Supporting Information

Carbazolylpyridine (*cp*)-Based Tetradentate Platinum(II) Complexes Containing Fused 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 125 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 NMR spectra were recorded with TMS (δ = 0.00 ppm) or $CDCl_3$ (δ = 7.26 ppm) as internal references; ^{13}C NMR spectra were recorded with TMS (δ = 0.00 ppm) or $CDCl_3$ (δ = 77.00 ppm) as internal references. If DMSO-d_6 was used as solvent, ^{1}H NMR spectra were recorded with TMS (δ = 0.00 ppm) or DMSO-d_6 (δ = 2.50 ppm) as internal references; ^{13}C NMR spectra were recorded with TMS (δ = 0.00 ppm) and DMSO-d_6 (δ = 39.52 ppm) as internal references. 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.

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.

Electrochemistry. Cyclic voltammetry and different pulsed voltammetry were performed using a CH1760E electrochemical analyzeraccording previous report. 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^+). The reversibility of reduction or oxidation was determined using CV. 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.

Photophysical Measurements. The absorption spectra were measured on an Agilent 8453 UV−VS Spectrometer. Steady state emission experiments and lifetime measurements were performed on an Edinburgh FS5 Spectrofluorometer. Quantum efficiencies of the samples were measured using an Edinburgh FS5 Spectrofluorometer equipped with an integrating sphere.

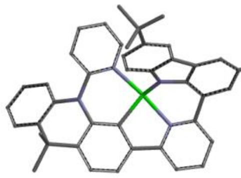
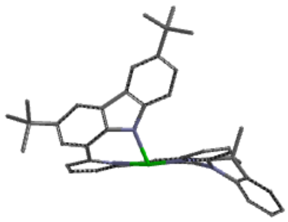
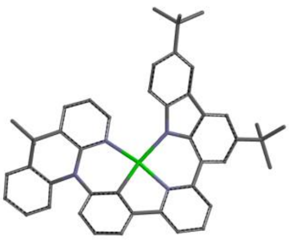
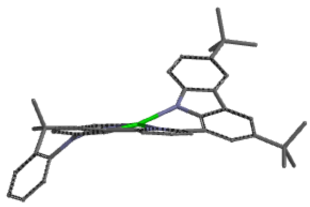
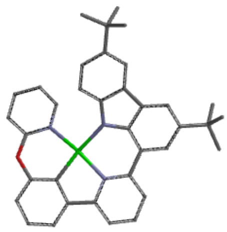
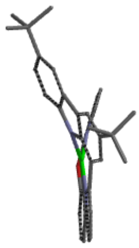
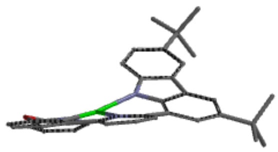
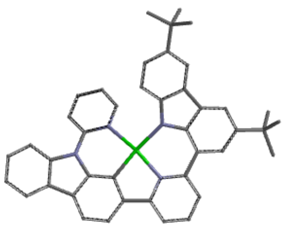
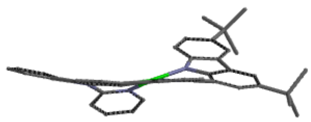
X-ray Crystallography. X-ray diffraction data were collected at 170 K on a Bruker D8 Venture diffractometer using graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å) from a rotating anode generator.

Table S1. Crystal Data and Structure Refinement for Pt(*cp*-1).

Identification code	240830_Pt_cp_1
Empirical formula	$C_{45}H_{42}N_4Pt$
Formula weight	833.91
Temperature/K	170.00
Crystal system	monoclinic
Space group	C2/c
a/Å	38.7590(18)
b/Å	19.3350(9)
c/Å	12.2485(6)
α/°	90
β/°	100.097(2)
γ/°	90
Volume/Å^3	9036.9(7)
Z	8
ρ_{calc}g/cm^3	1.226
μ/mm^{-1}	4.138
F(000)	3344.0
Crystal size/mm^3	0.05 × 0.03 × 0.02
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	7.488 to 121.746
Index ranges	$-50 \le h \le 50$, $-25 \le k \le 11$, $-15 \le l \le 15$
Reflections collected	38379
Independent reflections	10392 [R_{int} = 0.0603, R_{sigma} = 0.0879]
Data/restraints/parameters	10392/81/488
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0445, wR_2 = 0.1035
Final R indexes [all data]	R_1 = 0.0681, wR_2 = 0.1130
Largest diff. peak/hole / e Å^{-3}	1.57/-1.43

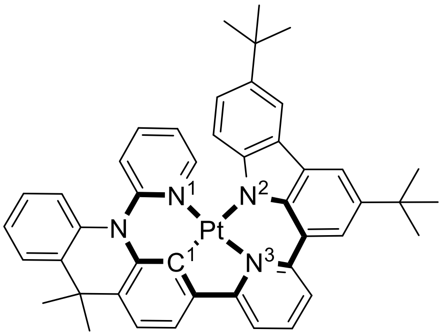
Table S2. Crystal Data and Structure Refinement for Pt(*cp*-2).

Identification code	240830_Pt_cp_2
Empirical formula	$C_{45}H_{42}N_4Pt$
Formula weight	833.91
Temperature/K	170.00
Crystal system	triclinic
Space group	P-1
a/Å	12.2751(6)
b/Å	16.9466(7)
c/Å	19.2822(8)
α/°	80.219(2)
β/°	87.400(2)
γ/°	74.135(2)
Volume/$Å^3$	3802.2(3)
Z	4
$\rho_{calc}g/cm^3$	1.457
μ/mm^{-1}	4.917
F(000)	1672.0
Crystal size/mm^3	0.05 × 0.03 × 0.01
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	4.046 to 107.804
Index ranges	$-14 \le h \le 14, -20 \le k \le 20, -23 \le l \le 22$
Reflections collected	48123
Independent reflections	13879 [R_{int} = 0.0739, R_{sigma} = 0.1460]
Data/restraints/parameters	13879/174/979
Goodness-of-fit on F^2	0.799
Final R indexes [I>=2σ (I)]	R_1 = 0.0425, wR_2 = 0.1131
Final R indexes [all data]	R_1 = 0.0604, wR_2 = 0.1273
Largest diff. peak/hole / e $Å^{-3}$	1.65/-1.02

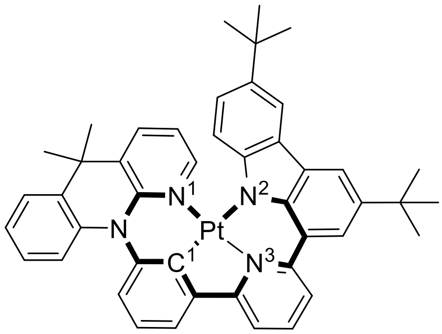
Table S3. DFT Calculations for Pt(II) Complexes[a]			
Complexes	Front view	Side view	Top view
Pt(*cp*-1)			
Pt(*cp*-2)			
Pt(*cp*-3)			
Pt(*cp*-4)			

[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.

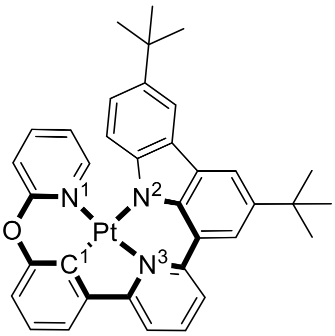
Table S4. Selected Bond Lengths (Å), Bond Angles (°) and Dihedral Angles (°) for Tetradentate Pt(II) Complexes Based on the DFT Calculations.



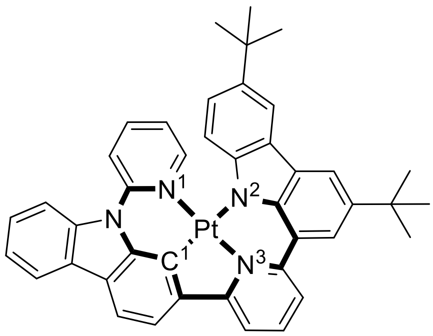
Pt(CzPyAcPy)
Pt(*cp*-1)



Pt(CzPyPhAAc)
Pt(*cp*-2)



Pt(CzPyPhOPy)
Pt(*cp*-3)



Pt(CzPyCzPy)
Pt(*cp*-4)

metal complexes	Pt–N^1	Pt –N^2	Pt –N^3	Pt –C^1
Pt(*cp*-1)	2.077	2.016	2.128	1.992
Pt(*cp*-2)	2.084	2.145	2.058	1.970
Pt(*cp*-3)	2.078	2.113	2.060	1.970
Pt(*cp*-4)	2.103	2.114	2.062	1.956

metal complexes	N^1– Pt – C^1	C^1– Pt – N^3	N^3–Pt–N^2	N^2–Pt–N^1	N^1–Pt–N^3	C^1–Pt–N^2	dihedral angle^a
Pt(*cp*-1)	93.49	80.87	83.86	92.38	170.73	117.68	48.52
Pt(*cp*-2)	91.21	82.12	88.64	99.51	170.02	163.74	36.99
Pt(*cp*-3)	89.88	81.87	91.15	98.94	165.73	167.45	44.41
Pt(*cp*-4)	89.60	81.17	91.59	99.58	164.65	167.27	51.88

[a]Dihedral angle between terminal pyridine and carbazole 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.

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

excited state	energy [eV]	wavelength [nm]	*f*	major contributions
S_1	2.193	565	0.0433	HOMO → LUMO (99%)
S_2	2.596	478	0.0713	HOMO → LUMO+1 (97%)
T_1	2.018	614	0.0000	HOMO→ LUMO (85%) HOMO → LUMO+1 (10%)
T_2	2.290	541	0.0000	HOMO→ LUMO (11%) HOMO → LUMO+1 (62%) HOMO → LUMO+2 (18%)
T_3	2.534	489	0.0000	HOMO-3 → LUMO+2 (3%) HOMO-2 → LUMO (6%) HOMO → LUMO+1 (19%) HOMO → LUMO+2 (63%)
T_4	2.608	475	0.0000	HOMO-1 → LUMO (23%) HOMO-1 → LUMO+1 (30%) HOMO-1 → LUMO+2 (9%)
T_5	2.632	471	0.0000	HOMO-3 → LUMO (8%) HOMO-2 → LUMO (48%) HOMO-1→ LUMO+1 (11%)
T_6	2.759	449	0.0000	HOMO-3 → LUMO (30%) HOMO-2 → LUMO (18%)
T_7	2.934	423	0.0000	HOMO-3 → LUMO (3%) HOMO-1 → LUMO (6%) HOMO → LUMO+3 (75%)
T_8	2.954	420	0.0000	HOMO-3 → LUMO (7%) HOMO-1 → LUMO (58%) HOMO-1 → LUMO+1 (8%)

Table S6. TD-B3LYP/SV/SVP/def2-TZVP results of **Pt(*cp*-2)** at optimized S_0 geometry.

excited state	energy [eV]	wavelength [nm]	*f*	major contributions
S_1	2.230	556	0.0449	HOMO → LUMO (98%)
S_2	2.603	476	0.0835	HOMO → LUMO+1 (96%)
T_1	2.016	615	0.0000	HOMO→ LUMO (81%) HOMO → LUMO+1 (15%)
T_2	2.270	546	0.0000	HOMO-3→ LUMO+1 (2%) HOMO → LUMO (15%) HOMO → LUMO+1 (74%)
T_3	2.570	482	0.0000	HOMO-2 → LUMO (5%) HOMO → LUMO+2 (83%)
T_4	2.645	469	0.0000	HOMO-3 → LUMO (21%) HOMO-2 → LUMO (31%)
T_5	2.668	465	0.0000	HOMO-1 → LUMO (17%) HOMO-1→ LUMO+1 (52%)
T_6	2.812	441	0.0000	HOMO-3 → LUMO (23%) HOMO-2 → LUMO (37%)
T_7	3.039	408	0.0000	HOMO-2 → LUMO+1 (10%) HOMO-1 → LUMO (60%)
T_8	3.081	402	0.0000	HOMO-2 → LUMO (6%) HOMO → LUMO+3 (55%) HOMO → LUMO+4 (7%)

Table S7. TD-B3LYP/SV/SVP/def2-TZVP results of **Pt(*cp*-3)** at optimized S_0 geometry.

excited state	energy [eV]	wavelength [nm]	*f*	major contributions
S_1	2.213	560	0.0387	HOMO → LUMO (98%)
S_2	2.568	483	0.0817	HOMO → LUMO+1 (96%)
T_1	2.002	619	0.0000	HOMO→ LUMO (84%) HOMO → LUMO+1 (12%)
T_2	2.269	546	0.0000	HOMO→ LUMO (13%) HOMO → LUMO+1 (58%) HOMO → LUMO+2 (22%)
T_3	2.498	496	0.0000	HOMO → LUMO+1 (25%) HOMO → LUMO+1 (68%)
T_4	2.588	479	0.0000	HOMO-1 → LUMO (22%) HOMO-1 → LUMO+1 (41%) HOMO-1 → LUMO+2 (18%)
T_5	2.678	463	0.0000	HOMO-2 → LUMO (52%) HOMO-2→ LUMO+2 (15%)
T_6	2.940	422	0.0000	HOMO-2 → LUMO (8%) HOMO-1 → LUMO (64%) HOMO-1 → LUMO+1 (8%)
T_7	3.033	409	0.0000	HOMO-2 → LUMO (7%) HOMO-1 → LUMO (9%) HOMO → LUMO+2 (50%)
T_8	3.101	400	0.0000	HOMO-2 → LUMO (19%) HOMO-2 → LUMO+1 (11%) HOMO-2 → LUMO+2 (17%)

Table S8. TD-B3LYP/SV/SVP/def2-TZVP results of **Pt(*cp*-4)** at optimized S_0 geometry.

excited state	energy [eV]	wavelength [nm]	*f*	major contributions
S_1	2.086	594	0.0427	HOMO → LUMO (98%)
S_2	2.495	497	0.0336	HOMO → LUMO+1 (96%)
T_1	1.907	650	0.0000	HOMO→ LUMO (90%) HOMO → LUMO+2 (4%)
T_2	2.232	555	0.0000	HOMO→ LUMO+1 (30%) HOMO → LUMO+2 (58%)
T_3	2.418	513	0.0000	HOMO-2 → LUMO (40%) HOMO → LUMO+1 (24%) HOMO → LUMO+1 (16%)
T_4	2.424	512	0.0000	HOMO-2 → LUMO (28%) HOMO → LUMO+1 (39%) HOMO → LUMO+2 (14%)
T_5	2.590	479	0.0000	HOMO-1 → LUMO (26%) HOMO-1→ LUMO+2 (47%)
T_6	2.856	446	0.0000	HOMO-3 → LUMO (27%) HOMO-2 → LUMO (13%) HOMO-1 → LUMO (21%) HOMO → LUMO+3 (14%)
T_7	2.886	434	0.0000	HOMO-1 → LUMO (29%) HOMO → LUMO+3 (48%)
T_8	3.101	430	0.0000	HOMO → LUMO (23%) HOMO-1 → LUMO+3 (22%) HOMO-3 → LUMO+3 (26%)

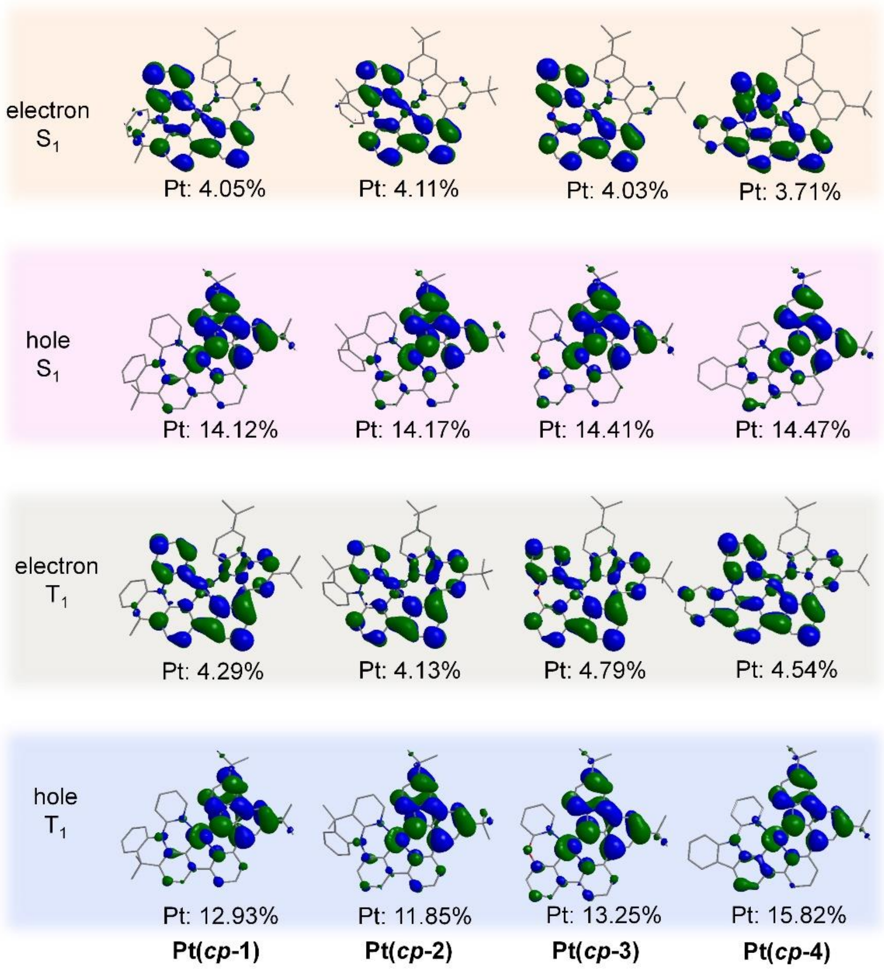


Figure S1. Natural transition orbital (NTO) analyses of *cp*-based Pt(II) complexes.

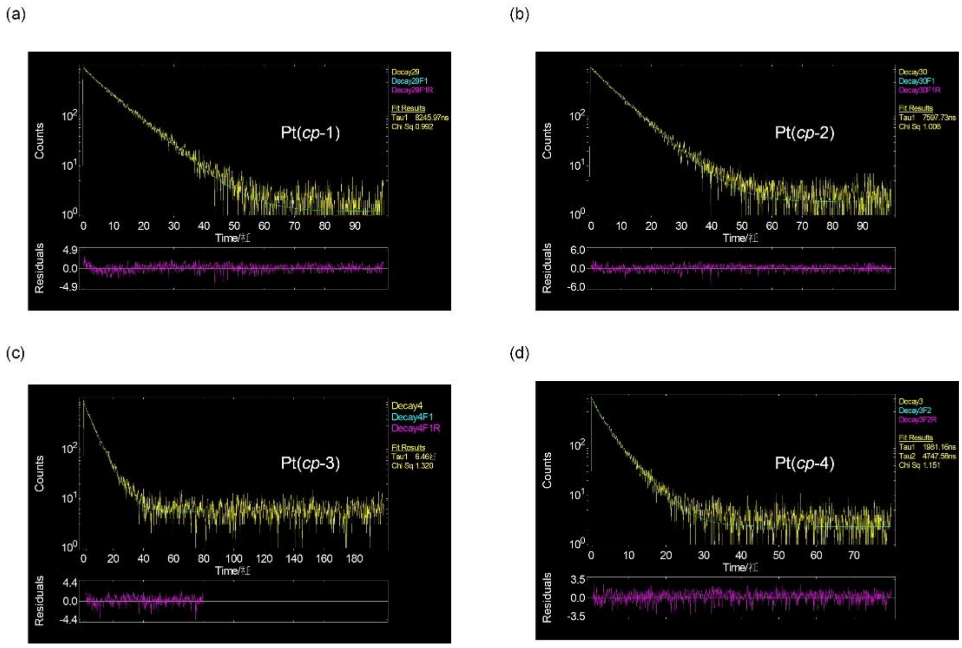
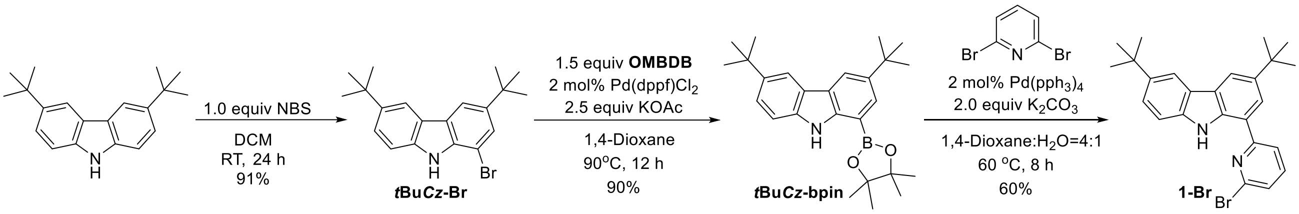


Figure S2. Time-resolved photoluminescence attenuation fitting of *cp*-based Pt(II) complexes in PMMA.

Experimental Procedures

1-bpin[1], **2-bpin**[1], **3-bpin**[2]**and 4-bpin**[3] were prepared according to previous reports.



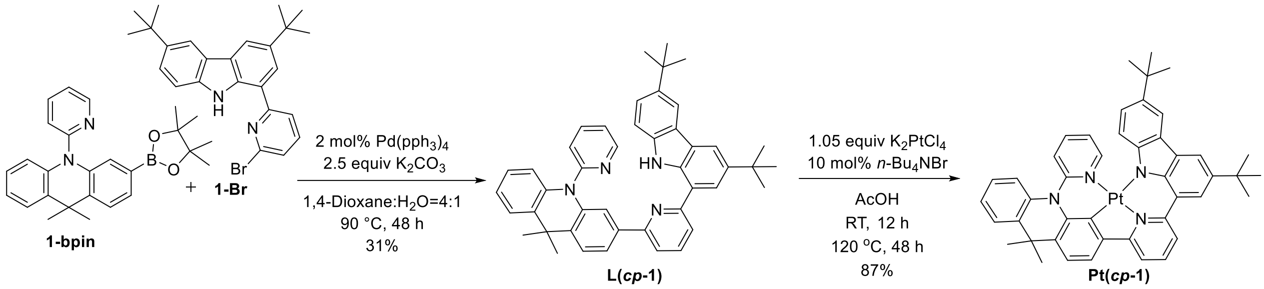
Synthesis of ***t*****Bu*****Cz*****-*****Br***: 3,6-di-*tert*-butyl-9*H*-carbazole (3.00 g, 10.74 mmol, 1.0 equiv), NBS (1.91 g, 10.74 mmol, 1.0 equiv) were added to a dry three-necked flask equipped with a magnetic stir bar. Then dichloromethane (30 mL) was added into the flask at room temperature. Then the flask was placed in an oil bath and the reaction mixture was stirred at room temperature for 24 hours, the reaction was monitored by TLC until the reaction was completed. The solvent was concentrated under reduced pressure and the residue was purified through column chromatography on silica gel (eluent: petroleum ether/dichloromethane = 30:1−10:1) to obtain the desired product as a white solid 3.5 g in 91% yield. ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 1.39 (d, J = 1.0 Hz, 18H), 7.45 (dd, J = 9.0, 0.5 Hz, 1H), 7.49 (dd, J = 8.5, 1.5 Hz, 1H), 7.57 (d, J = 2.0 Hz, 1H), 8.17 (d, J = 2.0 Hz, 1H), 8.19 (d, J = 1.5 Hz, 1H), 11.10 (s, 1H).

Synthesis of ***t*****Bu*****Cz*****-bpin: *t*****Bu*****Cz*****-Br** (3.50 g, 9.77 mmol, 1.0 equiv), **OMBDB** (3.72 g, 14.65 mmol, 1.5 equiv), KOAc (2.40 g, 24.42 mmol, 2.5 equiv) and Pd(dppf)Cl_2 (143 mg, 0.20 mmol, 2 mol%) 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) was added into the flask under nitrogen atmosphere at room temperature. Then the flask was placed in an oil bath and the reaction mixture was stirred at 90 °C for 12 hours, the reaction was monitored by TLC until the reaction was completed. The reaction 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 (eluent: petroleum ether/dichloromethane = 100:1) to obtain the desired product as a white solid 3.56 g in 90% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 1.44 (s, 12H), 1.46 (s, 9H), 1.48 (s, 9H), 7.40 (d, J = 9.0 Hz, 1H), 7.47 (dd, J = 8.5, 2.0 Hz, 1H), 7.89 (d, J = 2.0 Hz, 1H), 8.08 (d, J = 2.0 Hz, 1H), 8.22 (d, J = 1.5 Hz, 1H), 8.97 (s, 1H).

Synthesis of **1-Br**: ***t*****Bu*****Cz*****-bpin** (3.10 g, 7.65 mmol, 1.0 equiv), 2,6-dibromopyridine (1.99 g, 8.41

mmol, 1.1 equiv), K_2CO_3 (2.11 g, 15.29 mmol, 2.0 equiv), $Pd(PPh_3)_4$ (177 mg, 0.15 mmol, 2 mol%) 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 (40 mL) and H_2O (10 mL) were added into the flask under nitrogen atmosphere at room temperature. Then the flask was placed in an oil bath and the reaction mixture was stirred and heated at 60 °C for 8 hours, the reaction was monitored by TLC until the reaction was completed. The reaction mixture was cooled down to room temperature, and diluted with ethyl acetate. 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/dichloromethane = 30:1−20:1) to obtain the desired product as a white solid 2.00 g in 60% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 1.47 (s, 9H), 1.51 (s, 9H), 7.41 (dd, J = 7.5, 0.5 Hz, 1H), 7.49 (dd, J = 8.5, 1.0 Hz, 1H), 7.53 (dd, J = 8.5, 1.5 Hz, 1H), 7.67 (t, J = 7.5 Hz, 1H), 7.96 (d, J = 2.0 Hz, 1H), 8.00 (d, J = 7.5 Hz, 1H), 8.12 (t, J = 1.0 Hz, 1H), 8.21 (d, J = 1.0 Hz, 1H), 10.66 (s, 1H).

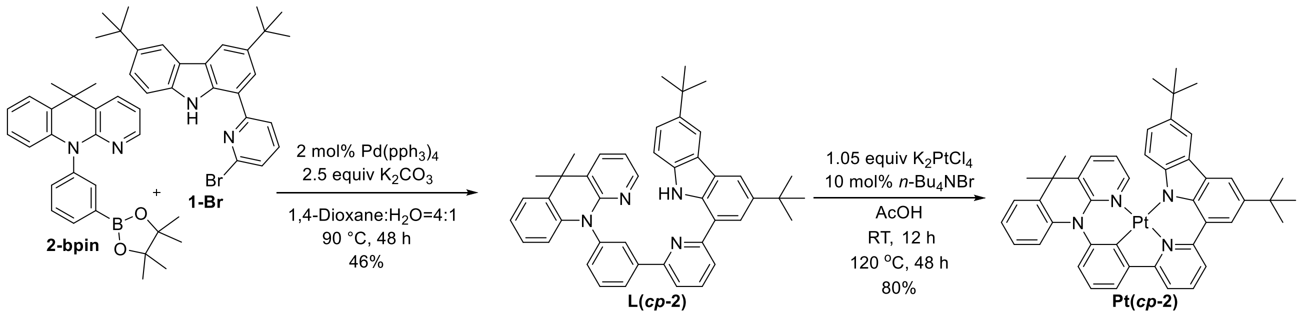
Scheme 2:



Synthesis of **L(*cp*-1)**: **1-Br** (278 mg, 0.64 mmol, 1.0 equiv), **1-bpin**[1] (290 mg, 0.70 mmol, 1.1 equiv), $Pd(pph_3)_4$ (14.76 mg, 0.01 mmol, 2 mol%), K_2CO_3 (220 mg, 1.60 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 (10 mL) and H_2O (2.5 mL) were added into the flask under nitrogen atmosphere at room temperature. Then the flask was placed in an oil bath and the reaction mixture was stirred and heated at 90 °C for 48 hours, the reaction was monitored by TLC until the reaction was completed. The reaction mixture was cooled down to room temperature, filtered and washed with ethyl acetate. 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 = 50:1−30:1) to obtain the desired product as a white solid 127 mg in 31% yield. ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 1.44 (s, 9H), 1.48 (s, 9H), 1.69 (s, 6H), 6.46 (dd, J = 8.0, 1.5 Hz, 1H), 7.03 (td, J = 7.5, 1.5 Hz, 1H), 7.07 (td, J = 7.5, 1.5 Hz, 1H), 7.22 (ddd, J = 7.5, 5.0, 1.0 Hz, 1H),7.43 (d, J = 2.0 Hz, 1H), 7.51 (dd, J = 9.0, 2.0 Hz, 1H), 7.55 (d, J = 8.5 Hz, 2H), 7.56 (dd, J = 8.0, 2.0 Hz, 1H), 7.72 (d, J = 2.0 Hz, 2H), 7.75 (dd, J = 4.5, 2.0 Hz, 1H), 7.77 (td, J = 7.5, 2.0 Hz, 1H), 7.95 (d, J = 1.5 Hz, 1H), 8.0 (t, J = 7.5 Hz, 1H), 8.07 (d, J = 7.5 Hz, 1H), 8.24 (d, J =1.5 Hz, 1H), 8.31−8.32 (m, 1H), 8.46 (ddd, J = 5.0, 2.5, 1.0 Hz, 1H),10.94 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 30.24, 32.09, 32.15, 34.72, 34.81, 36.61, 110.88, 115.41, 115.96, 116.91, 117.80, 118.17, 118.34, 119.60, 120.59, 120.68, 121.74, 121.86, 122.17, 122.45, 123.63, 124.73, 124.90, 125.53, 126.41, 133.16, 134.26, 137.20, 137.26, 138.20, 138.51, 139.28, 140.46, 141.00, 141.34, 141.87, 150.55, 155.21, 156.87, 157.83. HRMS (ESI): calcd for $C_{45}H_{45}N_4$ $[M+H]^+$ 641.3639, found 641.3621.

Synthesis of **Pt (*cp*-1)**: **L (*cp*-1)** (80 mg, 0.12 mmol, 1.0 equiv), K_2PtCl_4 (54.40 mg, 0.13 mmol, 1.05 equiv), *n*-Bu_4NBr (4.02 mg, 0.01 mmol, 10 mol%) 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 (10 mL) was 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 the reaction mixture was stirred and heated at 120 °C for 48 hours. The reaction mixture was cooled down to room temperature, filtered and washed with dichloromethane. The filtrate was concentrated under reduced pressure and the residue was purified through column chromatography on silica gel (eluent: petroleum ether/dichloromethane = 3:1−2:1) to obtain the desired product as a red solid 90.57 mg in 87% yield. ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 1.34 (s, 3H), 1.42 (s, 9H), 1.57 (s, 9H), 1.96 (s, 3H), 6.90−6.93(m, 1H), 7.07 (d, J = 8.5 Hz, 1H), 7.24 (dd, J = 8.5, 2.0 Hz, 1H), 7.30 (dd, J = 7.0, 1.0 Hz, 1H), 7.33 (d, J = 8.0 Hz, 1H), 7.38 (td, J = 7.5, 1.5 Hz, 1H), 7.53 (dd, J = 7.5, 0.5 Hz, 1H), 7.62 (d, J = 10.5 Hz, 1H), 7.64 (dd, J = 7.5, 1.0 Hz, 1H), 7.80 (d, J = 8.5 Hz, 1H), 7.97−8.00 (m, 1H), 8.19 (dd, J = 8.0, 1.0 Hz, 1H), 8.26 (d, J = 2.0 Hz, 1H), 8.29 (t, J = 8.0 Hz, 1H), 8.48 (d, J = 1.0 Hz, 1H), 8.50 (d, J = 1.5 Hz, 1H), 8.76 (dd, J = 6.0, 1.5 Hz, 1H), 8.81(d, J = 8.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 22.88, 32.18, 32.39, 32.56, 34.59, 34.86, 36.94, 115.17, 115.49, 115.75, 117.44, 118.01, 118.25, 119.57, 119.80, 120.04, 120.13, 120.86, 121.74, 122.04, 124.13, 124.86, 125.71, 126.66, 127.11, 134.39, 134.82, 135.64, 137.12, 137.22, 137.93, 139.15, 140.13, 140.72, 140.89, 143.38, 147.13, 152.20, 153.14, 156.68, 166.92. HRMS (ESI): calcd for $C_{45}H_{43}N_4Pt$ $[M+H]^+$ 834.3130, found 834.3116.

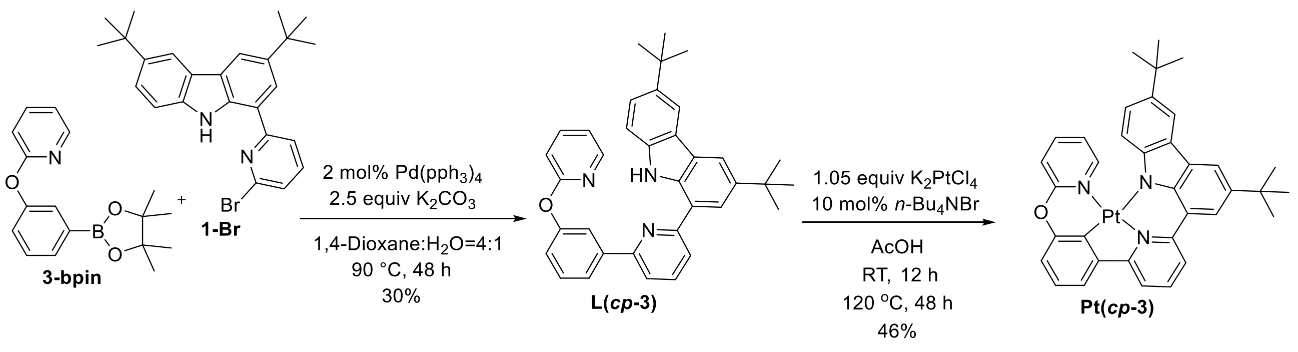
Scheme 3:



Synthesis of **L (*cp*-2)**: **1-Br** (300 mg, 0.69 mmol, 1.0 equiv), **2-bpin**[1] (313 mg, 0.76 mmol, 1.1 equiv), $Pd(pph_3)_4$ (16 mg, 0.01 mmol, 2 mol%), K_2CO_3 (238 mg, 1.72 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 (8 mL) and H_2O (2 mL) were added into the flask under nitrogen atmosphere at room temperature. Then the flask was placed in an oil bath and the reaction mixture was stirred and heated at 90 °C for 48 hours, the reaction was monitored by TLC until the reaction was completed. The reaction mixture was cooled down to room temperature, filtered and washed with ethyl acetate. 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 = 50:1−30:1) to obtain the desired product as a white solid 203 mg in 46% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 1.37 (s, 9H), 1.44 (s, 9H), 1.60 (s, 6H), 6.39 (dd, J = 9.5, 2.5 Hz, 1H), 6.62 (d, J =10.5 Hz, 1H), 6.80 (dd, J = 9.5, 6.0 Hz, 1H), 6.96 (td, J = 6.0, 3.5 Hz, 1H), 6.99 (td, J = 9.0, 2.5 Hz, 1H), 7.20 (dd, J = 10.5, 2.5 Hz, 1H), 7.43 (dd, J = 8.0, 1.5 Hz, 1H), 7.45 (dd, J = 9.5, 1.5 Hz, 1H), 7.61 (d, J = 5.5 Hz, 1H), 7.63 (dd, J = 7.5, 2.5 Hz, 1H), 7.74 (t, J = 9.5 Hz, 1H), 7.81 (t, J = 9.5 Hz, 1H), 7.94 (d, J =10.5 Hz, 1H), 7.96 (d, J = 2.5 Hz, 1H), 7.99 (dd, J = 6.0, 2.0 Hz, 2H), 8.08−8.10 (m, 2H), 8.12 (dt, J =10.0, 2.0 Hz, 1H), 11.11 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 31.07, 32.05, 32.14, 34.63, 34.80, 36.32, 110.50, 115.14, 115.89, 116.69, 118.03, 118.20, 118.48, 119.28, 120.69, 121.60, 122.34, 123.56, 124.81, 124.97, 125.16, 126.28, 127.01, 129.34, 130.09, 130.73, 131.94, 133.11, 137.17, 137.51, 138.12, 140.91, 141.38, 141.59, 141.78, 142.34, 145.67, 151.71, 155.81, 158.00. HRMS (ESI): calcd for $C_{45}H_{45}N_4$ $[M+H]^+$ 641.3639, found 641.3628.

Synthesis of **Pt (*cp*-2)**: A mixture of **L(*cp*-2)** (100 mg, 0.16 mmol, 1.0 equiv), K_2PtCl_4 (68 mg, 0.16 mmol, 1.05 equiv), *n*-Bu_4NBr (5.03 mg, 0.02 mmol, 10 mol%) 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 (10 mL) was 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 the reaction mixture was stirred and heated at 120 °C for 48 hours. The reaction mixture was cooled down to room temperature, filtered and washed with dichloromethane. The filtrate was concentrated under reduced pressure and the residue was purified through column chromatography on silica gel (eluent: petroleum ether/dichloromethane = 3:1−2:1) to obtain the desired product as a orange solid 104 mg in 80% yield. ^1H NMR (500 MHz, $CDCl_3$): δ (ppm) 1.39 (s, 3H), 1.40 (s, 9H), 1.60 (s, 9H), 2.00 (s, 3H), 6.67 (dd, J = 9.5, 7.5 Hz, 1H), 6.82 (d, J = 11.0 Hz, 1H), 7.04 (dd, J = 11.0, 2.5 Hz, 1H), 7.16 (s, 1H), 7.17 (d, J = 2.5 Hz, 1H), 7.26−7.29 (m, 2H), 7.47−7.49 (m, 1H), 7.54−7.59 (m, 2H), 7.87−7.90 (m, 2H), 8.10 (t, J = 9.5 Hz, 1H), 8.18 (d, J = 2.0 Hz, 1H), 8.42 (s, 1H), 8.44 (d, J = 2.5 Hz, 1H), 8.57 (d, J =10.0 Hz, 1H), 8.82 (dd, J = 8.0, 2.0 Hz, 1H). HRMS (ESI): calcd for $C_{45}H_{43}N_4Pt$ $[M+H]^+$ 834.3130, found 834.3110.

Scheme 4:



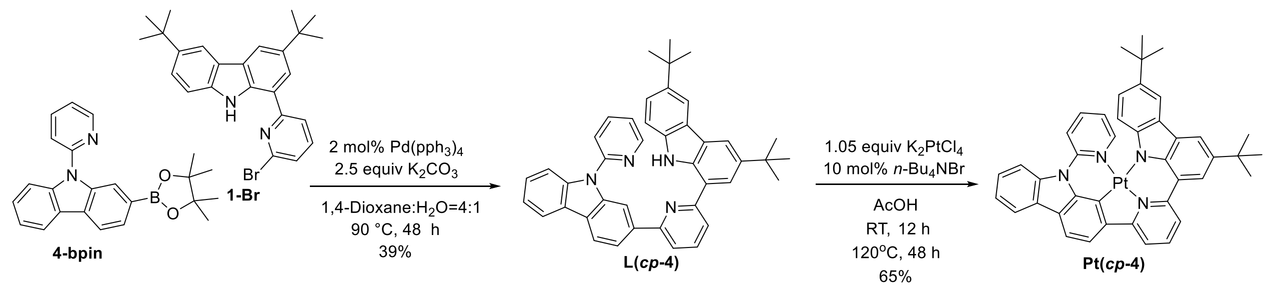
Synthesis of **L(*cp*-3)**: **1-Br** (300 mg, 0.69 mmol, 1.0 equiv), **3-bpin**[2] (224 mg, 0.76 mmol, 1.1 equiv), K_2CO_3 (238 mg, 1.72 mmol, 2.5 equiv), $Pd(PPh_3)_4$ (16 mg, 0.01 mmol, 2 mol%) were added sequentially to a dry three-necked flask equipped with a magnetic stir bar. The flask was evacuated and backfilled with nitrogen, this evacuation and backfill procedure was repeated twice. Then 1,4-

dioxane (10 mL) and H_2O (2.5 mL) were added into the flask under nitrogen atmosphere at room temperature. Then the flask was placed in an oil bath and the reaction mixture was stirred and heated at 90 °C for 48 hours, the reaction was monitored by TLC until the reaction was completed. The reaction mixture was cooled down to room temperature, filtered and washed with ethyl acetate. 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 = 50:1−30:1) to obtain the desired product as a white solid 109 mg in 30% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.46 (s, 9H), 1.53 (s, 9H), 7.02 (dd, J = 7.2, 0.8 Hz, 1H), 7.03 (d, J = 8.4 Hz, 1H), 7.24−7.26 (m, 1H), 7.30 (ddd, J = 8.0, 2.0, 0.8 Hz, 1H), 7.45 (dd, J = 2.0, 8.4 Hz, 1H), 7.62 (t, J = 8.0 Hz, 1H), 7.64 (dd, J = 7.6, 0.4 Hz, 1H), 7.73 (ddd, J = 2.0, 7.6, 8.4 Hz, 1H), 7.88 (t, J = 2.4 Hz, 1H), 7.91 (d, J = 8.0 Hz, 1H), 7.95 (ddd, J = 7.6, 1.6, 1.2 Hz, 1H), 8.01 (d, J = 7.2 Hz, 1H), 8.04 (d, J = 1.6 Hz, 1H), 8.12 (d, J = 2.0 Hz, 1H), 8.19 (d, J = 1.6 Hz, 1H), 8.23 (ddd, J = 4.8, 2.0, 0.8 Hz, 1H), 11.12 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 32.06, 32.14, 34.69, 34.82, 110.46, 111.78, 116.10, 118.01, 118.43, 118.63, 118.72, 119.49, 119.87, 120.84, 121.97, 122.54, 123.28, 123.64, 124.79, 130.26, 137.18, 137.52, 138.18, 139.55, 141.49, 141.92, 142.03, 147.83, 154.91, 156.04, 158.08, 163.72. HRMS (ESI): calcd for $C_{36}H_{36}N_3O$ $[M+H]^+$ 526.2853, found 526.2841.

Synthesis of **Pt (*cp*-3)**: A mixture of **L (*cp*-3)** (100 mg, 0.19 mmol, 1.0 equiv), K_2PtCl_4 (83 mg, 0.20 mmol, 1.05 equiv), *n*-Bu_4NBr (6.13 mg, 0.02 mmol, 10 mol%) 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 (20 mL) was 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 the reaction mixture was stirred and heated at 120 °C for 48 hours. The reaction mixture was cooled down to room temperature, filtered and washed with dichloromethane. The filtrate was concentrated under reduced pressure and crude product was recrystallized with dichloromethane/ethyl acetate obtain the desired product as a yellow solid 63 mg in 46% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ(ppm) 1.45 (s, 9H), 1.59 (s, 9H), 6.65–6.68 (m, 1H), 6.99 (d, J = 9.0 Hz, 1H), 7.18 (dd, J = 8.5, 2.0 Hz, 1H), 7.19 (dd, J = 12.0, 0.5 Hz, 1H), 7.27 (t, J = 7.5 Hz, 1H), 7.36 (dd, J = 8.0, 1.0 Hz, 1H), 7.60

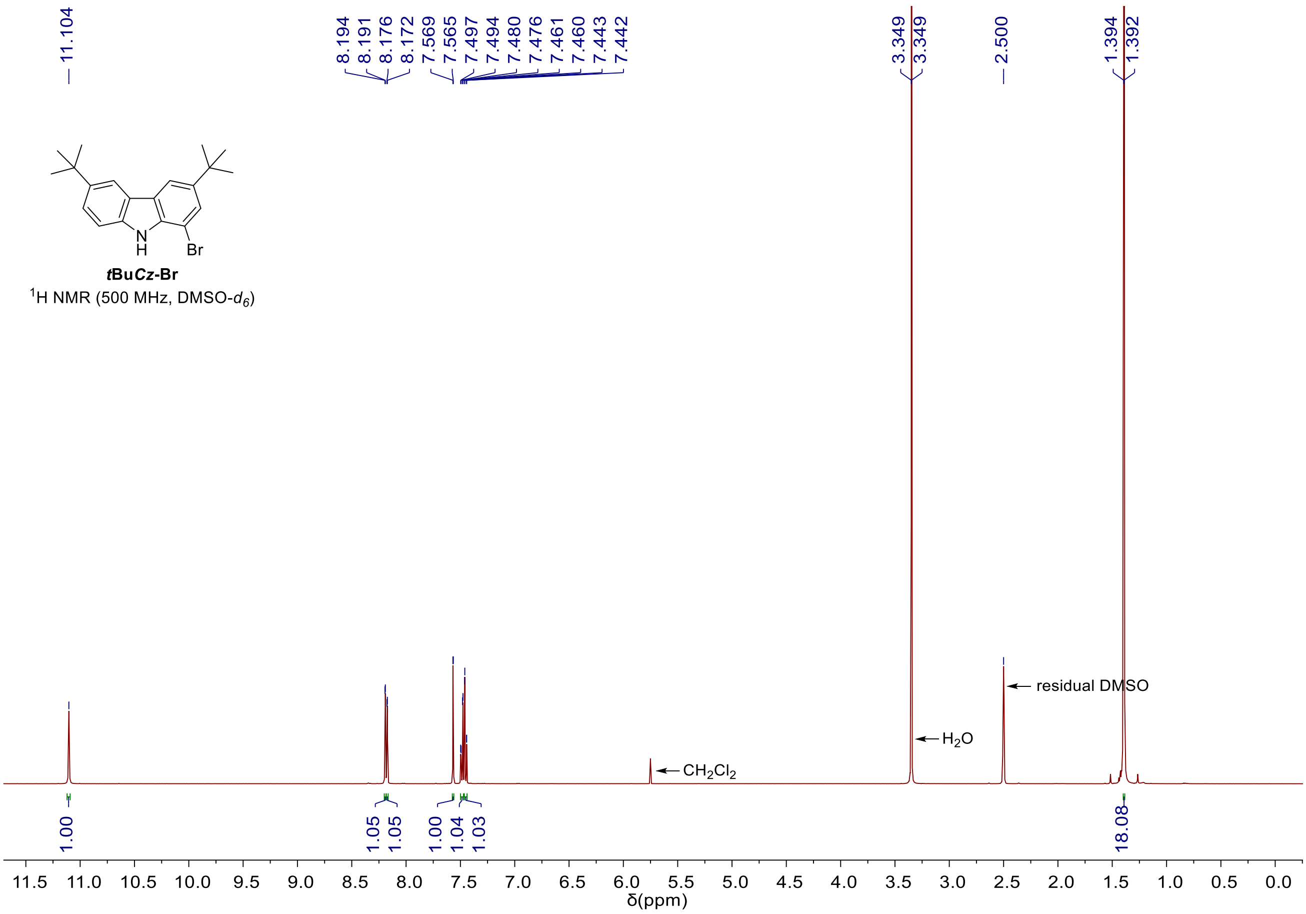
(d, J = 7.5 Hz, 1H), 7.82 (dd, J = 7.5, 1.0 Hz, 1H), 7.86–7.90 (m, 1H), 8.05 (t, J = 7.5 Hz, 1H), 8.20 (d, J = 2.0 Hz, 1H), 8.32 (d, J = 1.0 Hz, 1H), 8.43 (d, J = 1.5 Hz, 1H), 8.44 (s, 1H), 8.75 (dd, J = 6.0, 1.5 Hz, 1H). HRMS (ESI): calcd for $C_{36}H_{34}N_3OPt$ $[M+H]^+$ 719.2344, found 719.2330.

Scheme 5:



Synthesis of **L(*cp*-4)**: **1-Br** (300 mg, 0.69 mmol, 1.0 equiv), **4-bpin**[3] (281 mg, 0.76 mmol, 1.1 equiv), K_2CO_3 (238 mg, 1.72 mmol, 2.5 equiv), $Pd(PPh_3)_4$ (16 mg, 0.01 mmol, 2 mol%) 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 (8 mL) and H_2O (2 mL) were added into the flask under nitrogen atmosphere at room temperature. Then the flask was placed in an oil bath and the reaction mixture was stirred and heated at 90 °C for 48 hours, the reaction was monitored by TLC until the reaction was completed. The reaction mixture was cooled down to room temperature, filtered and washed with ethyl acetate. 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 = 50:1−30:1) to obtain the desired product as a white solid 161 mg in 39% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 1.44 (s, 9H), 1.49 (s, 9H), 7.31 (d, J = 8.8 Hz, 1H), 7.34 (ddd, J = 6.4, 5.6, 1.2 Hz, 1H), 7.37−7.41 (m, 1H), 7.46 (dd, J = 8.8, 2.0 Hz, 1H), 7.50−7.54 (m, 1H), 7.85 (d, J = 8.4 Hz, 1H), 7.87 (td, J = 7.2, 2.0 Hz, 1H), 7.99 (dt, J = 8.0, 0.8 Hz, 1H), 8.04 (d, J = 1.6 Hz, 1H), 8.07 (d, J = 4.0 Hz, 1H), 8.09 (d, J = 2.0 Hz, 1H), 8.11−8.15 (m, 1H), 8.16 (dd, J = 8.4, 1.6 Hz, 1H), 8.24 (d, J = 1.6 Hz, 1H), 8.32 (t, J = 2.0 Hz, 1H), 8.35 (d, J = 7.6 Hz, 1H), 8.45 (d, J = 8.4 Hz, 1H), 8.61 (ddd, J = 4.8, 2.0, 0.8 Hz, 1H), 8.77 (d, J = 0.8 Hz, 1H), 11.22 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 32.08, 32.17, 34.70, 34.84, 109.94, 110.56, 111.22, 116.00, 117.89, 118.07, 118.59, 118.97, 119.63, 120.01, 120.54, 120.57, 120.73, 121.18, 121.48, 122.48, 123.66, 123.96, 124.78, 125.00, 126.66, 137.28, 137.43, 138.14, 138.42, 138.51, 140.34, 141.47, 141.87, 149.85, 151.61, 157.26, 157.91. HRMS (ESI): calcd for $C_{42}H_{39}N_4$ $[M+H]^+$ 599.3169, found 599.3165.

Synthesis of **Pt (*cp*-4)**: A mixture of **L (*cp*-4**) (100 mg, 0.19 mmol, 1.0 equiv), K_2PtCl_4 (83 mg, 0.20 mmol, 1.05 equiv), *n*-Bu_4NBr (6.13 mg, 0.02 mmol, 10 mol%) 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 (10 mL) was 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 the reaction mixture was stirred and heated at 120 °C for 48 hours. The reaction mixture was cooled down to room temperature, filtered and washed with dichloromethane. The filtrate was concentrated under reduced pressure and crude product was recrystallized with dichloromethane/ethyl acetate obtain the desired product as orange solid 86 mg in 65% yield. ^1H NMR (500 MHz, $CDCl_3$): δ (ppm) 1.47 (s, 9H), 1.60 (s, 9H), 6.64–6.67 (m, 1H), 7.25–7.26(m, 1H), 7.34 (d, J = 8.5 Hz, 1H), 7.42 (t, J = 7.5 Hz, 1H), 7.53–7.56 (m, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.81 (d, J = 7.0 Hz, 1H), 7.86–7.90 (m, 1H), 8.02 (t, J = 8.0 Hz, 1H), 8.07 (d, J = 8.5 Hz, 1H), 8.11 (d, J = 7.0 Hz, 1H), 8.21 (d, J = 8.5 Hz, 1H), 8.24 (d, J = 1.5 Hz, 1H), 8.35 (s, 1H), 8.39 (d, J = 8.0 Hz, 1H), 8.45 (d, J = 1.5 Hz, 1H), 9.23 (dd, J = 6.5, 1.5 Hz, 1H). HRMS (ESI): calcd for $C_{42}H_{37}N_4Pt$ $[M+H]^+$ 792.2661, found 792.2646.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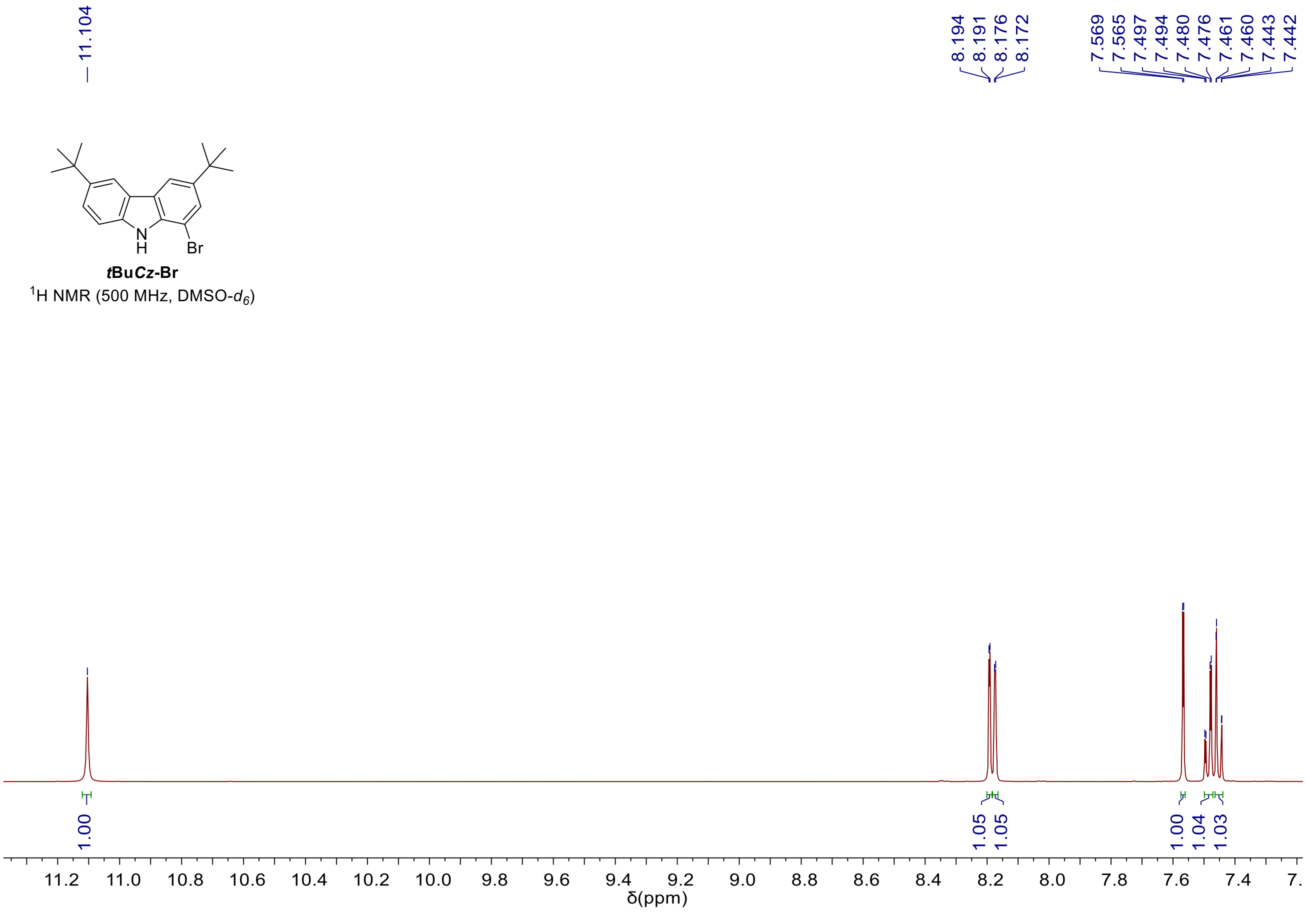
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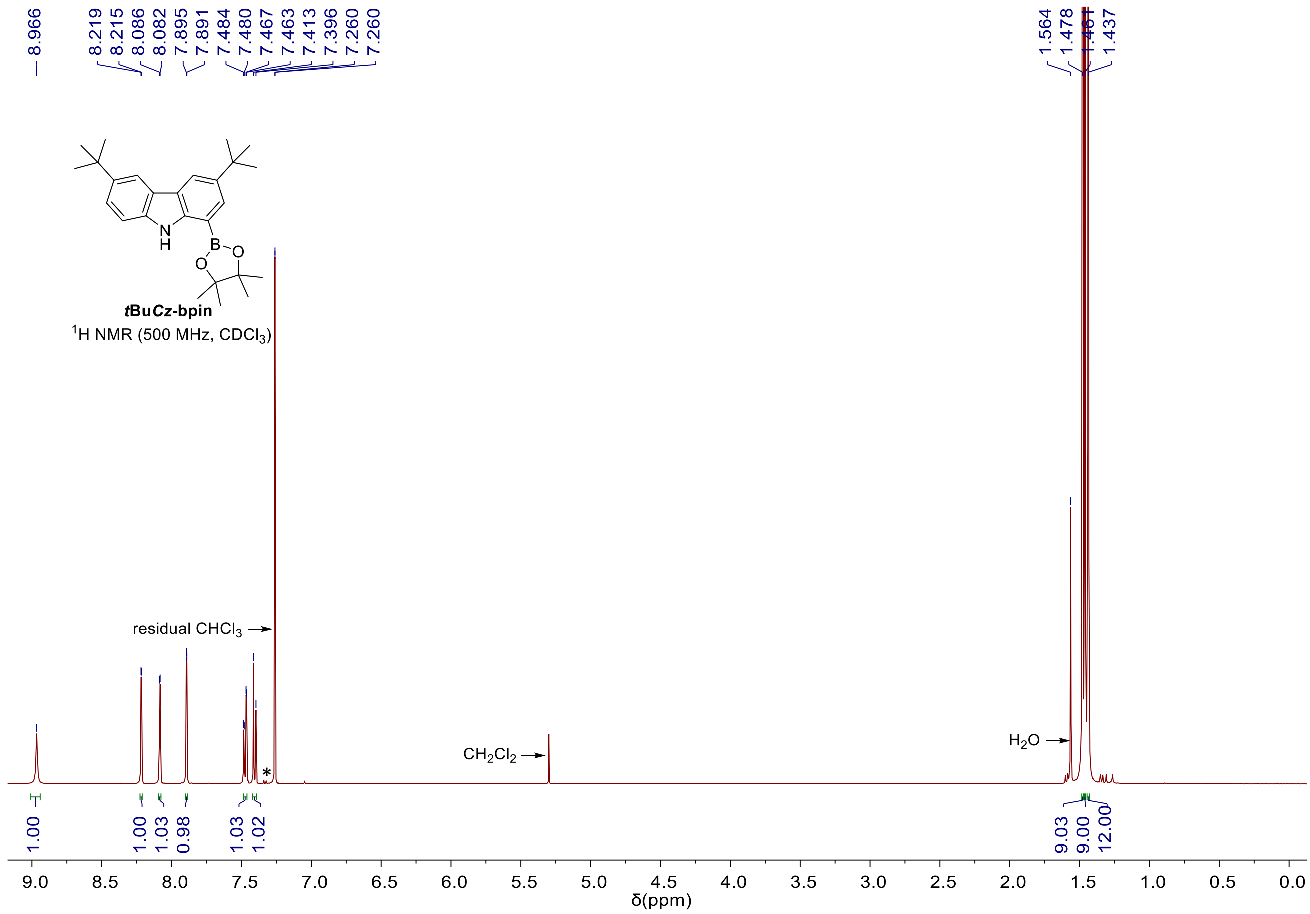
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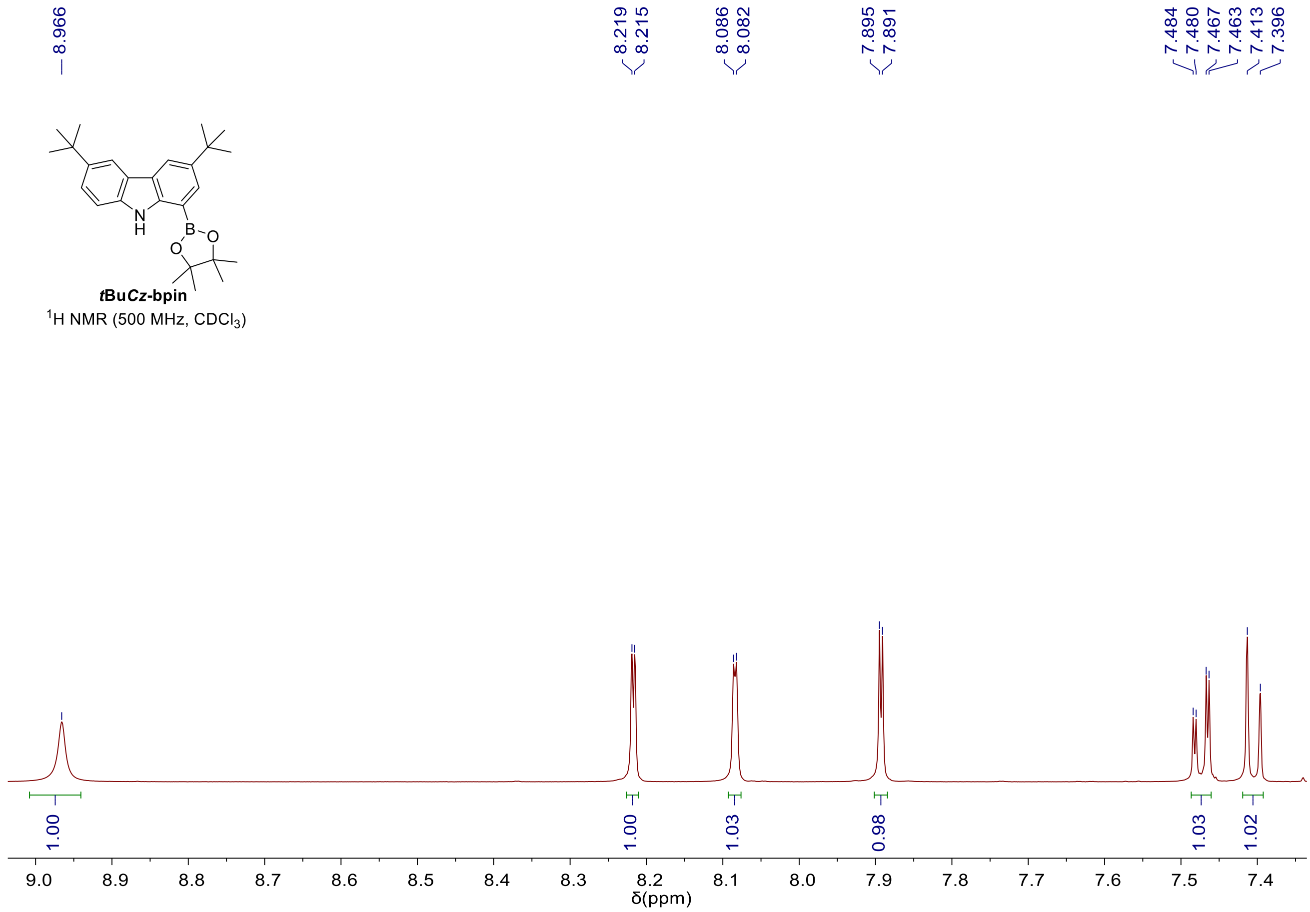
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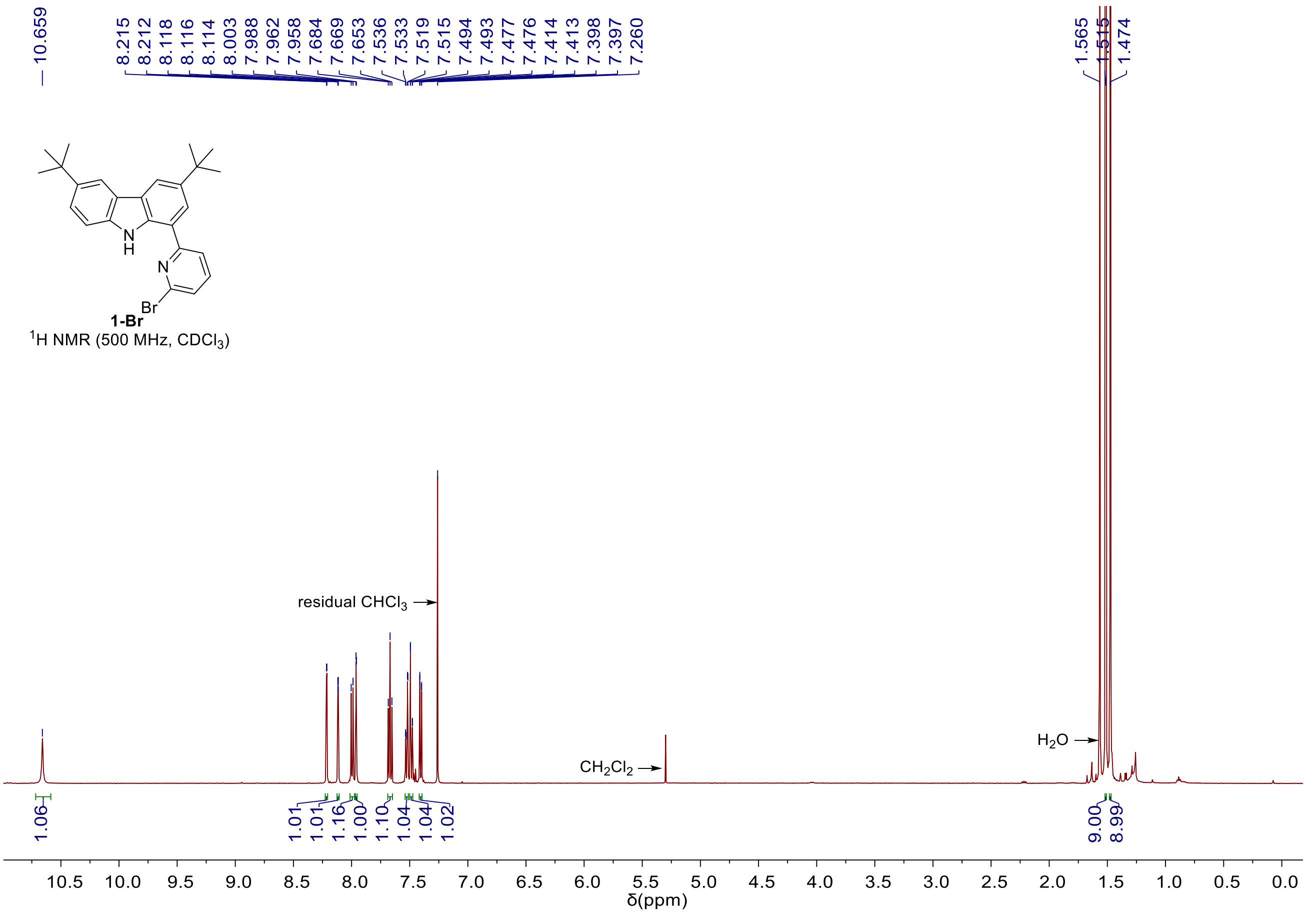
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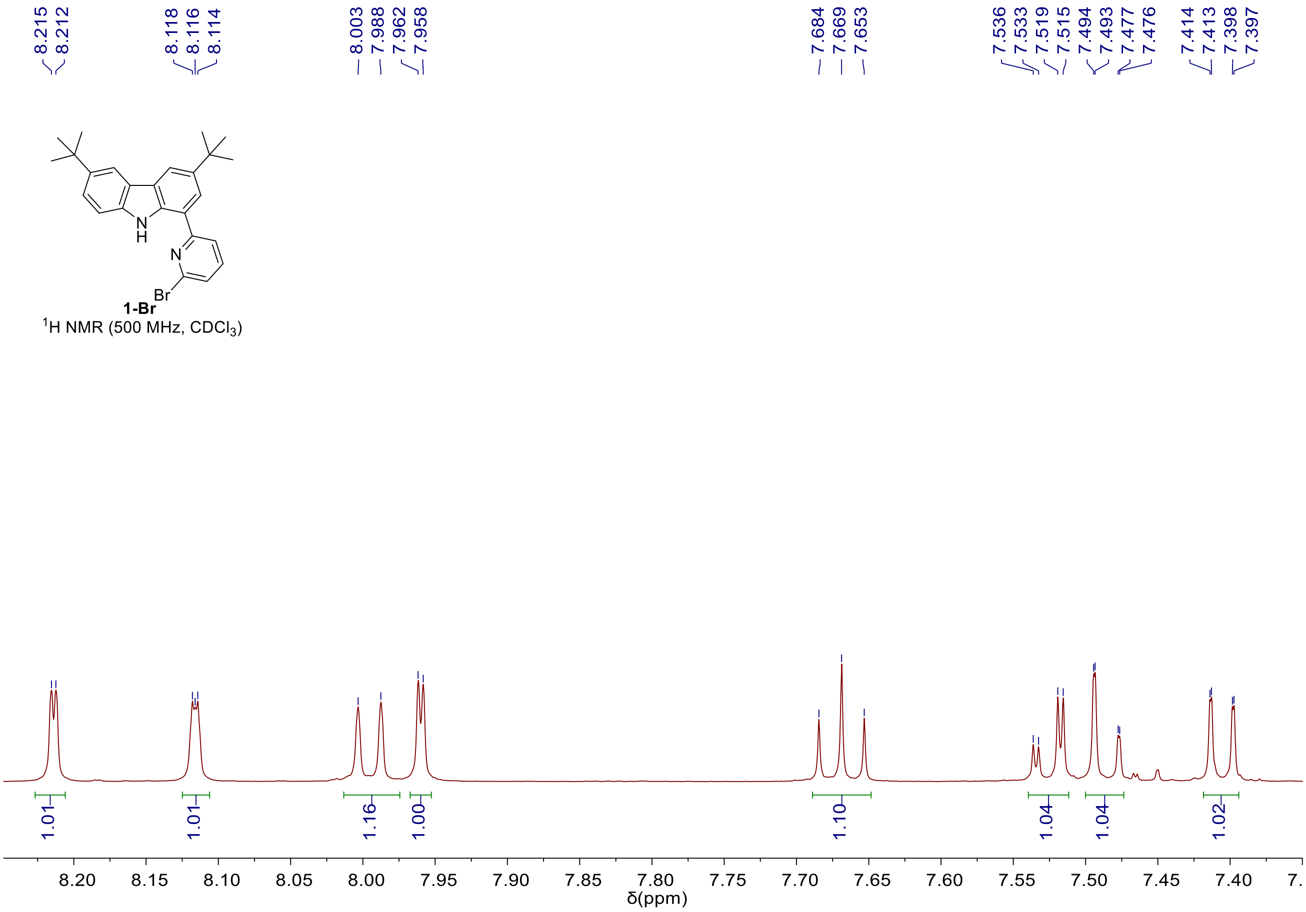
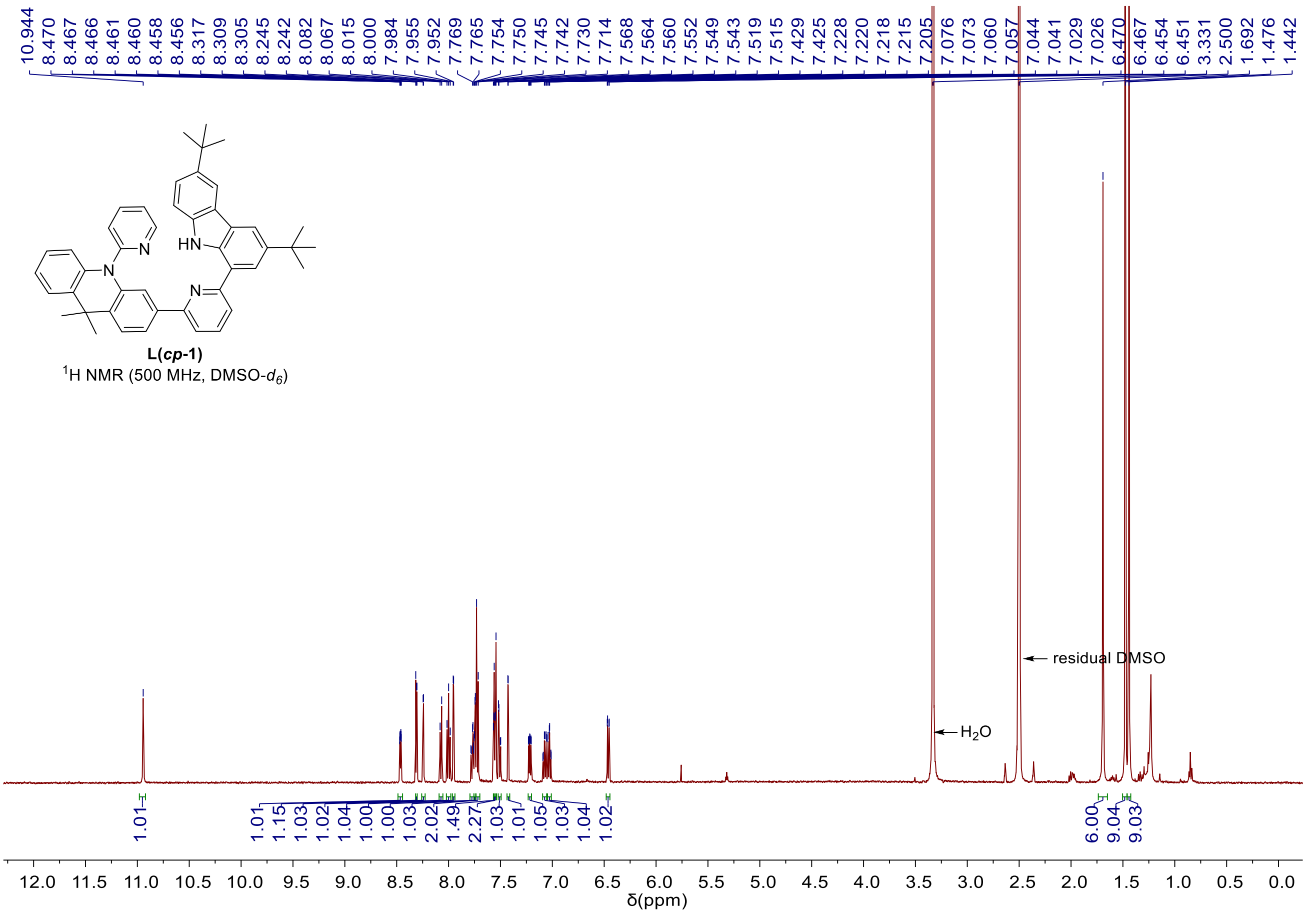
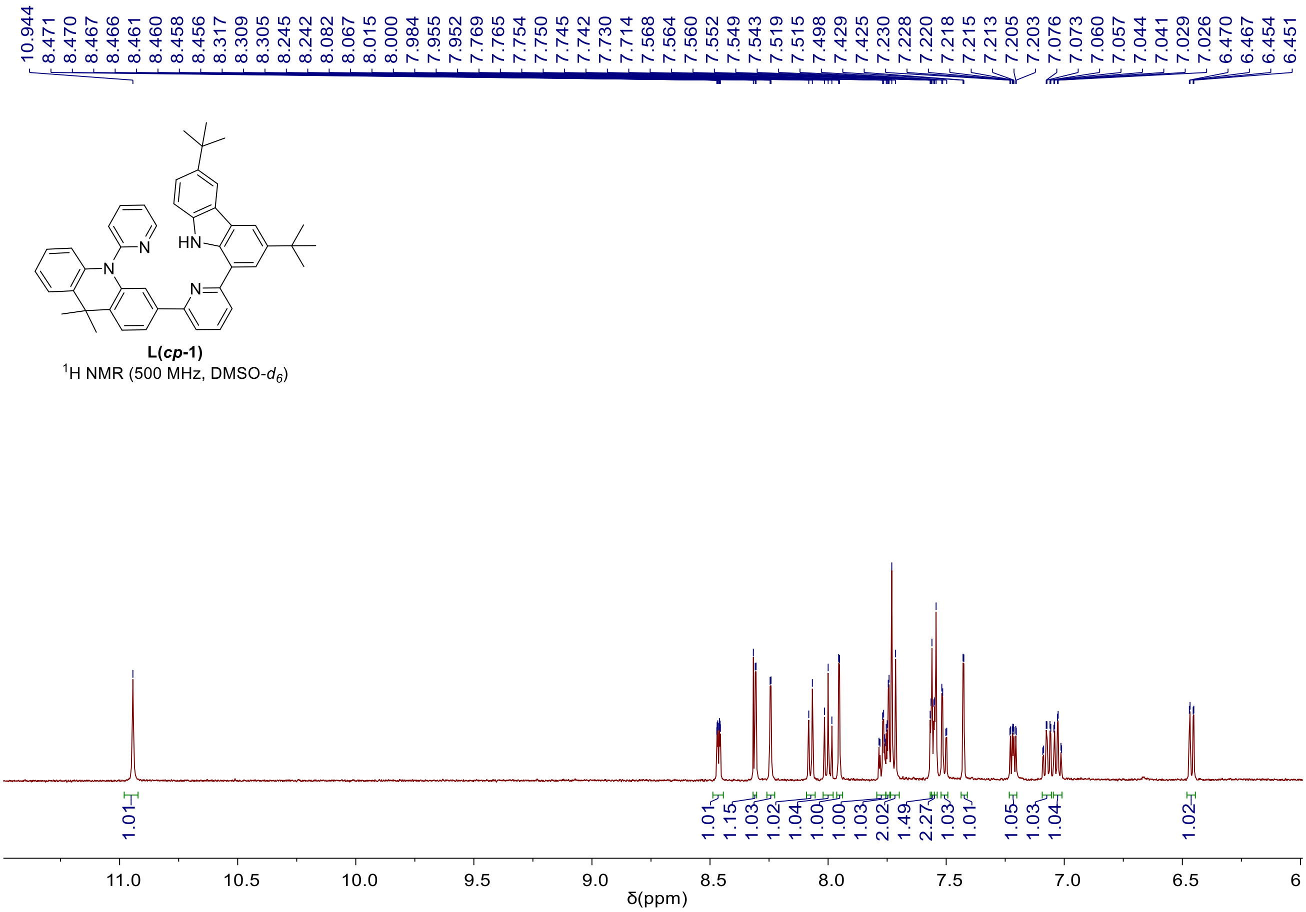
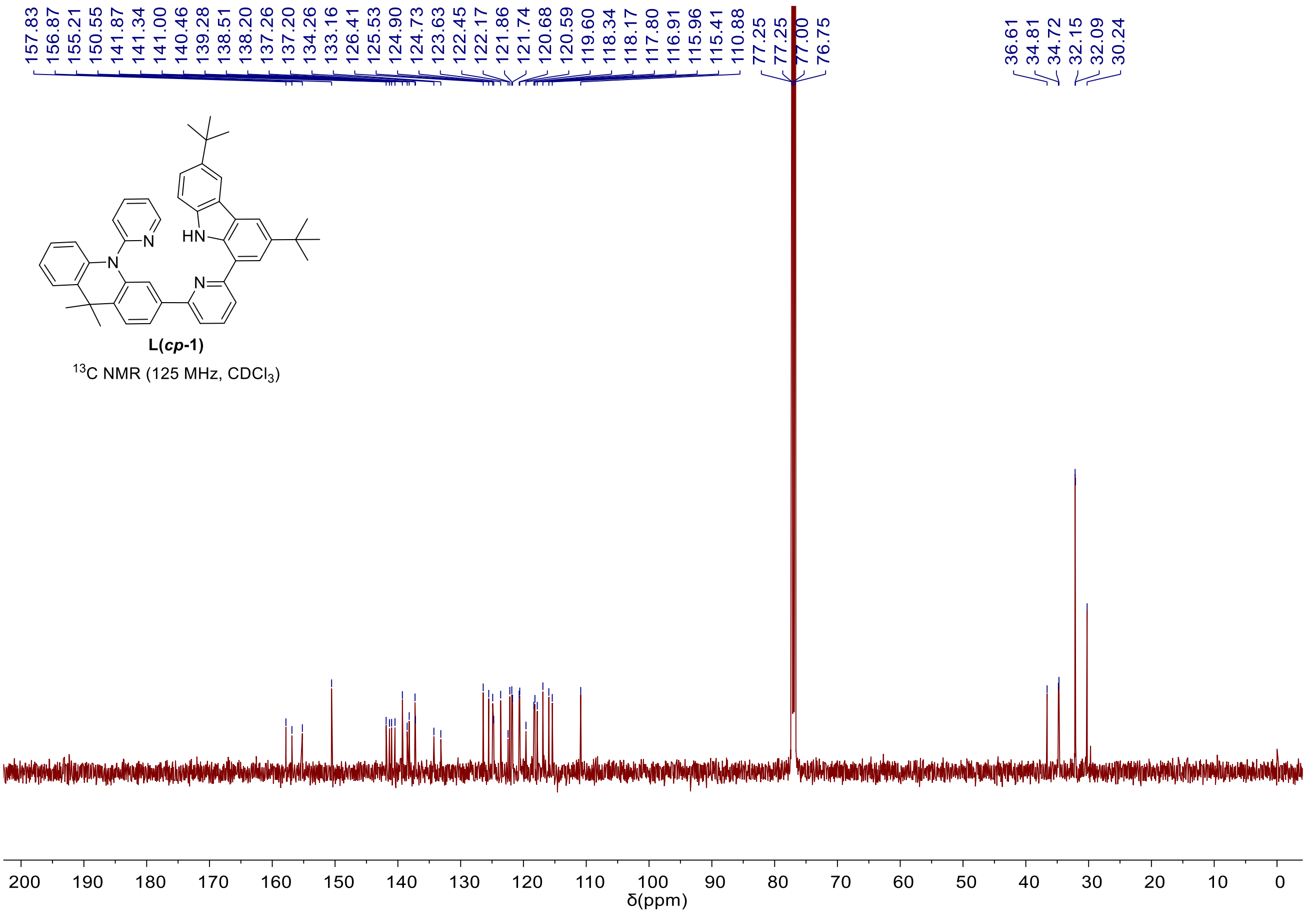
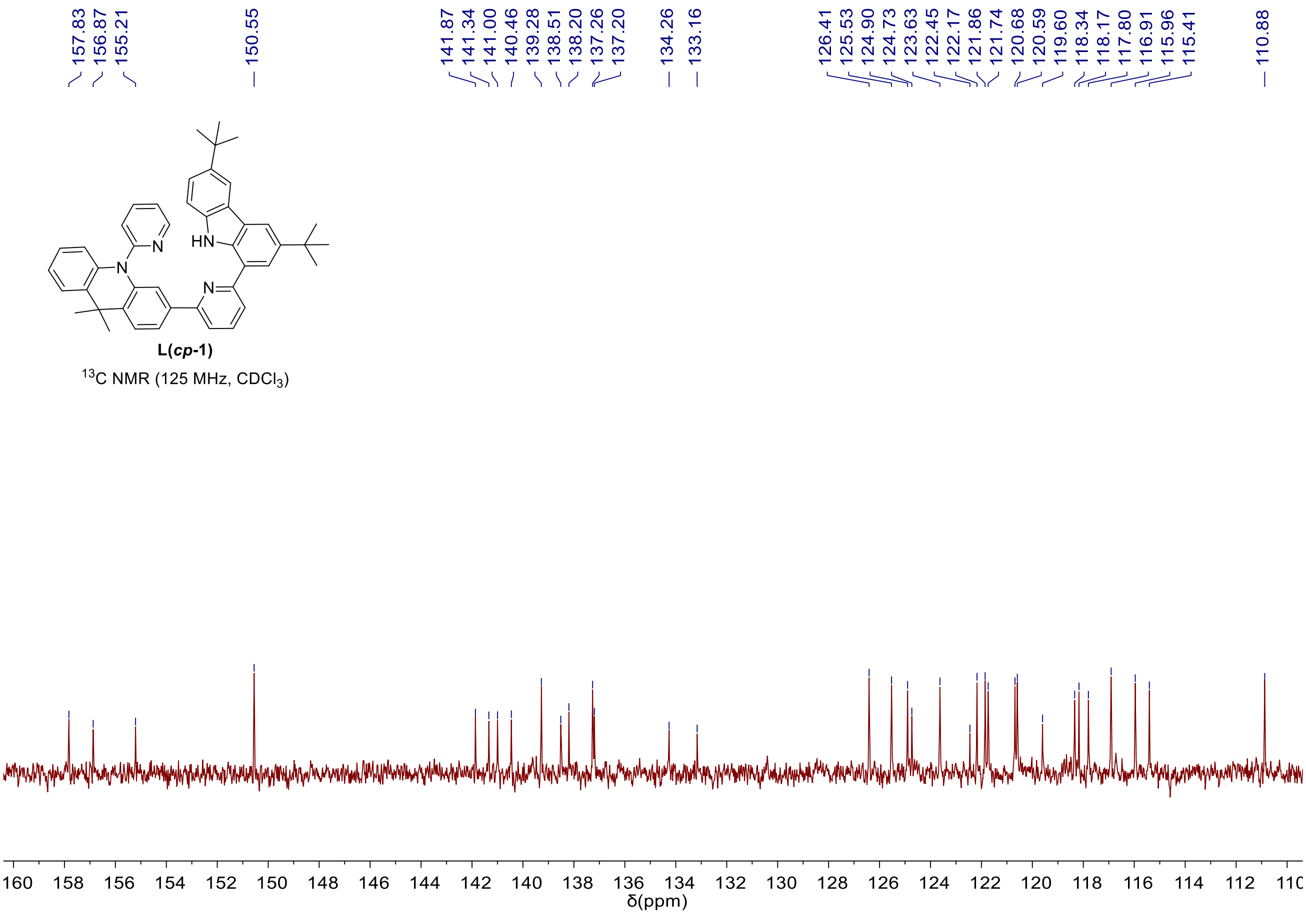
N
Br
1-Br
^{1}H NMR (500 MHz, $CDCl_3$)
residual $CHCl_3$
CH_2Cl_2
H_2O
1.06
1.01
1.01
1.16
1.00
1.10
1.04
1.04
1.02
9.00
8.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ(ppm)

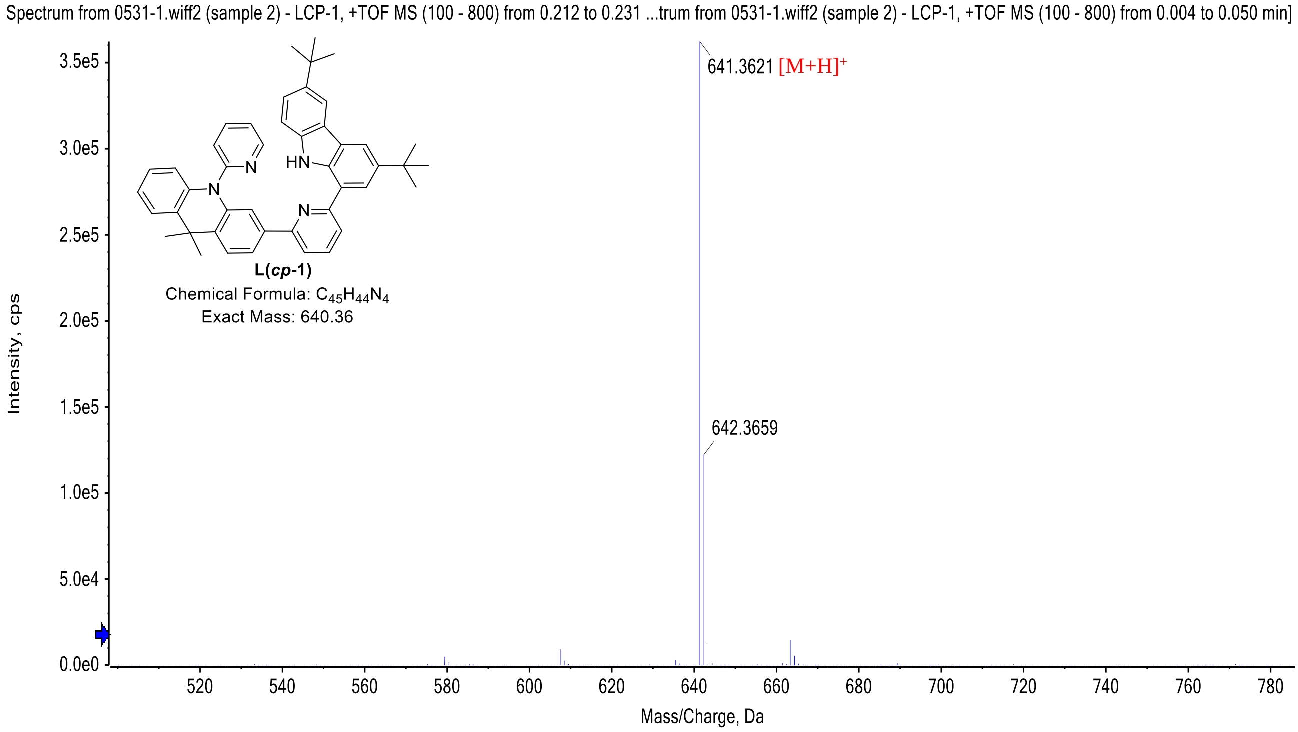

8.215
8.212
8.118
8.116
8.114
8.003
7.988
7.962
7.958
7.684
7.669
7.653
7.536
7.533
7.519
7.515
7.494
7.493
7.477
7.476
7.414
7.413
7.398
7.397
H
N
Br
1-Br
^{1}H NMR (500 MHz, $CDCl_3$)
1.01
1.01
1.16
1.00
1.10
1.04
1.04
1.02
8.20 8.15 8.10 8.05 8.00 7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.
δ(ppm)

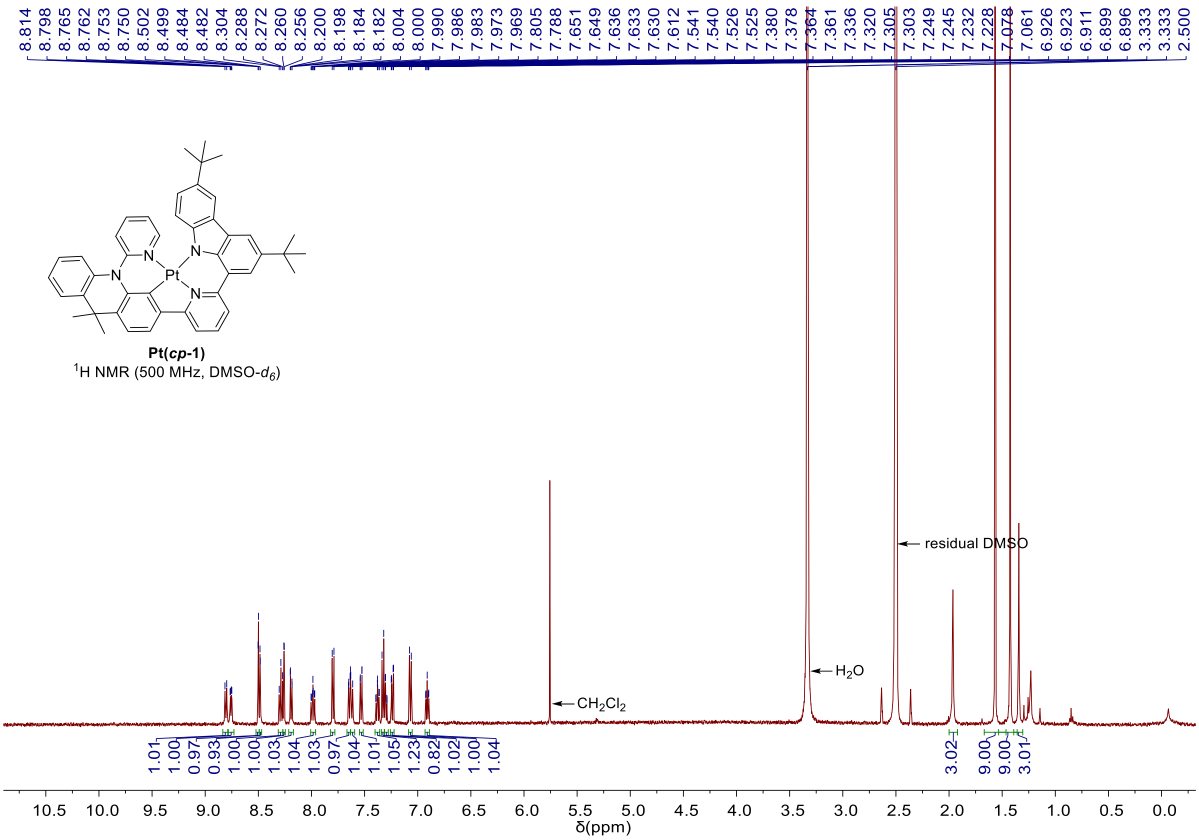

L(cp-1)
1H NMR (500 MHz, DMSO-d6)
residual DMSO
H2O
δ(ppm)


L(cp-1)
1H NMR (500 MHz, DMSO-d6)
δ(ppm)

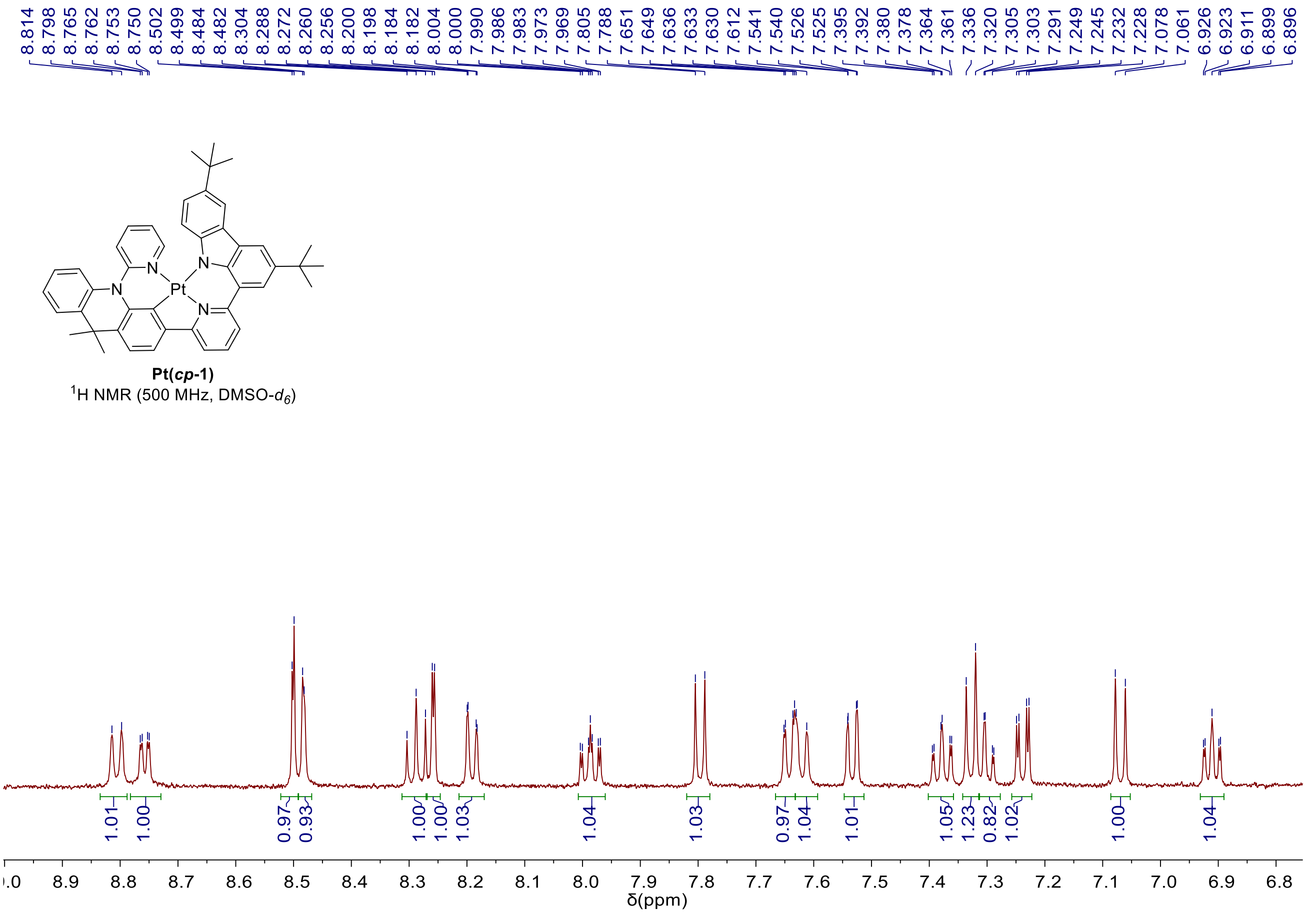

157.83 156.87 155.21 150.55 141.87 141.34 141.00 140.46 139.28 138.51 138.20 137.26 137.20 134.26 133.16 126.41 125.53 124.90 124.73 123.63 122.45 122.17 121.86 121.74 120.68 120.59 119.60 118.34 118.17 117.80 116.91 115.96 115.41 110.88
77.25 77.25 77.00 76.75
36.61 34.81 34.72 32.15 32.09 30.24
HN
N
N
N
L(cp-1)
13C NMR (125 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ(ppm)

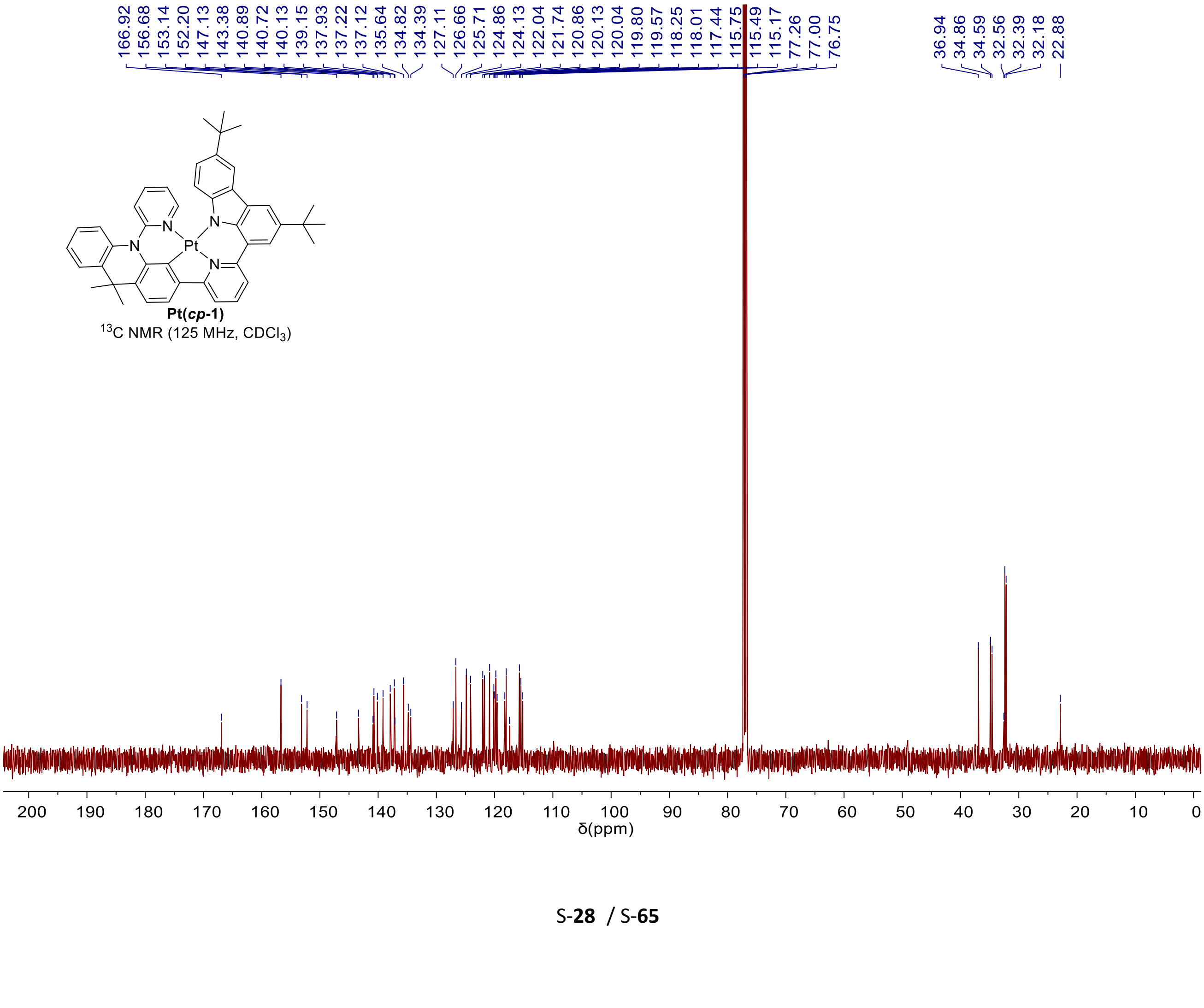

157.83 156.87 155.21 150.55 141.87 141.34 141.00 140.46 139.28 138.51 138.20 137.26 137.20 134.26 133.16 126.41 125.53 124.90 124.73 123.63 122.45 122.17 121.86 121.74 120.68 120.59 119.60 118.34 118.17 117.80 116.91 115.96 115.41 110.88
HN
N
N
N
L(cp-1)
13C NMR (125 MHz, CDCl3)
160 158 156 154 152 150 148 146 144 142 140 138 136 134 132 130 128 126 124 122 120 118 116 114 112 110
δ(ppm)

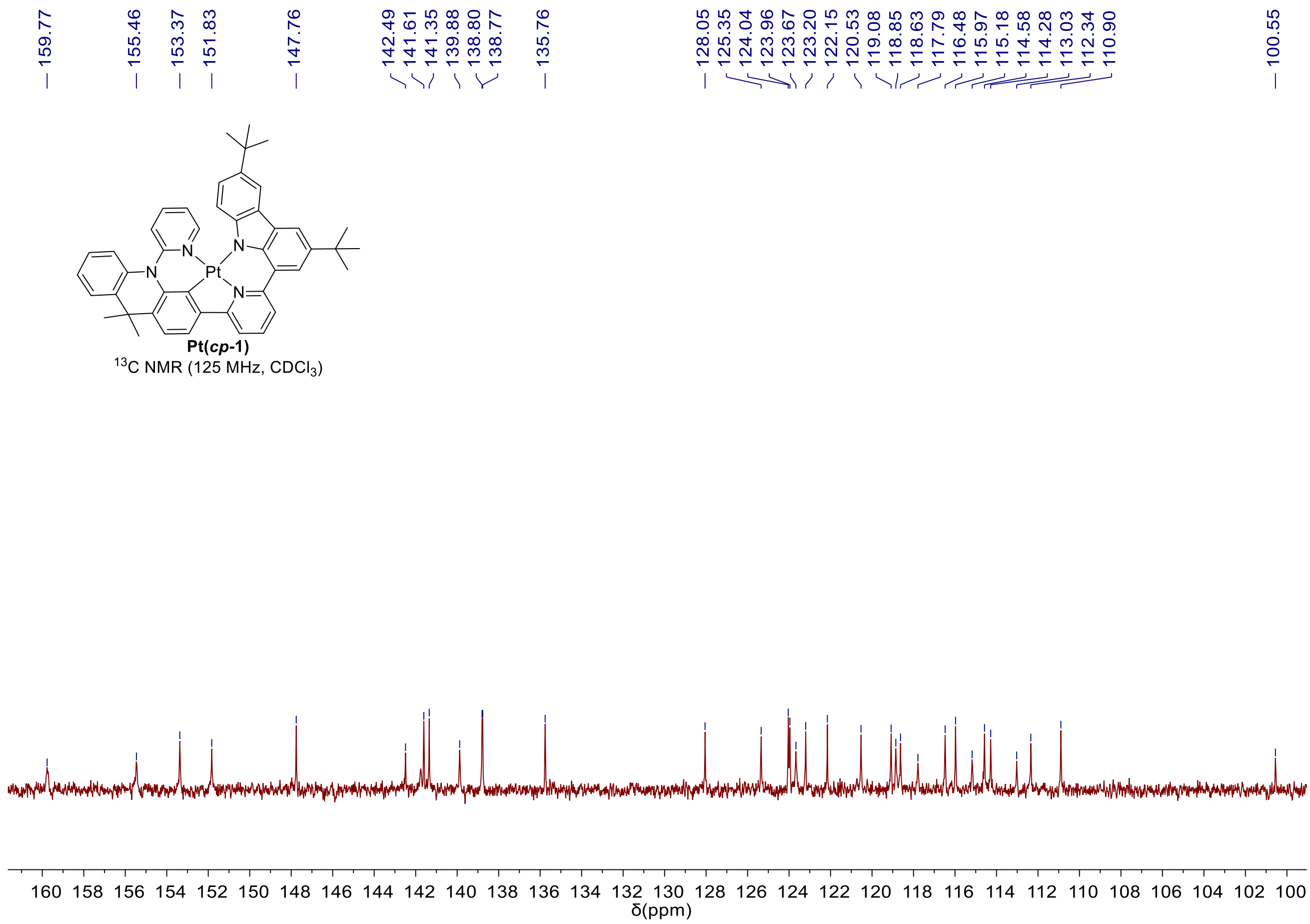

Spectrum from 0531-1.wiff2 (sample 2) - LCP-1, +TOF MS (100 - 800) from 0.212 to 0.231 ...trum from 0531-1.wiff2 (sample 2) - LCP-1, +TOF MS (100 - 800) from 0.004 to 0.050 min]
641.3621 [M+H]+
642.3659
L(cp-1)
Chemical Formula: C45H44N4
Exact Mass: 640.36
Intensity, cps
Mass/Charge, Da

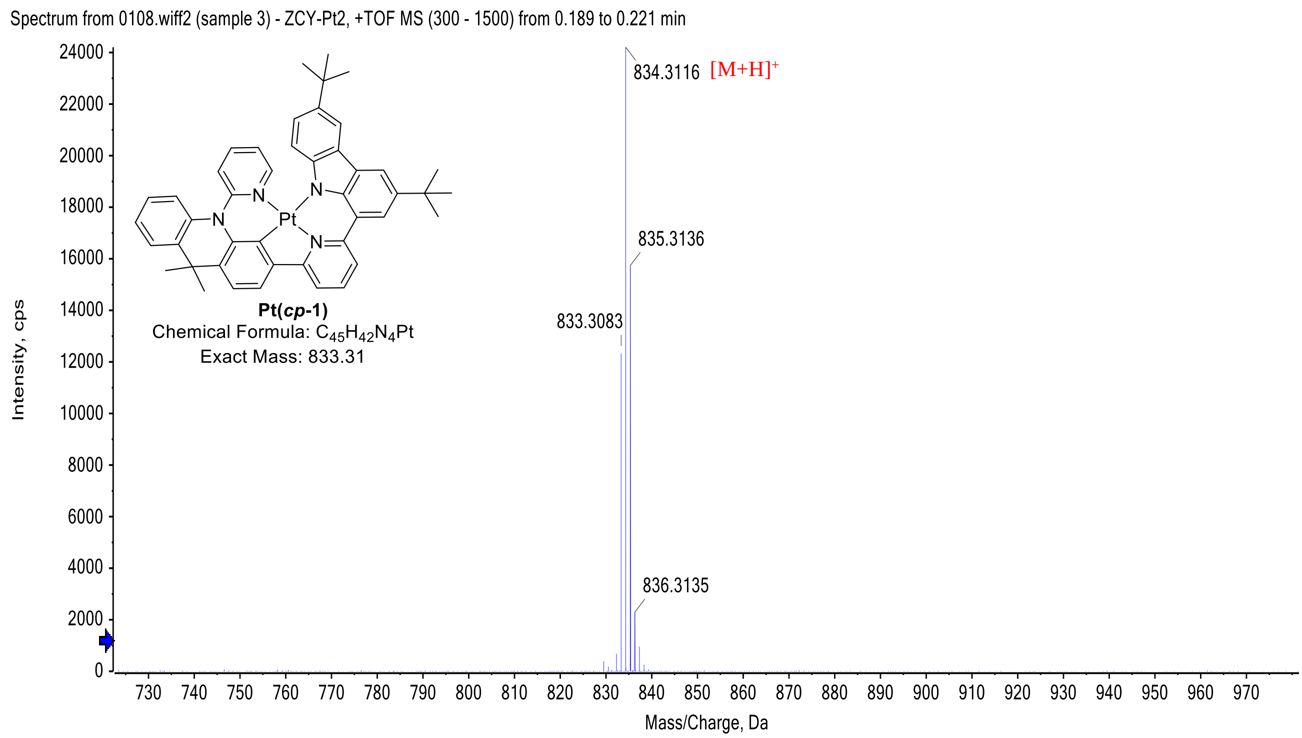

8.814 8.798 8.765 8.762 8.753 8.750 8.502 8.499 8.484 8.482 8.304 8.288 8.272 8.260 8.256 8.200 8.198 8.184 8.182 8.004 8.000 7.990 7.986 7.983 7.973 7.969 7.805 7.788 7.651 7.649 7.636 7.633 7.630 7.612 7.541 7.540 7.526 7.525 7.380 7.378 7.364 7.361 7.336 7.320 7.305 7.303 7.249 7.245 7.232 7.228 7.078 7.061 6.926 6.923 6.911 6.899 6.896 3.333 3.333 2.500
Pt(cp-1)
1H NMR (500 MHz, DMSO-d6)
residual DMSO
H2O
CH2Cl2
1.01 1.00 0.97 0.93 1.00 1.00 1.03 1.04 1.03 0.97 1.04 1.01 1.05 1.23 0.82 1.02 1.00 1.04
3.02 9.00 9.00 3.01
δ(ppm)

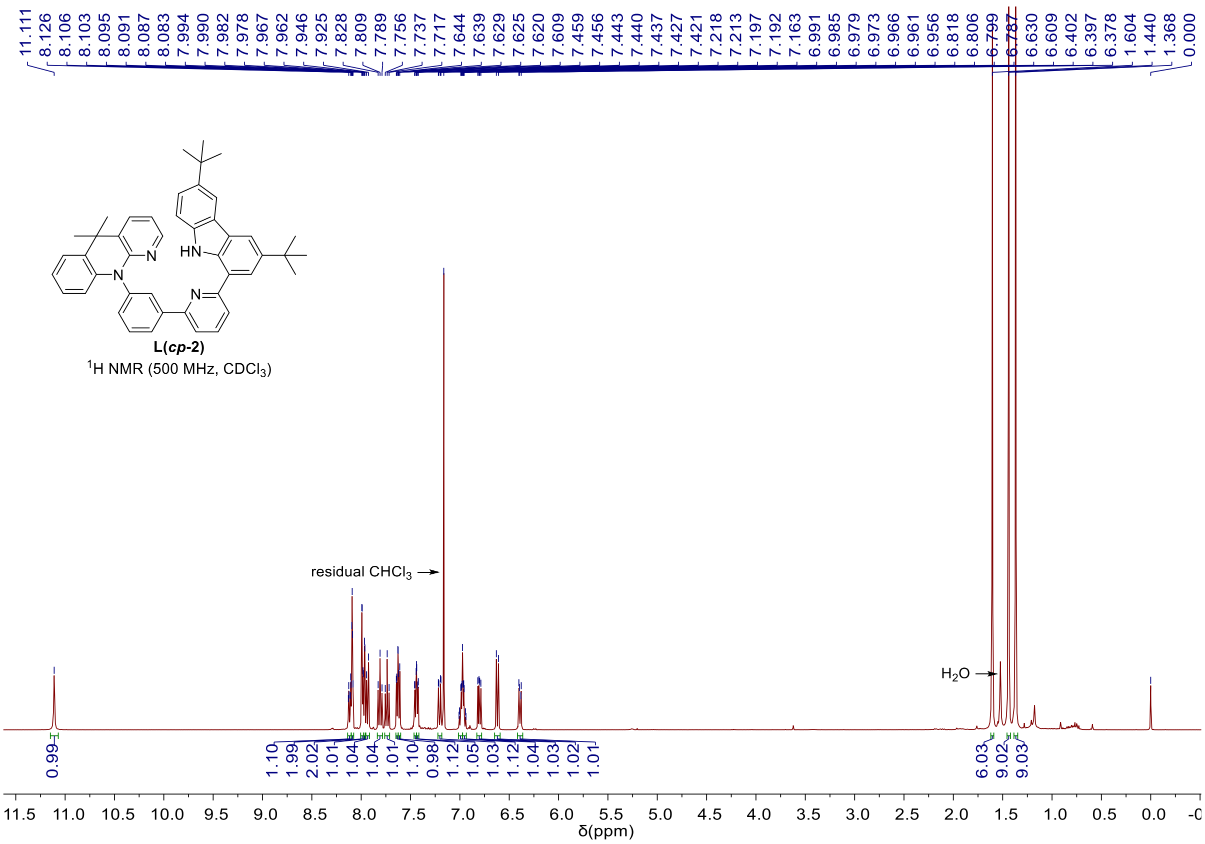
13

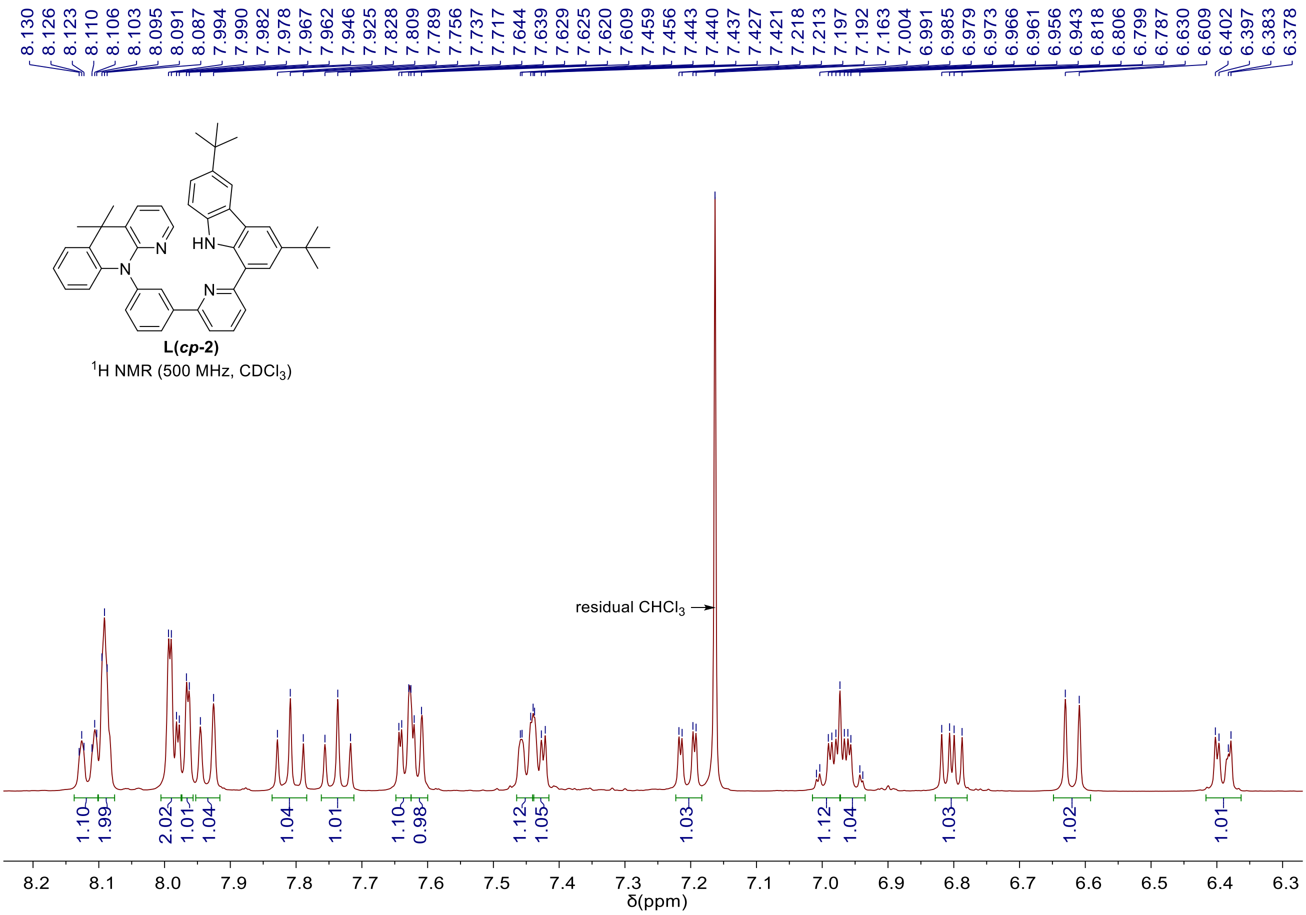

8.814 8.798 8.765 8.762 8.753 8.750 8.502 8.499 8.484 8.482 8.304 8.288 8.272 8.260 8.256 8.200 8.198 8.184 8.182 8.004 8.000 7.990 7.986 7.983 7.973 7.969 7.805 7.788 7.651 7.649 7.636 7.633 7.630 7.612 7.541 7.540 7.526 7.525 7.395 7.392 7.380 7.378 7.364 7.361 7.336 7.320 7.305 7.303 7.291 7.249 7.245 7.232 7.228 7.078 7.061 6.926 6.923 6.911 6.899 6.896
N
Pt
N
N
N
Pt(cp-1)
1H NMR (500 MHz, DMSO-d6)
1.01 1.00 0.97 0.93 1.00 1.00 1.03 1.04 1.03 0.97 1.04 1.01 1.05 1.23 0.82 1.02 1.00 1.04
.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 6.9 6.8
δ(ppm)

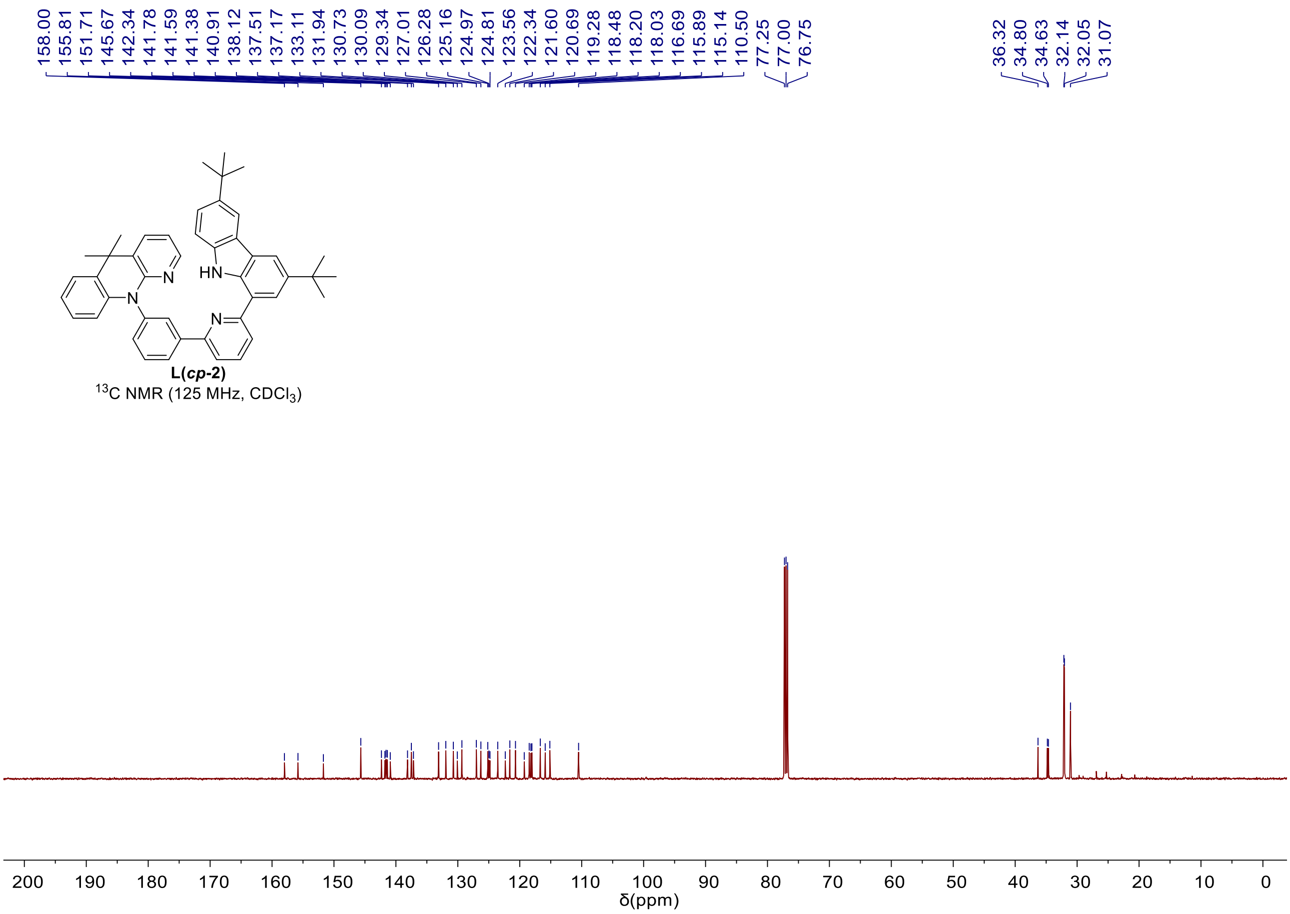

166.92 156.68 153.14 152.20 147.13 143.38 140.89 140.72 140.13 139.15 137.93 137.22 137.12 135.64 134.82 134.39 127.11 126.66 125.71 124.86 124.13 122.04 121.74 120.86 120.13 120.04 119.80 119.57 118.25 118.01 117.44 115.75 115.49 115.17 77.26 77.00 76.75
36.94 34.86 34.59 32.56 32.39 32.18 22.88
N
Pt
N
N
N
Pt(cp-1)
13C NMR (125 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ(ppm)

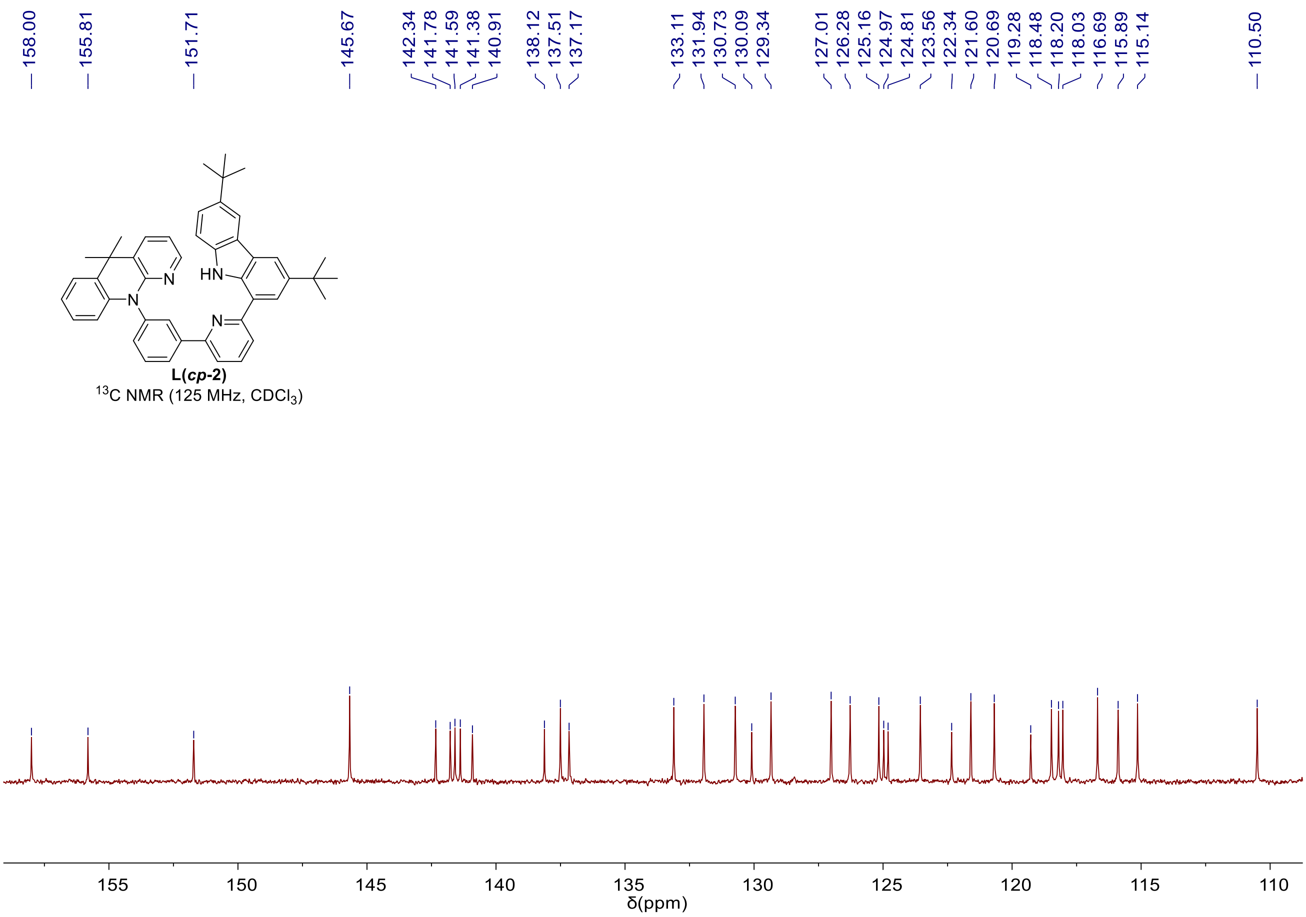

159.77
155.46
153.37
151.83
147.76
142.49
141.61
141.35
139.88
138.80
138.77
135.76
128.05
125.35
124.04
123.96
123.67
123.20
122.15
120.53
119.08
118.85
118.63
117.79
116.48
115.97
115.18
114.58
114.28
113.03
112.34
110.90
100.55
Pt(cp-1)
13C NMR (125 MHz, CDCl3)
δ(ppm)

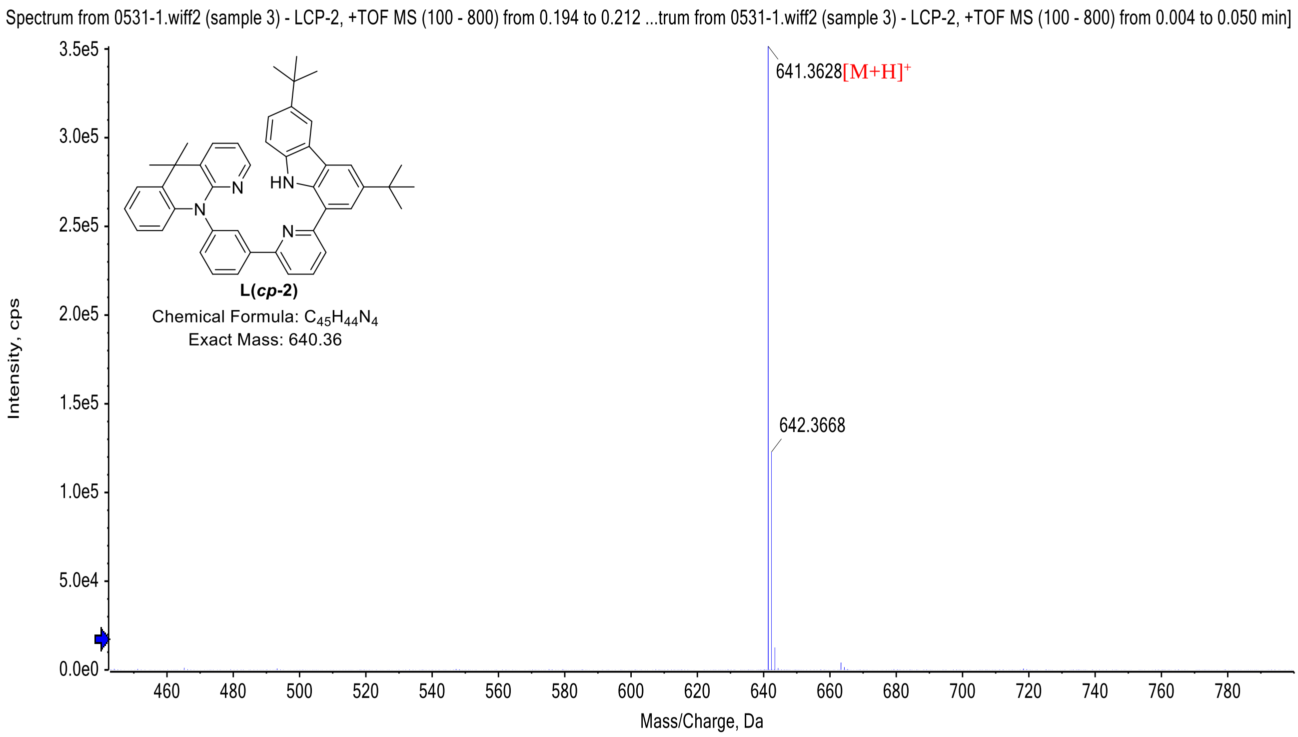

Spectrum from 0108.wiff2 (sample 3) - ZCY-Pt2, +TOF MS (300 - 1500) from 0.189 to 0.221 min
834.3116 [M+H]+
835.3136
833.3083
836.3135
Pt(cp-1)
Chemical Formula: C45H42N4Pt
Exact Mass: 833.31
Intensity, cps
Mass/Charge, Da


11.111 8.126 8.106 8.103 8.095 8.091 8.087 8.083 7.994 7.990 7.982 7.978 7.967 7.962 7.946 7.925 7.828 7.809 7.789 7.756 7.737 7.717 7.644 7.639 7.629 7.625 7.620 7.609 7.459 7.456 7.443 7.440 7.437 7.427 7.421 7.218 7.213 7.197 7.192 7.163 6.991 6.985 6.979 6.973 6.966 6.961 6.956 6.818 6.806 6.799 6.787 6.630 6.609 6.402 6.397 6.378 1.604 1.440 1.368 0.000
HN
N
N
N
L(*cp*-2)
^{1}H NMR (500 MHz, $CDCl_3$)
residual $CHCl_3$
H_2O
0.99
1.10 1.99 2.02 1.01 1.04 1.04 1.01 1.10 0.98 1.12 1.05 1.03 1.12 1.04 1.03 1.02 1.01
6.03 9.02 9.03
11.5 11.0 10.5 10.0 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
δ(ppm)

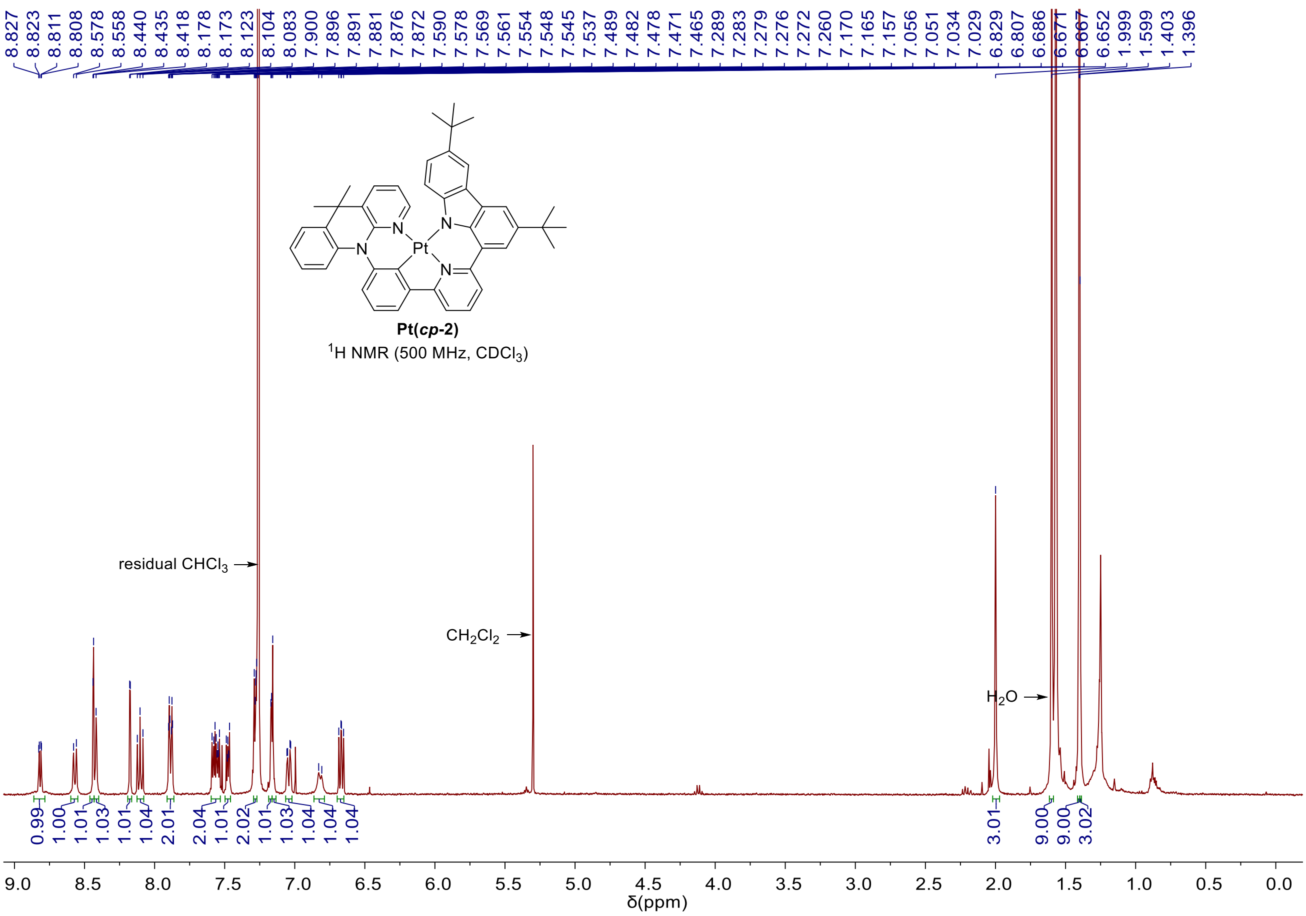

8.130 8.126 8.123 8.110 8.106 8.103 8.095 8.091 8.087 7.994 7.990 7.982 7.978 7.967 7.962 7.946 7.925 7.828 7.809 7.789 7.756 7.737 7.717 7.644 7.639 7.629 7.625 7.620 7.609 7.459 7.456 7.443 7.440 7.437 7.427 7.421 7.218 7.213 7.197 7.192 7.163 7.004 6.991 6.985 6.979 6.973 6.966 6.961 6.956 6.943 6.818 6.806 6.799 6.787 6.630 6.609 6.402 6.397 6.383 6.378
HN
N
N
N
L(*cp*-2)
^{1}H NMR (500 MHz, $CDCl_3$)
residual $CHCl_3$
1.10 1.99 2.02 1.01 1.04 1.04 1.01 1.10 0.98 1.12 1.05 1.03 1.12 1.04 1.03 1.02 1.01
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 6.5 6.4 6.3
δ(ppm)


158.00
155.81
151.71
145.67
142.34
141.78
141.59
141.38
140.91
138.12
137.51
137.17
133.11
131.94
130.73
130.09
129.34
127.01
126.28
125.16
124.97
124.81
123.56
122.34
121.60
120.69
119.28
118.48
118.20
118.03
116.69
115.89
115.14
110.50
77.25
77.00
76.75
36.32
34.80
34.63
32.14
32.05
31.07
N
HN
N
N
L(cp-2)
^{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
δ(ppm)

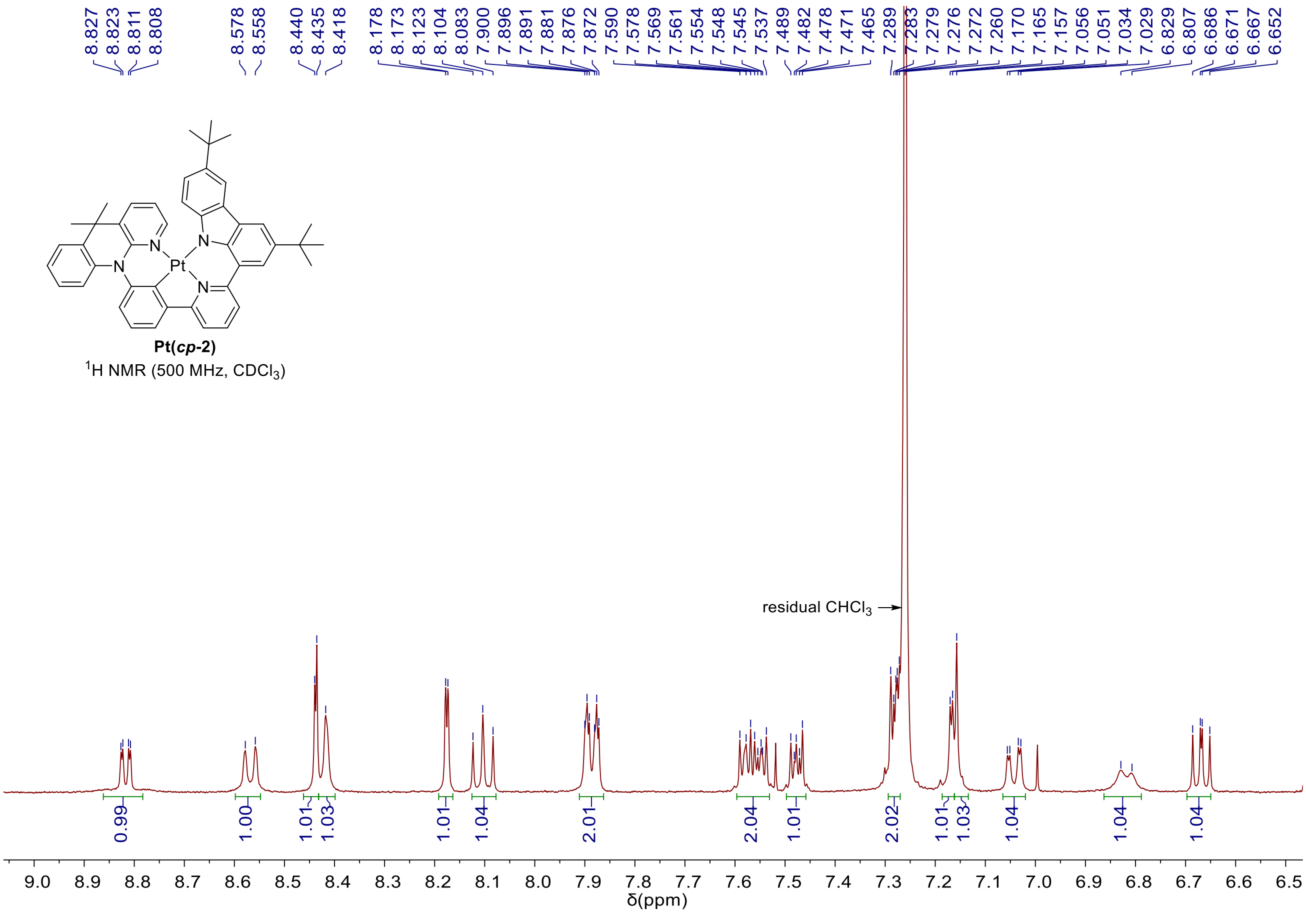

158.00
155.81
151.71
145.67
142.34
141.78
141.59
141.38
140.91
138.12
137.51
137.17
133.11
131.94
130.73
130.09
129.34
127.01
126.28
125.16
124.97
124.81
123.56
122.34
121.60
120.69
119.28
118.48
118.20
118.03
116.69
115.89
115.14
110.50
N
HN
N
N
L(cp-2)
^{13}C NMR (125 MHz, CDCl$_3$)
155 150 145 140 135 130 125 120 115 110
δ(ppm)

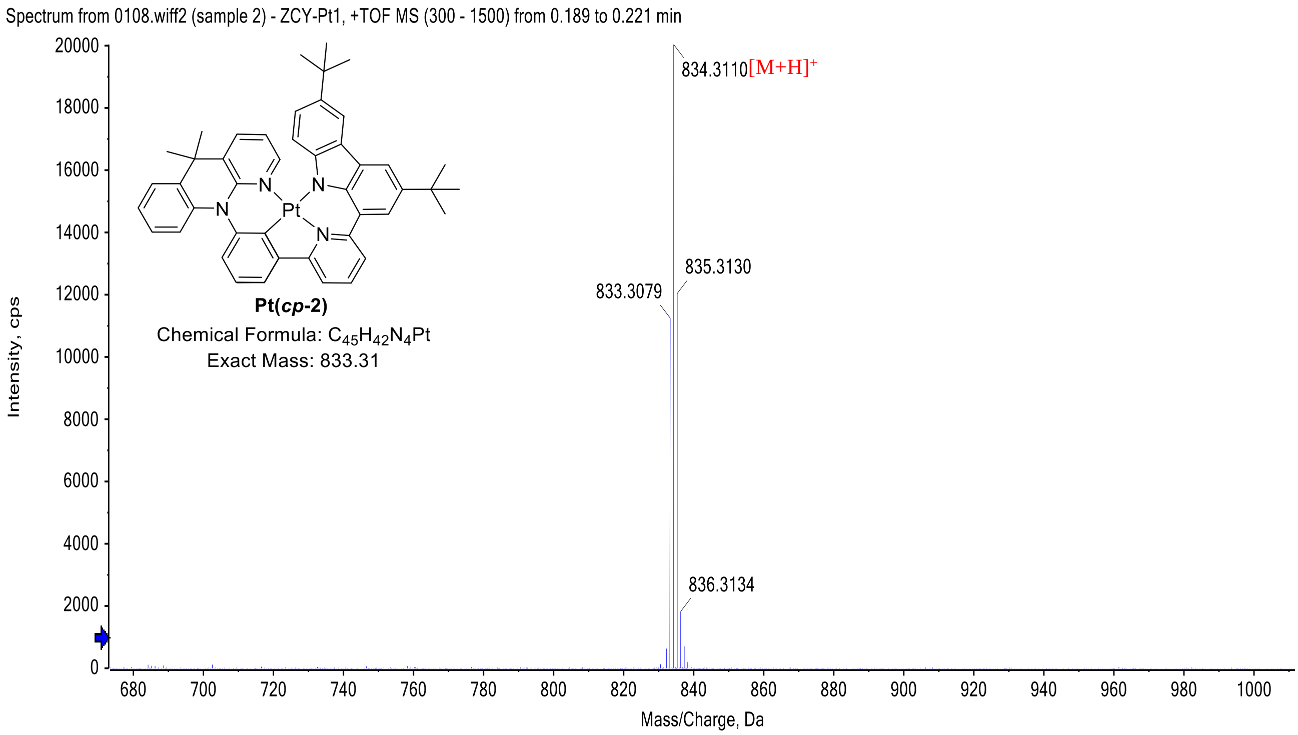


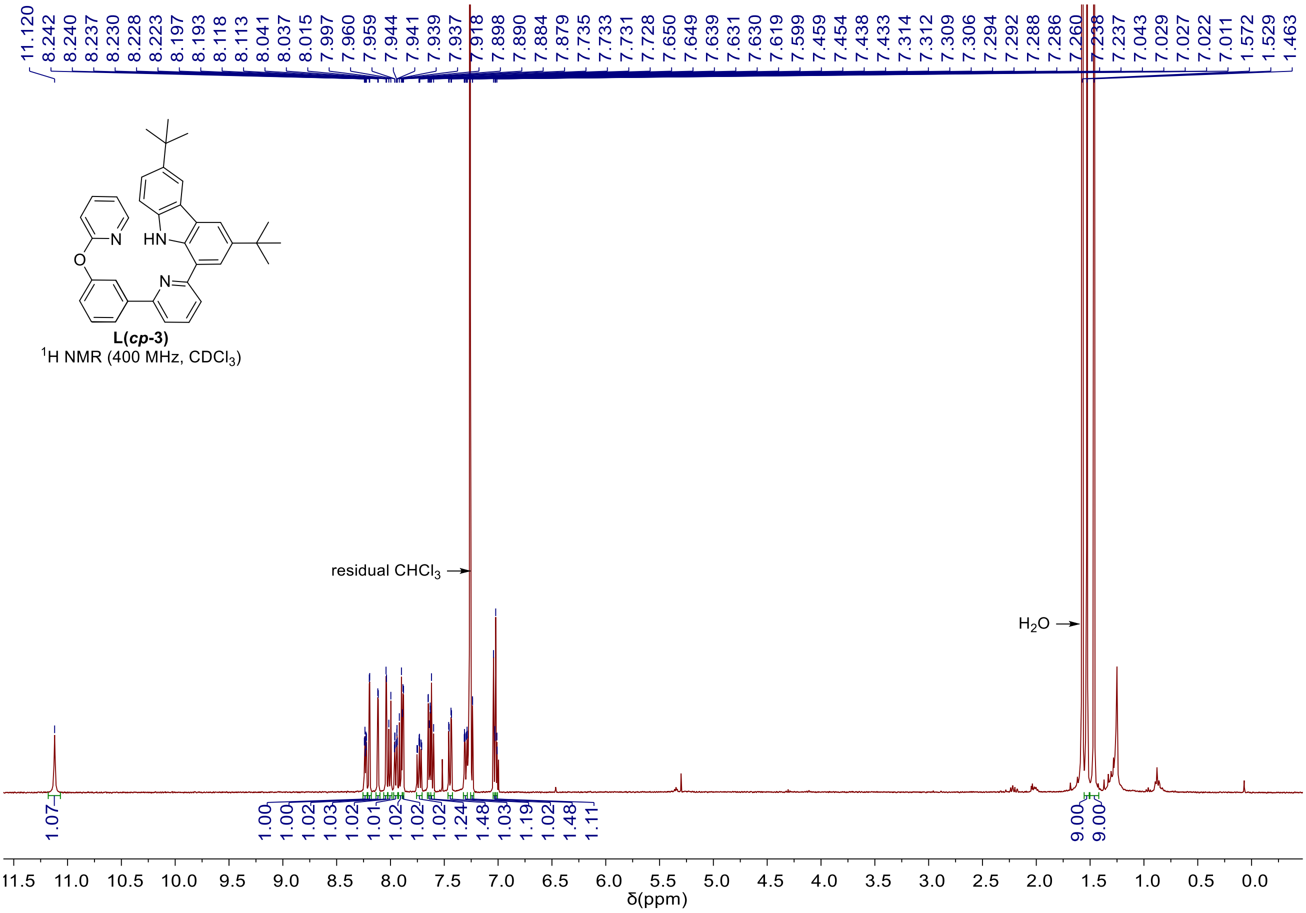
Spectrum from 0531-1.wiff2 (sample 3) - LCP-2, +TOF MS (100 - 800) from 0.194 to 0.212 ...trum from 0531-1.wiff2 (sample 3) - LCP-2, +TOF MS (100 - 800) from 0.004 to 0.050 min]
641.3628[M+H]+
642.3668
Intensity, cps
Mass/Charge, Da
L(cp-2)
Chemical Formula: C45H44N4
Exact Mass: 640.36

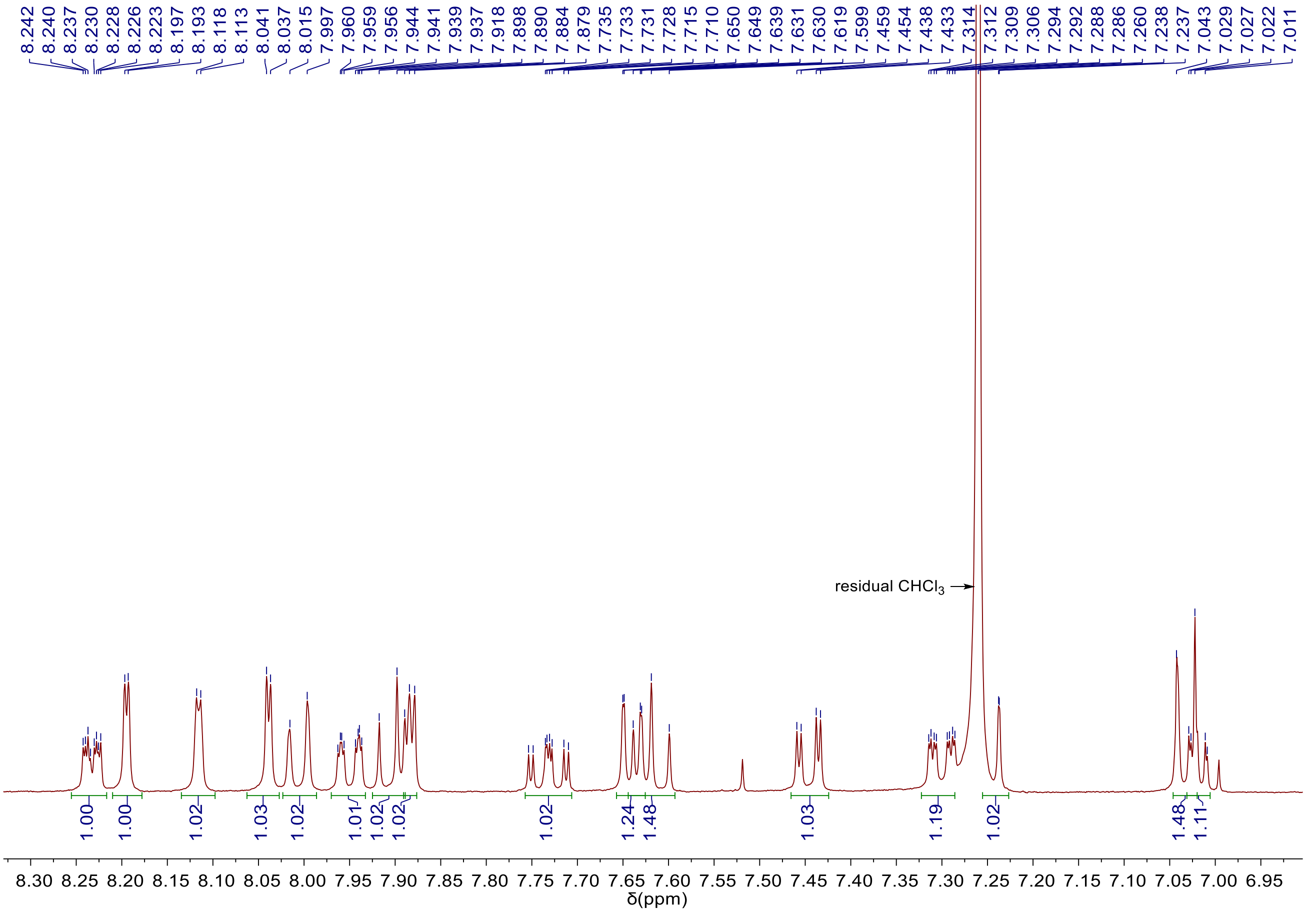


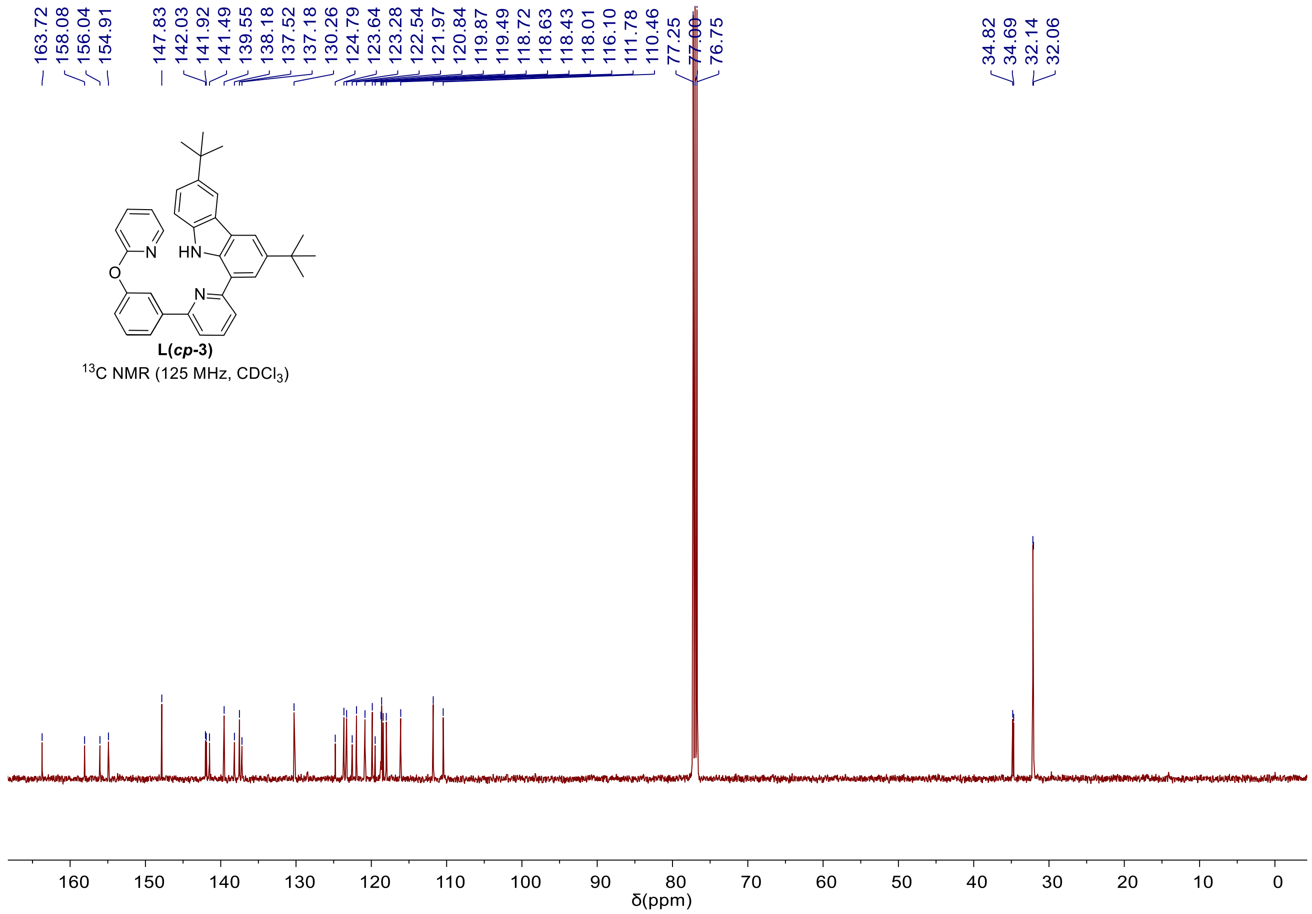
8.827 8.823 8.811 8.808 8.578 8.558 8.440 8.435 8.418 8.178 8.173 8.123 8.104 8.083 7.900 7.896 7.891 7.881 7.876 7.872 7.590 7.578 7.569 7.561 7.554 7.548 7.545 7.537 7.489 7.482 7.478 7.471 7.465 7.289 7.283 7.279 7.276 7.272 7.260 7.170 7.165 7.157 7.056 7.051 7.034 7.029 6.829 6.807 6.686 6.671 6.667 6.652 1.999 1.599 1.403 1.396
Pt(cp-2)
1H NMR (500 MHz, CDCl3)
residual CHCl3
CH2Cl2
H2O
0.99 1.00 1.01 1.03 1.01 1.04 2.01 2.04 1.01 2.02 1.01 1.03 1.04 1.04 1.04 3.01 9.00 9.00 3.02
δ(ppm)

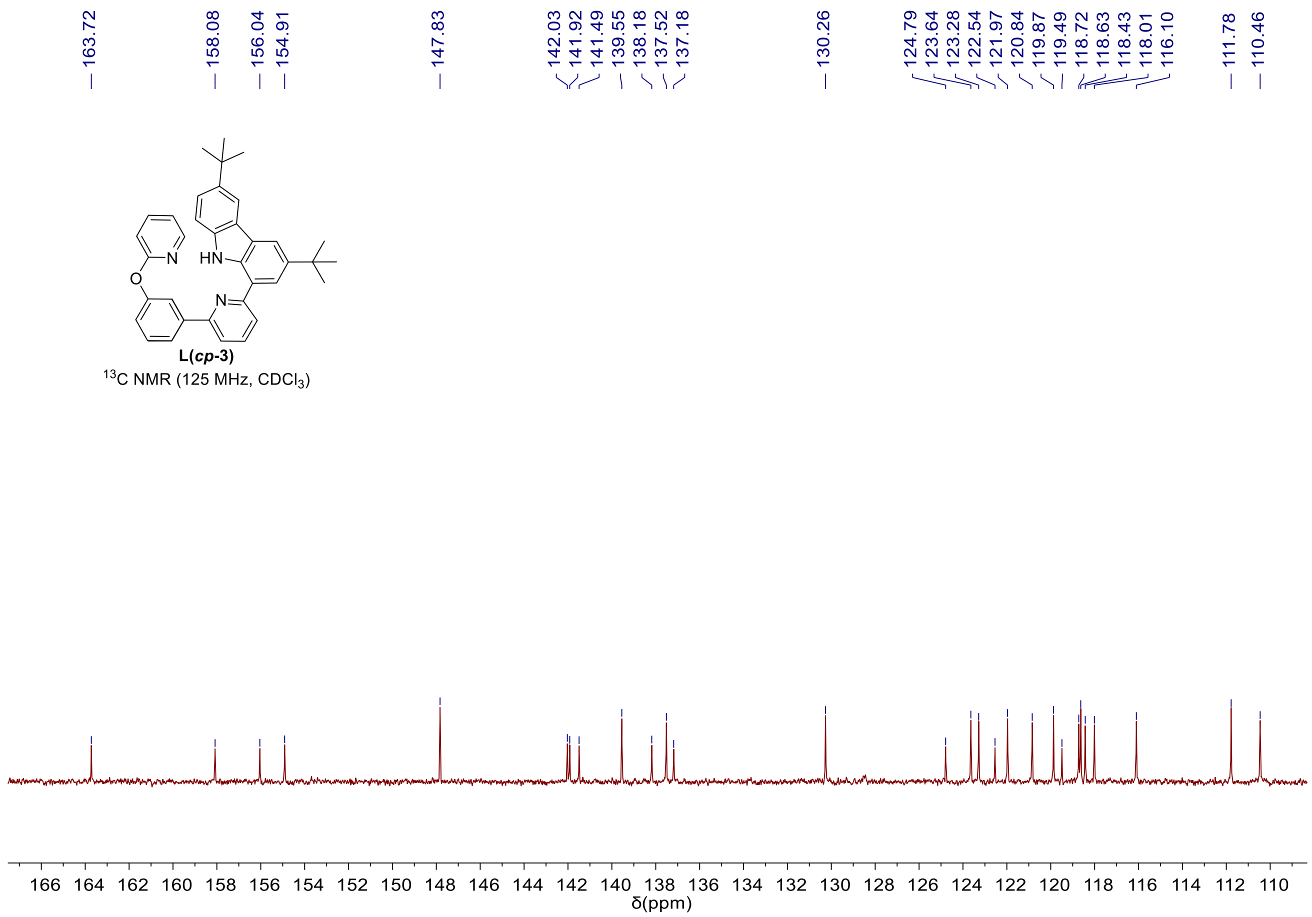

8.827 8.823 8.811 8.808 8.578 8.558 8.440 8.435 8.418 8.178 8.173 8.123 8.104 8.083 7.900 7.896 7.891 7.881 7.876 7.872 7.590 7.578 7.569 7.561 7.554 7.548 7.545 7.537 7.489 7.482 7.478 7.471 7.465 7.289 7.283 7.279 7.276 7.272 7.260 7.170 7.165 7.157 7.056 7.051 7.034 7.029 6.829 6.807 6.686 6.671 6.667 6.652
Pt(cp-2)
1H NMR (500 MHz, CDCl3)
residual CHCl3
0.99 1.00 1.01 1.03 1.01 1.04 2.01 2.04 1.01 2.02 1.01 1.03 1.04 1.04 1.04
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 6.9 6.8 6.7 6.6 6.5
δ(ppm)

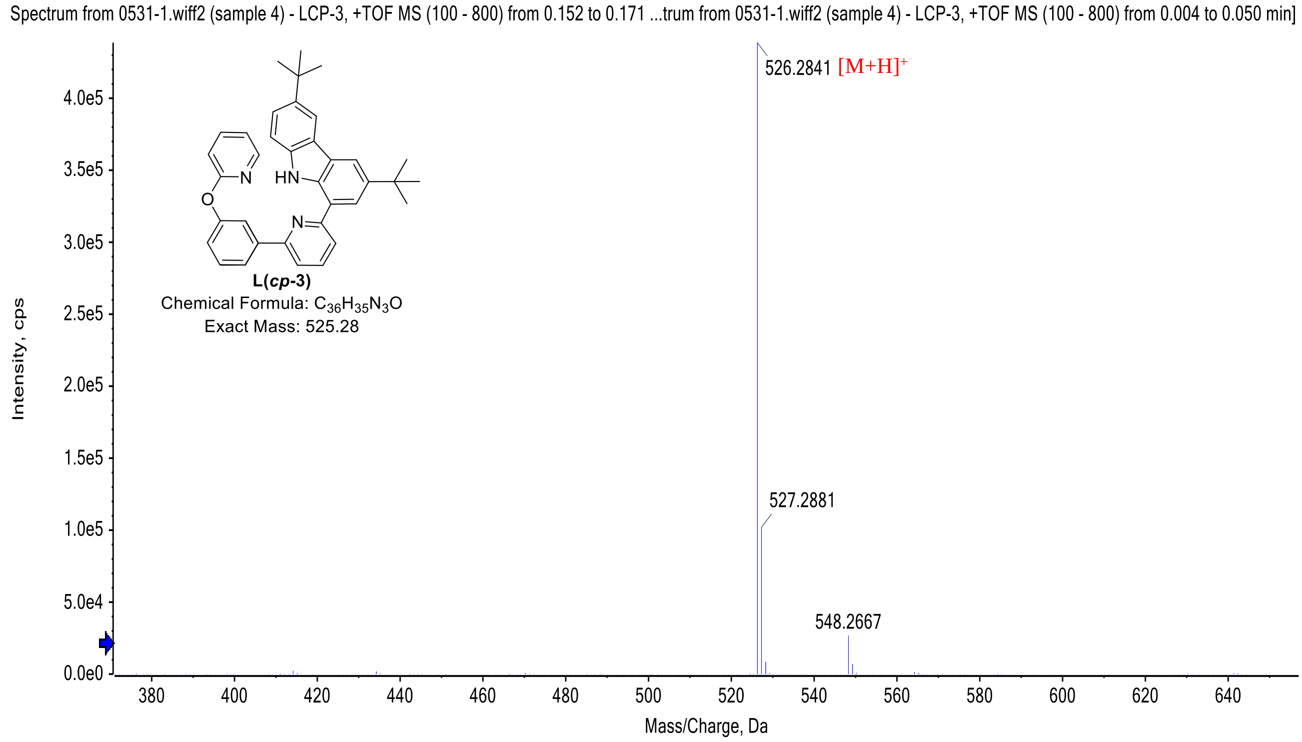

Spectrum from 0108.wiff2 (sample 2) - ZCY-Pt1, +TOF MS (300 - 1500) from 0.189 to 0.221 min
834.3110[M+H]+
835.3130
833.3079
836.3134
Pt(cp-2)
Chemical Formula: C45H42N4Pt
Exact Mass: 833.31
Intensity, cps
Mass/Charge, Da

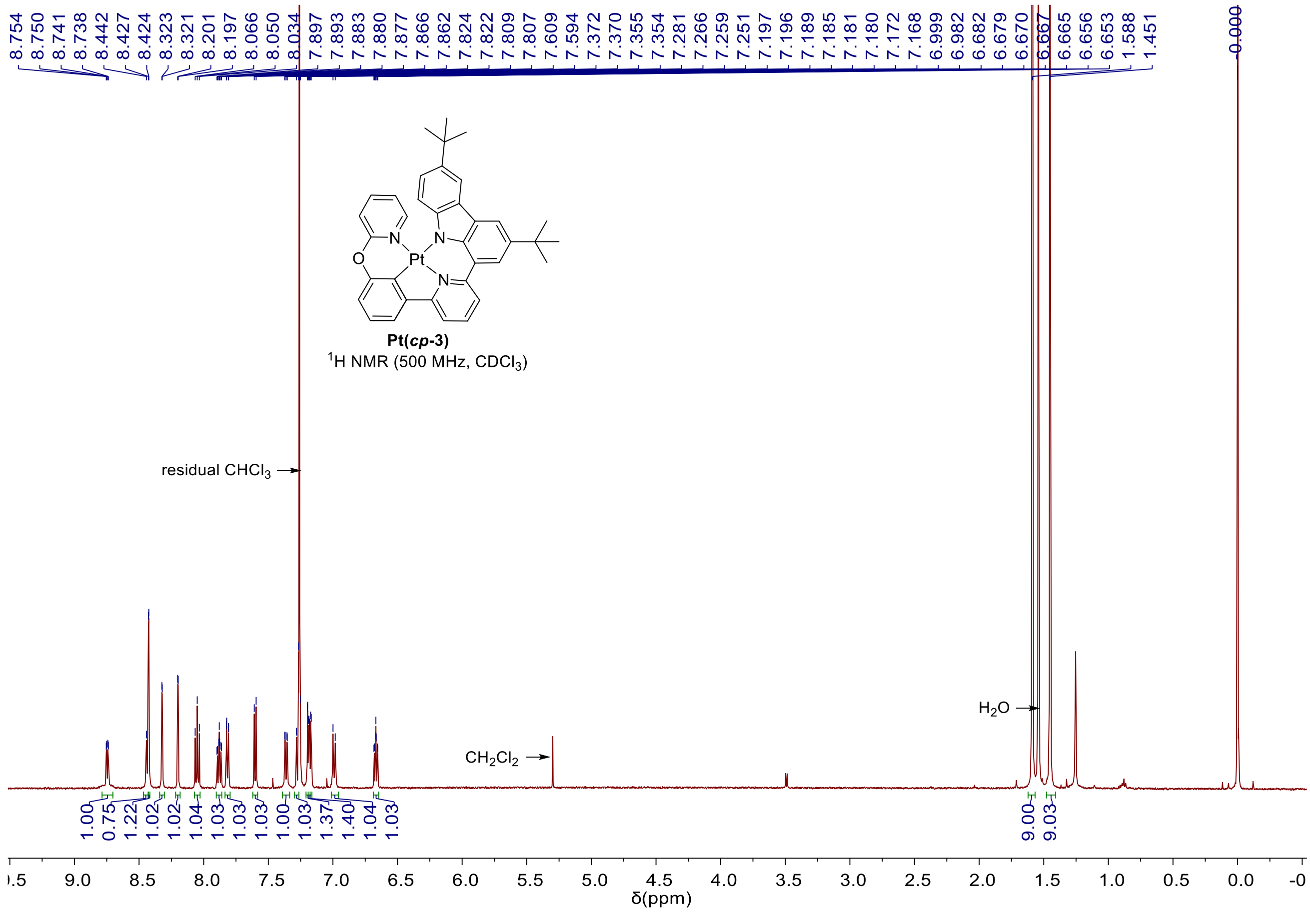

11.120 8.242 8.240 8.237 8.230 8.228 8.223 8.197 8.193 8.118 8.113 8.041 8.037 8.015 7.997 7.960 7.959 7.944 7.941 7.939 7.937 7.918 7.898 7.890 7.884 7.879 7.735 7.733 7.731 7.728 7.650 7.649 7.639 7.631 7.630 7.619 7.599 7.459 7.454 7.438 7.433 7.314 7.312 7.309 7.306 7.294 7.292 7.288 7.286 7.260 7.238 7.237 7.043 7.029 7.027 7.022 7.011 1.572 1.529 1.463
HN
N
O
N
L(*cp*-3)
^{1}H NMR (400 MHz, $CDCl_3$)
residual $CHCl_3$
H_2O
1.07
1.00 1.00 1.02 1.03 1.02 1.01 1.02 1.02 1.02 1.24 1.48 1.03 1.19 1.02 1.48 1.11
9.00 9.00
11.5 11.0 10.5 10.0 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
δ(ppm)

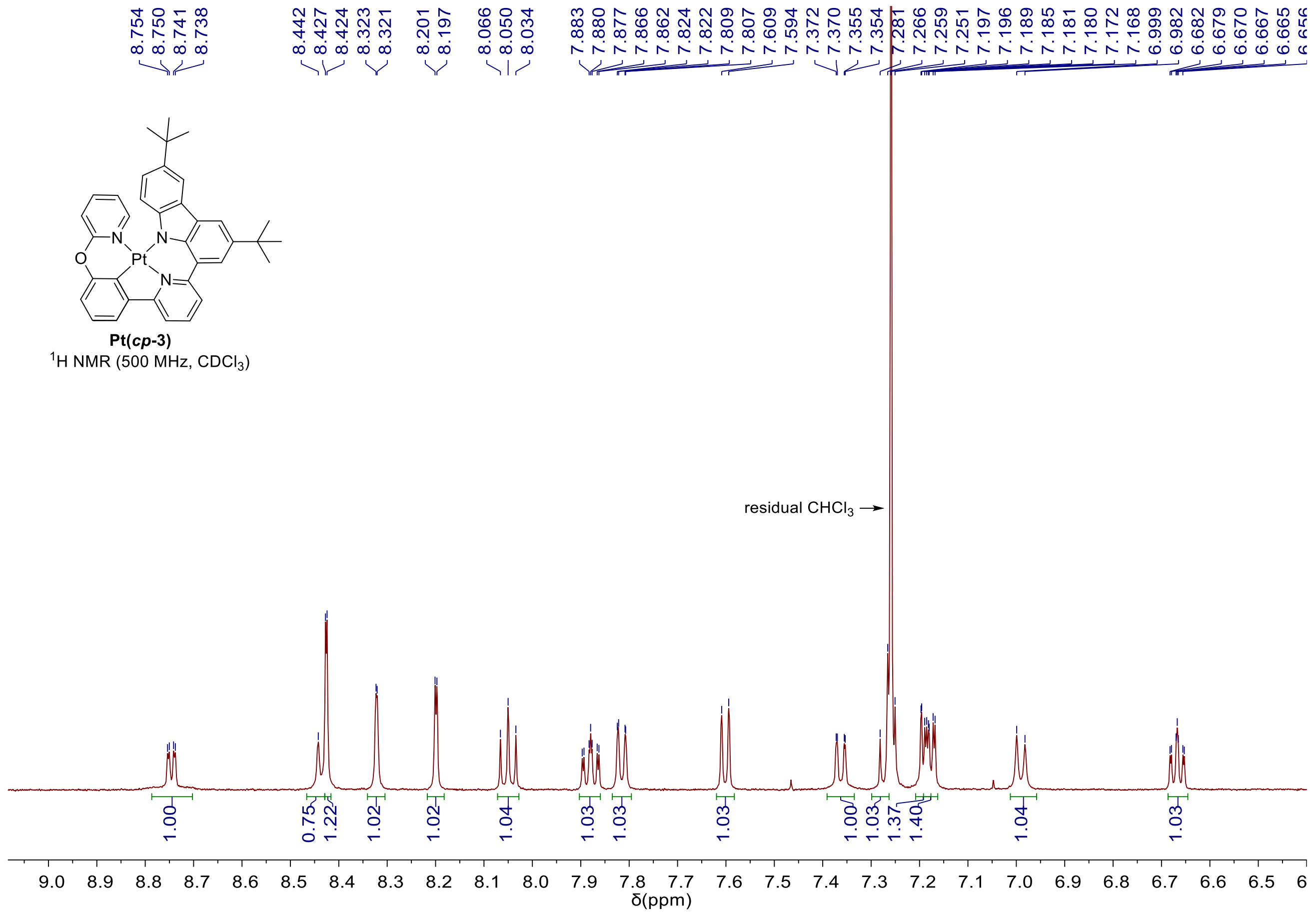

8.242 8.240 8.237 8.230 8.228 8.226 8.223 8.197 8.193 8.118 8.113 8.041 8.037 8.015 7.997 7.960 7.959 7.956 7.944 7.941 7.939 7.937 7.918 7.898 7.890 7.884 7.879 7.735 7.733 7.731 7.728 7.715 7.710 7.650 7.649 7.639 7.631 7.630 7.619 7.599 7.459 7.454 7.438 7.433 7.314 7.312 7.309 7.306 7.294 7.292 7.288 7.286 7.260 7.238 7.237 7.043 7.029 7.027 7.022 7.011
residual $CHCl_3$
1.00 1.00 1.02 1.03 1.02 1.01 1.02 1.02 1.02 1.24 1.48 1.03 1.19 1.02 1.48 1.11
8.30 8.25 8.20 8.15 8.10 8.05 8.00 7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95
δ(ppm)


163.72
158.08
156.04
154.91
147.83
142.03
141.92
141.49
139.55
138.18
137.52
137.18
130.26
124.79
123.64
123.28
122.54
121.97
120.84
119.87
119.49
118.72
118.63
118.43
118.01
116.10
111.78
110.46
77.25
77.00
76.75
34.82
34.69
32.14
32.06
HN
N
O
N
L(*cp*-3)
^{13}C NMR (125 MHz, CDCl$_3$)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ(ppm)


163.72
158.08
156.04
154.91
147.83
142.03
141.92
141.49
139.55
138.18
137.52
137.18
130.26
124.79
123.64
123.28
122.54
121.97
120.84
119.87
119.49
118.72
118.63
118.43
118.01
116.10
111.78
110.46
HN
N
O
N
L(*cp*-3)
^{13}C NMR (125 MHz, CDCl$_3$)
166 164 162 160 158 156 154 152 150 148 146 144 142 140 138 136 134 132 130 128 126 124 122 120 118 116 114 112 110
δ(ppm)


Spectrum from 0531-1.wiff2 (sample 4) - LCP-3, +TOF MS (100 - 800) from 0.152 to 0.171 ...trum from 0531-1.wiff2 (sample 4) - LCP-3, +TOF MS (100 - 800) from 0.004 to 0.050 min]
526.2841 [M+H]+
527.2881
548.2667
Intensity, cps
Mass/Charge, Da
L(cp-3)
Chemical Formula: C36H35N3O
Exact Mass: 525.28


Pt(cp-3)
1H NMR (500 MHz, CDCl3)
residual CHCl3
CH2Cl2
H2O
δ(ppm)


8.754
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8.424
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8.201
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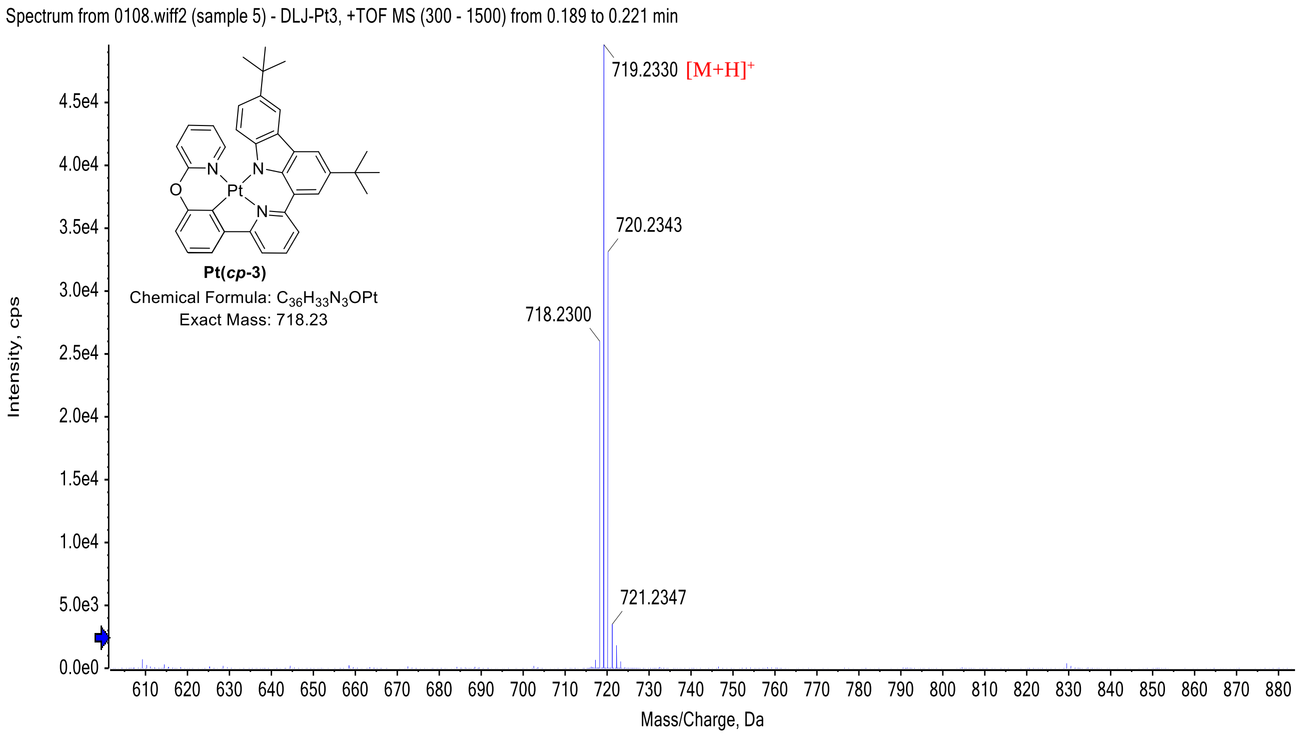
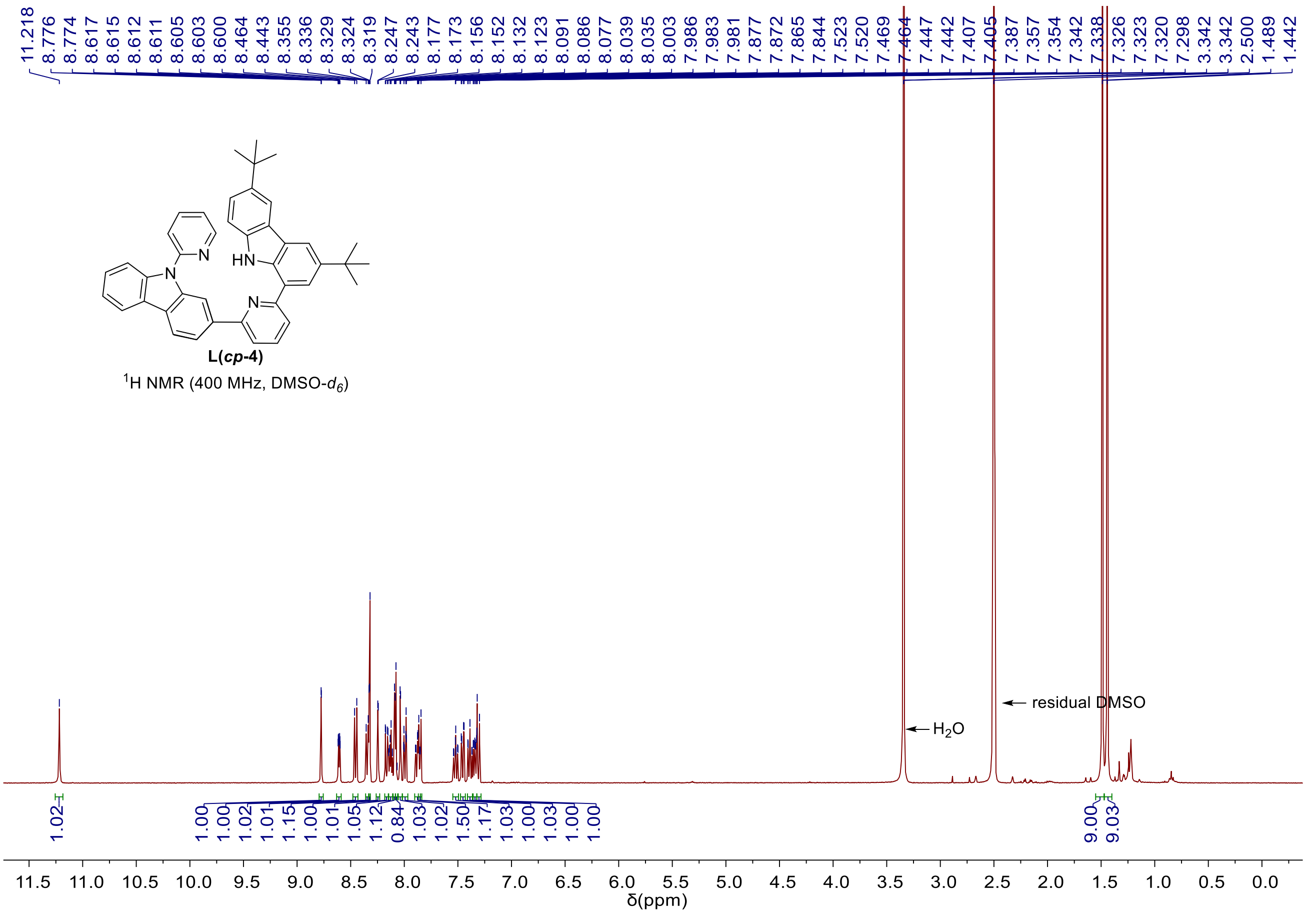
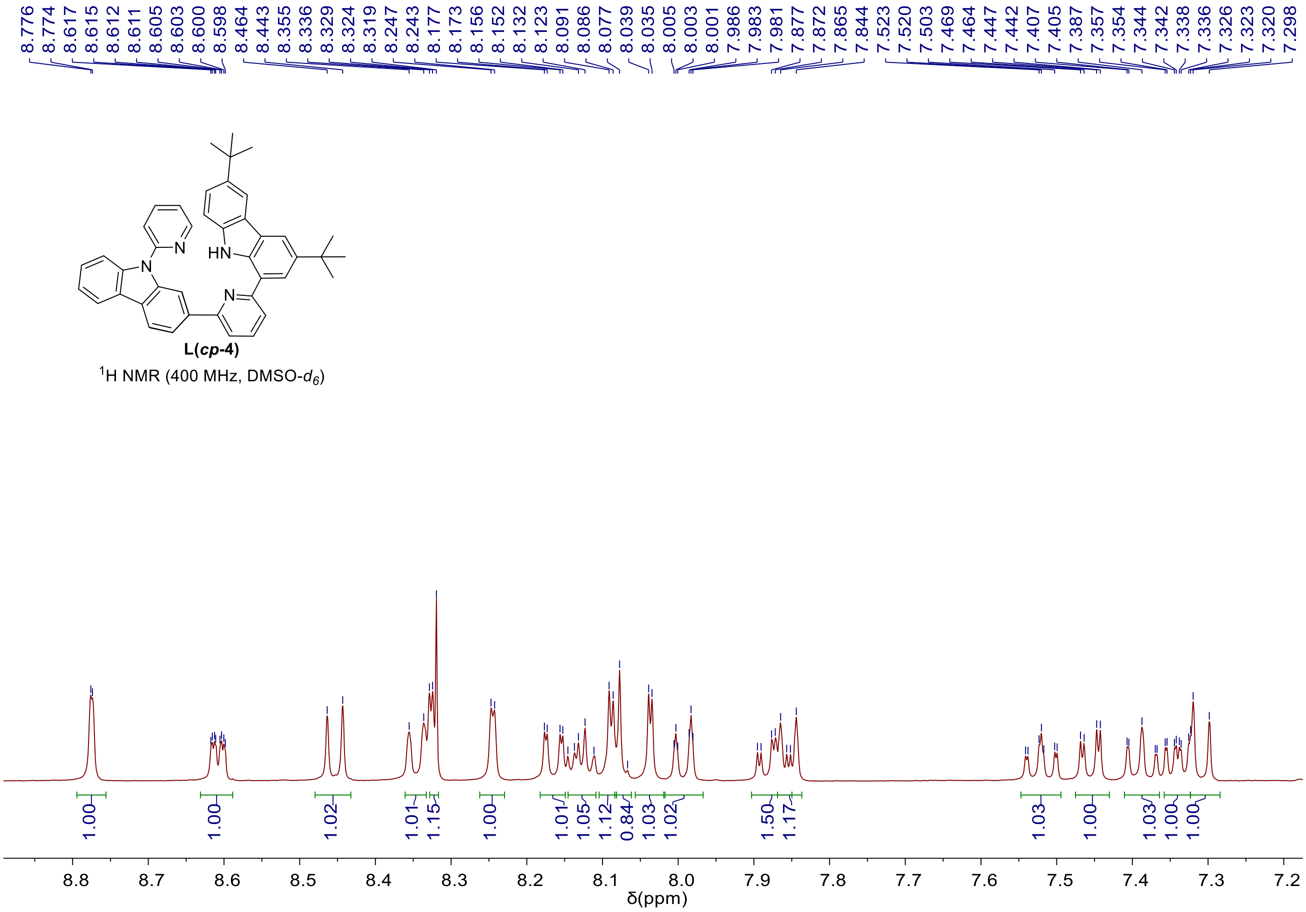
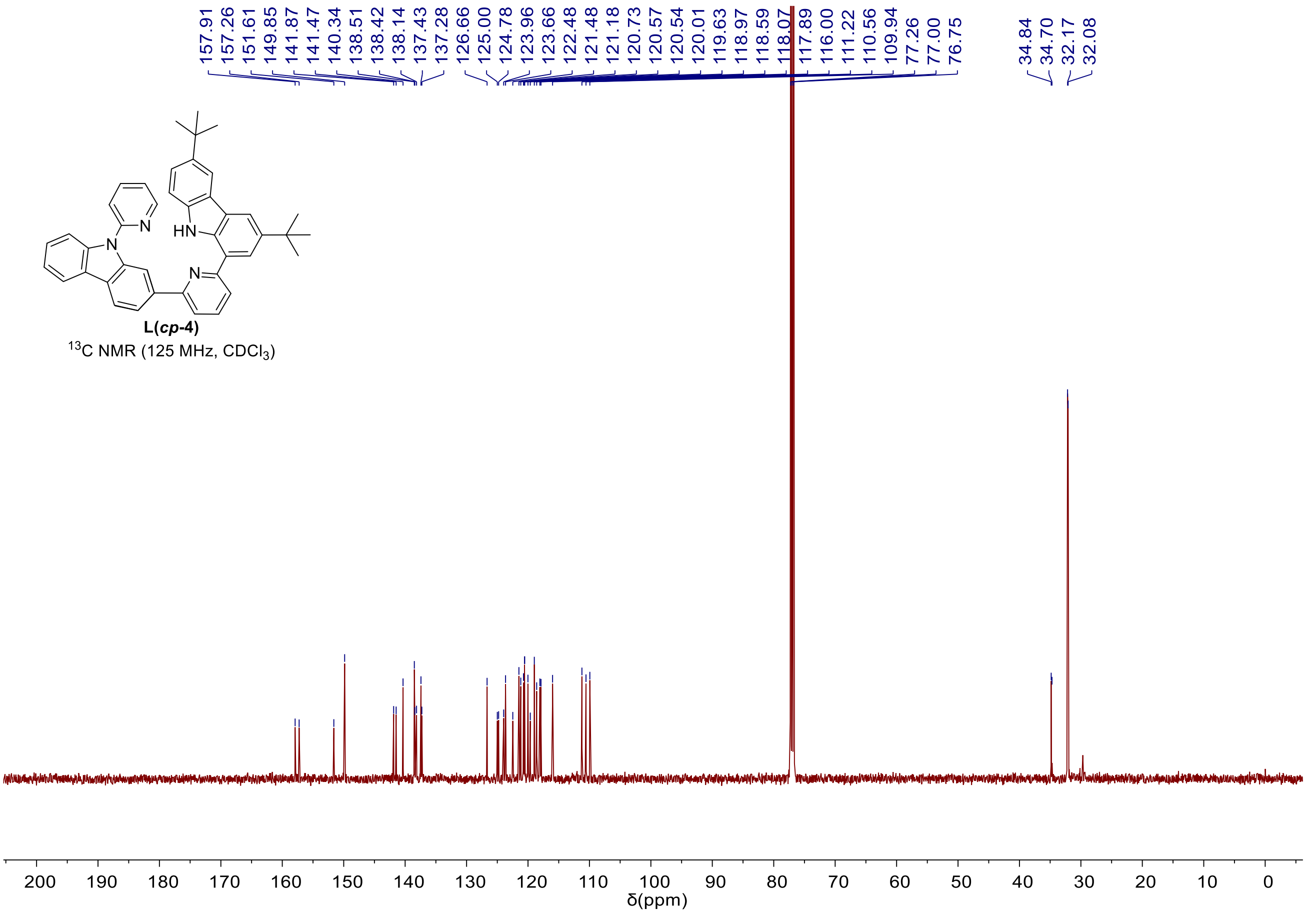
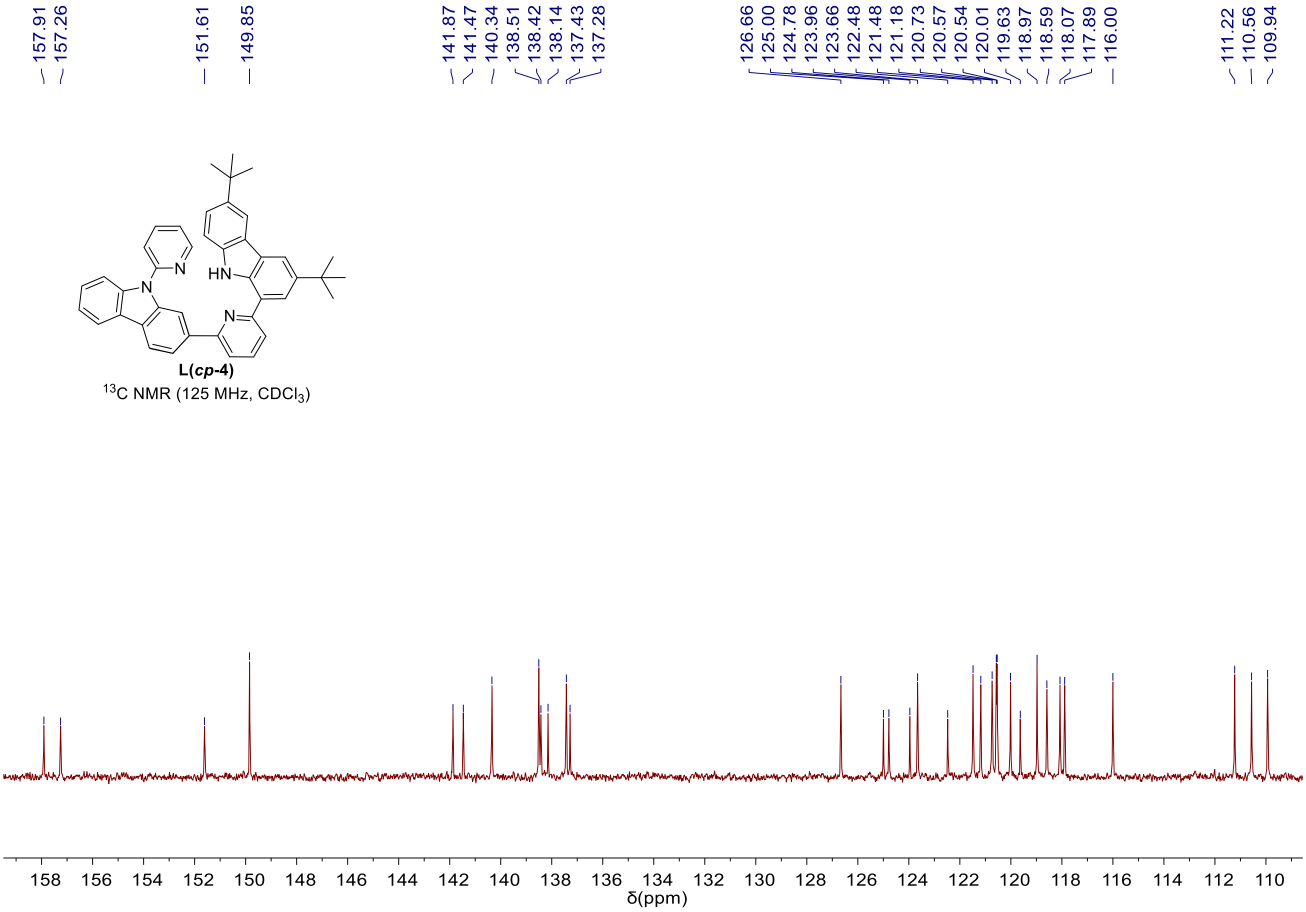
8.034
7.883
7.880
7.877
7.866
7.862
7.824
7.822
7.809
7.807
7.609
7.594
7.372
7.370
7.355
7.354
7.281
7.266
7.259
7.251
7.197
7.196
7.189
7.185
7.181
7.180
7.172
7.168
6.999
6.982
6.682
6.679
6.670
6.667
6.665
Pt(cp-3)
1H NMR (500 MHz, CDCl3)
residual CHCl3
1.00
0.75
1.22
1.02
1.02
1.04
1.03
1.03
1.03
1.00
1.03
1.37
1.40
1.04
1.03
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 6.9 6.8 6.7 6.6 6.5 6
δ(ppm)


Spectrum from 0108.wiff2 (sample 5) - DLJ-Pt3, +TOF MS (300 - 1500) from 0.189 to 0.221 min
719.2330 [M+H]+
720.2343
718.2300
721.2347
Pt(cp-3)
Chemical Formula: C36H33N3OPt
Exact Mass: 718.23
Intensity, cps
4.5e4
4.0e4
3.5e4
3.0e4
2.5e4
2.0e4
1.5e4
1.0e4
5.0e3
0.0e0
610 620 630 640 650 660 670 680 690 700 710 720 730 740 750 760 770 780 790 800 810 820 830 840 850 860 870 880
Mass/Charge, Da

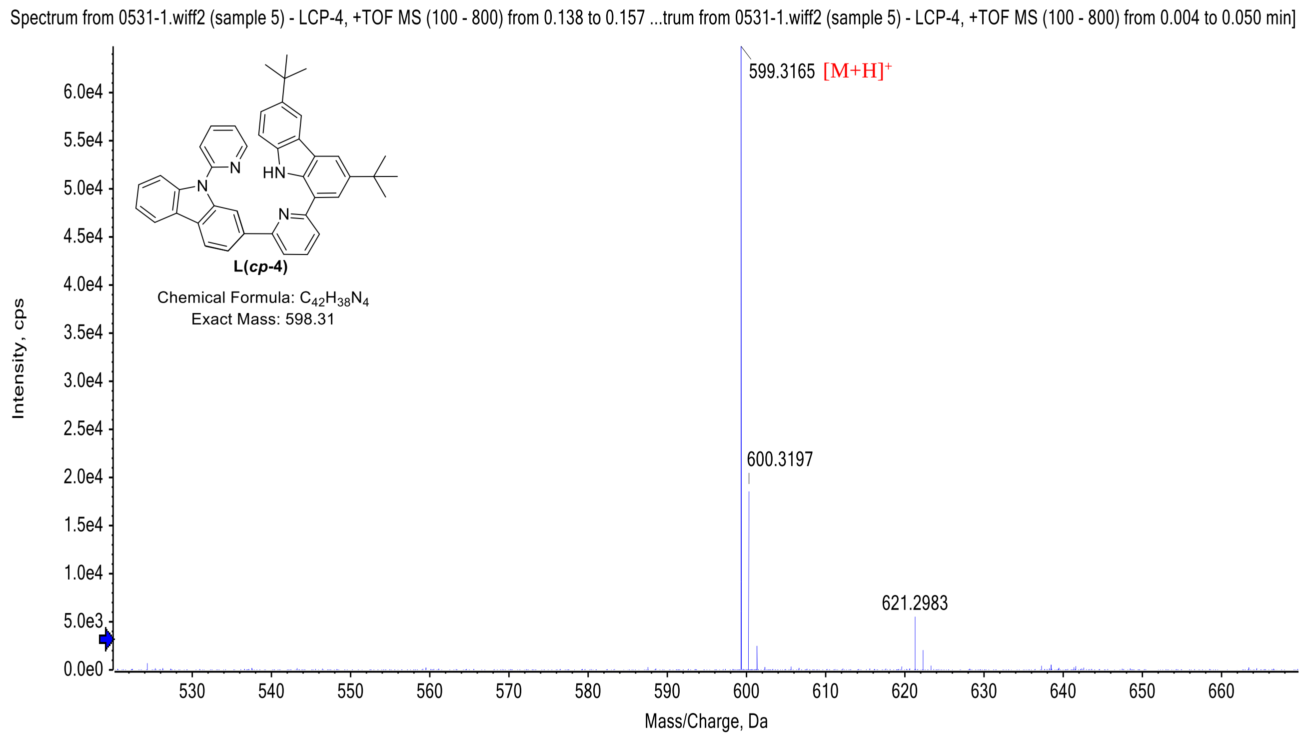

L(cp-4)
^{1}H NMR (400 MHz, DMSO-d_6)
H$_2$O
residual DMSO
δ(ppm)

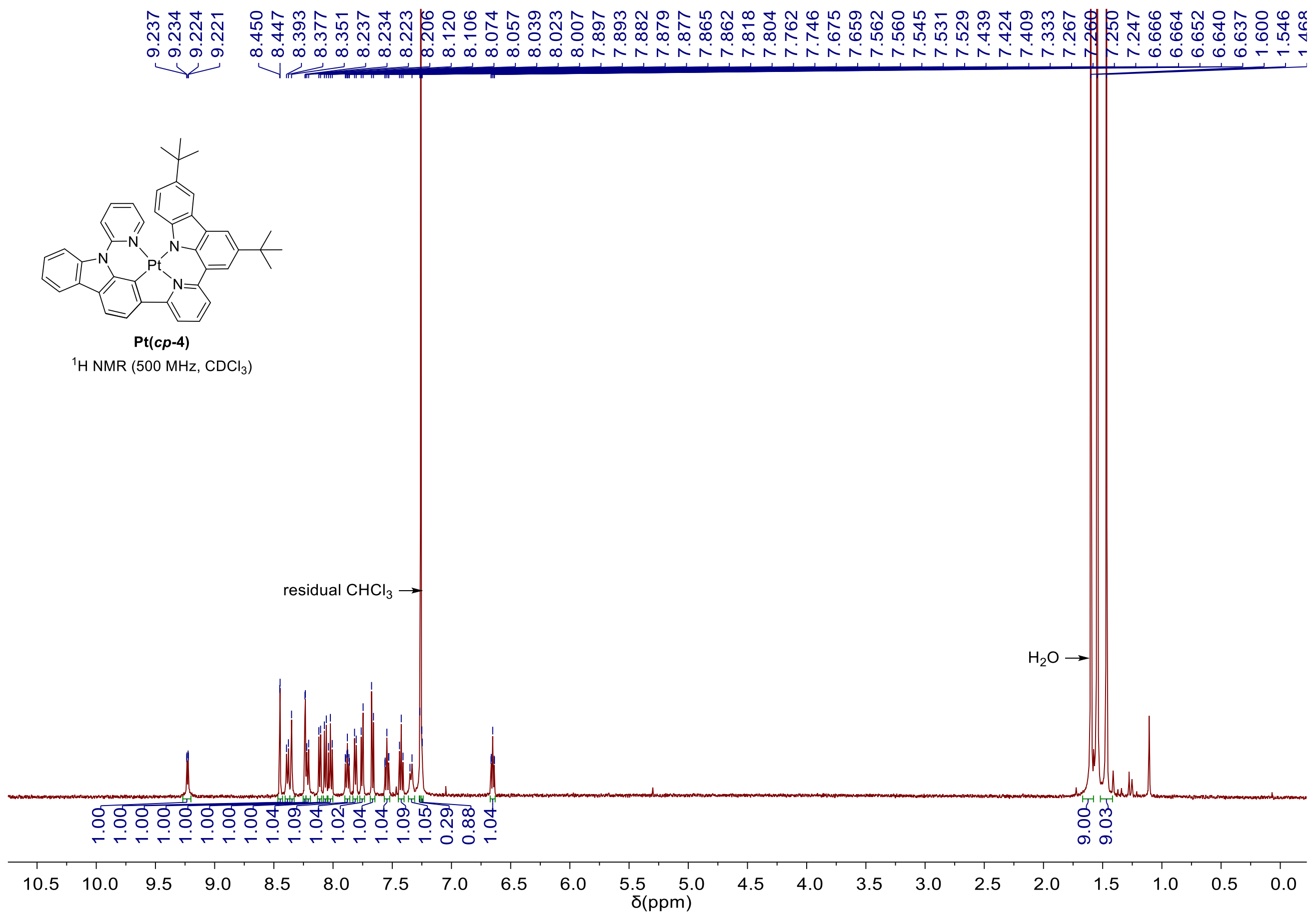

L(cp-4)
^{1}H NMR (400 MHz, DMSO-d_6)
δ(ppm)

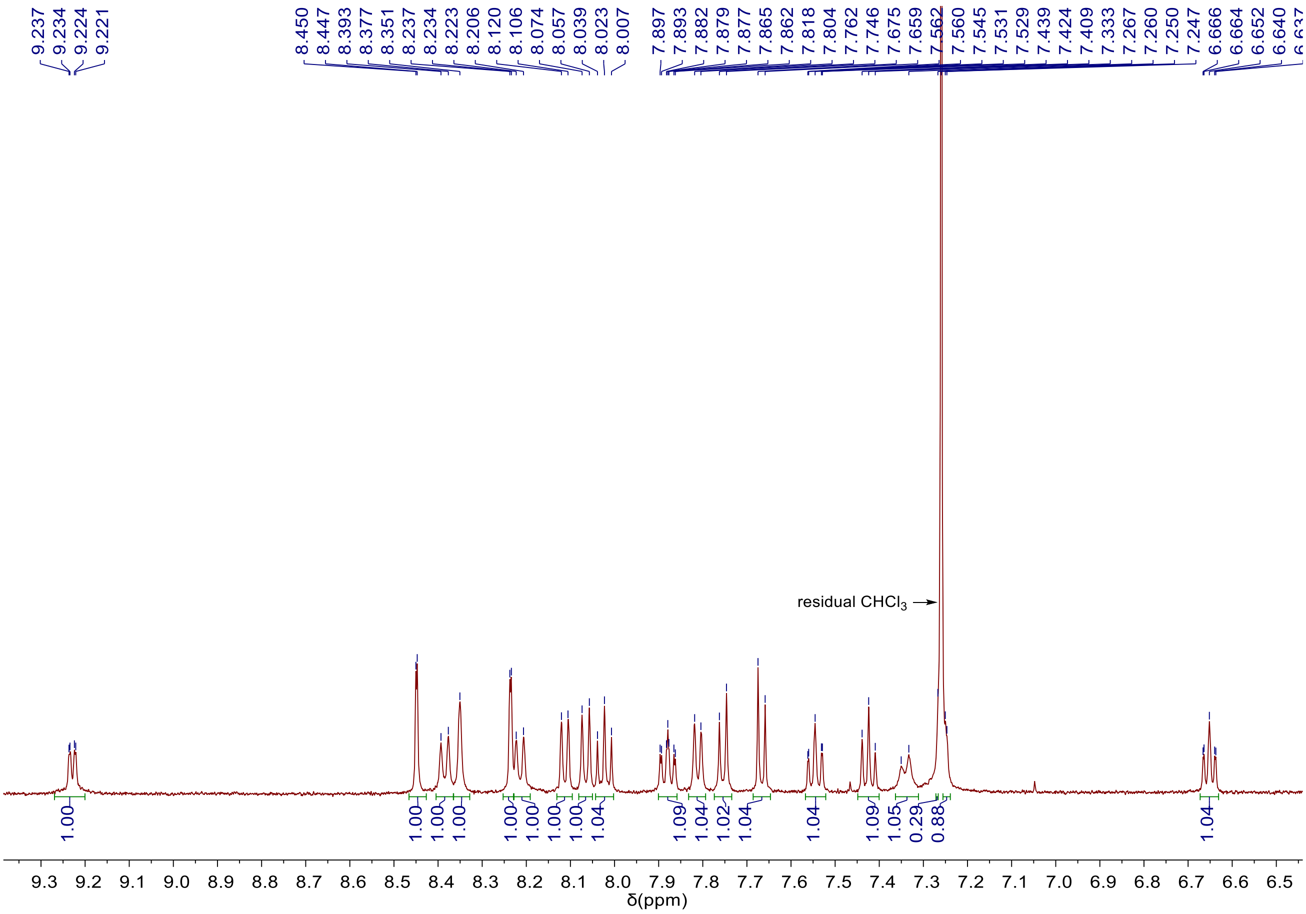

157.91 157.26 151.61 149.85 141.87 141.47 140.34 138.51 138.42 138.14 137.43 137.28 126.66 125.00 124.78 123.96 123.66 122.48 121.48 121.18 120.73 120.57 120.54 120.01 119.63 118.97 118.59 118.07 117.89 116.00 111.22 110.56 109.94 77.26 77.00 76.75
34.84 34.70 32.17 32.08
HN
N
L(*cp*-4)
^{13}C NMR (125 MHz, CDCl$_3$)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ(ppm)


157.91 157.26 151.61 149.85 141.87 141.47 140.34 138.51 138.42 138.14 137.43 137.28 126.66 125.00 124.78 123.96 123.66 122.48 121.48 121.18 120.73 120.57 120.54 120.01 119.63 118.97 118.59 118.07 117.89 116.00 111.22 110.56 109.94
HN
N
L(*cp*-4)
^{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
δ(ppm)

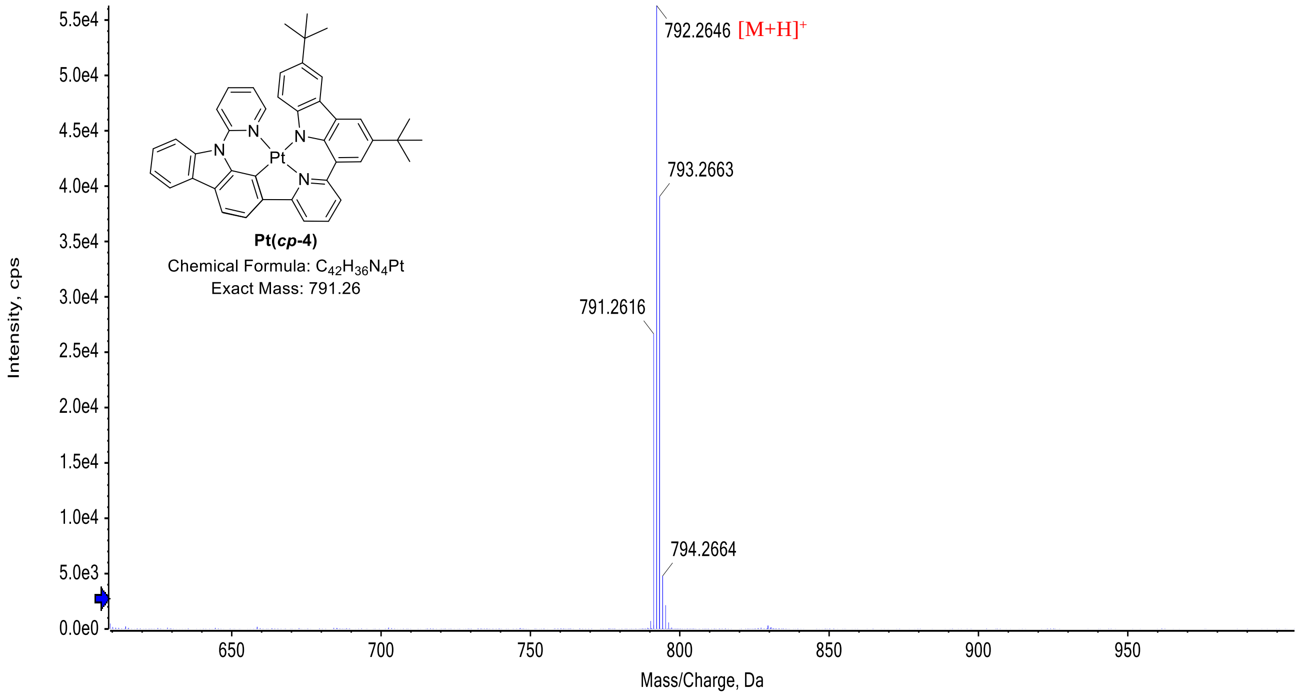
Spectrum from 0531-1.wiff2 (sample 5) - LCP-4, +TOF MS (100 - 800) from 0.138 to 0.157 ...trum from 0531-1.wiff2 (sample 5) - LCP-4, +TOF MS (100 - 800) from 0.004 to 0.050 min]







Spectrum from 0108.wiff2 (sample 4) - DLJ-Pt2, +TOF MS (300 - 1500) from 0.189 to 0.221 min



Cartesian coordinates of the structures

Pt(*cp*-1)_S_0

C	4.57388600	2.19102600	0.28968000
C	1.89621200	2.50751200	1.13305800
C	3.66706900	1.12751600	0.18447400
C	4.16499100	3.42126500	0.80962700
C	2.81787900	3.54291400	1.23450000
C	2.30883500	1.28601000	0.57846400
H	2.48457400	4.47913200	1.67497600
H	0.88135700	2.63598900	1.49871700
C	3.79328700	-0.25221200	-0.22132400
C	3.42784800	-2.95877700	-0.61980800
C	4.84559500	-1.02000200	-0.71279500
C	2.49974100	-0.82665500	-0.00642100
C	2.34058000	-2.23173900	-0.09362800
C	4.66336300	-2.38820500	-0.96848900
H	5.80446100	-0.54688600	-0.89728100
H	3.29975200	-4.02506600	-0.77304100
N	1.58547800	0.11299700	0.38122900
H	5.60179800	2.03845500	-0.02351600
C	5.11483500	4.62495100	0.95701500
C	6.53613300	4.31635500	0.44826800
H	6.99942900	3.49652000	1.00891800
H	7.17337900	5.20045800	0.56819400
H	6.53850900	4.04755300	-0.61436000
C	5.21967200	5.02994700	2.44693800
H	5.62111100	4.20523900	3.04691500
H	4.24461900	5.30086400	2.86535900
H	5.88574400	5.89433600	2.56550000
C	4.56729600	5.82125100	0.14186500

H	3.56876800	6.11975800	0.47893000
H	4.49835500	5.56782900	-0.92257900
H	5.22757200	6.69228100	0.24239500
C	5.76426400	-3.27684300	-1.58104100
C	7.05120000	-2.48444300	-1.88226700
H	7.48920600	-2.05648500	-0.97316400
H	6.86983400	-1.66807100	-2.59069100
H	7.79998900	-3.14947800	-2.32799700
C	6.12909400	-4.42069900	-0.60445700
H	6.49620000	-4.01979800	0.34727300
H	6.91426300	-5.05712800	-1.03206800
H	5.26786800	-5.06180700	-0.38644600
C	5.25673400	-3.88501100	-2.91036700
H	4.35959400	-4.49553000	-2.76110600
H	6.02593400	-4.52536000	-3.36090500
H	5.00528000	-3.09671600	-3.62920700
C	1.19923800	-2.94316700	0.50001700
C	-0.92780300	-4.35562200	1.63255800
C	1.36803900	-4.27109000	0.95108800
N	-0.00979100	-2.34030600	0.68962400
C	-1.07620700	-3.04028600	1.20420500
C	0.31695400	-4.96903700	1.51823700
H	2.34608400	-4.72701200	0.88378300
H	0.46316400	-5.98670300	1.86946100
H	-1.77782300	-4.89196100	2.03648700
N	-3.59748300	0.81150400	-0.42077100
C	-2.57365800	1.72873100	-0.63802600
C	-0.65594500	3.57015300	-1.44664900
C	-2.94161200	3.05315800	-0.98126800

N	-1.25246100	1.39893900	-0.55038700
C	-0.34213500	2.30131500	-1.00638800
C	-1.99418000	3.97161900	-1.38354300
H	-3.98826000	3.32390700	-0.93582100
H	0.67902600	1.95722100	-0.99401700
H	0.13439400	4.22726600	-1.79022200
Pt	-0.50110100	-0.40499200	0.18037200
H	-2.29217400	4.98343200	-1.64286400
C	-4.81371300	0.93402400	-1.17595900
C	-7.18621200	1.02269200	-2.64761200
C	-4.79255500	1.30060800	-2.52884100
C	-6.02038700	0.56320800	-0.55682700
C	-7.19666700	0.61439100	-1.31445000
C	-5.97719000	1.35999000	-3.25718300
H	-3.84838500	1.53023300	-3.01084200
H	-8.13879100	0.32813300	-0.86043600
H	-5.94860800	1.64788500	-4.30429000
H	-8.11486600	1.06007700	-3.20990100
C	-2.35214100	-2.31792700	1.18704200
C	-4.71867000	-0.81336200	0.98566300
C	-3.54098600	-2.80034400	1.74380400
C	-2.32583500	-1.07187000	0.51730100
C	-3.52214700	-0.37215900	0.38258600
C	-4.70514000	-2.04160100	1.65696400
H	-3.57066300	-3.75160400	2.26742400
H	-5.60971100	-2.41674000	2.12104300
C	-5.95440100	0.09119300	0.89749500
C	-5.75339700	1.31801200	1.83483700
H	-6.61257100	1.99498600	1.76048700

H	-4.85105200	1.88117600	1.58260300
H	-5.66343800	0.98493500	2.87480000
C	-7.24170300	-0.62580900	1.33582500
H	-7.45407500	-1.50588300	0.71954700
H	-8.09932200	0.05183300	1.27671600
H	-7.16519200	-0.94571800	2.37936400

Pt(*cp*-1)_T_1

C	4.47639900	2.28034400	0.31996500
C	1.74855800	2.49775600	1.05133700
C	3.62344200	1.19005600	0.17083200
C	3.98933600	3.49405100	0.83880700
C	2.62457200	3.56709900	1.20884200
C	2.24467300	1.30504500	0.50969300
H	2.23942400	4.48568800	1.64086800
H	0.71199600	2.57626000	1.36278700
C	3.81696900	-0.19349500	-0.23572400
C	3.54771700	-2.91366300	-0.64227100
C	4.92344600	-0.91672500	-0.66787300
C	2.54928900	-0.81321400	-0.07059100
C	2.40913100	-2.22535500	-0.12625400
C	4.77374900	-2.30327500	-0.92140100
H	5.87276600	-0.41864800	-0.82192800
H	3.44928900	-3.97662500	-0.82590800
N	1.58038800	0.11298600	0.26238900
H	5.52065600	2.18084300	0.04512200
C	4.88799000	4.72905600	1.02929800
C	6.33794500	4.48019800	0.57124100
H	6.81517000	3.67702300	1.14407200
H	6.93155100	5.38911600	0.72075200

H	6.39093800	4.22183300	-0.49251100
C	4.91860400	5.11931800	2.52727100
H	5.32711300	4.30421900	3.13533800
H	3.91979000	5.35286300	2.90995000
H	5.54917900	6.00455400	2.67620400
C	4.32120500	5.91010700	0.20418300
H	3.30212600	6.16963800	0.50914500
H	4.29932200	5.66613200	-0.86425900
H	4.94664800	6.80151100	0.33646200
C	5.92643200	-3.15535300	-1.48814900
C	7.20121600	-2.32656600	-1.74120200
H	7.59209100	-1.88552400	-0.81709900
H	7.02594500	-1.51788700	-2.45982000
H	7.98406300	-2.97241900	-2.15486800
C	6.28186100	-4.28432300	-0.49041000
H	6.59505600	-3.87015500	0.47477000
H	7.10546900	-4.89368400	-0.88283400
H	5.43218600	-4.95017200	-0.30827000
C	5.48763700	-3.78110900	-2.83425100
H	4.60924100	-4.42400300	-2.71829300
H	6.29810000	-4.39162600	-3.25172300
H	5.23681900	-3.00305300	-3.56428100
C	1.28532800	-2.94145700	0.45446400
C	-0.82948900	-4.37757900	1.58542900
C	1.46531700	-4.26038600	0.90127200
N	0.04797600	-2.32427000	0.65315800
C	-1.01301000	-3.07535000	1.16188800
C	0.43440300	-4.98367800	1.48457500
H	2.44988600	-4.70428700	0.81836600

H	0.59978300	-5.99219300	1.84914200
H	-1.67297400	-4.93138000	1.98271900
N	-3.60440300	0.76086900	-0.40337200
C	-2.59415100	1.68425400	-0.65682500
C	-0.72796500	3.51153600	-1.59554400
C	-2.97790300	3.00846800	-0.97224000
N	-1.26638200	1.34602400	-0.63448700
C	-0.38914600	2.24757700	-1.16963700
C	-2.05858900	3.92760700	-1.43799500
H	-4.02085300	3.27753800	-0.86411800
H	0.63013900	1.90134500	-1.23415500
H	0.03754300	4.15978900	-2.00693300
Pt	-0.47952800	-0.43168000	0.13224600
H	-2.36742800	4.94078600	-1.67634300
C	-4.83848500	0.87770600	-1.13081000
C	-7.24185500	0.95566900	-2.55400300
C	-4.84787500	1.24847100	-2.48310300
C	-6.03019300	0.49729300	-0.48874600
C	-7.22220500	0.54406800	-1.22222200
C	-6.04705500	1.30170200	-3.18724800
H	-3.91539400	1.48648200	-2.98323100
H	-8.15285200	0.25133100	-0.74876500
H	-6.04124000	1.59204000	-4.23413800
H	-8.18214500	0.98964900	-3.09704200
C	-2.29653200	-2.38128500	1.15273600
C	-4.68879600	-0.88562800	1.00284400
C	-3.48359100	-2.88181000	1.70230000
C	-2.29552500	-1.11416200	0.51428000
C	-3.49887900	-0.42298000	0.39275500

C	-4.65317100	-2.12906400	1.64228800
H	-3.50307400	-3.84645500	2.20094600
H	-5.54941700	-2.52291000	2.10833600
C	-5.92720500	0.01617700	0.95933200
C	-5.71238200	1.23710700	1.90108000
H	-6.57592700	1.91147800	1.85262800
H	-4.81849000	1.80661700	1.63286200
H	-5.59620500	0.89566800	2.93582900
C	-7.20030300	-0.71038700	1.42249500
H	-7.42526400	-1.58413300	0.80164900
H	-8.06194500	-0.03551200	1.39371200
H	-7.09445500	-1.04289100	2.45960700

Pt(*cp*-2)_S_0

C	-4.07561600	2.67041400	-0.21577100
C	-1.41908800	2.52085900	-1.16425700
C	-3.36049200	1.46854100	-0.13563100
C	-3.48326200	3.81160300	-0.76244900
C	-2.15330500	3.69902500	-1.23951900
C	-2.01308400	1.39012400	-0.58369300
H	-1.68096700	4.56339600	-1.69914100
H	-0.41199400	2.47232600	-1.56845600
C	-3.70436700	0.13232400	0.29238600
C	-3.78795800	-2.59708800	0.72391500
C	-4.84601900	-0.44204700	0.83323100
C	-2.53526300	-0.65836100	0.03440100
C	-2.61289100	-2.06708700	0.14093000
C	-4.88989900	-1.82316900	1.10608500
H	-5.70791000	0.18480600	1.04931000
H	-3.82703800	-3.66542500	0.89263900

N	-1.49306200	0.11082100	-0.40086200
H	-5.10102100	2.69636100	0.13873300
C	-4.21960700	5.15972200	-0.87992500
C	-5.65361600	5.09405600	-0.32102900
H	-6.26826100	4.36656800	-0.86338500
H	-6.13599300	6.07368500	-0.41971700
H	-5.66380500	4.82477700	0.74142900
C	-4.30568800	5.58240900	-2.36632200
H	-4.85603400	4.83712900	-2.95184900
H	-3.31346200	5.69207300	-2.81649700
H	-4.82472800	6.54462400	-2.46408300
C	-3.44839800	6.24290600	-0.08769200
H	-2.42591600	6.36747100	-0.46028700
H	-3.38679400	5.97898000	0.97463100
H	-3.95361800	7.21399500	-0.16840900
C	-6.13878000	-2.42755500	1.77675500
C	-7.38255900	-2.17066600	0.89235600
H	-7.26736200	-2.64241800	-0.09039300
H	-7.55348500	-1.10134000	0.72945000
H	-8.28305200	-2.58274500	1.36537300
C	-6.01847600	-3.94813100	1.99443600
H	-5.91286100	-4.48963600	1.04689400
H	-6.92291800	-4.32337700	2.48719300
H	-5.16456600	-4.20277300	2.63282500
C	-6.35151100	-1.76422800	3.15880900
H	-5.49086500	-1.94274200	3.81370900
H	-7.24459600	-2.17201100	3.64935600
H	-6.48379100	-0.68051000	3.07195300
C	-1.63488000	-2.96987300	-0.47935600

C	0.17323900	-4.73811300	-1.66944100
C	-2.04013800	-4.26223900	-0.88407600
N	-0.35254100	-2.58107000	-0.74003200
C	0.55555400	-3.45660000	-1.28797200
C	-1.14777000	-5.13598800	-1.47724800
H	-3.07480600	-4.55028600	-0.75924700
H	-1.47597900	-6.12324500	-1.79022100
H	0.90205400	-5.41585700	-2.09696800
C	1.93314000	-2.95329400	-1.35865700
C	4.49154300	-1.86427300	-1.33223000
C	2.98022200	-3.62739900	-1.99732100
C	2.14927400	-1.71470500	-0.70334100
C	3.44975600	-1.21218000	-0.64978700
C	4.25526800	-3.06454700	-1.99934200
H	2.81011500	-4.56689000	-2.51503800
H	5.06996000	-3.55814700	-2.52099900
H	5.49043100	-1.44035800	-1.32756900
H	0.72603800	3.87573500	1.75532500
C	1.36798600	3.11498200	1.32651500
H	3.17732500	4.27647400	1.39527200
C	2.73572500	3.32020600	1.13914900
N	1.55161600	0.91571000	0.35554900
C	3.52244200	2.30470800	0.61847800
C	0.82244900	1.92460700	0.89706400
C	2.90670300	1.05194400	0.32651400
H	-0.23603100	1.73539200	0.96938700
C	5.66474200	1.23189200	0.98279000
C	6.83869200	1.26338700	1.74384400
C	4.99776200	0.00775300	0.82118900

H	4.94972000	-2.08651900	1.33118200
N	3.76257900	-0.02246000	0.08625600
C	7.35026100	0.10534600	2.32745300
H	7.36399500	2.20210900	1.88357100
H	8.26867900	0.14949300	2.90573400
C	6.66836900	-1.10294000	2.17402000
H	7.04159900	-2.00834300	2.64428200
C	5.49087200	-1.15313700	1.43327900
Pt	0.47962400	-0.75088000	-0.29562600
C	5.01858200	2.45090200	0.32856900
C	5.58797900	3.77411900	0.86366700
H	6.65356800	3.85044400	0.62724000
H	5.47219700	3.86707200	1.94890400
H	5.09676100	4.62828800	0.38645100
C	5.25901300	2.41701100	-1.20855900
H	6.33271500	2.48123200	-1.41762900
H	4.76145900	3.26762300	-1.68829000
H	4.87900300	1.49884400	-1.66355100

Pt(*cp*-2)_T_1

C	-4.00112100	2.72903200	-0.24217800
C	-1.30538900	2.50068900	-1.08500100
C	-3.33090600	1.51267800	-0.11742700
C	-3.34534300	3.84584400	-0.78640900
C	-2.00076400	3.69725000	-1.21253500
C	-1.96536900	1.40248200	-0.51556100
H	-1.49017900	4.54189600	-1.66477500
H	-0.28430300	2.40834500	-1.44120700
C	-3.72691900	0.18442100	0.31420400
C	-3.88339000	-2.54681700	0.76806400

C	-4.91975300	-0.34979600	0.78845700
C	-2.58112400	-0.63141300	0.11167600
C	-2.66304200	-2.05192500	0.18165700
C	-4.97879900	-1.74881200	1.06768800
H	-5.77929700	0.28828400	0.96438400
H	-3.93381000	-3.60376800	0.98757600
N	-1.49592600	0.12156000	-0.28891500
H	-5.03585300	2.80025100	0.07416000
C	-4.03681600	5.21164100	-0.94430300
C	-5.49243700	5.19822700	-0.43940500
H	-6.11062600	4.48475900	-0.99597400
H	-5.93707000	6.19141000	-0.56951200
H	-5.55295300	4.94644500	0.62562900
C	-4.05201800	5.61522300	-2.43904600
H	-4.60393200	4.88086300	-3.03655000
H	-3.04134500	5.69066200	-2.85331200
H	-4.53754200	6.59091500	-2.56477900
C	-3.25884000	6.27800600	-0.13491700
H	-2.22115200	6.36965000	-0.47229600
H	-3.24338200	6.02509200	0.93157600
H	-3.73380500	7.26086700	-0.24418400
C	-6.26412800	-2.32091800	1.69058700
C	-7.45594200	-2.05492900	0.73857400
H	-7.30210500	-2.55061700	-0.22676100
H	-7.59816000	-0.98669400	0.54595500
H	-8.38457100	-2.44171400	1.17643800
C	-6.18704700	-3.83829600	1.94379200
H	-6.03824700	-4.39984300	1.01449200
H	-7.12571900	-4.18447700	2.39157000

H	-5.37621600	-4.09551600	2.63451200
C	-6.52700500	-1.62264300	3.04757600
H	-5.70229600	-1.80492400	3.74600200
H	-7.44905000	-2.00784900	3.50056900
H	-6.63620100	-0.53915900	2.93541100
C	-1.70738100	-2.94652100	-0.42526600
C	0.09336000	-4.73134400	-1.62423300
C	-2.10422800	-4.25280800	-0.78975300
N	-0.40434900	-2.53741200	-0.74214000
C	0.48810500	-3.45462500	-1.28088800
C	-1.23988700	-5.13800000	-1.40189000
H	-3.13318000	-4.54468300	-0.61898000
H	-1.57599600	-6.12577000	-1.70036400
H	0.81715000	-5.42161400	-2.04240600
C	1.86701200	-2.96488600	-1.38110800
C	4.44136100	-1.88496600	-1.40109100
C	2.89939300	-3.63153900	-2.05055500
C	2.11188200	-1.72953700	-0.72567900
C	3.41485300	-1.23532800	-0.68723600
C	4.17746300	-3.07374400	-2.07558700
H	2.71123800	-4.56323200	-2.57582200
H	4.97518300	-3.56549100	-2.62529800
H	5.44122400	-1.46469500	-1.41732600
H	0.82146500	3.78538200	1.98855900
C	1.43908400	3.03963500	1.50105800
H	3.25873700	4.19189300	1.53701500
C	2.80150800	3.24735700	1.26593600
N	1.56622200	0.87676300	0.43410600
C	3.55799300	2.24556000	0.67870000

C	0.86928300	1.87218300	1.04621200
C	2.92284800	1.00679600	0.36772400
H	-0.18765500	1.68928500	1.15577600
C	5.69971400	1.14793100	0.93813400
C	6.89532700	1.15005500	1.66568600
C	5.01633000	-0.06555000	0.76566100
H	4.96002000	-2.17045600	1.22754800
N	3.75918700	-0.06573700	0.06667600
C	7.41067900	-0.02653400	2.20706500
H	7.43399100	2.08008800	1.81285800
H	8.34554100	-0.00531000	2.75981500
C	6.71140200	-1.22395300	2.04563800
H	7.08762100	-2.14374400	2.48453100
C	5.51339900	-1.24530800	1.33712200
Pt	0.45662700	-0.75925600	-0.26135900
C	5.04365900	2.38917100	0.33810400
C	5.64269500	3.69324600	0.88737700
H	6.69976900	3.76824800	0.61489500
H	5.56665600	3.75779600	1.97813000
H	5.14104000	4.56318500	0.45102000
C	5.22969800	2.39450600	-1.20677900
H	6.29580400	2.45815100	-1.45189800
H	4.72158600	3.26067900	-1.64612400
H	4.82838700	1.49072600	-1.67198600

Pt(*cp*-3)_S_0

C	3.95953200	-1.31775500	-0.37343200
C	1.39518200	-2.41660100	-0.82140500
C	2.81422700	-0.51972500	-0.24919000
C	3.84764900	-2.66713800	-0.71663800

C	2.54744300	-3.18446500	-0.94372800
C	1.51889200	-1.06982000	-0.44858400
H	2.43648600	-4.22350500	-1.24265800
H	0.42219000	-2.84687000	-1.03941700
C	2.60283300	0.88276700	0.02015500
C	1.56561700	3.41831100	0.31903900
C	3.45830900	1.93844000	0.31643900
C	1.18578000	1.07840600	-0.06807300
C	0.65497000	2.39300500	-0.01931900
C	2.94216600	3.22892900	0.51353100
H	4.52332500	1.74912600	0.40202500
H	1.17628100	4.42013900	0.45617300
N	0.53266400	-0.10371800	-0.27148900
H	4.93403900	-0.86732600	-0.21409800
C	5.06900100	-3.59132500	-0.88034600
C	6.39614500	-2.86583400	-0.58723300
H	6.56293600	-2.02938100	-1.27545900
H	7.23406000	-3.56289200	-0.70493200
H	6.42937100	-2.47703900	0.43709800
C	5.12742900	-4.12609700	-2.33159900
H	5.21810300	-3.30069300	-3.04691200
H	4.22841900	-4.69447000	-2.59259400
H	5.99195500	-4.78925600	-2.46408300
C	4.95295000	-4.78573900	0.09721400
H	4.04350800	-5.36944500	-0.08075100
H	4.92845300	-4.43801100	1.13669400
H	5.81016200	-5.46201100	-0.01508400
C	3.82368500	4.42939000	0.91288800
C	5.30801600	4.03955100	1.05267600

H	5.72116100	3.66177300	0.11031100
H	5.45717700	3.27409300	1.82271900
H	5.89564700	4.91849600	1.34198500
C	3.72461700	5.54049600	-0.15985300
H	4.05540700	5.17096000	-1.13721400
H	4.35494200	6.39650400	0.11269400
H	2.69918600	5.90930200	-0.27270800
C	3.34826400	4.99184100	2.27390000
H	2.30573700	5.32594500	2.23435300
H	3.96261800	5.85092700	2.57256700
H	3.42281900	4.23020300	3.05851400
C	-0.72018700	2.74629500	-0.40684300
C	-3.32851000	3.53328800	-1.03831300
C	-1.00761200	4.07300500	-0.80374100
N	-1.73444200	1.83008900	-0.43242000
C	-3.03222500	2.21925200	-0.69603200
C	-2.29547900	4.46355500	-1.11736200
H	-0.19772300	4.78306700	-0.89073800
H	-2.49734900	5.48651600	-1.42226600
H	-4.35218700	3.81975700	-1.24605700
C	-2.85969200	-2.81865100	0.82920400
C	-0.67123900	-3.76296400	2.20484800
C	-2.92666300	-4.07094700	1.46865300
N	-1.72365700	-2.08638300	0.81759700
C	-0.66387000	-2.55687600	1.53492000
C	-1.82873600	-4.55012300	2.15545600
H	-3.86394600	-4.61182600	1.41615200
H	0.20548500	-1.91661500	1.53507400
H	0.21354600	-4.07616900	2.74693300

Pt	-1.56815200	-0.17920200	0.00015800
H	-1.87451500	-5.51030900	2.66062500
C	-4.04144600	1.16051000	-0.56919000
C	-5.77004700	-1.02753800	-0.37471400
C	-5.40430800	1.31503400	-0.86360200
C	-3.52972900	-0.08761900	-0.15032100
C	-4.41188800	-1.15494600	-0.08585200
C	-6.26366700	0.22195000	-0.75730800
H	-5.80292500	2.27088400	-1.19035200
H	-7.31958600	0.33638500	-0.98310700
H	-6.41881800	-1.89527800	-0.30425800
O	-4.00456400	-2.45428800	0.23164400

Pt(*cp*-3)_T_1

C	3.78829300	-1.70852700	-0.27971300
C	1.09900600	-2.49637000	-0.67443400
C	2.75977900	-0.76748000	-0.22716600
C	3.49486800	-3.05654200	-0.53602600
C	2.14106800	-3.41683100	-0.73647500
C	1.41383000	-1.15947800	-0.41222700
H	1.89458300	-4.45323300	-0.94847500
H	0.06981600	-2.80020500	-0.83680000
C	2.72397700	0.66906800	-0.00806300
C	2.05227500	3.31571100	0.27265900
C	3.72651400	1.59355500	0.25812400
C	1.35374800	1.05220400	-0.10292600
C	1.00312400	2.42553600	-0.03090600
C	3.39777300	2.94539900	0.43265100
H	4.75327900	1.25441700	0.34130400
H	1.79889800	4.35993200	0.41216800

N	0.55206300	-0.07221400	-0.28648200
H	4.81264600	-1.38786600	-0.12381300
C	4.58439000	-4.14248900	-0.60557300
C	5.99638300	-3.57423500	-0.36602200
H	6.26777700	-2.82609900	-1.11960000
H	6.73435300	-4.38248800	-0.42285000
H	6.08790200	-3.11275000	0.62396200
C	4.56695900	-4.80747200	-2.00332900
H	4.76888700	-4.07120800	-2.78963100
H	3.60012400	-5.27226200	-2.22269400
H	5.33425300	-5.58949100	-2.06345500
C	4.31207400	-5.21795200	0.47413400
H	3.33689400	-5.69662200	0.33607100
H	4.32950500	-4.77763800	1.47778600
H	5.07782400	-6.00254000	0.43299400
C	4.44451300	4.01845600	0.78751900
C	5.86689300	3.43365000	0.88645000
H	6.19280500	2.99044500	-0.06157500
H	5.93957300	2.66747500	1.66666100
H	6.57603800	4.22993700	1.13954800
C	4.45700600	5.12071800	-0.29876400
H	4.70867700	4.70191700	-1.27982900
H	5.20179900	5.88835000	-0.05494700
H	3.48593600	5.61946500	-0.38787500
C	4.08945100	4.65048800	2.15491000
H	3.10018900	5.12015900	2.14259600
H	4.82267000	5.42180800	2.42169000
H	4.08871600	3.89311600	2.94707900
C	-0.34131600	2.99105300	-0.31784500

C	-2.87629500	4.02773700	-0.78684700
C	-0.48927100	4.32939700	-0.72993600
N	-1.43898700	2.21477800	-0.20481800
C	-2.69436500	2.69141700	-0.41572500
C	-1.76041900	4.84204900	-0.95541400
H	0.38175200	4.94879300	-0.90118300
H	-1.88059800	5.87137600	-1.28186500
H	-3.86980600	4.41311500	-0.98239800
C	-3.43122300	-2.69155100	0.52543500
C	-1.64205100	-4.30819100	1.82787800
C	-3.70776300	-4.06867500	0.61741800
N	-2.32417500	-2.14502400	1.02287600
C	-1.45488200	-2.94309500	1.67488900
C	-2.79698200	-4.87994500	1.27438500
H	-4.62702700	-4.45162300	0.18860400
H	-0.57288400	-2.44451600	2.06706300
H	-0.90824300	-4.90697100	2.35704300
Pt	-1.47097000	-0.02957200	-0.14191900
H	-2.98541900	-5.94605100	1.36583100
C	-3.80151200	1.71555400	-0.27026000
C	-5.85352800	-0.16872400	-0.07598200
C	-5.13883300	2.13240800	-0.22291100
C	-3.45204900	0.33443400	-0.20197400
C	-4.51577600	-0.57148400	-0.10582800
C	-6.16155600	1.18899300	-0.12944500
H	-5.39781600	3.18675700	-0.24339000
H	-7.19853500	1.51064600	-0.09343700
H	-6.63315200	-0.92176400	-0.01239600
O	-4.37533900	-1.96290600	-0.11268600

Pt(*cp*-4)_S_0

C	-3.93087900	2.51909400	-0.45372500
C	-1.12909200	2.62667400	-0.80916500
C	-3.15395900	1.36064800	-0.31881900
C	-3.32963300	3.74184700	-0.76141900
C	-1.92371600	3.75924500	-0.94368000
C	-1.74192200	1.41039100	-0.47229000
H	-1.43755500	4.69292200	-1.21456000
H	-0.05918400	2.67935300	-0.98873200
C	-3.46756400	-0.02551200	-0.06517900
C	-3.41841700	-2.76180800	0.25215100
C	-4.65399300	-0.70240200	0.19599000
C	-2.21259600	-0.71647100	-0.11226200
C	-2.18896600	-2.13437500	-0.04771800
C	-4.64197600	-2.09077200	0.39985600
H	-5.58195000	-0.14245700	0.25102000
H	-3.41899300	-3.83537800	0.39845600
N	-1.17380500	0.15466700	-0.28366400
H	-5.00659100	2.44896000	-0.32819300
C	-4.12977500	5.04776700	-0.92684400
C	-5.63748900	4.84591900	-0.68292600
H	-6.07422900	4.13803400	-1.39656400
H	-6.16348400	5.80062100	-0.80040600
H	-5.83991900	4.47851000	0.32978100
C	-3.94738000	5.59393400	-2.36347700
H	-4.31157400	4.87231900	-3.10362100
H	-2.89587400	5.79976700	-2.58998300
H	-4.50677300	6.52917600	-2.49449900
C	-3.62110900	6.10205100	0.08572900
H	-2.55743200	6.32165600	-0.05552600

H	-3.75557100	5.75018100	1.11532500
H	-4.17381900	7.04355000	-0.02730900
C	-5.90969500	-2.89299800	0.75637400
C	-7.15499500	-1.99183500	0.86694600
H	-7.37690200	-1.48482800	-0.07920500
H	-7.03729500	-1.22804600	1.64416100
H	-8.02935000	-2.59889600	1.12869300
C	-6.18757400	-3.95441400	-0.33493100
H	-6.33924300	-3.48018500	-1.31131900
H	-7.08892700	-4.53141900	-0.09190400
H	-5.35835000	-4.66343700	-0.43419800
C	-5.71229400	-3.60130500	2.11795400
H	-4.86579800	-4.29622100	2.09692100
H	-6.60774500	-4.17595100	2.38718700
H	-5.52322900	-2.87188500	2.91385800
C	-1.01658400	-2.96478100	-0.37455500
C	1.15937500	-4.64359900	-0.90393100
C	-1.20862300	-4.31241800	-0.75867000
N	0.25860600	-2.47449200	-0.35435700
C	1.34352200	-3.30545800	-0.57536700
C	-0.13498500	-5.14334200	-1.01862800
H	-2.21481700	-4.68722900	-0.87931400
H	-0.30277200	-6.17579900	-1.31219300
H	2.02016500	-5.27902700	-1.07449000
N	3.90716100	0.75930100	0.31656800
C	2.96442600	1.50302900	1.02643300
C	1.12693500	2.97767100	2.49402300
C	3.39988700	2.51430600	1.90576800
N	1.63301600	1.21300500	0.91568000

C	0.75821700	1.94235700	1.65586500
C	2.48664800	3.25991400	2.62963500
H	4.46057700	2.66290800	2.04728800
H	-0.27777200	1.65739200	1.54740800
H	0.36458400	3.52240700	3.03885700
Pt	0.80053000	-0.52983500	0.06853800
H	2.83522100	4.03009200	3.31150800
C	5.25759100	1.10619400	0.06059900
C	7.95705000	1.25169200	-0.62566700
C	5.88556000	2.35507000	0.04314800
C	5.96357800	-0.06625300	-0.32383900
C	7.31987400	0.01387500	-0.65528200
C	7.23880300	2.40968500	-0.29510400
H	5.34447700	3.27094400	0.24886600
H	7.86325400	-0.88027700	-0.94807300
H	7.73712300	3.37481300	-0.31168300
H	9.00999800	1.32543400	-0.88157000
C	2.65475000	-2.66769100	-0.43240400
C	5.01085600	-1.15841400	-0.35224100
C	3.89762800	-3.25801000	-0.75870800
C	2.58514600	-1.32682500	-0.01141400
C	3.76875500	-0.61644100	0.01646300
C	5.07273800	-2.51376300	-0.72127900
H	3.94738800	-4.29368700	-1.08291600
H	6.01746300	-2.96938300	-1.00305400

Pt(*cp*-4)_T_1

C	-4.05342300	2.46308700	-0.41762900
C	-1.27080600	2.58754200	-0.91931600
C	-3.26312700	1.31836300	-0.31101200

C	-3.47177800	3.68809000	-0.77923300
C	-2.07959000	3.71557400	-1.03113800
C	-1.86973900	1.38100600	-0.54286100
H	-1.61437500	4.64956500	-1.33275200
H	-0.20805300	2.63029300	-1.13928400
C	-3.54806300	-0.07503600	-0.00945200
C	-3.49173000	-2.79104800	0.38295200
C	-4.72513200	-0.73061600	0.33120200
C	-2.30552100	-0.76692600	-0.11527700
C	-2.27833100	-2.18086500	0.01000500
C	-4.70840500	-2.11290800	0.56581500
H	-5.64313800	-0.16064000	0.42502300
H	-3.48170000	-3.86027700	0.55752800
N	-1.27269100	0.13587900	-0.36359700
H	-5.11903700	2.39449800	-0.22703600
C	-4.29110200	4.98447100	-0.92026700
C	-5.78542400	4.77165400	-0.61124100
H	-6.24573000	4.05117100	-1.29702300
H	-6.32311100	5.72040200	-0.72034000
H	-5.94387000	4.41855400	0.41424400
C	-4.17294300	5.51739900	-2.36881400
H	-4.55721900	4.78488300	-3.08771500
H	-3.13504600	5.73709800	-2.63960500
H	-4.75086800	6.44294500	-2.48332400
C	-3.74682300	6.05011500	0.06174400
H	-2.69274200	6.27840200	-0.12751200
H	-3.83380800	5.70661800	1.09906100
H	-4.31337100	6.98456900	-0.03605000
C	-5.96021700	-2.89978500	0.99785900

C	-7.19532500	-1.99033200	1.14597000
H	-7.45947100	-1.50337700	0.20015500
H	-7.03957500	-1.21107800	1.90079300
H	-8.05827300	-2.58778600	1.46090800
C	-6.28796800	-3.98222300	-0.05869500
H	-6.48151500	-3.52847500	-1.03736100
H	-7.18012600	-4.54810600	0.23699200
H	-5.46720200	-4.69749100	-0.17890700
C	-5.69900200	-3.57950600	2.36343400
H	-4.85785900	-4.27939800	2.31769700
H	-6.58362600	-4.14317700	2.68498000
H	-5.47093500	-2.83479100	3.13443100
C	-1.11487000	-3.05441800	-0.30090900
C	1.09508200	-4.65438700	-0.82606600
C	-1.29546700	-4.40784000	-0.64866900
N	0.13190000	-2.54727400	-0.28198300
C	1.23827700	-3.29085100	-0.54003100
C	-0.18263800	-5.20166300	-0.89402400
H	-2.28990200	-4.82224200	-0.75231500
H	-0.31115800	-6.24886100	-1.15426000
H	1.96113400	-5.27636200	-1.01549900
N	4.09988900	0.76663100	0.24938300
C	3.30509400	1.59896000	1.07258900
C	1.75028300	3.20970700	2.66427400
C	3.85993100	2.14550800	2.24425300
N	2.02997100	1.81059600	0.71910700
C	1.27716500	2.59213800	1.51268800
C	3.07417700	2.96941800	3.03928500
H	4.87955500	1.90789800	2.52306500

H	0.24725900	2.72479100	1.19477800
H	1.09687300	3.84559900	3.25281600
Pt	0.68427000	-0.36637700	-0.16324100
H	3.48391200	3.39973700	3.94892400
C	5.48365600	0.94788600	0.07906700
C	8.20810100	0.82157500	-0.47674700
C	6.25625300	2.10376200	0.23472100
C	6.06137800	-0.26205800	-0.37497700
C	7.43280300	-0.32149200	-0.64915200
C	7.61951000	2.02222200	-0.04480600
H	5.81248700	3.04250000	0.54842100
H	7.88289600	-1.24625900	-1.00038900
H	8.23492600	2.91074300	0.06688800
H	9.27332700	0.79046900	-0.68720200
C	2.53797300	-2.57434700	-0.50226200
C	4.98655500	-1.22250500	-0.47585500
C	3.73726800	-3.24721100	-0.81110900
C	2.52110700	-1.17851800	-0.19207500
C	3.78015000	-0.56298300	-0.13088700
C	4.95494900	-2.57657800	-0.82286200
H	3.73048700	-4.30027500	-1.07296400
H	5.86858500	-3.10181800	-1.08764700

References:

(1) G. Li, F. Zhan, J. Zheng, Y.-F. Yang, Q. Wang, Q. Chen, G. Shen and Y. She, *Inorg. Chem.*, 2020, **59,** 3718−3729.

(2) G. Li, J. Wen, F. Zhan, W. Lou, Y.-F. Yang, Y. Hu and Y. She, *Inorg. Chem.*, 2022, **61,** 11218−11231.

(3) G. Li, G. Shen, X. Fang, Y.-F. Yang, F. Zhan, J. Zheng, W. Lou, Q. Zhang and Y. She, *Inorg. Chem.*, 2020, **59,** 18109−18121.