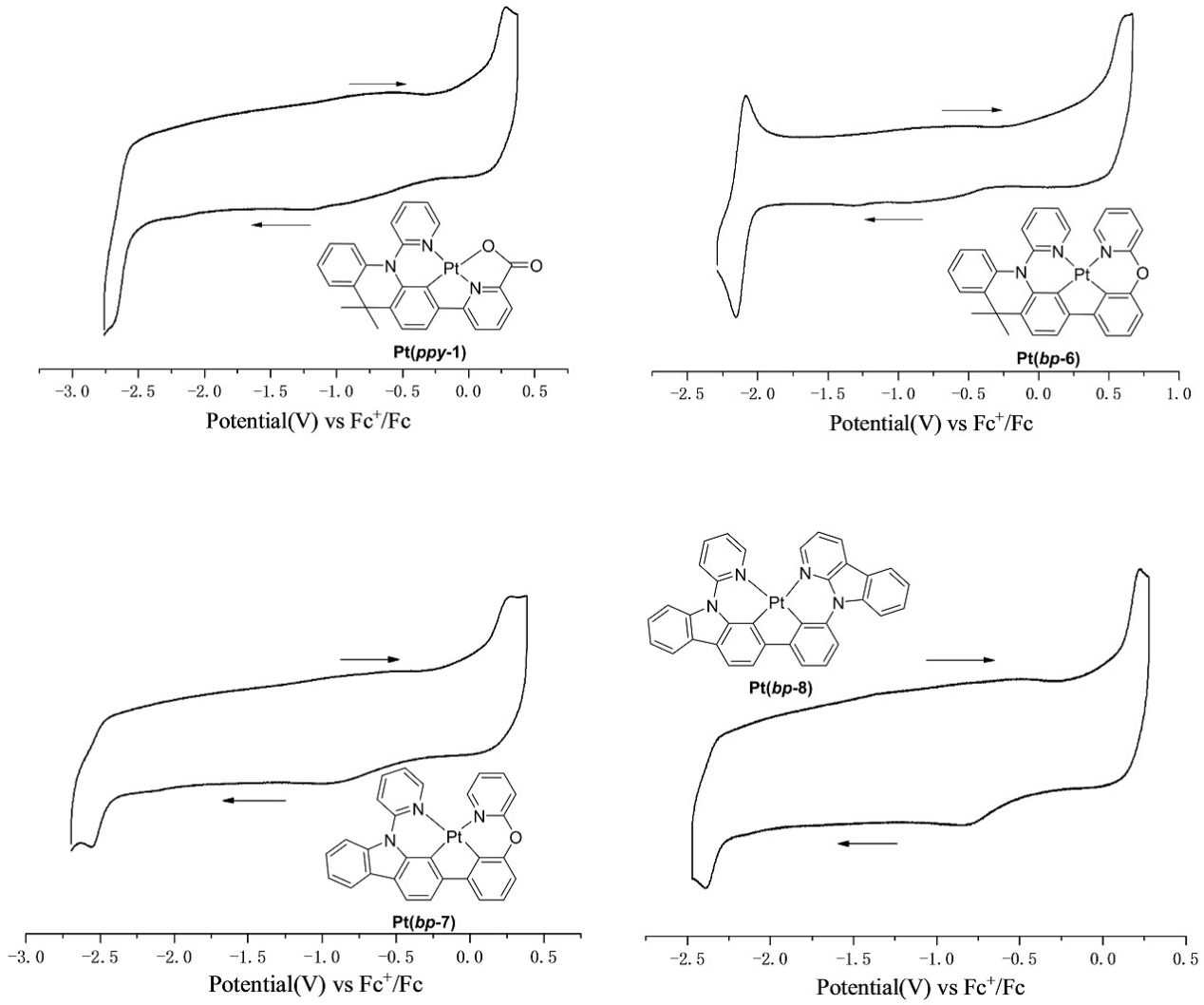


Figure S2. Cyclic voltammograms of Pt(II) complexes in *N*,*N*-dimethylformamide.

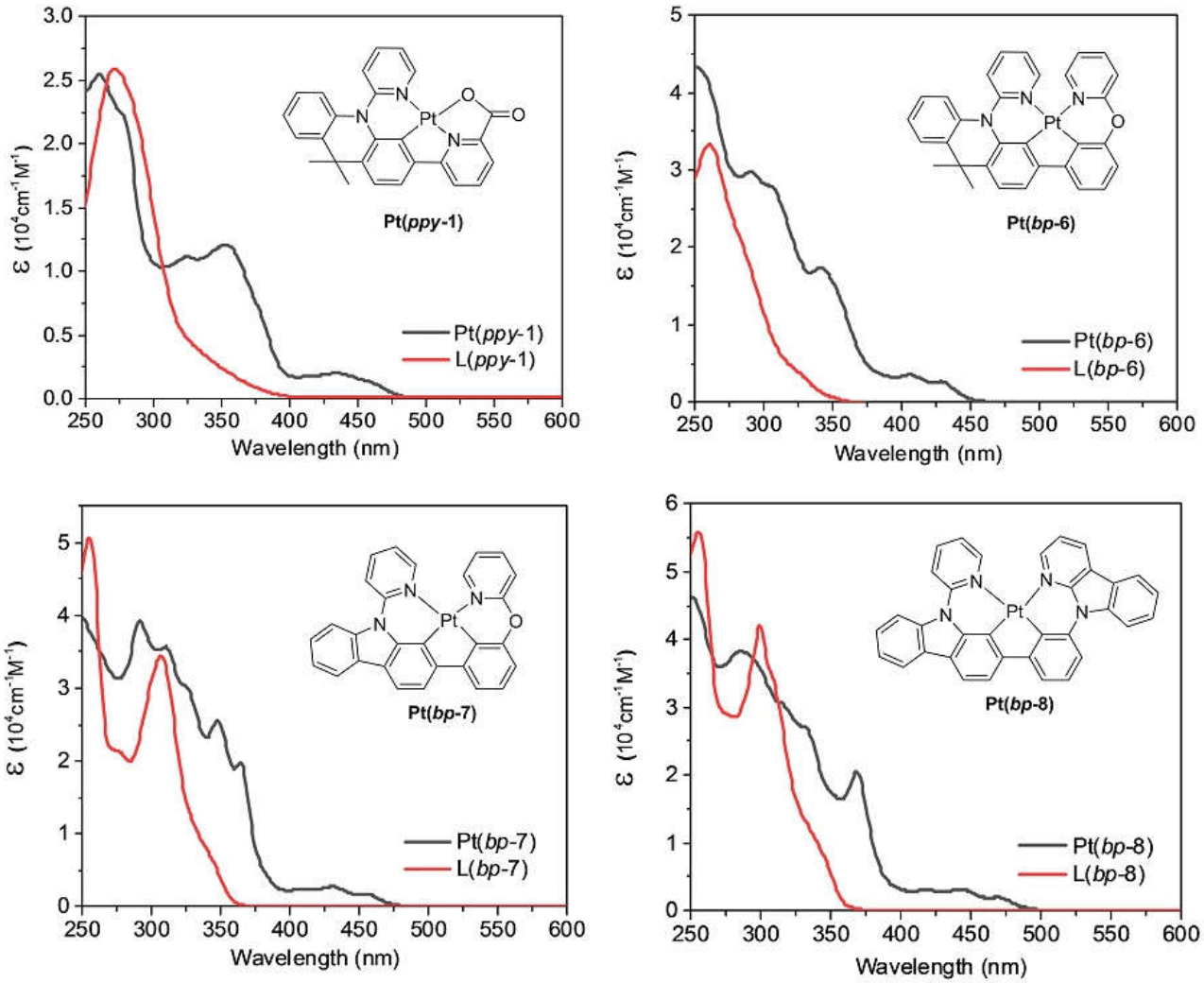


Figure S3. Absorption spectra of Pt(II) complexes and their ligands in dichloromethane solution.

Table S5. TD-B3LYP/SV/SVP/def2-TZVP results of **Pt(*ppy*-1)** at optimized S_0 geometry.

excited state	energy [eV]	wavelength [nm]	f	major contributions
T_1	2.472	502	0.0000	HOMO → LUMO (87%)
S_1	2.716	457	0.0196	HOMO → LUMO (96%)
T_2	2.759	449	0.0000	HOMO-1 → LUMO (39%) HOMO-1 → LUMO+2 (4%) HOMO → LUMO (8%) HOMO → LUMO+1 (25%)
S_2	3.222	385	0.0158	HOMO → LUMO+1 (88%) HOMO → LUMO+2 (7%)

Table S6. TD-B3LYP/SV/SVP/def2-TZVP results of **Pt(*bp*-6)** at optimized S_0 geometry.

excited state	energy [eV]	wavelength [nm]	f	major contributions
T_1	2.472	502	0.0000	HOMO → LUMO (80%) HOMO → LUMO+4 (6%)
T_2	2.587	479	0.0000	HOMO-1 → LUMO (11%) HOMO → LUMO (4%) HOMO → LUMO+1 (70%) HOMO → LUMO+4 (5%)
S_1	2.669	465	0.0212	HOMO → LUMO (97%)
S_2	2.764	449	0.0075	HOMO → LUMO+1 (96%)

Table S7. TD-B3LYP/SV/SVP/def2-TZVP results of **Pt(*bp*-7)** at optimized S_0 geometry.

excited state	energy [eV]	wavelength [nm]	f	major contributions
T_1	2.249	551	0.0000	HOMO → LUMO (72%) HOMO → LUMO+2 (7%) HOMO → LUMO+3 (9%)
T_2	2.519	492	0.0000	HOMO-1 → LUMO (6%) HOMO → LUMO (8%) HOMO → LUMO+1 (73%) HOMO → LUMO+3 (5%)
S_1	2.519	492	0.0073	HOMO → LUMO (97%)
S_2	2.687	461	0.0081	HOMO → LUMO+1 (96%)

Table S8. TD-B3LYP/SV/SVP/def2-TZVP results of **Pt(*bp*-8)** at optimized S_0 geometry.

excited state	energy [eV]	wavelength [nm]	f	major contributions
T_1	2.196	565	0.0000	HOMO → LUMO (57%) HOMO → LUMO+1 (21%) HOMO → LUMO+2 (8%) HOMO → LUMO+3 (5%)
T_2	2.344	529	0.0000	HOMO → LUMO (32%) HOMO → LUMO+1 (55%)
S_1	2.407	515	0.0338	HOMO → LUMO (94%)
S_2	2.533	490	0.0002	HOMO → LUMO+1 (95%)

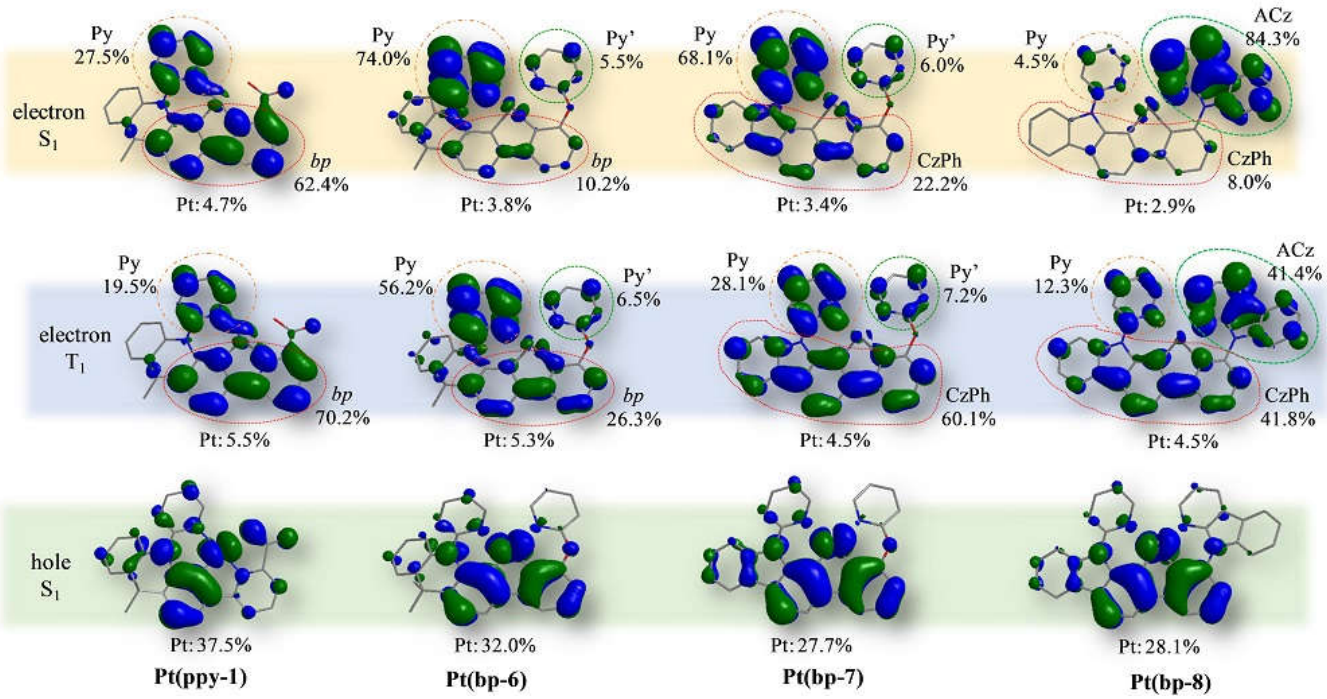


Figure S4. Natural transition orbitals (NTOs) of the S_1 and T_1 states for Pt(II) complexes based on optimized S_0 geometry. All the H atoms are omitted for clarity.

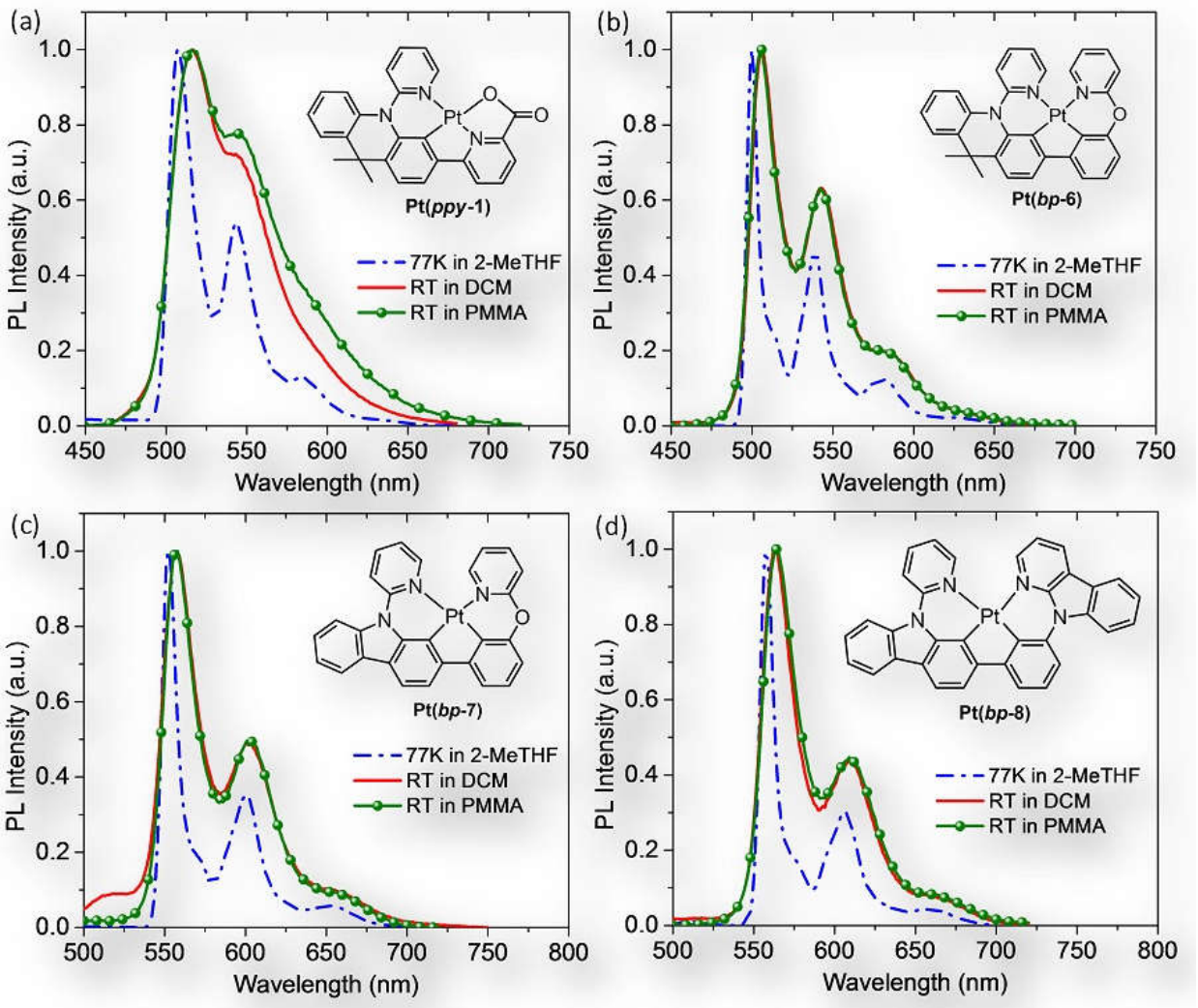


Figure S5. Luminescence spectra of (a) Pt(*ppy*-1), (b) Pt(*bp*-6), (c) Pt(*bp*-7), and (d) Pt(*bp*-8) at 77K in 2-MeTHF (dash-dotted lines), at RT in DCM solution (solid lines) and at RT in PMMA film (solid-ball lines). The chemical structure of each Pt(II) complex is shown in the inset.

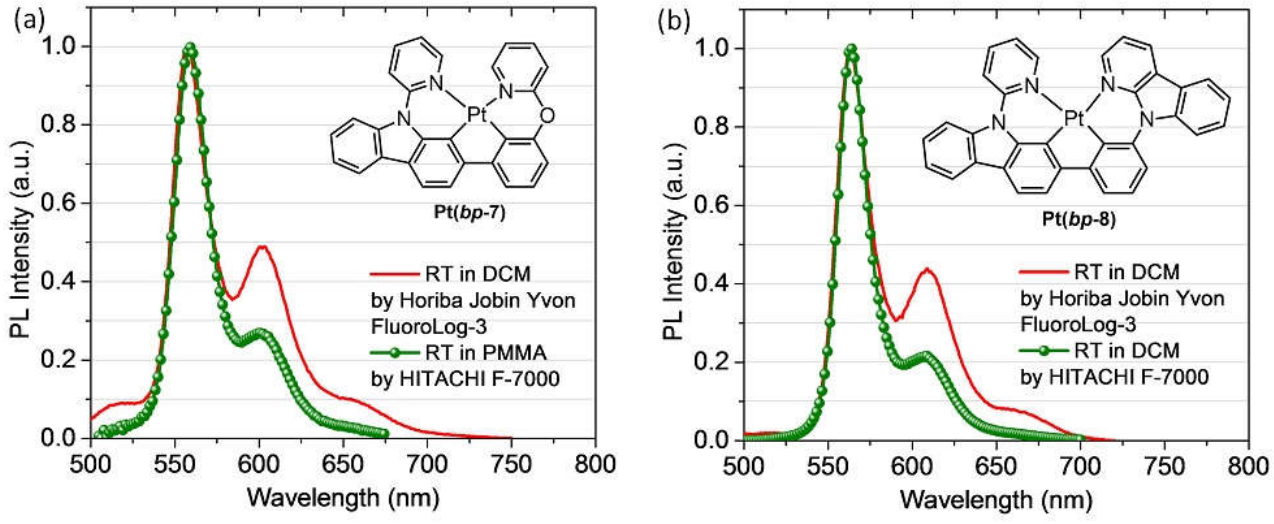
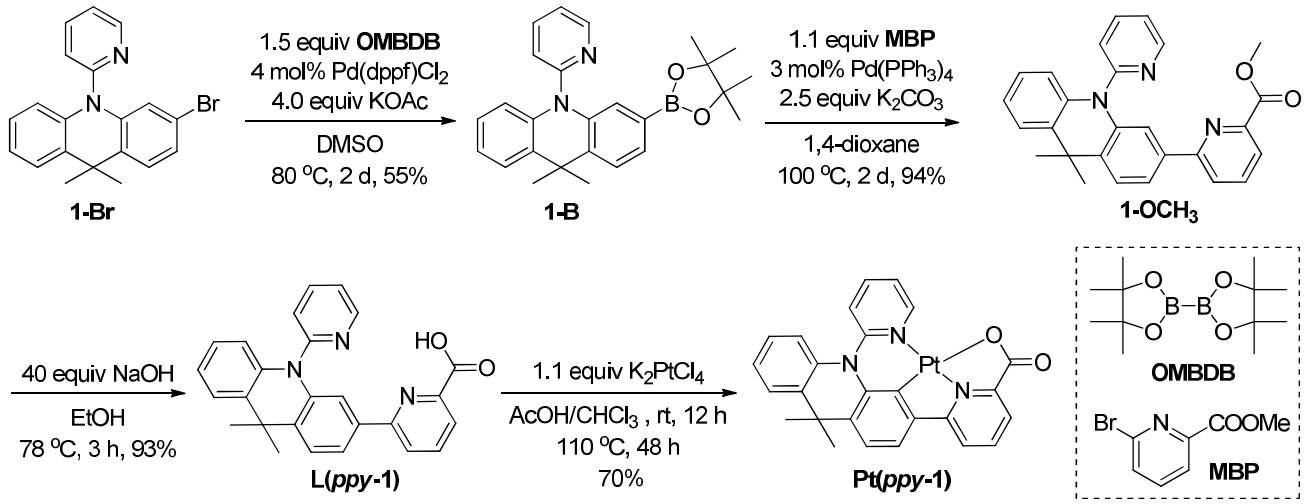


Figure S6. Luminescence spectra comparison measured by different spectrometers.

Experimental Procedures

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



Synthesis of **1-B**: 3-Bromo-9,9-dimethyl-10-(pyridin-2-yl)-9,10-dihydroacridine **1-Br**[5] (1.50 g, 4.11 mmol, 1.0 equiv), **OMBDB** (1.56 g, 6.15 mmol, 1.5 equiv), $Pd(dppf)Cl_2$ (121 mg , 0.16 mmol, 4 mol%), KOAc (1.61 g, 16.50 mmol, 4.0 equiv) were added sequentially to a dry three-necked flask equipped with a magnetic stir bar. The flask was evacuated and backfilled with nitrogen, this evacuation and backfill procedure was repeated twice. Then DMSO (25 mL) were added under nitrogen atmosphere, and then the flask was placed in an oil bath and heated at 80 °C with stirring. The reaction was monitored by TLC until the reaction was completed. After 2 days, the resulting mixture was cooled down to room temperature, filtered and washed with ethyl acetate. The organic layer was washed with water, and then dried over Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The residue was purified through column chromatography on silica gel using petroleum ether/ethyl acetate = 10:1–5:1 as eluent to afford the desired product as a white solid 896 mg in 55% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.28 (s, 12H), 1.62 (s, 6H), 7.01−7.05 (m, 2H), 7.10 (td, *J* = 8.0, 1.5 Hz, 1H), 7.17 (ddd, *J* = 7.0, 4.5, 0.5 Hz, 1H), 7.28 (d, *J* = 8.5 Hz, 1H), 7.39 (s, 1H), 7.43 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.46 (d, *J* =8.0 Hz, 1H), 7.50 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.76 (td, *J* = 8.0, 2.0 Hz, 1H), 8.62 (dd, *J* = 5.0, 1.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) : δ 24.76, 29.07, 36.97, 83.57, 118.93, 119.11, 120.07, 122.56, 123.90, 124.29, 124.74, 126.08, 129.26, 135.32, 138.75, 138.80, 139.94, 140.43, 149.68, 155.58. HRMS (ESI): calcd for $C_{26}H_{30}N_2O_2B$ $[M+H]^+$ 413.2395, found 413.2415.

Synthesis of **1-OCH$_3$**: **1-B** (0.68 g, 1.65 mmol, 1.0 equiv), 6-bromopyridine-2-carboxylic acid

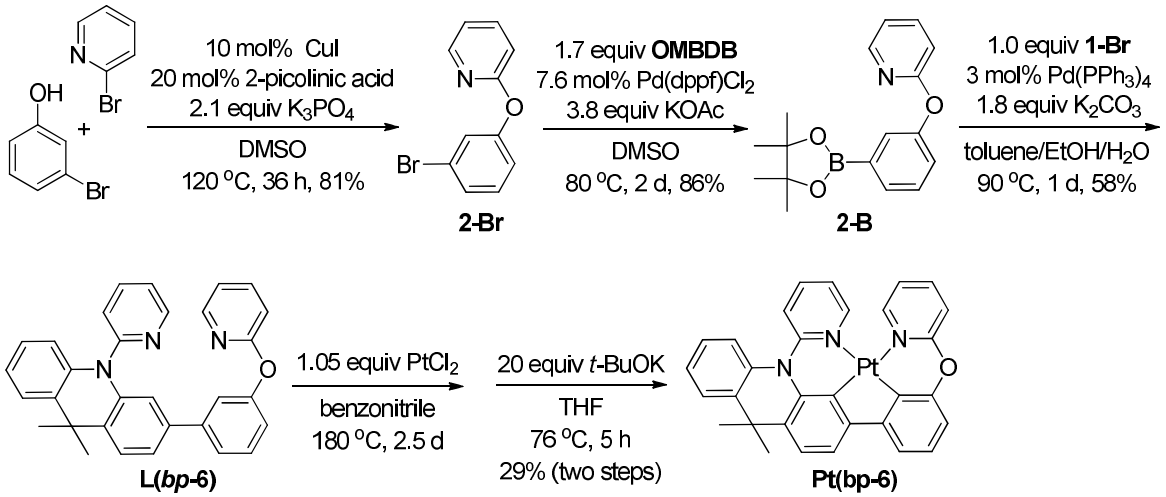
methyl ester (0.39 g, 1.81 mmol, 1.1 equiv), $Pd(PPh_3)_4$ (57 mg , 0.05 mmol, 3 mol%), K_2CO_3 (0.57 g, 4.12 mmol, 2.5 equiv) were added sequentially to a dry three-necked flask equipped with a magnetic stir bar. The flask was evacuated and backfilled with nitrogen, this evacuation and backfill procedure was repeated twice. Then 1,4-dioxane (30 mL) were added under nitrogen atmosphere, and then the flask was placed in an oil bath and heated at 100 ^oC with stirring. The reaction was monitored by TLC until the reaction was completed. After 2 days, the resulting mixture was cooled down to room temperature, filtered and washed with ethyl acetate. The filtrate was concentrated under reduced pressure and the residue was purified through column chromatography on silica gel using petroleum ether/ethyl acetate = 10:1−3:1 as eluent to afford the desired product as a yellow oily solid 640 mg in 92% yield. ^1H NMR (500 MHz, DMSO-d_6): δ 1.69 (s, 6H), 4.00 (S, 3H), 6.82 (dd, J = 8.0, 1.0, 1H), 7.05 (td, J = 7.5, 1.5 Hz, 1H), 7.12 (m, 1H), 7.28−7.31(m, 1H), 7.38 (dt, J = 8.0, 1.0, 1H), 7.48−7.50 (m, 2H), 7.58 (d, J = 8.5 Hz, 1H), 7.31−7.31(m, 2H), 7.83 (t, J = 2.5 Hz, 1H), 7.87−7.88 (m,1H), 8.00 (dd, J = 7.5, 1.0 Hz, 1H), 8.72−8.74 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) : δ 29.80, 36.60, 52.61, 116.14, 117.59, 121.12, 121.15, 122.33, 123.02, 123.52, 124.67, 125.27, 126.26, 133.84, 135.44, 136.67, 137.44, 139.13, 140.28, 140.71, 147.77, 150.11, 155.48, 157.60, 165.97. HRMS (ESI): calcd for $C_{27}H_{24}N_3O_2$ $[M+H]^+$ 422.1877, found 422.1873.

Synthesis of **L(*ppy*-1)**: **1-OCH$_3$** (0.64 g, 1.55 mmol, 1.0 equiv) and NaOH (2.48g, 62.00 mmol, 40 equiv) were added sequentially to a dry three-necked flask equipped with a magnetic stir bar. Then EtOH (30 mL) was added and the flask was placed in an oil bath and heated at 78 ^oC with stirring. The reaction was monitored by TLC until the reaction was completed. After 3 hours, the resulting mixture was cooled down to room temperature, filtered and add hydrochloric acid to adjust pH to 6, washed with CH_2Cl_2. The organic layer was separated and dried over Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The residue was purified through column chromatography on silica gel using petroleum ether/ethyl acetate = 3:1 and then ethyl acetate/CH_3OH = 10:1 as eluent to afford the desired product as a maroon solid 587 mg in 93% yield. ^1H NMR (500 MHz, DMSO-d_6): δ 1.63 (s, 6H), 6.64 (dd, J = 8.0, 1.5 Hz, 1H), 7.03 (td, J = 7.5, 1.5 Hz, 1H), 7.09 (td, J = 8.0, 2.0 Hz, 1H), 7.40 (d, J = 2.0 Hz, 1H), 7.43−7.46 (m, 2H), 7.53 (dd, J = 7.5, 1.5 Hz, 1H), 7.65 (d, J = 8.5 Hz, 1H), 7.77 (dd, J = 8.5, 2.0 Hz, 1H), 7.90−7.93 (m, 2H), 7.99 (t, J = 7.5 Hz, 1H), 8.03 (td, J = 7.5, 2.0 Hz, 1H), 8.67−8.69 (m, 1H), 12.73 (br, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 30.18, 36.81, 115.71, 117.18, 120.52, 121.72, 121.96, 121.99, 122.64, 124.69, 125.05,

125.69, 126.67, 133.35, 135.15, 135.90, 139.29, 139.58, 140.28, 141.18, 145.79, 150.55, 155.45, 156.39, 164.23. HRMS (ESI): calcd for $C_{26}H_{21}N_3O_2Na$ $[M+Na]^+$ 430.1526, found 430.1520.

Synthesis of **Pt(*ppy*-1)**: A mixture of **L(*ppy*-1)** (300 mg, 0.74 mmol, 1.00 equiv) and K_2PtCl_4 (336 mg, 0.81 mmol, 1.10 equiv) were added sequentially to a dry three-necked flask equipped with a magnetic stir bar. The flask was evacuated and backfilled with nitrogen, this evacuation and backfill procedure was repeated twice. Then AcOH (40 mL) and $CHCl_3$ (4mL) were added into the flask under nitrogen atmosphere. The reaction mixture was bubbled with nitrogen for 15 minutes and then stirred at room temperature for 12 h. Then the flask was placed in an oil bath and heated at 110 ^oC with stirring. After 48 hours, the resulting mixture was cooled down to room temperature and concentrated in vacuum and the residue was diluted with dichloromethane. The mixture was washed with water, the organic layer was separated and dried over Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The residue was purified through column chromatography on silica gel using petroleum ether/dichloromethane= 2:1, and then dichloromethane/ethyl acetate/CH_3OH =1:1:0.1 as eluent to afford the desired product as a yellow solid 309 mg in 70% yield. m.p.: >320 ^oC. ^1H NMR (500 MHz, DMSO-d_6): δ 1.34 (s, 3H), 1.88 (s, 3H), 7.20−7.24 (m, 2H), 7.25−7.28 (m, 3H), 7.57 (dd, J = 7.5, 1.5 Hz, 1H), 7.60−7.63 (m, 2H), 7.66 (dd, J = 7.0, 1.5 Hz, 1H), 8.03−8.07 (m, 1H), 8.08−8.13 (m, 2H), 8.85 (dd, J = 6.0, 1.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 22.96, 31.32, 37.26, 118.29, 118.94, 119.87, 120.92, 121.29, 121.34, 122.37, 122.79, 124.31, 125.51, 126.73, 135.59, 137.12, 138.36, 139.32, 139.53, 141.41, 142.46, 150.93, 151.24, 151.79, 162.62, 172.86. HRMS (ESI): calcd for $C_{26}H_{19}N_3O_2Na^{195}Pt$ $[M+Na]^+$ 623.1017, found 623.1008. Anal. for $C_{26}H_{19}N_3O_2Pt$, Calcd.: C, 52.00, H, 3.19, N, 7.00; Found: C, 51.65, H, 3.20, N, 6.95.

Synthesis of **Pt(*bp*-6)**:



Synthesis of **2-Br**: CuI (440 mg, 2.31 mmol, 10 mol%), 2-picolinic acid (568 mg, 4.62 mmol, 20 mol%) and K_3PO_4 (10.31 g, 48.55 mmol, 2.1 equiv) were added sequentially to a dry three-necked flask equipped with a magnetic stir bar. The flask was evacuated and backfilled with nitrogen, this evacuate ion and backfill procedure was repeated twice. Then *m*-bromophenol (4.00 g, 23.12 mmol, 1.00 equiv), 2-bromopyridine (5.48 g, 34.68 mmol, 1.50 equiv) and DMSO (30 mL) were added under nitrogen atmosphere, and then the flask was placed in an oil bath and heated at 120 ^oC with stirring. The reaction was monitored by TLC until the reaction was completed. After 36 hours, the resulting mixture was cooled down to room temperature, filtered and washed with ethyl acetate. The organic layer was washed with water, and then dried over Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The residue was purified through column chromatography on silica gel using petroleum ether/dichloromethane = 40:1−20:1 as eluent to afford the desired product as a white solid 4.67 g in 81% yield. ^1H NMR (500 MHz, $CDCl_3$): δ 7.08 (d, *J*= 8.5 Hz, 1H), 7.14−7.18 (m, 2H), 7.36−7.43 (m, 3H), 7.86−7.90 (m, 1H), 7.08 (ddd, *J*= 4.5, 2.0, 0.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) : δ 111.81, 118.96, 119.85, 122.58, 124.45, 127.66, 130.62, 139.61, 147.67, 154.84, 163.06. HRMS (ESI): calcd for $C_{11}H_9NOBr$ $[M+H]^+$ 249.9862, found 249.9862.

Synthesis of **2-B**: 2-(3-Bromophenoxy)pyridine **2-Br** (4.00 g, 16.00 mmol, 1.00 equiv), **OMBDB** (6.92 g, 27.25 mmol, 1.70 equiv), $Pd(dppf)Cl_2$ (886 mg , 1.21 mmol, 7.6 mol%), KOAc (5.94 g, 60.53 mmol, 3.8 equiv) were added sequentially to a dry three-necked flask equipped with a magnetic stir bar. The flask was evacuated and backfilled with nitrogen, this evacuation and backfill

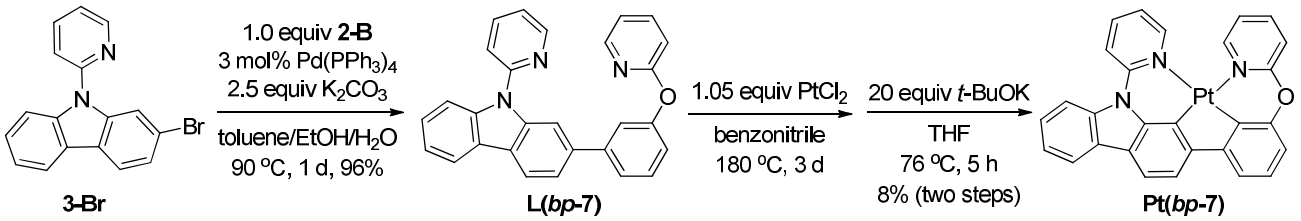
procedure was repeated twice. Then DMSO (45 mL) was added under nitrogen atmosphere, and then the flask was placed in an oil bath and heated at 80 ^{o}C with stirring. The reaction was monitored by TLC until the reaction was completed. After 2 days, the resulting mixture was cooled down to room temperature, filtered and washed with ethyl acetate. The organic layer was washed with water, and then dried over Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The residue was purified through column chromatography on silica gel using petroleum ether/ethyl acetate = 20:1−14:1 as eluent to afford the desired product as a white solid 4.07 g in 86% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.33 (s, 12 H), 6.87−6.89 (m, 1H), 6.95−6.99 (m, 1H), 7.24 (ddd, *J* = 4.0, 3.0, 1.5 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.56 (dd, *J* = 2.5, 1.0 Hz, 1H), 7.64−7.66 (m, 1H), 7.67−7.68 (m, 1H), 8.19 (ddd, *J* = 3.0, 2.0, 1.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) : δ 24.82, 83.88, 111.36, 118.22, 124.35, 127.16, 129.15, 131.15, 139.33, 147.67, 153.62, 163.88. HRMS (ESI): calcd for $C_{17}H_{21}NO_3B$ $[M+H]^+$ 298.1609, found 298.1623.

Synthesis of **L(*bp*-6)**: 3-Bromo-9,9-dimethyl-10-(pyridin-2-yl)-9,10-dihydroa cridine **1-Br** (1.30 g, 3.57 mmol, 1.00 equiv), 2-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2yl)phenoxy) pyridine **2-B** (1.16 g, 3.93 mmol, 1.10 equiv), $Pd(PPh_3)_4$ (124 mg , 0.11 mmol, 3 mol%), K_2CO_3 (888 mg, 6.43 mmol, 1.8 equiv) were added sequentially to a dry three-necked flask equipped with a magnetic stir bar. Then toluene (25 mL), EtOH (5 mL) and H_2O (5 mL) were added, and then the flask was placed in an oil bath and heated at 90 ^{o}C with stirring. The reaction was monitored by TLC until the reaction was completed. After 1 day, the resulting mixture was cooled down to room temperature, filtered and washed with ethyl acetate. The organic layer was separated and washed with water, then dried over Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The residue was purified through column chromatography on silica gel using petroleum ether/ethyl acetate = 10:1−5:1 as eluent to afford the desired product as a white solid 950 mg in 58% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.68 (s, 6H), 6.78 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.89 (dt, *J* = 8.5, 1.5 Hz, 1H), 6.97−6.98 (m, 1H), 6.99−7.01 (m, 1H), 7.00−7.09 (m, 3H), 7.20−7.25 (m, 3H), 7.27 (dt, *J* = 6.5, 1.0 Hz, 1H), 7.33 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.47 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.48 (d, *J* = 9.5 Hz, 1H), 7.66−7.69 (m, 1H), 7.82 (td, *J* = 8.0, 2.0 Hz, 1H), 8.18−8.20 (m, 1H), 8.68 (dd, *J*= 9.5, 1.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 29.49, 35.86, 110.96, 115.53, 116.79, 117.90, 118.99, 119.16, 120.46, 120.69, 120.72, 121.64, 122.80, 124.16, 124.62, 125.66, 129.13, 132.75, 133.19,

138.05, 138.60, 138.80, 139.71, 140.06, 142.45, 147.24, 149.69, 153.86, 154.85, 163.11. HRMS (ESI): calcd for $C_{31}H_{26}N_3O$ $[M+H]^+$ 456.2070, found 456.2068.

Synthesis of **Pt(*bp*-6)**: A mixture of **L(*bp*-6)** (250 mg, 0.55 mmol, 1.00 equiv) and $PtCl_2$ (153 mg, 0.58 mmol, 1.05 equiv) were added sequentially to a dry three-necked flask equipped with a magnetic stir bar. The flask was evacuated and backfilled with nitrogen, this evacuation and backfill procedure was repeated twice. Then benzonitrile (30 mL) was added into the flask, and the flask was placed in an oil bath and heated at 180 ^oC with stirring. After 2.5 days, the mixture was cooled to room temperature. THF (12 mL) and *t*-BuOK (1.23 g, 10.98 mmol, 20.00 equiv) were added to the mixture under nitrogen atmosphere and stirred in an oil bath held at 76 °C for 5 h. The resulting mixture was cooled down to room temperature and concentrated in vacuum. The residue was diluted with dichloromethane, and washed with water. The organic layer was separated, and the aqueous phase was extracted with dichloromethane twice. The combined organic layer was dried over anhydrous Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The crude solid was purified through column chromatography on silica gel using petroleum ether/dichloromethane = 3:1−1:1 as eluent to afford the desired product as a yellow solid 104 mg in 29% yield. m.p.: 314.5–315.5 ^oC. ^1H NMR (500 MHz, DMSO-d_6): δ 1.27 (s, 3H), 1.84 (s, 3H), 6.75 (dd, *J* = 8.0, 1.0 Hz, 1H), 6.91−6.98 (m, 2H), 7.10−7.14 (m, 2H), 7.19 (td, *J* = 8.5, 1.5 Hz, 1H), 7.21−7.24 (m, 2H), 7.28 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.33−7.35 (m, 1H), 7.44 (d, *J* = 8.5 Hz, 1H), 7.48 (dt, *J* = 8.5,1.0 Hz, 1H), 7.53 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.93−7.98 (m, 1H), 8.16−8.21 (m, 1H), 8.60 (dd, *J*= 6.0, 2.0 Hz, 1H), 8.66 (dd, *J*= 6.0, 2.0 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 22.72, 32.33, 36.29, 113.26, 116.06, 116.18, 118.12, 119.75, 119.88, 120.53, 120.90, 123.80, 124.26, 122.80, 124.54, 126.48, 128.43, 132.33, 135.28, 137.09, 138.21, 139.27, 140.19, 141.48, 148.89, 150.39, 151.74, 154.07, 156.96, 157.51. HRMS (ESI): calcd for $C_{31}H_{23}N_3ONa^{195}Pt$ $[M+Na]^+$ 671.1381, found 671.1384. Anal. for $C_{31}H_{23}N_3OPt•0.5H_2O$, Calcd.: C, 56.62, H, 3.68, N, 6.39; Found: C, 56.65, H, 3.70, N, 6.26.

Synthesis of **Pt(*bp*-7)**:

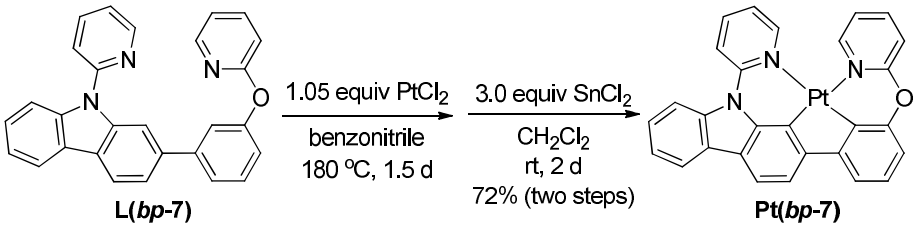


Synthesis of **L(*bp*-7)**: 2-(3-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2yl)phenoxy)pyridine **2-B** (1.00 g, 3.4 mmol, 1.0 equiv), 2-bromo-9-(pyridin-2-yl)-9*H*-carbazole **3-Br**[6] (1.20 g, 3.7 mmol, 1.1 equiv), $Pd(PPh_3)_4$ (116 mg , 0.10 mmol, 3 mol%), K_2CO_3 (1.16 g, 8.4 mmol, 2.5 equiv) were added sequentially to a dry three-necked flask equipped with a magnetic stir bar. The flask was evacuated and backfilled with nitrogen, this evacuation and backfill procedure was repeated twice. Then toluene (20 mL), EtOH(4 mL) and H_2O (4 mL) were added, and then the flask was placed in an oil bath and heated at 90 ^oC with stirring. The reaction was monitored by TLC until the reaction was completed. After 24 hours, the resulting mixture was cooled down to room temperature, filtered and washed with ethyl acetate. The organic layer was washed with water, and then dried over Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The residue was purified through column chromatography on silica gel using petroleum ether/ethyl acetate = 10:1−5:1 as eluent to afford the desired product as a white solid 1.32 g in 96% yield. ^1H NMR (500 MHz, $CDCl_3$): δ 6.94 (dd, *J* = 8.5 Hz, 1H), 7.00 (ddd, *J* = 6.0, 5.0, 1.0 Hz, 1H), 7.10−7.13 (m, 1H), 7.30−7.34 (m, 2H), 7.42−7.45 (m, 2H), 7.47 (d, *J* = 8.0, 1.0 Hz, 1H), 7.51 (dt, *J* = 7.5, 1.0 Hz, 1H), 7.55 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.64−7.66 (m, 1H), 7.67−7.70 (m, 1H), 7.82 (dd, *J*= 7.5, 1.0 Hz, 1H), 7.94 (td, *J*= 8.0 Hz, 1H), 8.02 (m, 1H), 8.12 (d, *J* = 7.5, 1.0 Hz, 1H),8.15 (d, *J* = 8.0 Hz, 1H), 8.20−8.23 (m, 1H), 8.72−8.75 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 109.95, 111.26, 111.66, 118.65, 119.36, 119.89, 120.40, 120.48, 120.55, 120.73, 121.20, 121.51, 123.88, 124.11, 124.14, 126.44, 129.99, 138.71, 139.08, 139.57, 140.21, 140.27, 144.04, 147.98, 149.89, 151.86, 154.67, 163.93. HRMS (ESI): calcd for $C_{28}H_{20}N_3O$ $[M+H]^+$ 414.1601, found 414.1596.

Synthesis of **Pt(*bp*-7)**: A mixture of **L(*bp*-7)** (350 mg, 0.85 mmol, 1.00 equiv) and $PtCl_2$ (236 mg, 0.89 mmol, 1.05 equiv) were added sequentially to a dry three-necked flask equipped with a magnetic stir bar. The flask was evacuated and backfilled with nitrogen, this evacuation and backfill procedure was repeated twice. Then benzonitrile (40 mL) was added into the flask ,and the flask was

placed in an oil bath and heated at 180 °C with stirring. After 3 days, the mixture was cooled to room temperature. THF (15 mL) and *t*-BuOK (1.90 g, 16.93 mmol, 20.00 equiv) were added to the mixture under nitrogen atmosphere and stirred in an oil bath at 76 °C for 5 h. The resulting mixture was cooled down to room temperature and concentrated in vacuum. The residue was diluted with dichloromethane, and washed with water. The organic layer was separated, and the aqueous phase was extracted with dichloromethane twice. The combined organic layer was dried over anhydrous Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The crude solid was purified through column chromatography on silica gel using petroleum ether/dichloromethane = 3:1−1:1 as eluent to afford the desired product as a yellow solid 40 mg in 8% yield. m.p.: 317.6–318.9 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 6.75 (dd, J = 8.0, 1.0 Hz, 1H), 6.94 (t, J = 7.5 Hz, 1H), 7.18 (dd, J = 7.5, 1.0 Hz, 1H), 7.31−7.34 (m, 2H), 7.35−7.41 (m, 2H), 7.45−7.49 (m, 1H), 7.52 (dd, J = 7.5, 1.0 Hz, 1H), 7.60 (d, J = 7.5 Hz, 1H), 8.03 (d, J = 8.0 Hz,1H), 8.10 (dd, J = 7.5, 1.5 Hz,1H), 8.15−8.22 (m, 2H), 8.28 (d, J = 8.5 Hz, 1H), 8.70 (dd, J = 6.0, 1.0 Hz, 1H), 8.78 (dd, J = 6.0, 1.5 Hz, 1H). ^{13}C NMR (150 MHz, DMSO-d_6): δ 113.91, 114.23, 114.91, 116.44, 116.50, 116.62, 120.16, 120.62, 120.95, 122.76, 124.94, 125.91, 127.67, 128.15, 129.11, 138.50, 139.54, 140.04, 140.64, 148.98, 152.17, 152.63, 152.68, 156.98, 158.37. HRMS (DART positive ion mode): calcd for $C_{28}H_{18}ON_3Pt$ $[M+H]^+$ 607.1092, found 607.1092. Anal. for $C_{28}H_{17}ON_3Pt•0.5CH_2Cl_2$, Calcd.: C, 52.74, H, 2.80, N, 6.47; Found: C, 53.05, H, 2.95, N, 6.44.

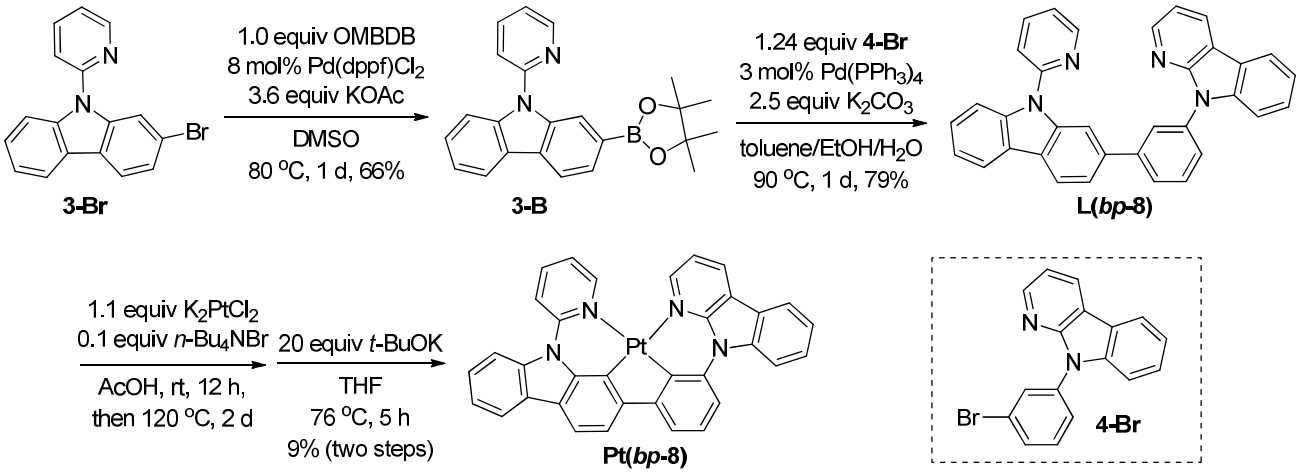
Improved synthesis of **Pt(*bp*-7)**:



A mixture of L(*bp*-7) (200 mg, 0.48 mmol, 1.00 equiv) and $PtCl_2$ (135 mg, 0.51 mmol, 1.05 equiv) were added sequentially to a dry three-necked flask equipped with a magnetic stir bar. The flask was evacuated and back-filled with nitrogen, this evacuation and backfill procedure was repeated twice. The flask was evacuated and backfilled with nitrogen, this evacuation and backfill procedure was repeated twice. Then benzonitrile (30 mL) was added into the flask , and the flask was placed in an oil bath and heated at 180 °C with stirring. After 36 hours, the mixture was cooled to

room temperature and concentrated in vacuum. The residue was diluted with dichloromethane, and washed with water. The organic layer was separated, and the aqueous phase was extracted with dichloromethane twice. The combined organic layer was dried over anhydrous Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The crude product and anhydrous $SnCl_2$ (274 mg, 1.45 mmol, 3.00 equiv) were added to a dry three-necked flask equipped with a magnetic stir bar. The flask was evacuated and backfilled with nitrogen, this evacuation and backfill procedure was repeated twice. Then dichloroethane (30 mL) was added under nitrogen atmosphere and stirred at room temperature for two days. Then the mixture was washed with water, separated and the aqueous phase was extracted with dichloromethane. The combined organic layer was dried over anhydrous Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The crude solid was purified through column chromatography on silica gel using petroleum ether/dichloromethane = 3:1−2:1 as eluent to afford the desired product as a yellow solid 213 mg in 72% yield.^{1}H NMR (500 MHz, DMSO−d_6) :^{1}H NMR (500 MHz, DMSO−d_6) : δ 6.75 (dd, J = 8.0, 1.0 Hz, 1H), 6.93 (t, J = 7.5 Hz, 1H), 7.17 (dd, J= 7.0, 1.0 Hz, 1H), 7.30−7.33 (m, 2H), 7.34−7.40 (m, 2H), 7.47 (td, J= 8.0, 1.0 Hz, 1H), 7.52 (dd, J= 8.5, 1.0 Hz, 1H), 7.60 (d, J= 7.5 Hz, 1H), 8.02 (d, J= 8.5 Hz,1H), 8.08−8.11 (m, 1H), 8.16−8.22 (m, 2H), 8.27 (d, J= 8.5 Hz, 1H), 8.69 (dd, J= 6.0, 2.0 Hz, 1H), 8.78 (dd, J= 6.0, 2.0 Hz, 1H). The ^{1}H NMR is agreement with the data obtained above.

Synthesis of **Pt(*bp*-8)**:



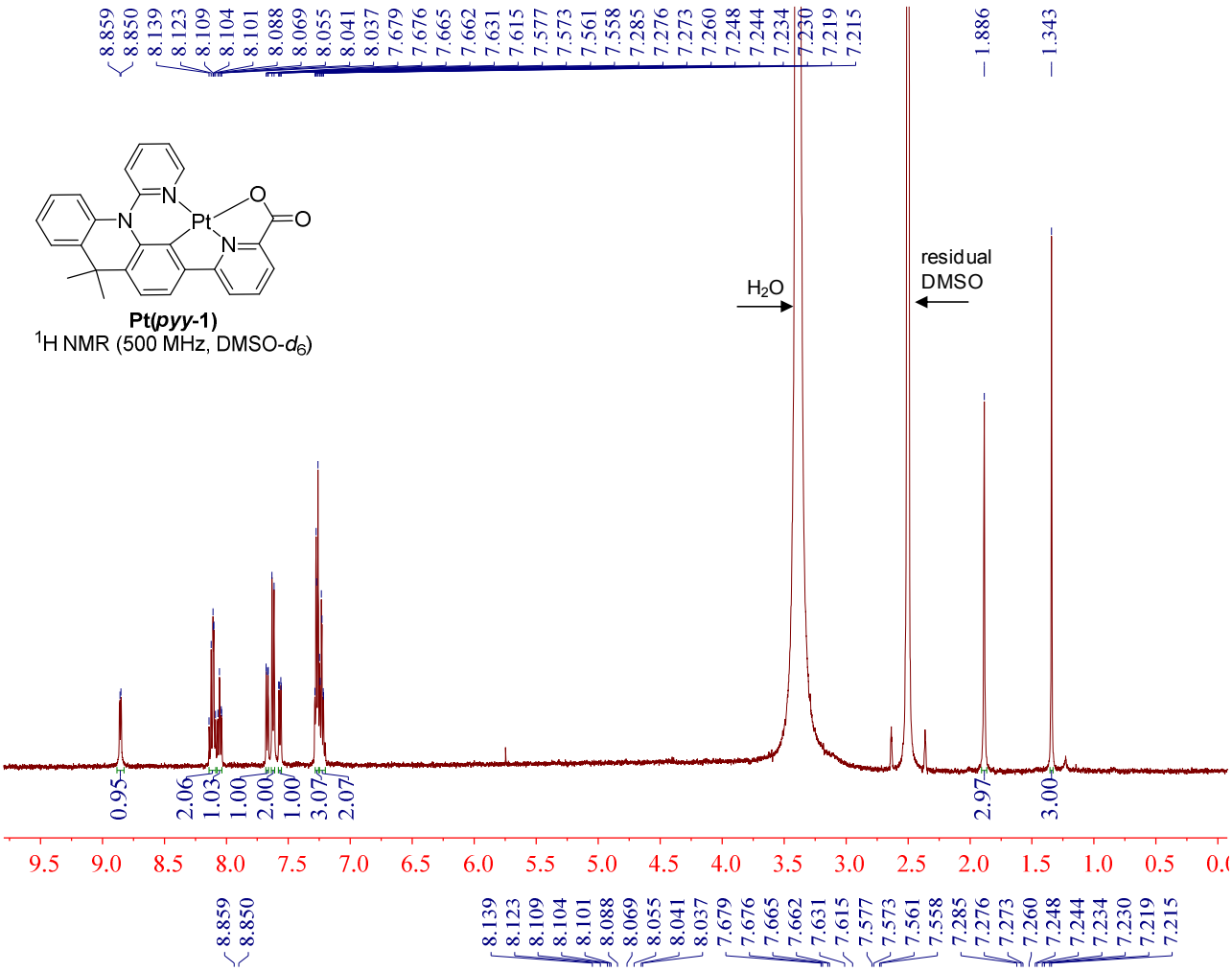
Synthesis of **3-B**: 2-Bromo-9-(pyridin-2-yl)-9*H*-carbazole **3-Br**[6] (1.50 g, 4.64 mmol, 1.02 equiv), **OMBDB** (1.15 g, 4.53 mmol, 1.00 equiv), Pd(dppf)Cl_2 (263 mg, 0.36 mmol, 8 mol%), KOAc (1.62 g, 16.48 mmol, 3.6 equiv) were added sequentially to a dry three-necked flask equipped with a

magnetic stir bar. The flask was evacuated and backfilled with nitrogen, this evacuation and backfill procedure was repeated twice. Then DMSO (20 mL) were added under nitrogen atmosphere, and then the flask was placed in an oil bath and heated at 80 ^{o}C with stirring. The reaction was monitored by TLC until the reaction was completed. After 1day, the resulting mixture was cooled down to room temperature, filtered and washed with ethyl acetate. The organic layer was washed with water, and then dried over Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The residue was purified through column chromatography on silica gel using petroleum ether/ethyl acetate = 20:1−10:1 as eluent to afford the desired product as a white solid 1.10 g in 72% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.34 (s, 12H), 7.22 (dd, *J* = 7.5, 5.0 Hz, 1H), 7.30−7.34 (m, 1H), 7.42 (dt, *J* = 8.0, 1.0Hz, 1H), 7.45−7.48 (m, 1H), 7.63 (t, *J* = 8.0 Hz, 1H), 7.72 (ddd, *J* = 7.5, 2.0, 1.0 Hz, 1H), 7.92 (dt, *J* = 7.5, 1.5 Hz, 1H), 8.03 (dd, *J* = 2.5, 1.0 Hz, 1H), 8.12 (dt, *J* = 7.5, 1.0 Hz, 1H), 8.38 (dd, *J* = 7.5, 1.5 Hz, 1H), 8.48 (dd, *J* = 4.5, 1.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) : δ 24.87, 83.76, 111.19, 117.04, 119.47, 119.49, 120.54, 120.82, 121.30, 123.94, 126.77, 127.07, 138.61, 139.12, 140.13, 149.67, 151.64.HRMS (ESI): calcd for $C_{23}H_{24}N_2O_2B$ $[M+H]^+$ 371.1925, found 371.1945.

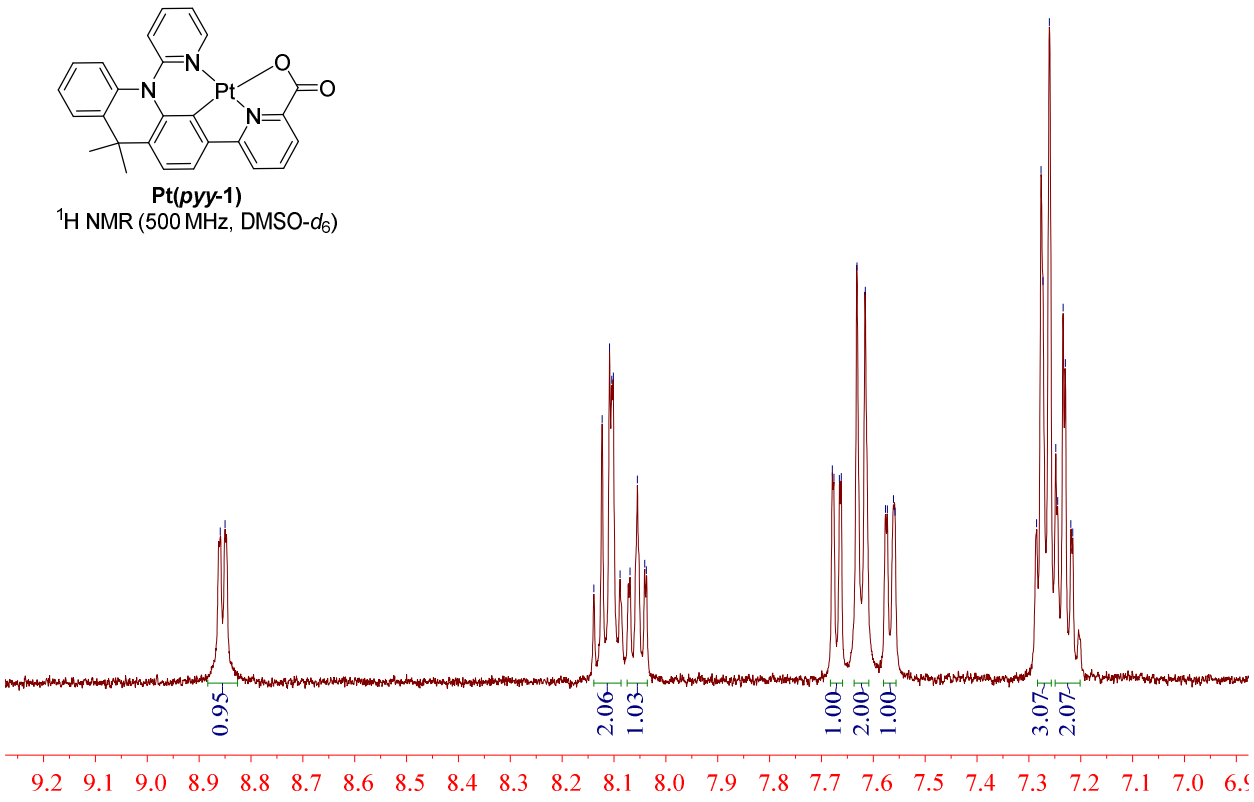
Synthesis of **L(*bp*-8)**: **3-B** (1.00 g, 2.70 mmol, 1.00 equiv), **4-Br**[5] (1.08 g, 3.34 mmol, 1.24 equiv), $Pd(PPh_3)_4$ (94 mg , 0.08 mmol, 3 mol%), K_2CO_3 (933 mg, 6.75 mmol, 2.50 equiv) were added sequentially to a dry three-necked flask equipped with a magnetic stir bar. Then toluene (20 mL), EtOH (4 mL) and H_2O (4 mL) were added, then the flask was placed in an oil bath and heated at 90 ^{o}C with stirring. The reaction was monitored by TLC until the reaction was completed. After 24 hours, the resulting mixture was cooled down to room temperature, filtered and washed with ethyl acetate. The organic layer was washed with water, and then dried over Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The residue was purified through column chromatography on silica gel using petroleum ether/ethyl acetate = 10:1−3:1 as eluent to afford the desired product as a white solid 1.04 g in 79% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.28−7.34 (m, 2H), 7.33−7.37 (m, 2H), 7.43−7.46 (m, 1H), 7.46−7.49 (m, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.63 (dd, *J* = 8.0, 1.5 Hz, 2H), 7.66−7.71 (m, 2H), 7.77 (dt, *J* = 3.0, 1.5 Hz, 1H), 7.83 (d, *J*= 8.0 Hz, 1H), 7.91−7.95 (m, 2H), 8.08 (d, *J* = 1.0 Hz,1H), 8.14 (t, *J* =7.5, 1.5 Hz, 2H),8.18 (d, *J* = 8.0 Hz, 1H), 8.41 (dd, *J* = 7.5, 1.5Hz, 1H), 8.49 (d, *J* = 5.0, 2.0 Hz, 1H), 8.71 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 109.99, 110.55, 111.15, 116.11, 116.41, 119.24, 120.32, 120.53, 120.71, 120.78, 120.89, 120.96, 121.10, 121.40, 123.85, 124.01, 126.08, 126.37, 126.51, 126.96, 127.00, 128.32, 129.98,

136.68, 138.59, 138.88, 140.14, 140.17, 140.18, 143.74, 146.54, 149.77, 151.73, 152.03. HRMS (ESI): calcd for $C_{34}H_{23}N_4$ $[M+H]^+$ 487.1917, found 487.1914.

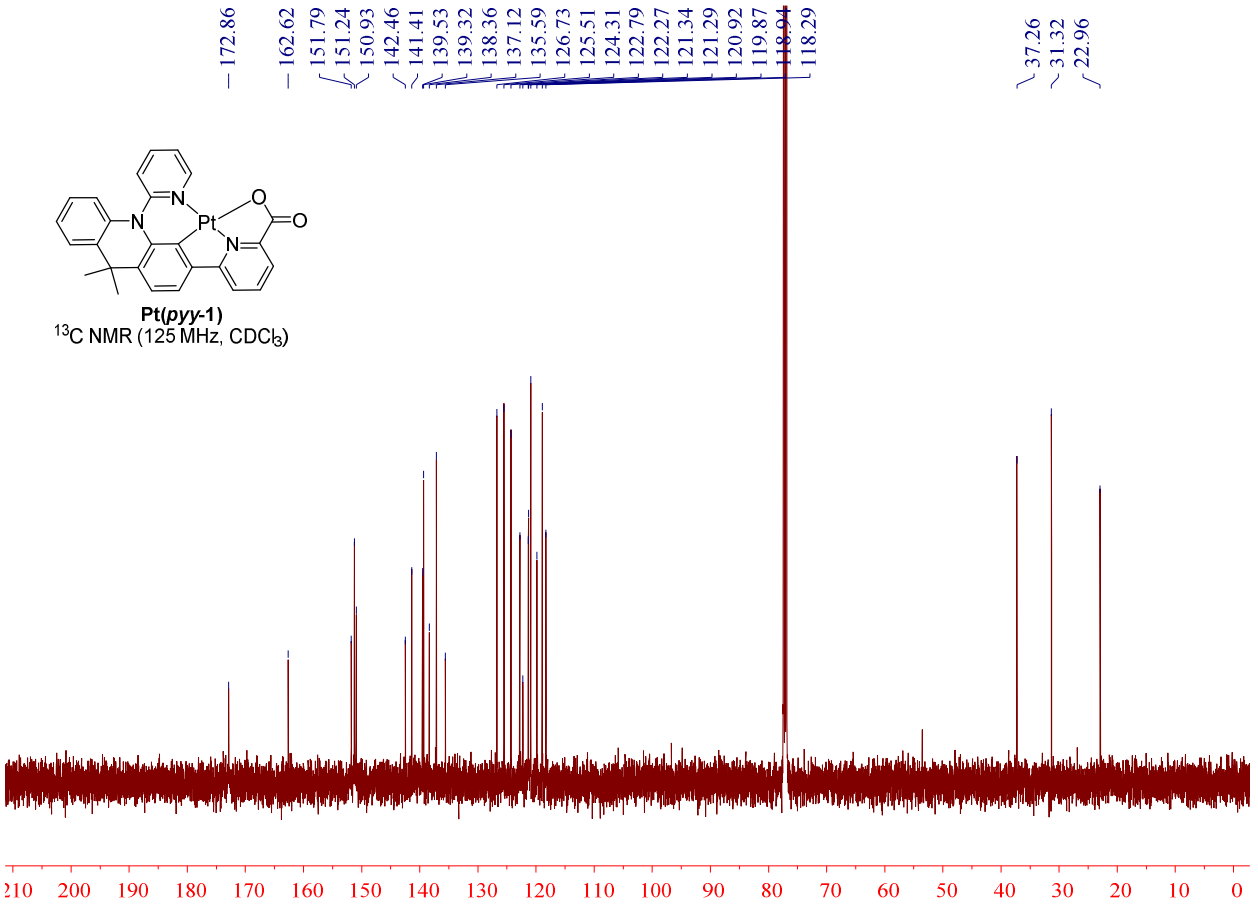
Synthesis of **Pt(*bp*-8)**: A mixture of **L(*bp*-8)** (200 mg, 0.41 mmol, 1.00 equiv), K_2PtCl_4 (188 mg, 0.45 mmol, 1.10 equiv) and *n*-Bu_4NBr (13 mg, 0.04 mmol, 0.1 equiv) were added sequentially to a dry three-necked flask equipped with a magnetic stir bar. The flask was evacuated and backfilled with nitrogen, this evacuation and backfill procedure was repeated twice. Then AcOH (30 mL) were added into the flask under nitrogen atmosphere at room temperature. The reaction mixture was bubbled with nitrogen for 30 minutes and then stirred at room temperature for 12 h. Then the flask was placed in an oil bath and heated at 120 ^oC with stirring. After two days, the resulting mixture was cooled down to room temperature and concentrated in vacuum and the residue was diluted with dichloromethane. The mixture was washed with water, the organic layer was separated and dried over anhydrous Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The residue obtained in last step, THF (15 mL) and *t*-BuOK (460 mg, 4.1 mmol, 10.00 equiv) were added to the mixture under nitrogen atmosphere and stirred in an oil bath at 76 °C for 5 h. The resulting mixture was cooled down to room temperature and concentrated in vacuum. The residue was diluted with dichloromethane, and washed with water. The organic layer was separated, and the aqueous phase was extracted with dichloromethane twice. The combined organic layer was dried over anhydrous Na_2SO_4, filtered, and the filtrate was concentrated under reduced pressure. The crude solid was purified through column chromatography on silica gel using petroleum ether/dichloromethane = 3:1−1:1 as eluent to afford the desired product as a yellow solid 25 mg in 9% yield. m.p.: 221.1–222.0 ^oC. ^1H NMR (500 MHz, DMSO-d_6): δ 7.07−7.11 (m, 1H),7.23−7.27 (m, 1H), 7.32 (d, J = 7.0 Hz, 1H), 7.37 (t, J = 8.0 Hz, 1H), 7.42 (d, J = 8.0 Hz, 1H), 7.46−7.50 (m, 1H),7.51−7.54 (t, J = 7.5 Hz, 1H), 7.61−7.66 (m, 3H), 7.69−7.73 (m, 1H), 8.04 (d, J = 8.5 Hz, 1H), 8.11−8.13 (m, 1H), 8.15−8.19 (m, 1H), 8.25−8.31 (t, J = 6.5 Hz, 2H), 8.45−8.48 (m, 1H), 8.53−8.56 (dd, J = 6.0, 2.0 Hz, 1H), 8.88 (dd, J = 5.5, 1.5 Hz, 1H), 9.05 (dd, J = 7.5, 1.5 Hz, 1H). ^{13}C NMR (150 MHz, DMSO-d_6): δ 113.97, 114.89, 115.60, 116.42, 116.66, 116.73, 118.38, 119.64, 119.84, 120.65, 120.88, 121.97, 122.16, 122.36, 122.71, 124.43, 125.88, 127.85, 128.11, 129.50, 130.50, 135.63, 136.10, 138.26, 138.30, 139.36, 139.68, 146.39, 146.44, 149.00, 152.44, 153.61, 157.00. HRMS (DART positive ion mode): calcd for $C_{34}H_{21}N_4Pt$ $[M+H]^+$ 680.1408, found 680.1411. Anal. for $C_{34}H_{20}N_4Pt$, Calcd.: C, 60.09, H, 2.97, N, 8.24; Found: C, 59.60, H, 3.30, N, 7.88.



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



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


172.86
162.62
151.79
151.24
150.93
142.46
141.41
139.53
139.32
138.36
137.12
135.59
126.73
125.51
124.31
122.79
122.27
121.34
121.29
120.92
119.87
118.94
118.29
37.26
31.32
22.96
N
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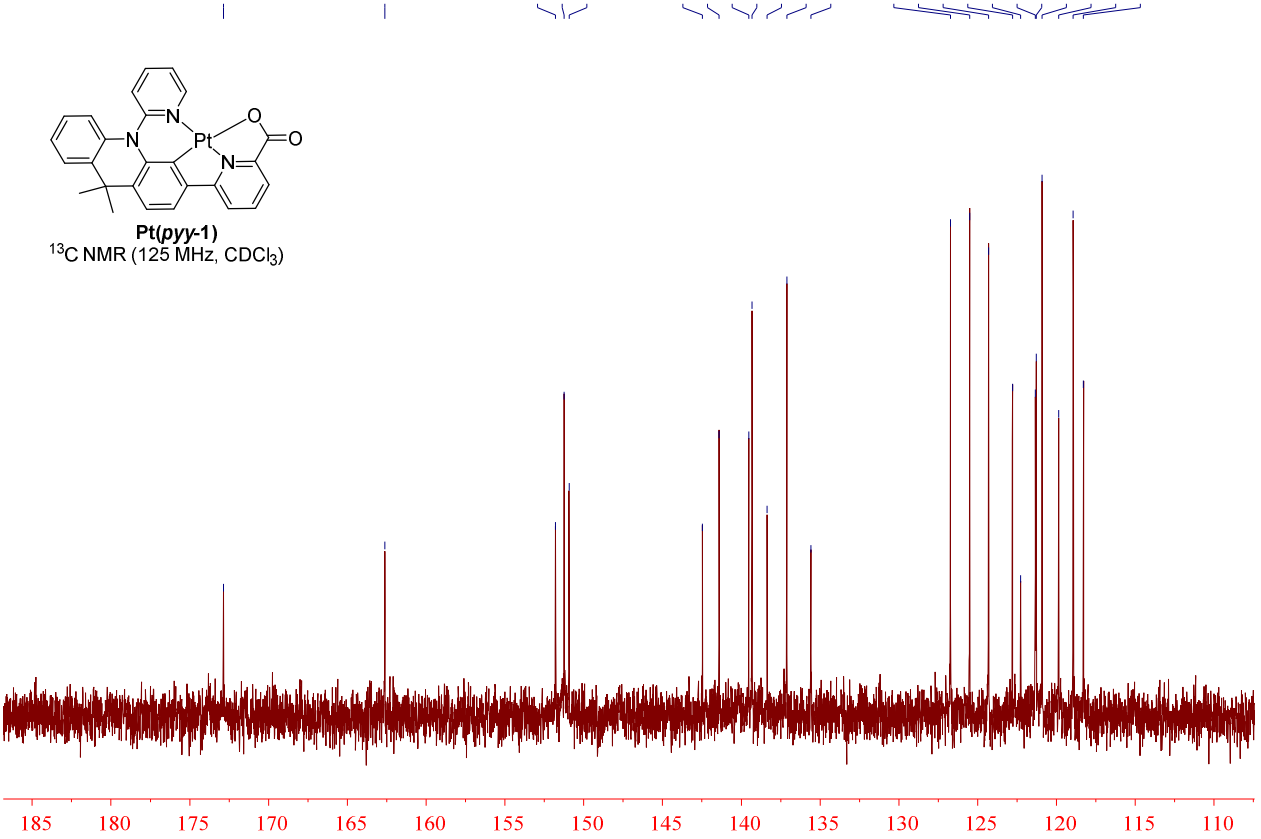
Pt(pyy-1)
13C NMR (125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


172.86
162.62
151.79
151.24
150.93
142.46
141.41
139.53
139.32
138.36
137.12
135.59
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125.51
124.31
122.79
122.27
121.34
121.29
120.92
119.87
118.94
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N
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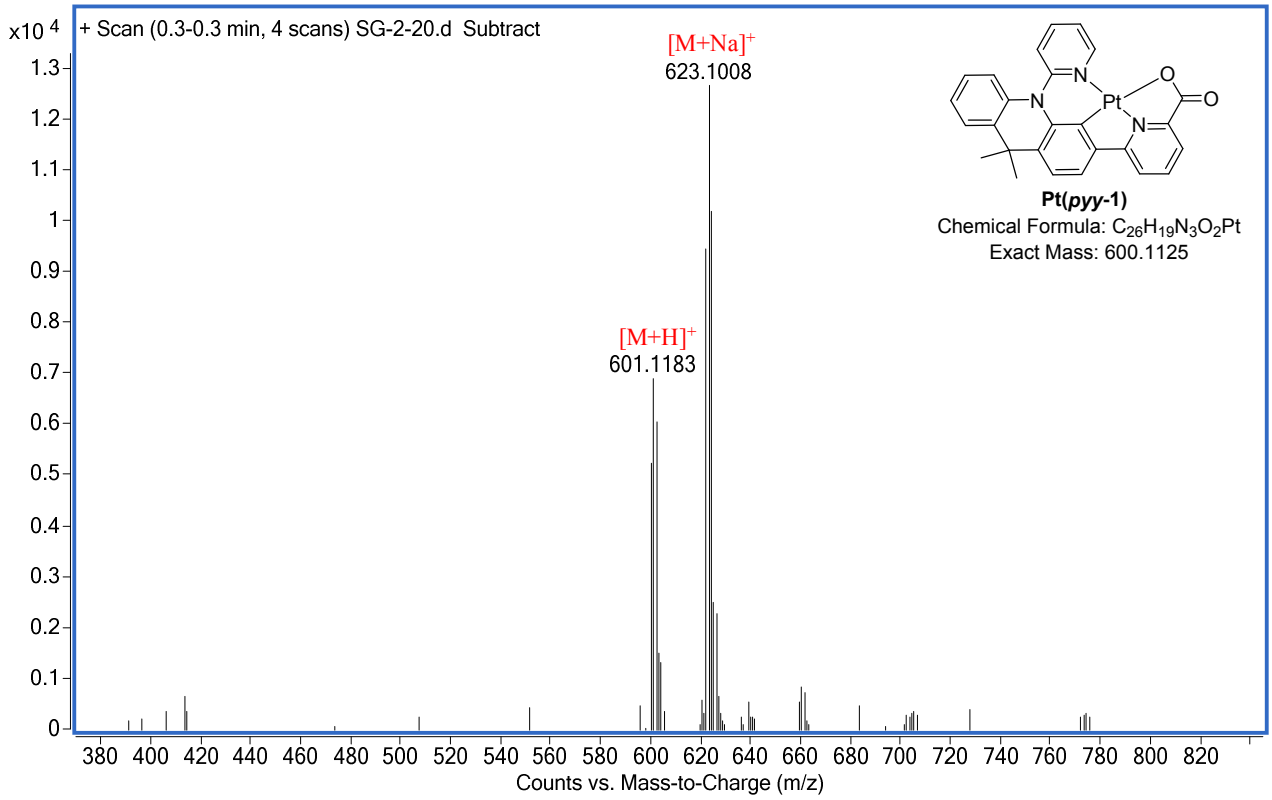
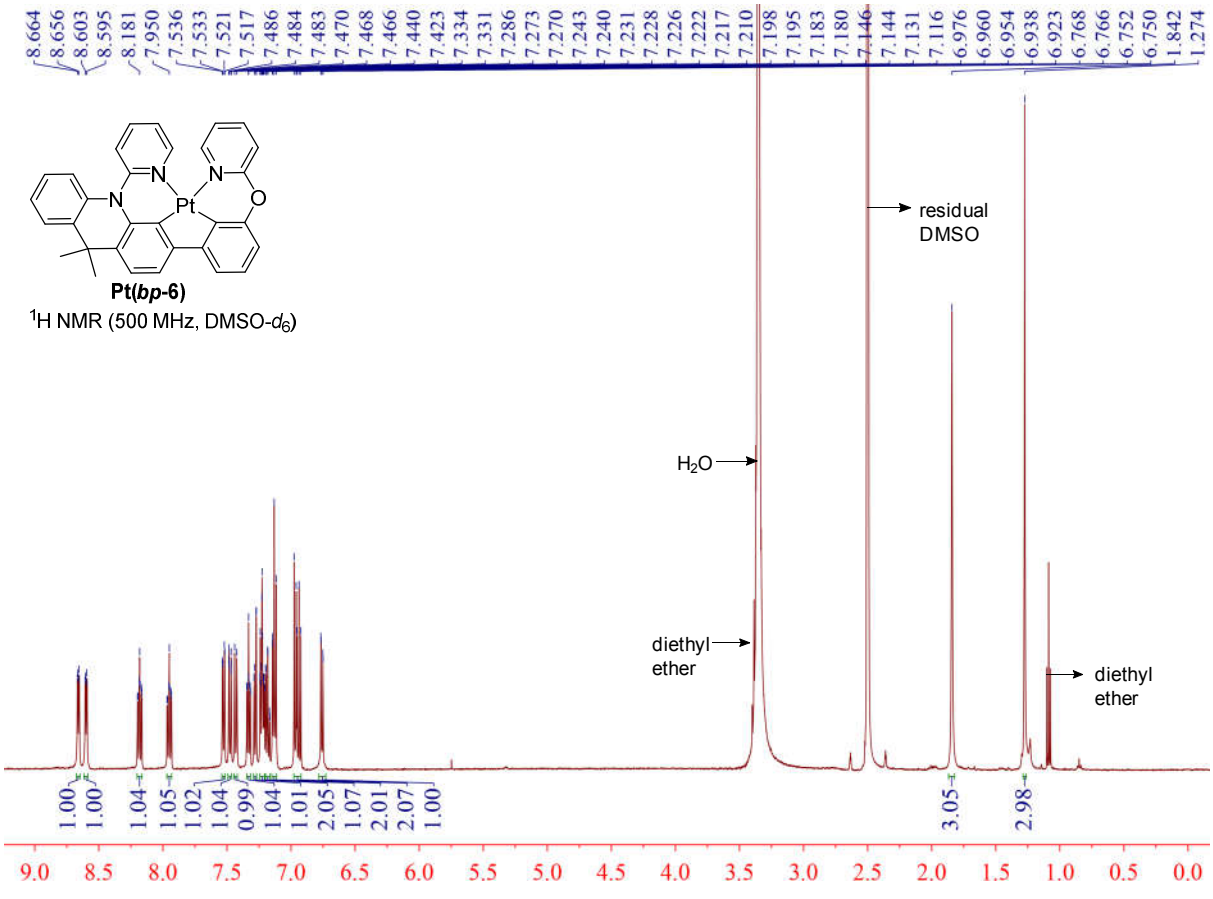
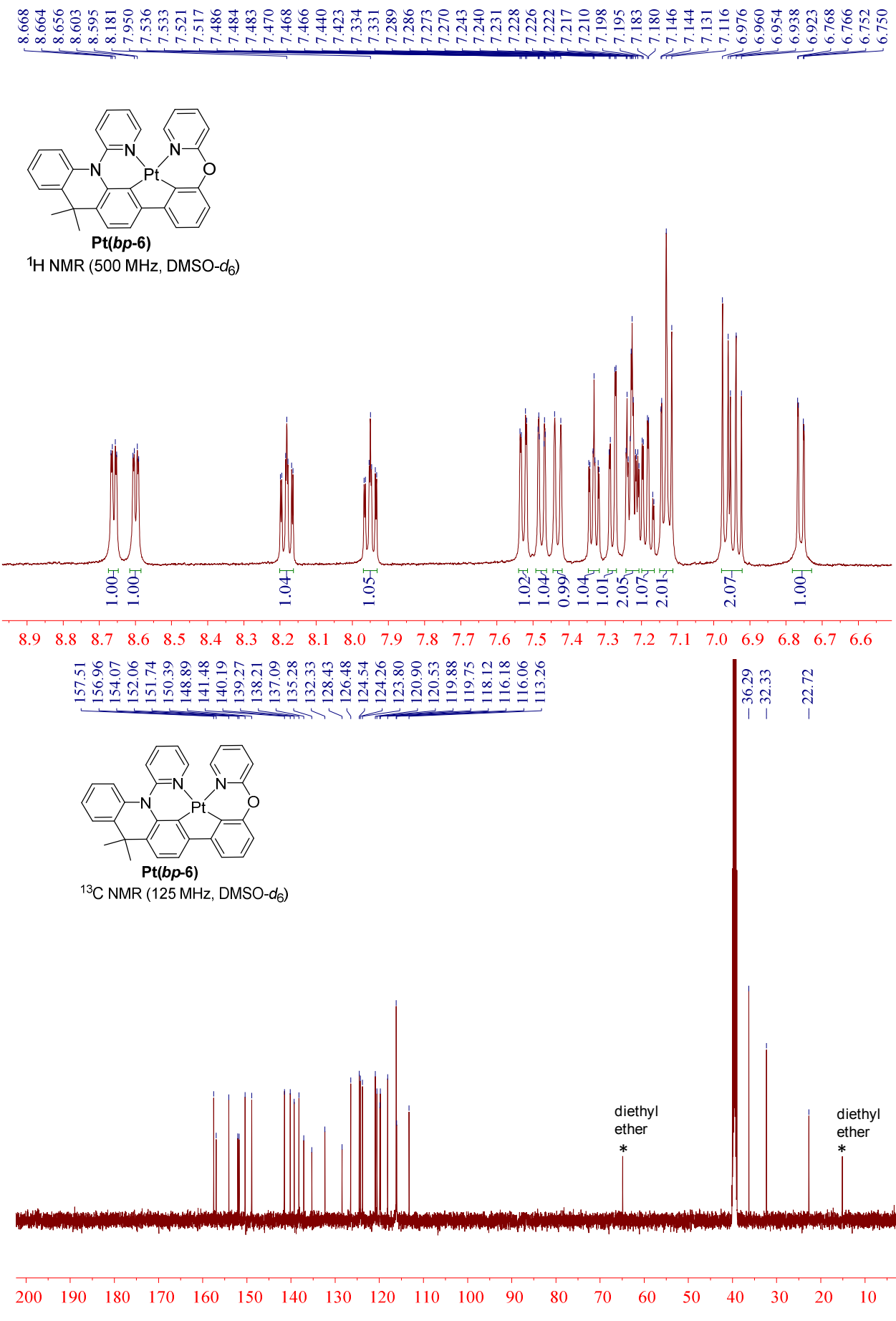
Pt(pyy-1)
13C NMR (125 MHz, CDCl3)
185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110



Fomula(M)	Ion Formula	m/z	Calc m/z	Error (ppm)
$C_{26}H_{19}N_3O_2$ [^{195}Pt]	$C_{26}H_{19}N_3NaO_2$ [^{195}Pt]	623.1008	623.1017	1.54

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8.656
8.603
8.595
8.181
7.950
7.536
7.533
7.521
7.517
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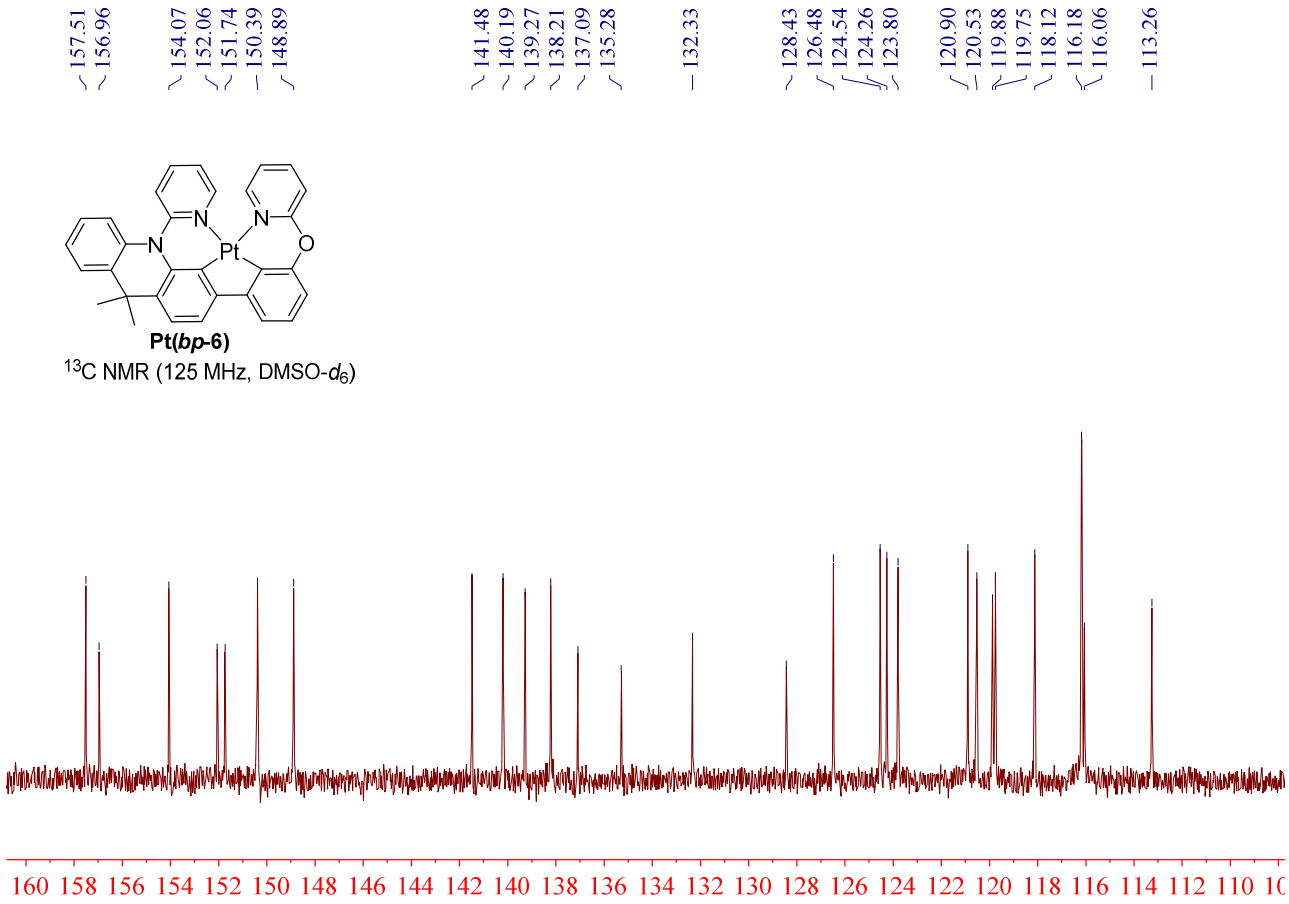
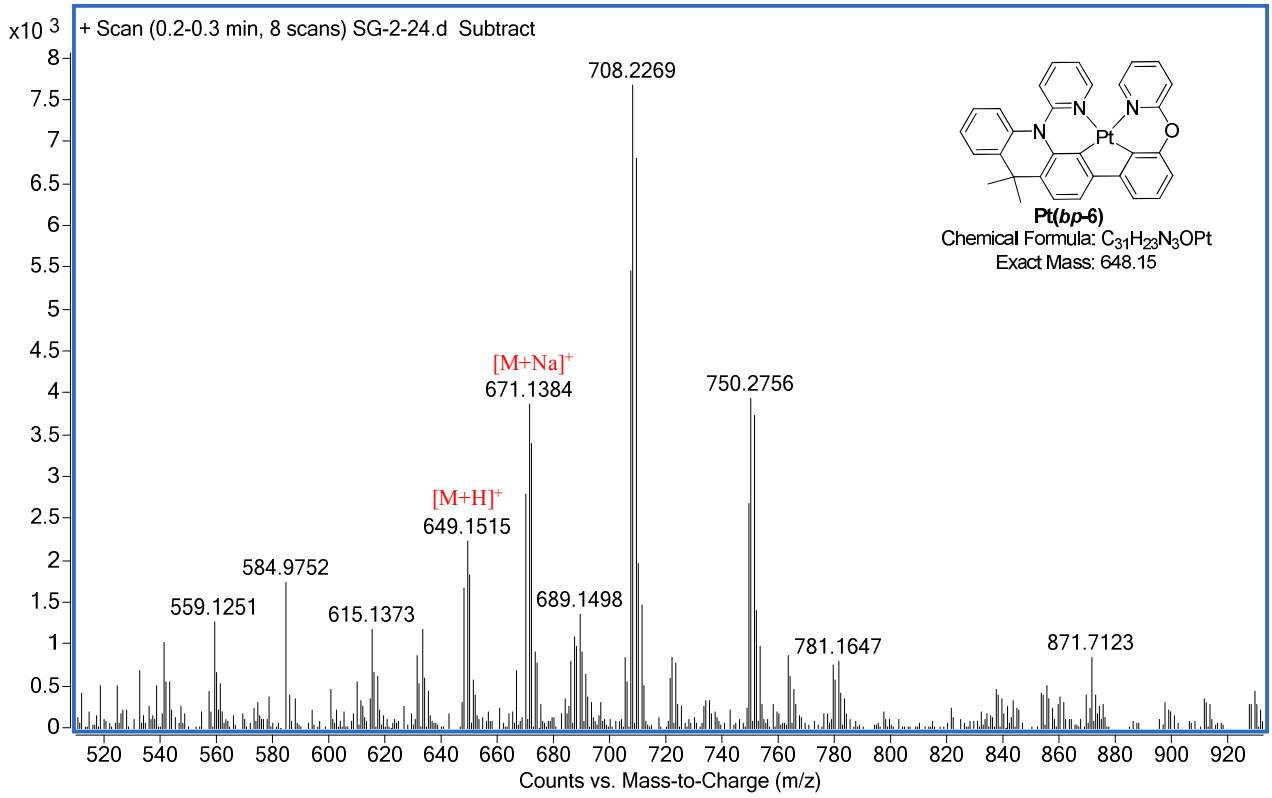
7.483
7.470
7.468
7.466
7.440
7.423
7.334
7.331
7.289
7.286
7.273
7.270
7.243
7.240
7.231
7.228
7.226
7.222
7.217
7.210
7.198
7.195
7.183
7.180
7.146
7.144
7.131
7.116
6.976
6.960
6.954
6.938
6.923
6.768
6.766
6.752
6.750
N
N
Pt
N
O
Pt(bp-6)
1H NMR (500 MHz, DMSO-d6)
1.00
1.00
1.04
1.05
1.02
1.04
0.99
1.04
1.01
2.05
1.07
2.01
2.07
1.00
8.9 8.8 8.7 8.6 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 6.8 6.7 6.6
157.51
156.96
154.07
152.06
151.74
150.39
148.89
141.48
140.19
139.27
138.21
137.09
135.28
132.33
128.43
126.48
124.54
124.26
123.80
120.90
120.53
119.88
119.75
118.12
116.18
116.06
113.26
36.29
32.33
22.72
N
N
Pt
O
Pt(bp-6)
13C NMR (125 MHz, DMSO-d6)
diethyl ether
*
diethyl ether
*
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

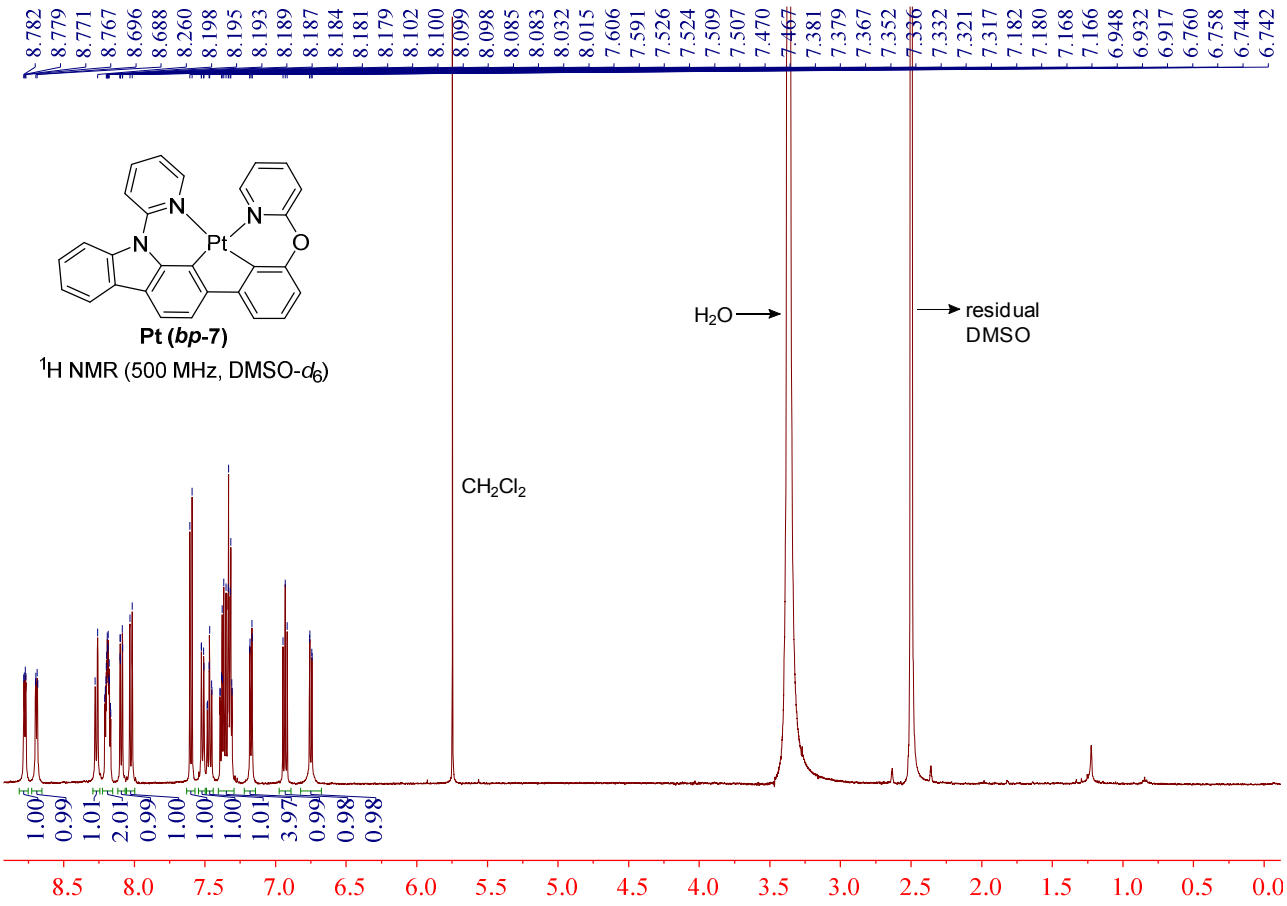


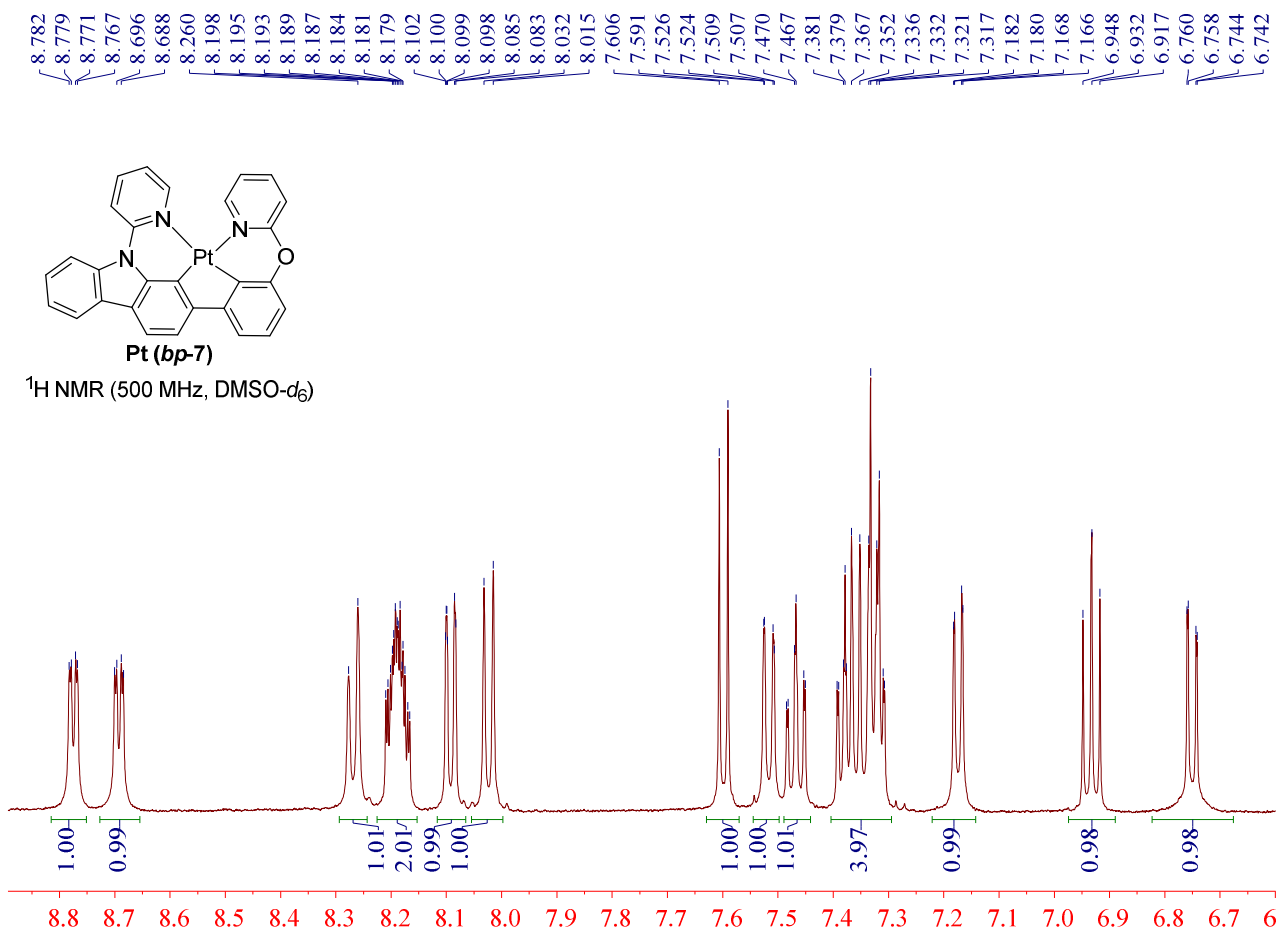
Pt(*bp*-6)

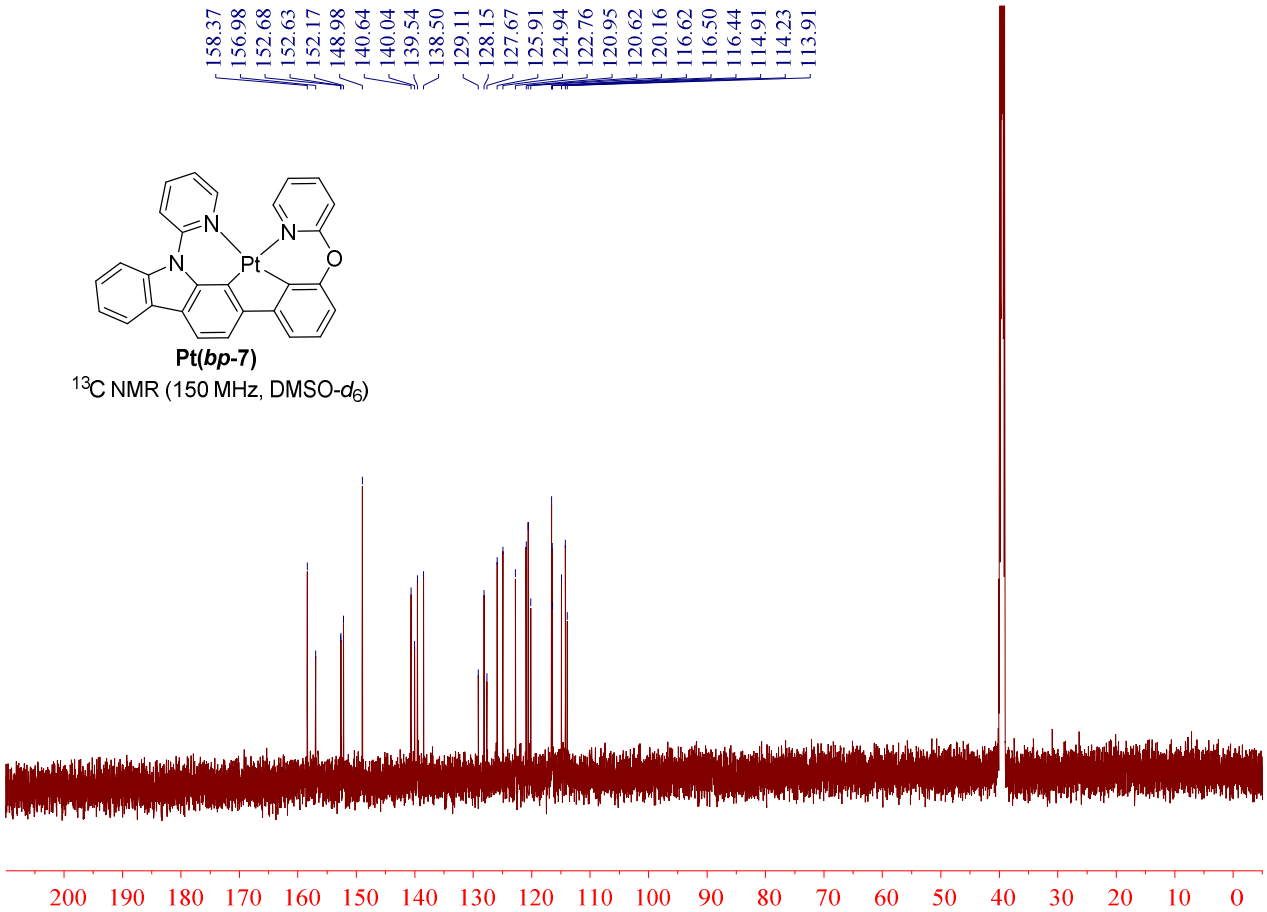
^{13}C NMR (125 MHz, DMSO-d_6)



Fomula(M)	Ion Formula	m/z	Calc m/z	Error (ppm)
$C_{31}H_{23}N_3O$ [^{195}Pt]	$C_{31}H_{23}N_3NaO$ [^{195}Pt]	671.1384	671.1381	-0.45

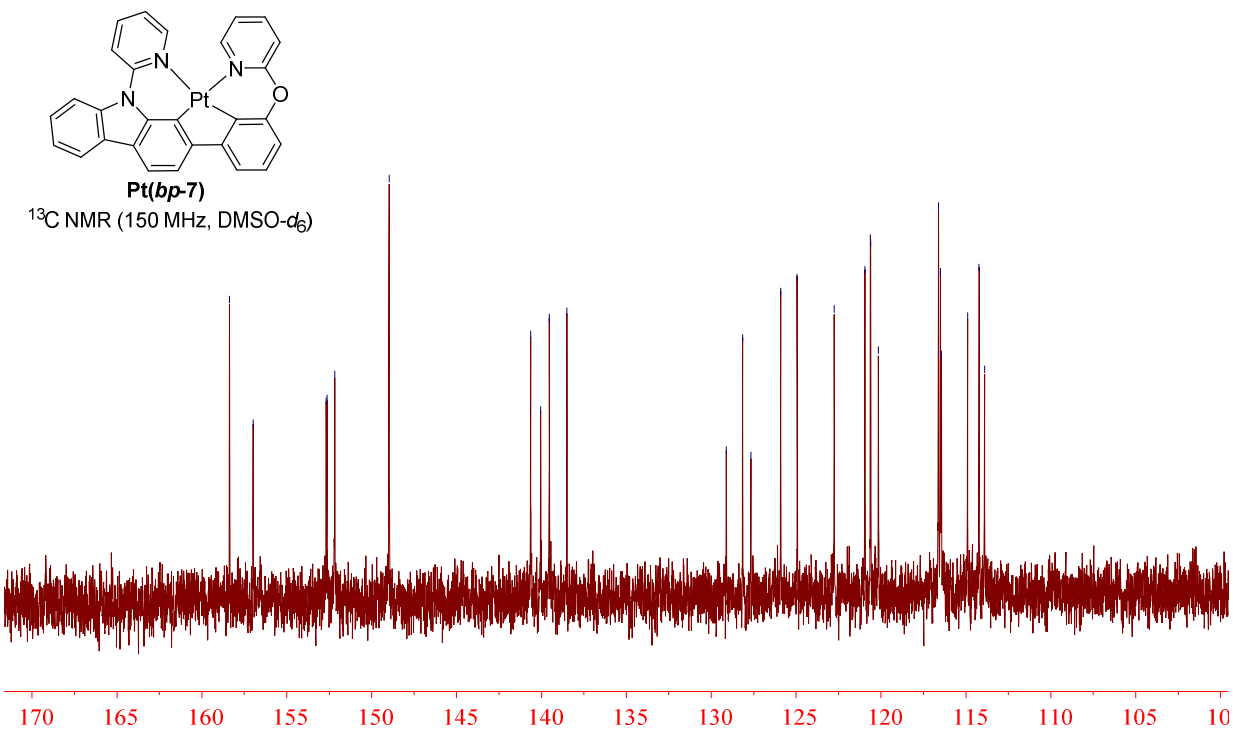

8.782 8.779 8.771 8.767 8.696 8.688 8.260 8.198 8.195 8.193 8.189 8.187 8.184 8.181 8.179 8.102 8.100 8.099 8.098 8.085 8.083 8.032 8.015 7.606 7.591 7.526 7.524 7.509 7.507 7.470 7.467 7.381 7.379 7.367 7.352 7.336 7.332 7.321 7.317 7.182 7.180 7.168 7.166 6.948 6.932 6.917 6.760 6.758 6.744 6.742
Pt (bp-7)
1H NMR (500 MHz, DMSO-d6)
H2O
residual DMSO
CH2Cl2
1.00 0.99 1.01 2.01 0.99 1.00 1.00 1.00 1.01 3.97 0.99 0.98 0.98
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


8.782 8.779 8.771 8.767 8.696 8.688 8.260 8.198 8.195 8.193 8.189 8.187 8.184 8.181 8.179 8.102 8.100 8.099 8.098 8.085 8.083 8.032 8.015 7.606 7.591 7.526 7.524 7.509 7.507 7.470 7.467 7.381 7.379 7.367 7.352 7.336 7.332 7.321 7.317 7.182 7.180 7.168 7.166 6.948 6.932 6.917 6.760 6.758 6.744 6.742
Pt (bp-7)
1H NMR (500 MHz, DMSO-d6)
1.00 0.99 1.01 2.01 0.99 1.00 1.00 1.00 1.01 3.97 0.99 0.98 0.98
8.8 8.7 8.6 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 6.8 6.7 6



Pt(*bp*-7)

^{13}C NMR (150 MHz, DMSO-d_6)



Pt(*bp*-7)

^{13}C NMR (150 MHz, DMSO-d_6)

Card Serial Number : D172118

Sample Serial Number: Z-9-2

Operator : DONG Date: 2017/12/20

Operation Mode: DART POSITIVE Ion Mode

Elemental composition search on mass 607.11

m/z= 602.11-612.11

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
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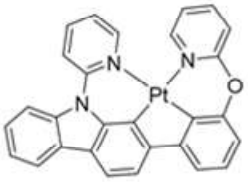
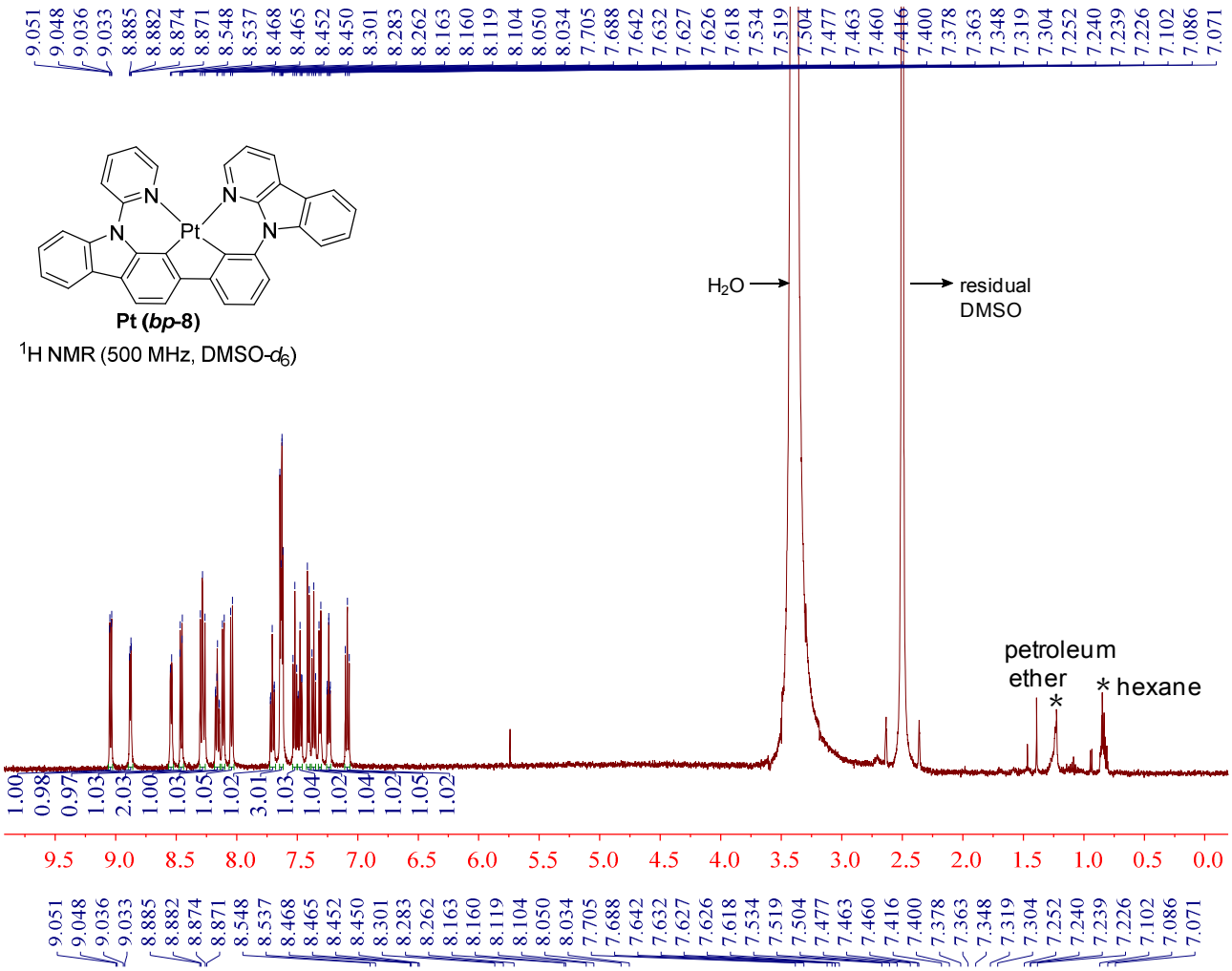
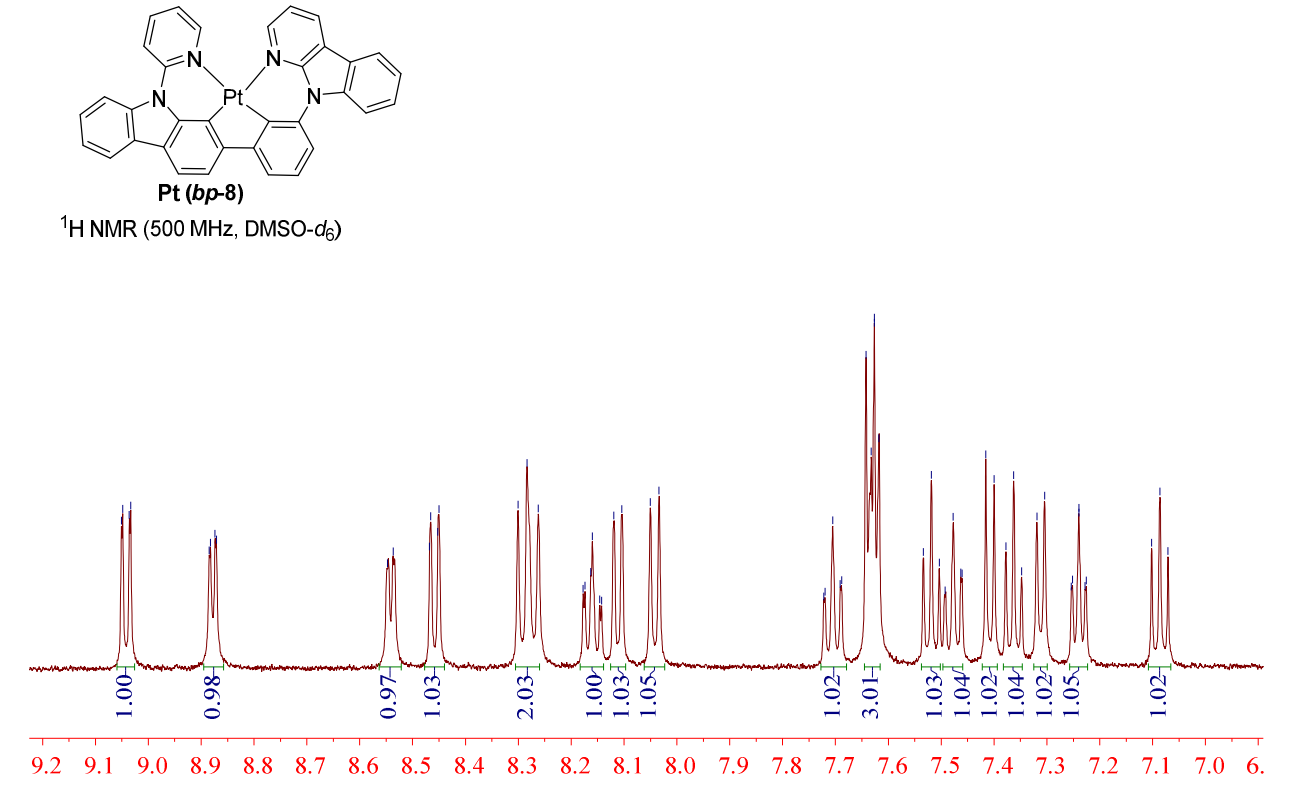
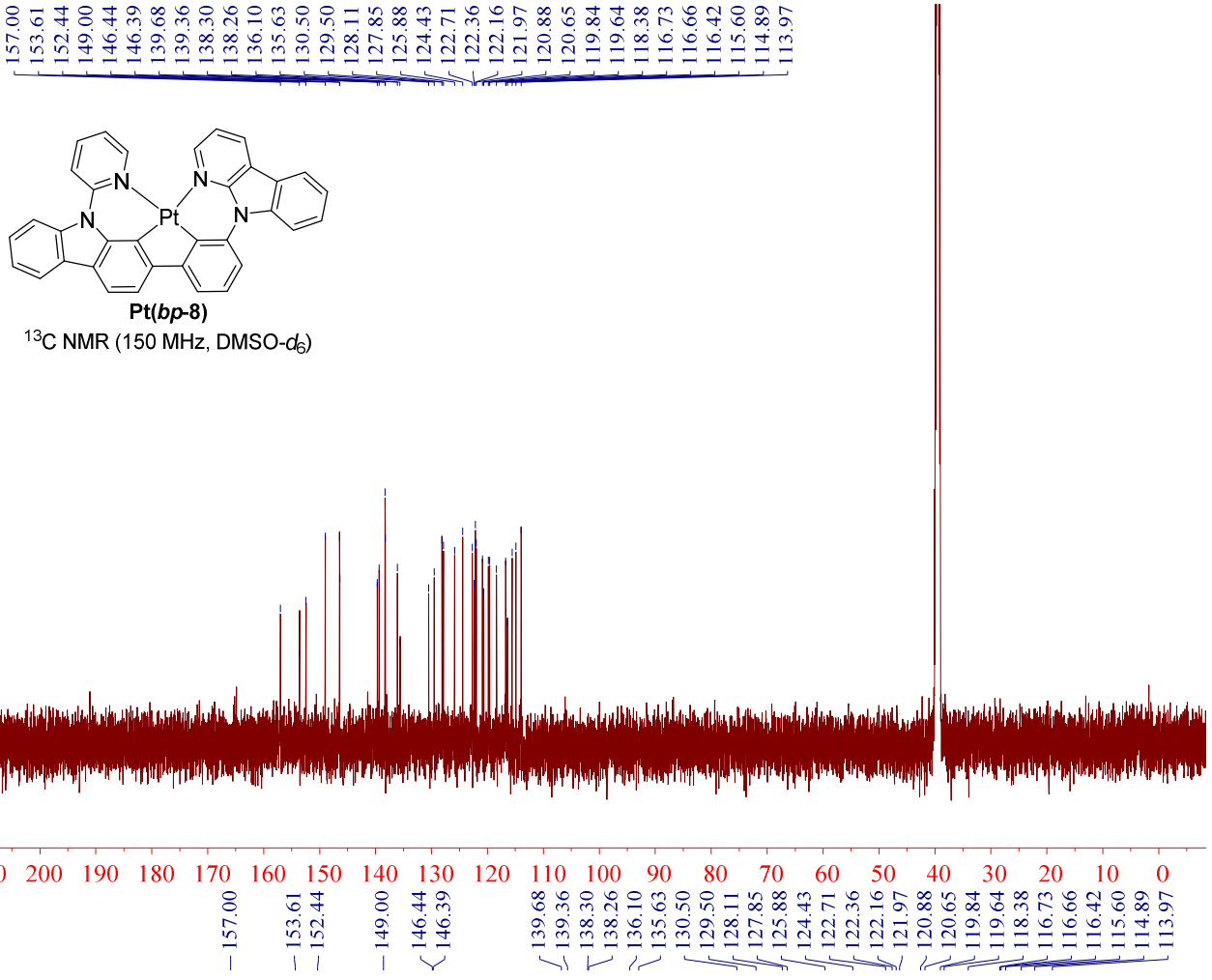
	607.1097	-0.88	33.0	$C_{38}H_{17}O_2N_5S$
	607.1086	1.07	12.5	$C_{20}H_{22}O_3N_5PtS$
	607.1099	-1.14	12.0	$C_{22}H_{24}O_4N_2PtS$
	607.1106	-2.22	21.0	$C_{30}H_{20}O_2Pt$
	607.1077	2.46	37.5	$C_{43}H_{15}O_3N_2$
	607.1111	-3.10	32.5	$C_{40}H_{19}O_3N_2S$
	607.1071	3.53	28.5	$C_{35}H_{19}O_5N_4S$
	607.1065	4.41	17.0	$C_{25}H_{20}O_4N_2Pt$
	607.1064	4.67	38.0	$C_{41}H_{13}O_2N_5$



Pt(*bp*-7)

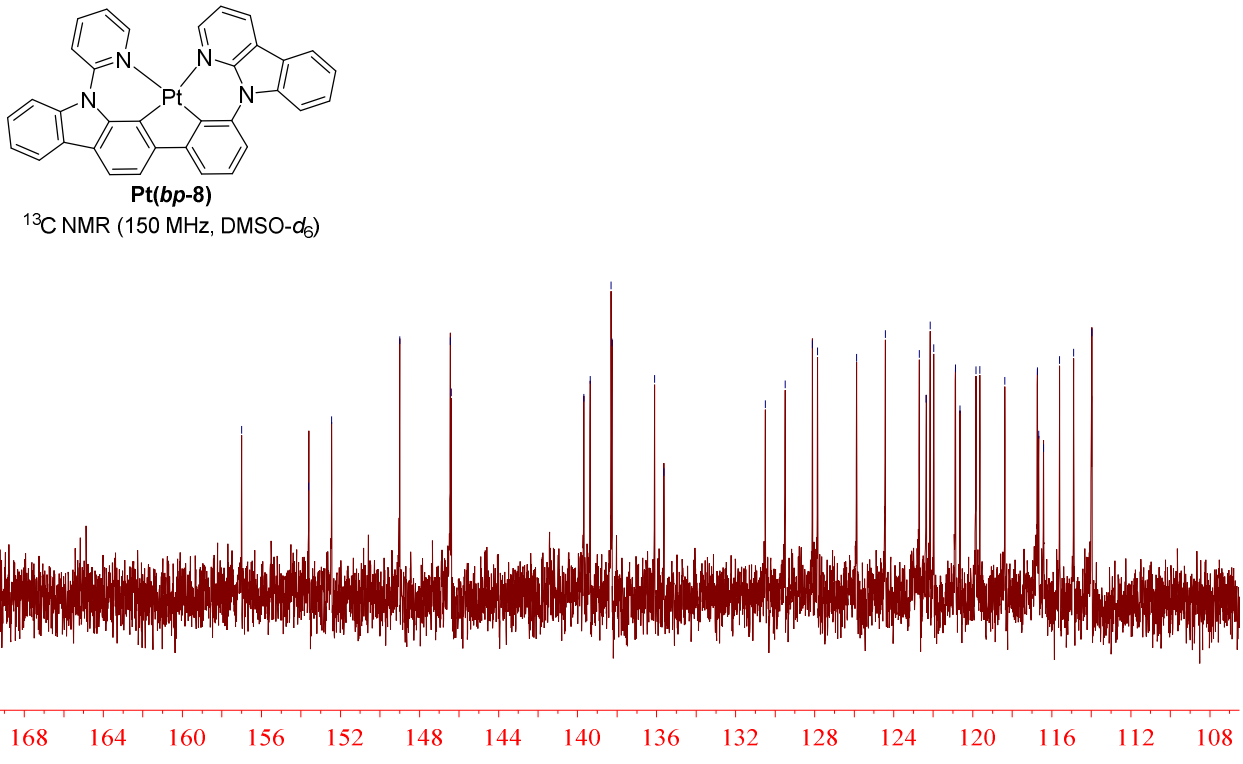

9.051 9.048 9.036 9.033 8.885 8.882 8.874 8.871 8.548 8.537 8.468 8.465 8.452 8.450 8.301 8.283 8.262 8.163 8.160 8.119 8.104 8.050 8.034 7.705 7.688 7.642 7.632 7.627 7.626 7.618 7.534 7.519 7.504 7.477 7.463 7.460 7.416 7.400 7.378 7.363 7.348 7.319 7.304 7.252 7.240 7.239 7.226 7.102 7.086 7.071
N
N
Pt
N
N
Pt (bp-8)
1H NMR (500 MHz, DMSO-d6)
H2O
residual DMSO
petroleum ether
*
* hexane
1.00 0.98 0.97 1.03 2.03 1.00 1.03 1.05 1.02 3.01 1.03 1.04 1.02 1.04 1.02 1.05 1.02
9.5 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


9.051 9.048 9.036 9.033 8.885 8.882 8.874 8.871 8.548 8.537 8.468 8.465 8.452 8.450 8.301 8.283 8.262 8.163 8.160 8.119 8.104 8.050 8.034 7.705 7.688 7.642 7.632 7.627 7.626 7.618 7.534 7.519 7.504 7.477 7.463 7.460 7.416 7.400 7.378 7.363 7.348 7.319 7.304 7.252 7.240 7.239 7.226 7.102 7.086 7.071
N
N
Pt
N
N
Pt (bp-8)
1H NMR (500 MHz, DMSO-d6)
1.00 0.98 0.97 1.03 2.03 1.00 1.03 1.05 1.02 3.01 1.03 1.04 1.02 1.04 1.02 1.05 1.02
9.2 9.1 9.0 8.9 8.8 8.7 8.6 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.



Pt(*bp*-8)

^{13}C NMR (150 MHz, DMSO-d_6)



Pt(*bp*-8)

^{13}C NMR (150 MHz, DMSO-d_6)

Card Serial Number : D172122

Sample Serial Number: Z-10-72

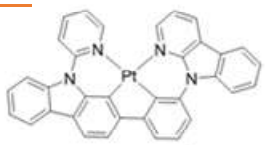
Operator : DONG Date: 2017/12/20

Operation Mode: DART POSITIVE Ion Mode

Elemental composition search on mass 680.14

m/z= 675.14-685.14

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
680.1411	680.1408	0.43	26.5	$C_{34}H_{21}N_4Pt$
	680.1415	-0.59	17.0	$C_{28}H_{27}O_3N_3PtS$
	680.1422	-1.54	26.0	$C_{36}H_{23}ONPt$
	680.1400	1.61	33.0	$C_{43}H_{24}O_5N_2S$
	680.1395	2.40	21.5	$C_{33}H_{25}O_4Pt$
	680.1429	-2.56	16.5	$C_{30}H_{29}O_4PtS$
	680.1387	3.59	33.5	$C_{41}H_{22}O_4N_5S$
	680.1382	4.37	22.0	$C_{31}H_{23}O_3N_3Pt$
	680.1442	-4.53	21.5	$C_{31}H_{25}N_4PtS$



Pt(*bp*-8)

Cartesian Coordinates of the Structures

Pt(*ppy*-1)_S_0

C	-3.53863900	1.78471700	-0.71644000
C	-4.01847400	0.74328600	0.30010000
C	-4.78225700	-1.22522200	2.16696900
C	-5.23098100	0.83379800	0.99444000
C	-3.18901600	-0.36432600	0.55728400
C	-3.56171200	-1.32713700	1.50590600
C	-5.62358700	-0.14280100	1.90925800
H	-5.88463600	1.68090500	0.82004600
H	-2.88881600	-2.14699600	1.73366200
H	-6.57408400	-0.04936200	2.42657500
H	-5.06023700	-1.97875900	2.89836900
C	-2.03968900	1.97843500	-0.46019400
C	0.75872900	2.20223200	-0.13528800
C	-1.24721100	0.83073800	-0.24559100
C	-1.40222000	3.22703900	-0.46763200
C	-0.02236100	3.34925000	-0.29160100
C	0.13335900	0.92355300	-0.13344100
H	-1.98725700	4.12748000	-0.61332300
H	0.42813300	4.33857100	-0.28676600
C	-4.32642000	3.10167700	-0.61849900
H	-5.38682100	2.93548300	-0.83275100
H	-3.96634700	3.81955600	-1.36155400
H	-4.24173900	3.55901300	0.37300300
C	-3.72979900	1.22040100	-2.15516500
H	-4.79296300	1.03765000	-2.34969100
H	-3.18865900	0.28093100	-2.29771700
H	-3.35928200	1.93922900	-2.89451600
N	-1.91320300	-0.43226100	-0.09210500

C	2.22139800	2.16962800	0.05931900
C	4.94144000	1.59160000	0.40321600
C	3.14791100	3.21372700	0.12335500
C	4.50381400	2.91528600	0.30004200
C	3.98994500	0.57744500	0.33597900
H	2.81778400	4.24307100	0.03201800
C	-1.38762200	-1.68833500	-0.42074700
C	-0.43889400	-4.24192700	-1.01961300
C	-2.27029300	-2.69321300	-0.87786400
N	-0.06009800	-1.96888900	-0.31729400
C	0.39082800	-3.21832400	-0.61062800
C	-1.80292800	-3.96043900	-1.17060100
H	-3.31731800	-2.44793300	-1.00250500
H	1.46195100	-3.34894300	-0.49578200
H	-2.49085500	-4.71979100	-1.53093000
H	-0.02629500	-5.22172100	-1.23113600
Pt	1.38622900	-0.56336600	0.03448100
H	5.22357800	3.72773500	0.34930100
H	5.98385400	1.32170100	0.52599200
N	2.69927900	0.90131600	0.18636000
C	4.28187700	-0.93389500	0.38648400
O	3.23915800	-1.70239400	0.25697000
O	5.44822700	-1.28005800	0.52992300

Pt(*ppy*-1)_T_1

C	3.53422300	-1.77954600	-0.73707700
C	4.02734700	-0.74329500	0.27820000
C	4.79885100	1.21325100	2.15836200
C	5.24616700	-0.83424300	0.96189100
C	3.19928400	0.36127100	0.55214900
C	3.57426800	1.31833500	1.50608800

C	5.64113600	0.13535600	1.88283400
H	5.90231900	-1.67634300	0.77319700
H	2.89911300	2.13240700	1.74682300
H	6.59649600	0.04123000	2.39107000
H	5.07964700	1.95962500	2.89573200
C	2.04298700	-1.96074400	-0.44886700
C	-0.81237100	-2.23419600	-0.10132900
C	1.25291700	-0.82088300	-0.23966800
C	1.37550300	-3.22001000	-0.43460500
C	0.00852300	-3.37083200	-0.25746600
C	-0.14346300	-0.90969600	-0.11960300
H	1.96743700	-4.11884800	-0.57194800
H	-0.41909100	-4.36929900	-0.24499700
C	4.31478200	-3.10167000	-0.64194300
H	5.37432400	-2.94475600	-0.86748200
H	3.94260400	-3.81981100	-1.37910800
H	4.23709100	-3.55525500	0.35207700
C	3.72475900	-1.21686000	-2.17634700
H	4.78762000	-1.03873500	-2.37987400
H	3.18775100	-0.27424500	-2.31676200
H	3.34499300	-1.93296800	-2.91386200
N	1.90880500	0.43175700	-0.07283000
C	-2.22174500	-2.18869000	0.08026200
C	-4.95859000	-1.54347500	0.38989900
C	-3.19501100	-3.21912800	0.14235000
C	-4.53046000	-2.90385800	0.29974900
C	-4.00351900	-0.54955000	0.32835800
H	-2.88148100	-4.25548500	0.05938800
C	1.38856500	1.69543200	-0.40183200
C	0.44068400	4.24183700	-0.99892800

C	2.27388600	2.69685500	-0.85287400
N	0.05763100	1.96512600	-0.30933100
C	-0.39195700	3.21946700	-0.59831900
C	1.80779500	3.96537800	-1.14859000
H	3.32156800	2.45182100	-0.97123900
H	-1.46361600	3.34982100	-0.48953700
H	2.49503500	4.72586700	-1.50635600
H	0.02757400	5.22204900	-1.20848600
Pt	-1.38850800	0.54571500	0.03015600
H	-5.26782900	-3.69940400	0.34646500
H	-6.00089500	-1.26799200	0.49870900
N	-2.70337600	-0.88151200	0.20375700
C	-4.25665500	0.95636300	0.36818300
O	-3.16786600	1.69881900	0.25385000
O	-5.39412100	1.38315000	0.48834400

Pt(*bp*-6)_S_0

C	-4.23357600	1.29923200	-0.33079600
C	-4.37509700	0.12043000	0.63702300
C	-4.52245600	-2.13246800	2.32851300
C	-5.49056000	-0.10147600	1.45334100
C	-3.32128100	-0.80980100	0.69276100
C	-3.39081100	-1.91977100	1.54626300
C	-5.57596900	-1.21861200	2.28525700
H	-6.31372400	0.60419200	1.43943300
H	-2.54938600	-2.60344300	1.60307000
H	-6.45803900	-1.36741200	2.90177200
H	-4.56749400	-2.99559800	2.98695300
C	-2.77841400	1.77909400	-0.24211500
C	-0.06460700	2.55923000	-0.17638900
C	-1.74380600	0.81484700	-0.20127300

C	-2.41435200	3.12821500	-0.23649400
C	-1.07431400	3.52011000	-0.18903300
C	-0.40016700	1.18059100	-0.21749600
H	-3.18055400	3.89510300	-0.25803200
H	-0.83356400	4.57951100	-0.14682600
C	-5.24107400	2.42009800	-0.02402200
H	-6.26870600	2.05436200	-0.11820000
H	-5.13360300	3.23929500	-0.74099200
H	-5.10827600	2.82557700	0.98459700
C	-4.51134400	0.79733900	-1.77872600
H	-5.53622900	0.41556700	-1.86125700
H	-3.82323800	-0.00125500	-2.06996300
H	-4.38807300	1.62165400	-2.49012600
N	-2.14655900	-0.56589200	-0.07552900
C	1.38401700	2.81308600	-0.04773600
C	4.17269100	2.99665200	0.15234600
C	2.15339300	1.62202700	0.07025500
C	2.00773600	4.06223400	-0.04644100
C	3.40133000	4.15080200	0.05765000
C	3.52926500	1.75218100	0.15308200
H	1.42031300	4.97204300	-0.14007200
C	-1.52035100	-1.63123900	-0.71787500
C	-0.33290000	-3.68823200	-2.15532700
C	-2.31521700	-2.65484100	-1.28810100
N	-0.16890300	-1.67441000	-0.82770400
C	0.38631000	-2.66391600	-1.57042600
C	-1.72516800	-3.68434500	-1.99469700
H	-3.39156900	-2.59780700	-1.18513200
H	1.46300500	-2.60689300	-1.68080200
H	-2.34102200	-4.45650800	-2.44707200

H	0.17759400	-4.45568300	-2.72668800
C	4.17267300	-0.62176400	0.45440700
C	3.92938700	-3.29932900	1.05436100
N	2.96228300	-1.20102900	0.33222000
C	5.31672200	-1.35994800	0.83151000
C	5.19724000	-2.70190200	1.12717600
C	2.86244700	-2.51614000	0.66209000
H	6.06876500	-3.27686800	1.42644000
H	1.86242900	-2.92831700	0.60263400
H	3.77385300	-4.34372200	1.30139300
Pt	1.14002200	-0.06729800	-0.12867000
H	3.88651300	5.12304700	0.05768300
H	5.25534700	3.03941800	0.22307000
O	4.42305900	0.67002900	0.21813500
H	6.26127400	-0.83220700	0.89183100

Pt(*bp*-6)_T_1

C	-4.22338300	1.25765600	-0.40716300
C	-4.37411700	0.11277500	0.60121000
C	-4.52484100	-2.07412200	2.37592800
C	-5.49170100	-0.07617300	1.42399800
C	-3.31975900	-0.81386900	0.69613300
C	-3.39138100	-1.89225900	1.58865600
C	-5.57776000	-1.16088400	2.29691500
H	-6.31536300	0.62781800	1.38036000
H	-2.55042200	-2.57369700	1.67010300
H	-6.46154300	-1.28745900	2.91603700
H	-4.57232300	-2.91190300	3.06607300
C	-2.77671400	1.74197700	-0.28908200
C	-0.05294100	2.58177100	-0.17257700

C	-1.74361800	0.78425700	-0.21701500
C	-2.41242100	3.12974900	-0.28583100
C	-1.11055200	3.54747900	-0.23293800
C	-0.39940500	1.15237900	-0.21592900
H	-3.19880400	3.87564700	-0.32274200
H	-0.88323200	4.60936100	-0.21176800
C	-5.24489200	2.38116700	-0.15884100
H	-6.26689700	2.00235200	-0.26100100
H	-5.12991300	3.17646500	-0.90147600
H	-5.13836200	2.82185300	0.83821800
C	-4.46943800	0.70731100	-1.84448700
H	-5.49247200	0.32170300	-1.93561900
H	-3.77496500	-0.09989000	-2.09239900
H	-4.33234100	1.50719900	-2.58118900
N	-2.13916000	-0.58962100	-0.06928900
C	1.31530800	2.83327800	-0.00686100
C	4.12957700	3.01215200	0.18212300
C	2.13266000	1.61281500	0.06861800
C	1.95840900	4.11701300	0.06454700
C	3.32468100	4.18880800	0.15135300
C	3.51020100	1.75983600	0.13633300
H	1.36431600	5.02544000	0.03186000
C	-1.50061400	-1.66941900	-0.68049300
C	-0.28309900	-3.75388600	-2.04451600
C	-2.27904700	-2.72111600	-1.20837800
N	-0.14387400	-1.68440700	-0.79543800
C	0.42224100	-2.69658600	-1.51105500
C	-1.67749200	-3.77313700	-1.87759700
H	-3.35583300	-2.67486300	-1.10297100
H	1.49543600	-2.62166000	-1.64065500

H	-2.28179400	-4.57140000	-2.29771500
H	0.23901200	-4.53179300	-2.59123400
C	4.17612100	-0.60582700	0.39977300
C	3.95149000	-3.27076100	1.03811100
N	2.95508500	-1.17816500	0.33264400
C	5.33138400	-1.33776400	0.73032100
C	5.22599900	-2.68081600	1.04483500
C	2.86816200	-2.49254800	0.68875200
H	6.10833200	-3.25511300	1.31009600
H	1.86563200	-2.90223700	0.68400600
H	3.80307600	-4.31134400	1.30576900
Pt	1.13631400	-0.05652500	-0.12629300
H	3.81793000	5.15625800	0.19557100
H	5.21070100	3.07509600	0.24335300
O	4.40962300	0.68981800	0.14004000
H	6.27762100	-0.80962800	0.74341500

Pt(*bp*-7)_S_0

C	-4.25611300	1.06317900	0.36138000
C	-6.19355600	-0.83478800	1.00410700
C	-5.55353900	1.48013400	0.67336100
C	-3.94640400	-0.32165900	0.33657700
C	-4.90502400	-1.27455300	0.69117600
C	-6.52270000	0.52705400	0.98104200
H	-5.79560100	2.53925600	0.69176800
H	-4.66430600	-2.32934100	0.75825100
H	-7.53324300	0.84175800	1.22573900
H	-6.94700900	-1.56726000	1.28009800
C	-3.02816000	1.78954900	0.10227000
C	-0.34706300	2.53706300	-0.21326700
C	-2.00812700	0.82786300	-0.05798800

C	-2.69326900	3.14819700	0.05583400
C	-1.35530000	3.51194000	-0.10893600
C	-0.67527100	1.15870300	-0.20199500
H	-3.45869000	3.91099600	0.17008500
H	-1.09305300	4.56699300	-0.11356000
N	-2.57038700	-0.47894000	0.02545200
C	1.11035100	2.77075700	-0.25975500
C	3.90924500	2.88808800	-0.40081800
C	1.86907200	1.56881300	-0.15797300
C	1.75595300	3.99919800	-0.41181200
C	3.15406900	4.05431400	-0.48062300
C	3.24644800	1.66431100	-0.23942800
H	1.17987900	4.91732300	-0.49524800
C	-1.97363300	-1.63421700	-0.47740400
C	-0.81098000	-3.92886200	-1.52200400
C	-2.77382900	-2.62517100	-1.08843800
N	-0.61999000	-1.77502900	-0.42782900
C	-0.08100500	-2.89684300	-0.96020000
C	-2.19794900	-3.77534100	-1.59591100
H	-3.83460200	-2.45133400	-1.19965700
H	1.00083600	-2.94265100	-0.93880200
H	-2.81994800	-4.52734900	-2.07303800
H	-0.30442400	-4.80231400	-1.91731900
C	3.88353800	-0.65543700	0.31480900
C	3.67279300	-3.14085000	1.48349500
N	2.65919400	-1.20055300	0.45392900
C	5.05292600	-1.34853100	0.69368200
C	4.94889300	-2.59733500	1.27291700
C	2.57716200	-2.41039000	1.06673300
H	5.84149200	-3.13562600	1.57814300

H	1.56962900	-2.77906400	1.21996700
H	3.53301300	-4.10305400	1.96366300
Pt	0.82492100	-0.11187500	-0.07004300
H	3.65481800	5.01079100	-0.60302000
H	4.99318300	2.90644600	-0.46105100
O	4.11186800	0.55505600	-0.21018000
H	6.00640200	-0.85925500	0.53292600

Pt(*bp*-7)_T_1

C	4.23435200	1.06387400	-0.33636200
C	6.17583400	-0.83330700	-1.02496000
C	5.54731400	1.48443100	-0.64751600
C	3.93223400	-0.33932400	-0.33085900
C	4.88941400	-1.28088700	-0.70927800
C	6.50322400	0.53647700	-0.97578400
H	5.79376800	2.54249300	-0.64514300
H	4.64934900	-2.33442700	-0.79427900
H	7.51384200	0.85223600	-1.22046500
H	6.92821900	-1.55668200	-1.32504600
C	3.03249300	1.76437000	-0.06742200
C	0.32877200	2.56524100	0.22611900
C	2.00422400	0.80079900	0.08842900
C	2.68561500	3.16338200	-0.00039100
C	1.37925100	3.54267100	0.15822100
C	0.67700000	1.12843200	0.21391200
H	3.46824400	3.91215100	-0.08639700
H	1.12917500	4.59954700	0.19033700
N	2.56683400	-0.50081800	-0.00109800
C	-1.06477700	2.78873100	0.23276700
C	-3.88370000	2.89746900	0.33619500

C	-1.85015400	1.56150900	0.15681400
C	-1.73710700	4.04464200	0.32341900
C	-3.11384800	4.08476400	0.37768000
C	-3.23151800	1.66790500	0.22887300
H	-1.16410600	4.96605100	0.37394300
C	1.95560800	-1.66531000	0.46374200
C	0.76531400	-3.97222400	1.44145800
C	2.74512000	-2.68746600	1.03088200
N	0.58997700	-1.77264200	0.42970400
C	0.04472500	-2.91261500	0.93403100
C	2.16256000	-3.84665300	1.50685200
H	3.80917100	-2.52850100	1.13589700
H	-1.03786500	-2.93945700	0.93693600
H	2.77621900	-4.62042600	1.95801000
H	0.24831200	-4.84957100	1.81442400
C	-3.87599100	-0.65100800	-0.29223500
C	-3.67270600	-3.12480600	-1.47631100
N	-2.64918100	-1.19055100	-0.44353700
C	-5.04643100	-1.33934500	-0.66014100
C	-4.94867200	-2.58820900	-1.24750800
C	-2.57210200	-2.39706900	-1.07010100
H	-5.84330800	-3.12624300	-1.54605300
H	-1.56626900	-2.76178200	-1.24049300
H	-3.53581900	-4.08307400	-1.96538100
Pt	-0.81781500	-0.10471700	0.08873900
H	-3.62725200	5.03913600	0.45780300
H	-4.96724700	2.92866400	0.38347200
O	-4.09206100	0.56097800	0.24486000
H	-5.99805700	-0.85078000	-0.48670900

Pt(*bp*-8)_S_0

C	-5.07770300	1.10717800	0.08530000
C	-7.09462400	-0.75960300	0.54530500
C	-6.39121100	1.54479500	0.27949400
C	-4.78824700	-0.28207000	0.08460700
C	-5.79034300	-1.21978800	0.34938000
C	-7.39928900	0.60728800	0.49539000
H	-6.61679800	2.60772500	0.27846100
H	-5.57472500	-2.27840300	0.43583200
H	-8.42288600	0.93776000	0.64756400
H	-7.88135300	-1.48040300	0.75002400
C	-3.82087300	1.81414900	-0.05959900
C	-1.11450100	2.52320700	-0.12505000
C	-2.80448900	0.83816500	-0.13765000
C	-3.46572900	3.16822400	-0.06404600
C	-2.11414000	3.51277200	-0.09943800
C	-1.45812400	1.15100400	-0.16958900
H	-4.22825800	3.94074100	-0.01352700
H	-1.83923800	4.56395200	-0.06705300
N	-3.39271700	-0.45812200	-0.10332300
C	0.34138400	2.74441900	-0.02591400
C	3.12100200	2.89425500	0.18200300
C	1.10230400	1.53988900	0.04408200
C	0.97130400	3.98874100	0.01518400
C	2.35899100	4.05712000	0.15324800
C	2.49798100	1.63566000	0.06170600
H	0.38913600	4.90498100	-0.03666100
N	3.32233500	0.45380900	0.01337200
C	5.48297600	1.33278600	-1.01835200
C	6.61192300	-1.09281500	-0.07387000

C	4.69871600	0.41737400	-0.30497900
C	6.82720200	1.02838900	-1.22322500
C	7.39835200	-0.16195500	-0.74269000
C	5.25683900	-0.81071700	0.13313900
H	7.44277400	1.72948100	-1.77995100
H	8.45123600	-0.36394100	-0.91583400
C	-2.76408600	-1.63309800	-0.51031400
C	-1.54162200	-3.98102800	-1.34117700
C	-3.51116800	-2.62798700	-1.17895000
N	-1.42701500	-1.79130300	-0.30869500
C	-0.85699400	-2.94209700	-0.73615800
C	-2.90681400	-3.80501300	-1.58071800
H	-4.54818200	-2.43776100	-1.41613100
H	0.21330400	-3.00768800	-0.58878200
H	-3.48638000	-4.56131900	-2.10242700
H	-1.01254600	-4.87748500	-1.64494200
C	2.99492100	-0.79275600	0.52189100
C	2.78485000	-3.25879600	1.66639300
N	1.75966100	-1.25143900	0.77935600
C	4.17145800	-1.58013700	0.68774200
C	4.05771300	-2.83376800	1.27554000
C	1.68121800	-2.45583500	1.39031200
H	4.93001100	-3.46213100	1.43223300
H	0.67860900	-2.78047700	1.64515800
H	2.63744000	-4.21619000	2.15444100
Pt	0.01458000	-0.12936800	0.09834400
H	2.85345200	5.02057700	0.24321700
H	5.06013300	2.23964100	-1.43041200
H	4.19045700	2.96695700	0.33166200

Pt(*bp*-8)_ T_1

C	5.04608700	1.11961400	-0.08208400
C	7.07085300	-0.73886800	-0.61190500
C	6.37097100	1.56538100	-0.28366900
C	4.76932600	-0.28717400	-0.10419300
C	5.77186000	-1.21072400	-0.40433000
C	7.36836200	0.63615900	-0.53359100
H	6.59652700	2.62783100	-0.25951500
H	5.55962800	-2.26813000	-0.51108400
H	8.38969100	0.97104700	-0.69353400
H	7.85848500	-1.44763000	-0.85009300
C	3.81243000	1.79810500	0.09042200
C	1.08441900	2.54932500	0.16224100
C	2.79344000	0.81749200	0.16444300
C	3.43984800	3.18881000	0.12822000
C	2.11780500	3.54526800	0.17609900
C	1.45163300	1.12233200	0.19218300
H	4.21401500	3.95092600	0.10665000
H	1.84905200	4.59779500	0.18613000
N	3.38482800	-0.47214900	0.11267500
C	-0.30607100	2.75501900	0.02541700
C	-3.09941200	2.87763600	-0.24685600
C	-1.08955000	1.52318800	-0.04209100
C	-0.96056300	4.01668000	-0.06672100
C	-2.32511200	4.06179900	-0.22768600
C	-2.49024300	1.62593300	-0.08056800
H	-0.38358800	4.93577800	-0.02511600
N	-3.31225000	0.45117400	-0.01328200
C	-5.48132800	1.35212500	0.97922200
C	-6.60425500	-1.08479800	0.05566800
C	-4.69376600	0.42422700	0.28957800

C	-6.83007300	1.05423500	1.17300600
C	-7.39605400	-0.14171000	0.70236700
C	-5.24584800	-0.80928400	-0.13986200
H	-7.45097100	1.76438500	1.71192500
H	-8.45149900	-0.33940200	0.86515200
C	2.75412000	-1.65437700	0.49922600
C	1.52378000	-4.00308800	1.30683900
C	3.50710800	-2.67419100	1.11804600
N	1.40135700	-1.78273300	0.33504400
C	0.83339800	-2.94447300	0.75622300
C	2.90483600	-3.85414300	1.51055700
H	4.55270000	-2.49806400	1.32807500
H	-0.24250900	-2.99245000	0.64917100
H	3.48778400	-4.62772500	2.00113600
H	0.99110600	-4.89890100	1.60658400
C	-2.98320200	-0.80185000	-0.50828100
C	-2.76042200	-3.27392900	-1.62657400
N	-1.74097800	-1.25537900	-0.75130300
C	-4.15564500	-1.58714100	-0.67440800
C	-4.03896500	-2.85140500	-1.24765400
C	-1.65908900	-2.46834400	-1.35940400
H	-4.90890600	-3.48190400	-1.40554900
H	-0.65637600	-2.79029000	-1.61491800
H	-2.60791100	-4.23459600	-2.10706400
Pt	-0.01088600	-0.12751600	-0.07236300
H	-2.83193800	5.01638000	-0.34148000
H	-5.05989000	2.26522700	1.37987700
H	-4.16392400	2.95134500	-0.42569300
H	-7.02712800	-2.02874000	-0.27760400

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