Supplementary Information (SI) for Journal of Materials Chemistry C.
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Electronic Supplementary Information

Synthesis and photophysical properties of *bis*-NHC platinum(II) complexes bearing bipyridine ligands furnished with two anionic *closo*-monocarborane clusters $[CB_{11}H_{12}]^-$

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General Information

Chemicals

All commercially chemicals are directly purchased without further purification. All commercial reagents were purchased from standard suppliers and were used without further purification.

Characterization

Thin-layer chromatography (TLC) was carried out using silica gel 60, F254 with a thickness of 0.25 mm. Column chromatography was performed on silica gel 60 (200-300 mesh).

NMR spectra were recorded on a Bruker AVANCE III 400 spectrometers (^{1}H NMR 400.13 MHz, ^{13}C NMR 100.62 MHz, ^{11}B NMR 128.38 MHz) at 25 °C. Data are reported as follows: Chemical shift in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, etc.), coup ling constant J in Hz, integration, and (where applicable) interpretation.

High-resolution MS data were recorded using ThermoFisher Scientific (USA) equipped with an electrospray ionization source (ESI). Accurate mass determination was corrected by calibration using sodium trifluoroacetate clusters as a reference.

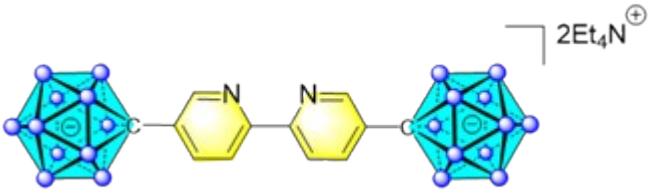
Single-crystal X-ray diffraction studies were performed on Bruker D8 Venture using Ga radiation. Olex2 was used in the determination of these structures.

UV−vis absorption measurements were carried out on an Agilent's Cary 100 UV−vis spectrophotometer. Emission spectrum, phosphorescence lifetime and quantum yield were measured directly using Edinburgh Instruments model FLS1000.

The theoretical calculations of the Pt (II) were performed using Gaussian 09 program.[1] The geometries of the ground state S_0 were optimized with the density functional theory (DFT) method with the B3LYP function. The 6-31G (d, p) basis set was used for the C, H, B and N atoms and LanL2DZ basis set was employed for the Pt atoms. Considering the solvent effect, the DCM was taken as the solvent into the polarizable continuum model (PCM) when the optimizations were conducted. The energies of the singlet and triplet excited states were obtained from the time-dependent density functional theory (TD-DFT) calculations. All molecular structures

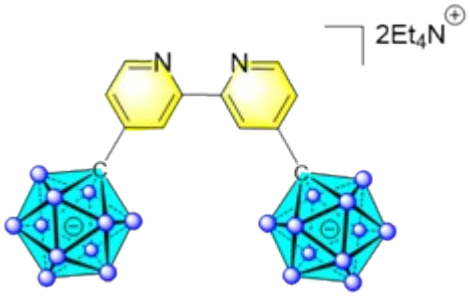
and orbital compositions were analyzed by Multiwfn [2] and visualized by VMD. [3]

Experimental Section



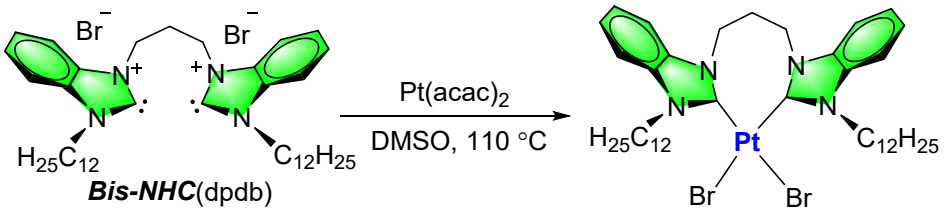
General procedure for synthesizing ligand L_1.

L_1 was prepared by following the reported procedure.[4] A flame-dried round bottomed flask was charged with $[Me_3NH][CB_{11}H_{12}]$ (600 mg, 2.96 mmol) and capped with a rubber septum. Anhydrous THF (15 mL) was then added to the flask and the resulting solution cooled to 0 °C in an ice bath. A solution of 1.6 M *n*-BuLi in hexane (4.07 mL, 6.51 mmol) was slowly added to the reaction flask. After 1 h of stirring at 0 °C, a slightly turbid, yellowish solution was obtained. Copper(I) iodide (628 mg, 3.30 mmol) was added and the mixture was stirred at room temperature for 30 min. A solution of palladium (II) acetate (80 mg, 0.36 mmol), tris(omethoxyphenyl) phosphine (348 mg, 0.988 mmol), and 5,5'-dibromo-2,2'-bipyridine (420 g, 1.34 mmol) in THF (8.0 mL) was then added dropwise at 0 °C. The obtained suspension was stirred overnight with increasing temperature from 0 °C to 25 °C. The reaction was quenched with water (5 mL) and the solution was concentrated on a rotary evaporator. The residue was dissolved in 1 M HCl and then extracted with methyl tert-butyl ether (3 x 30 mL). The combined organic extracts were evaporated under reduced pressure and the residue was dissolved in water/methanol (25 mL), which was neutralized to pH=7 with 1 M NaOH. $[Et_4N]Br$ (933mg, 4.44mmol) was added to the solution, and the resulting precipitate was collected by filtration and dried in a vacuum to give **L_1** as a white solid (509 mg, 54%).



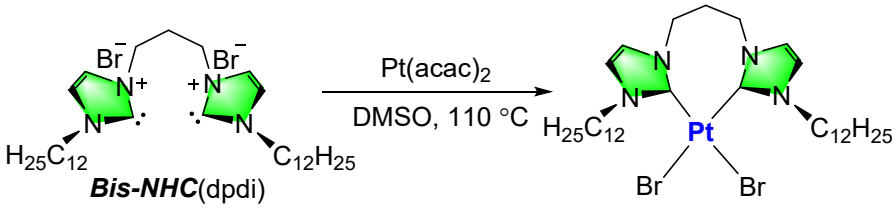
General procedure for synthesizing ligand L_2.

Following a similar procedure as for the preparation of L_1, using 4,4'-Dibromo-2,2'-bipyridine (420 g, 1.34 mmol), to afford compound **L_2** as a white solid (509 mg, 54%).



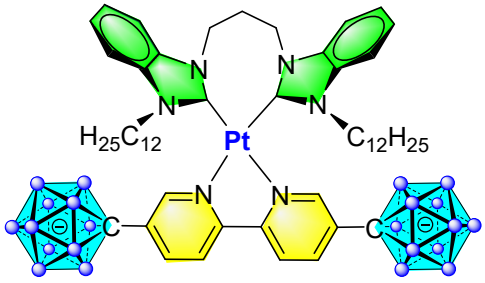
Synthetic procedure for complex Pt(*bis*-dpdb)Br_2. To a stirred solution of benzimidazolium salt (*bis*-dpdb)$^{2+}$ 2Br^- (2.00 g， 2.54 mmol) in dry dimethyl sulfoxide (20 mL) was added platinum bis(acetylacetonate) (1.00 g， 2.54 mmol). The reaction mixture was then heated to 110 °C for 24 h. All solvents were removed under reduced pressure and the crude product was passed through a silica column (eluent DCM) yielding a white solid. Yield: 3.5g， 72 %.

Pt(*bis*-dpdb)Br_2 ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33-7.30 (m, 4H), 7.24-7.21 (m, 4H), 5.61-5.54 (q, 2H), 5.01-4.93 (m, 2H), 4.57-4.49 (m, 4H), 2.72-2.65 (m, 1H), 2.33-2.18 (m, 2H), 2.10-2.00 (q, 1H), 1.80-1.69 (m, 2H), 1.57-1.28 (broad signal, 36H), 0.90-0.87 (t, 6H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 162.24, 134.22, 133.27, 123.60, 123.40, 111.00, 109.92, 48.92, 48.61, 31.95, 29.72, 29.67, 29.47, 29.39, 29.17, 27.24, 22.72, 14.14.



Synthetic procedure for complex Pt(*bis*-dpdi)Br_2. It was synthesized following the preparation procedure of Pt(*bis*-dpdb)Br_2. using imidazolium salt (*bis*-dpdi)$^{2+}$ 2Br^- (1.12g， 1.66 mmol) and platinum bis(acetylacetonate) (655mg，1.66 mmol)， white solid. Yield: 948mg， 66 %.

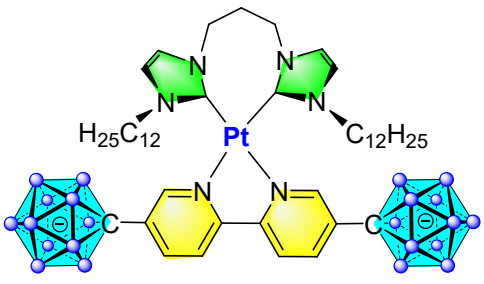
Pt(*bis*-dpdi)Br_2 ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.89 (s, 2H), 6.82 (s, 2H), 5.22-5.16 (t, 2H), 4.68-4.61 (m, 2H), 4.22-4.12 (m, 4H), 2.44 (d, *J*= 16.0 Hz,1H), 1.96-1.90 (broad signal, 2H), 1.90-1.86 (broad signal, 1H), 1.69-1.64 (q, 2H), 1.42-1.29 (broad signal, 36H), 0.89-0.86 (t, 6H).$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 149.98, 121.93, 119.41, 51.96, 50.55, 32.46, 30.66, 30.43, 29.69, 29.65, 29.62, 29.45, 26.93, 22.70, 14.12.



1a

General procedure for synthesis of compound 1a. An 100ml Schlenk tube was charged with Pt(*bis*-dpdb)Br_2 (126 mg, 0.130 mmol) and AgOTf (83 mg, 0.32 mmol) were resolved in 20ml dryTHF in nitrogen atmosphere. The solution was stirred at 80℃ in the dark for 1 hr. L_1 (100 mg, 0.143mmol) was added to the suspension and the mixture was stirred for another 8 hrs. The solution was filtered through celite. The solvent was removed under reduced pressure and the residue was purified with silica gel column chromatography using DCM/hexane as eluent to obtain the compound 1a (102mg, 63% yield).

1a ^{1}H NMR (400 MHz, Acetone-d6) δ 8.60 (d, J = 8.7 Hz, 2H), 8.43 (dd, J = 8.7, 2.2 Hz, 2H), 8.12 (d, J = 2.1 Hz, 2H), 7.90 – 7.86 (m, 4H), 7.48 – 7.45 (m, 4H), 5.55 (dd, J = 15.3, 10.8 Hz, 2H), 5.25 – 5.14 (m, 4H), 4.90 – 4.88 (m, 2H), 2.54 – 2.14 (broad signal, 8H), 1.94 – 1.36 (broad signal, 20H), 1.25 (s, 36H), 0.88 (t, 6H). ^{11}B NMR (128 MHz, Acetone-d6) δ − 6.02 (s, 2B), − 12.00 (s, 10B), − 13.55 (s, 10B). ^{13}C NMR (101 MHz, Acetone-d6) δ 155.40, 154.10, 150.02, 143.53, 141.13, 134.75, 133.64, 124.75, 124.61, 123.46, 112.28, 111.30, 49.48, 48.95, 31.78, 26.81, 22.46, 13.49. HRMS(ESI) m/z, Calcd. for $C_{53}H_{92}B_{22}N_6PtNa$, [M+ Na]+: 1268.9116; found: 1268.9128.

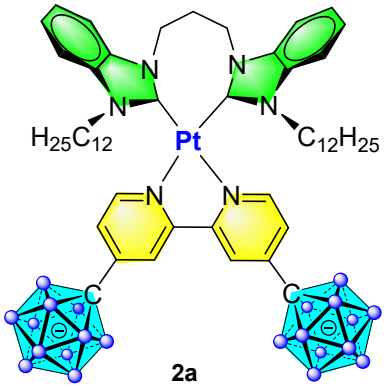


1b

General procedure for synthesis of compound 1b. The synthesis was similar to complex 1a, using Pt(*bis*-dpdi)Br_2（0.130 mmol,113 mg）to afford compound 1b (112mg, 75% yield).

1b ^{1}H NMR (400 MHz, Acetone-d_6) δ 8.53 (d, *J* = 8.7 Hz, 2H), 8.40 (dd, *J* = 8.6, 2.2 Hz, 2H), 8.05 (d, *J* = 2.2 Hz, 2H), 7.71 (dd, *J* = 22.5, 2.1 Hz, 4H), 5.17 (dd, *J* = 14.8, 10.8 Hz, 2H), 4.73 – 4.65 (m, 4H), 4.51 (ddd, *J* = 13.2, 11.3, 5.5 Hz, 2H), 2.76 – 2.12 (broad

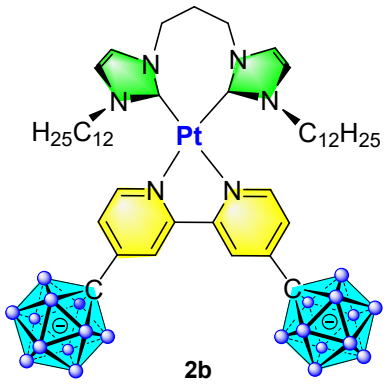
signal, 8H), 1.99 – 1.39 (broad signal, 20H), 1.24 (d, *J* = 8.0 Hz, 36H), 0.87 (t, 6H). ^{11}B NMR (128 MHz, Acetone-d_6) δ − 6.09 (s, 2B), − 11.91 (s, 10B), − 13.42 (s, 10B). ^{13}C NMR (100 MHz, Acetone-d_6) δ 154.03, 149.75, 144.29, 143.44, 140.84, 124.52, 123.29, 122.12, 66.24, 51.96, 50.97, 31.76, 30.53, 26.65, 22.45, 13.48. HRMS(ESI) *m/z*, Calcd. for $C_{45}H_{88}B_{22}N_6PtNa$, $[M+Na]^+$: 1168.8803; found: 1168.8804.



2a

General procedure for synthesis of compound 2a. The synthesis was similar to complex 1a, using L_2 to afford compound 2a (89.0mg, 55% yield).

2a ^{1}H NMR (400 MHz, Acetone-*d*6) δ 8.44 – 8.41 (m, 4H), 7.83 – 7.77 (m, 4H), 7.68 (dd, *J* = 6.0, 2.0 Hz, 2H), 7.44 –7.40 (M, 4H), 5.63 – 5.57 (m, 2H), 5.25 –5.19 (m, 2H), 5.09 (dd, *J* = 15.0, 5.9 Hz, 3H), 4.86 – 4.79 (m, 2H), 2.68 – 2.18 (broad signal, 8H), 2.01 – 1.37 (broad signal, 20H), 1.26 (d, *J* = 8.1 Hz, 36H), 0.88 (t, 6H). ^{11}B NMR (128 MHz, Acetone-*d*6) δ – 5.70 (s, 2B), − 11.85 (s, 10B), − 13.35 (s, 10B). ^{13}C NMR (101 MHz, Acetone-*d*6) δ 157.33, 155.72, 155.47, 151.63, 134.97, 133.91, 127.88, 124.45, 124.20, 122.79, 112.37, 111.26, 68.67, 49.33, 49.19, 31.79, 26.79, 22.47, 13.52. HRMS(ESI) *m/z*, Calcd. for C53H92B22N6PtNa, [M+Na]+: 1268.9116; found: 1268.9124.



2b

General procedure for synthesis of compound 2b. The synthesis was similar to complex 1b, using L_2 to afford compound 2b (92.6mg, 62% yield).

2b ^{1}H NMR (400 MHz, Acetone-d_6) δ 8.41 (d, *J* = 2.1 Hz, 2H), 8.15 (d, *J* = 6.0 Hz, 2H), 7.73 (dd, *J* = 6.0, 2.0 Hz, 2H), 7.63 (d, *J* = 1.7 Hz, 4H), 5.23 (dd, *J* = 14.9, 11.1 Hz, 2H), 4.80 – 4.75 (m, 2H), 4.61 (dd, *J* = 14.7, 6.1 Hz, 2H), 4.50 – 4.46 (m, 2H), 2.61 – 2.24 (broad signal, 8H), 1.72 – 1.35 (broad signal, 20H), 1.26 (d, *J* = 10.5 Hz, 36H), 0.89 (t, 6H). ^{11}B NMR (128 MHz, Acetone-d_6) δ – 5.32 (s, 2B), − 11.78 (s, 10B), − 13.27 (s, 10B). ^{13}C NMR (101 MHz, Acetone-d_6) δ 157.04, 155.40, 150.96, 144.45, 127.90, 124.32, 122.65, 121.88, 52.15, 50.73, 31.76, 30.21, 26.59, 22.45, 13.49. HRMS(ESI) *m/z*, Calcd. for $C_{45}H_{88}B_{22}N_6PtNa$, $[M+ Na]^+$: 1168.8803; found: 1168.8806.

Table S1. Crystal data and structure refinement for all the complexes

	1a	2a	2b
CCDC number	2168883	2168889	2168854
Empirical formula	$C_{56}H_{98}B_{22}N_6PtO$	$C_{53}H_{92}B_{22}N_6Pt$	$C_{54}H_{106}B_{22}N_6O_3Pt$
Formula weight	1304.31	1246.23	1320.35
Temperature/K	213.01	213.01	213.00
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	P-1	P-1	$P2_1/c$
a/Å	14.3504(2))	12.9019(13)	12.0464(5)
b/Å	14.5641(2))	15.2663(13)	18.6936(8)
c/Å	18.6103(2)	19.9007(17)	31.5101(13)
α/°	76.6580(10)	82.301(5)	90
β/°	67.4670(10)	84.738(6)	96.965(3)
γ/°	73.8900(10)	86.187(6)	90
Volume/Å^3	3417.45(8)	3862.2(6)	7043.4(5)
z	2	2	4
ρ_{calc} g/cm^3	1.268	1.072	1.245
μ/mm^{-1}	2.832	2.487	2.764
F(000)	1344.0	1280.0	2736.0
Crystal size/mm^3	0.08 × 0.06 × 0.05	0.06 × 0.05 × 0.05	0.07 × 0.07 × 0.05
2Θ range for data collection/°	6.874 to 109.862	5.994 to 111.066	6.41 to 110.156
Index ranges	-17 ≤ h ≤ 17, -17 ≤ k ≤ 17, -22≤ l ≤ 22	-12 ≤ h ≤ 15, -18 ≤ k ≤ 18, -24 ≤ l ≤ 24	-13 ≤ h ≤ 14, -22 ≤ k ≤ 21, -38 ≤ l ≤ 38
Reflections collected	47187	54436	70386
Independent reflections	12925[$R_{(int)}$=0.0349, R_{sigma} =0.0295]	14633[$R_{(int)}$=0.0673, R_{sigma} = 0.0590]	13411[R_{int}=0.0632, R_{sigma}=0.0510]
Data/restraints/parameters	12925/126/779	14633/172/741	13411/78/783
Goodness-of-fit on F^2	1.112	1.011	1.023
Final R indexes [I>=2σ (I)]	R1=0.0403, wR2 = 0.1230	R1 = 0.0743, wR2 = 0.2042	R1 = 0.0495, wR2 = 0.1144
Final R indexes [all data]	R1=0.0420, wR2 = 0.1260	R1 = 0.0924, wR2 = 0.2236	R1 = 0.0720, wR2 = 0.1260
Largest diff. peak/hole / e Å^{-3}	1.46/-1.32	1.21/-2.09	1.66/-1.51

Table S2. Selected Bond Lengths and Angles for **1a**, **2a** and **2b**

	bond length (Å)	bond angle (deg)			Dihedral angle
1a					
Pt(1)-C(1)	1.982(4)	C(1)-Pt(1)-N(1)	99.98(13)	(C2 Pt1 C1)-(N1 Pt1 N2)	3.0
Pt(1)-C(2)	1.983(4)	N(1)-Pt(1)-N(2)	79.63(12)	NHC-NHC	97.2
Pt(1)-N(1)	2.077(3)	C(2)-Pt(1)-N(2)	94.13(15)		
Pt(1)-N(2)	2.064(3)	C(1)-Pt(1)-C(2)	86.29(16)		
2a					
Pt(1)-C(16)	1.9824	C(16)-Pt(1)-N(1)	95.4	(C17 Pt1 C16)-(N1 Pt1 N2)	1.4
Pt(1)-C(17)	1.9721	N(1)-Pt(1)-N(2)	80.3	NHC-NHC	83.0
Pt(1)-N(1)	2.0675	C(17)-Pt(1)-N(2)	96.3		
Pt(1)-N(2)	2.0797	C(16)-Pt(1)-C(17)	87.9		
2b					
Pt(1)-C(1)	1.991(5)	C(1)-Pt(1)-N(1)	97.16(18)	(C2 Pt1 C1)-(N1 Pt1 N2)	3.9
Pt(1)-C(2)	1.985(5)	N(1)-Pt(1)-N(2)	79.22(15)	NHC-NHC	103.1
Pt(1)-N(1)	2.068(4)	C(2)-Pt(1)-N(2)	98.80(18)		
Pt(1)-N(2)	2.070(4)	C(1)-Pt(1)-C(2)	84.7(2)		

Table S3. Components of the frontier molecular orbitals of complexes at the singlet ground state (S_0).

Complexes	Orbital	Energy (eV)	Components (%)			
			Pt	bipyridine	carborane	*bis*-NHC
1a	HOMO - 1	-7.30	0.9	1.9	0.9	94.6
	HOMO	-7.18	12.4	1.9	0.4	80.6
	LUMO	-2.83	4.0	86.5	7.0	2.2
	LUMO + 1	-1.78	2.2	89.1	6.2	2.3
1b	HOMO - 1	-7.37	2.3	61.2	33.0	3.5
	HOMO	-7.23	20.8	3.6	1.0	74.6
	LUMO	-2.78	4.0	86.6	7.1	2.2
	LUMO + 1	-1.73	2.1	90.1	6.2	1.6
2a	HOMO - 1	-7.37	0.9	0.4	0.1	98.6
	HOMO	-7.25	13.0	1.8	0.2	84.9
	LUMO	-2.80	4.2	86.2	6.7	2.9
	LUMO + 1	-1.75	1.8	88.2	6.3	3.6
2b	HOMO - 1	-7.57	9.7	3.0	1.6	85.7
	HOMO	-7.31	21.4	2.6	0.3	75.7
	LUMO	-2.75	4.2	86.2	6.7	2.9
	LUMO + 1	-1.71	1.8	89.8	6.6	1.8

Table S4. Excited state properties of studied complexes calculated at the optimized S_0 geometry by TDDFT

Complex	State	E/eV	λcalc./nm	*f*	Antiition	Coefficient
1a	S0→S1	3.68	336.9	0.0207	HOMO→LUMO	0.67
					HOMO-5→LUMO	-0.18
	S0→S2	3.81	325.5	0.0108	HOMO-5→LUMO	0.60
	S0→S3	3.83	323.5	0.6183	HOMO-4→LUMO	0.57
					HOMO-1→LUMO	-0.32
1b	S0→S1	3.67	338.2	0.0154	HOMO→LUMO	0.63
					HOMO-3→LUMO	0.30
	S0→S2	3.77	329.2	0.0058	HOMO-3→LUMO	0.62
					HOMO→LUMO+1	-0.31
	S0→S3	3.85	321.6	0.6972	HOMO-1→LUMO	0.69
2a	S0→S1	3.77	328.5	0.0241	HOMO→LUMO	0.64
					HOMO-4→LUMO	0.22
	S0→S2	3.86	320.4	0.0148	HOMO-4→LUMO	0.47
					HOMO-5→LUMO	0.34
	S0→S3	4.02	308.8	0.0012	HOMO-1→LUMO	0.55
					HOMO-2→LUMO	0.35
					HOMO-3→LUMO	0.19
2b	S0→S1	3.75	330.5	0.0094	HOMO→LUMO	0.53
					HOMO-2→LUMO	-0.44
	S0→S2	3.83	323.6	0.0098	HOMO-2→LUMO	0.51
					HOMO→LUMO	0.46
					HOMO-1→LUMO	-0.16
	S0→S3	4.10	302.4	0.0116	HOMO-1→LUMO	0.49
					HOMO-3→LUMO	0.38
					HOMO-2→LUMO	0.17

Table S5. NBO(Natural Population Analysis) charges (*Q*) of the components of complexes

		Q (*e*)			Δ*Q* (*e*)	
complexes	components	S_0	S_1	T_1	S_1 - S_0	S_0 - T_1
1a	Pt	0.37	0.48	0.36	0.11	0.01
	bipyridine	0.57	-0.11	0.56	-0.68	0.01
	carborane	-2.00	-2.09	-1.97	-0.09	-0.03
	bis-NHC	1.06	1.72	1.05	0.66	0.01
1b	Pt	0.36	0.64	0.35	0.28	0.01
	bipyridine	0.56	-0.11	0.55	-0.67	0.01
	carborane	-2.01	-2.09	-1.98	-0.08	-0.03
	bis-NHC	1.09	1.56	1.08	0.47	0.01
2a	Pt	0.36	0.52	0.36	0.16	0.00
	bipyridine	0.57	-0.11	0.60	-0.68	-0.03
	carborane	-2.00	-2.08	-2.01	-0.08	0.01

	bis-NHC	1.07	1.67	1.05	0.60	0.02
2b	Pt	0.36	0.79	0.35	0.43	0.01
	bipyridine	0.56	-0.12	0.58	-0.68	-0.02
	carborane	-2.00	-2.07	-2.01	-0.07	0.01
	bis-NHC	1.08	1.40	1.08	0.32	0.00

Table S6. Excited state properties of studied complexes calculated at the optimized T_1 geometry by TDDFT.

Complex	State	E/eV	λcalc./nm	*f*	Antiition	Coefficient
1a	T1	1.89	652.9	0	HOMO→LUMO (89.8%)	0.67
	T2	3.22	384.9	0	HOMO-1→LUMO (76.3%)	0.62
					HOMO-5→LUMO (15.5%)	-0.28
1b	T1	1.90	652.1	0	HOMO→LUMO (91.5%)	0.68
	T2	3.19	388.6	0	HOMO-1→LUMO (53.6%)	0.52
					HOMO-3→LUMO (41.0%)	0.45
2a	T1	2.03	611.2	0	HOMO-1→LUMO (31.8%)	0.40
					HOMO-2→LUMO (27.2%)	0.37
	T2	3.22	384.5	0	HOMO→LUMO (51.2%)	0.51
					HOMO-6→LUMO (17.9%)	-0.30
2b	T1	2.04	609.1	0	HOMO-1→LUMO (89.8%)	0.67
	T2	3.21	385.8	0	HOMO→LUMO (44.2%)	0.47
					HOMO-3→LUMO (29.6%)	-0.38

References

1 Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

2 T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580-592.

3 W. Humphrey, A. Dalke and K. Schulten, *J. Mol. Graph.*, 1996, **14**, 33-38, 27-38.

4 R. Yang, Y. Zhou, H. Bian, G. Cheng, Y. Zhang, C.-M. Che, T. R. Cook and Y. Shen, *Chem. Eng. J.*, 2022, **447**, 137432.

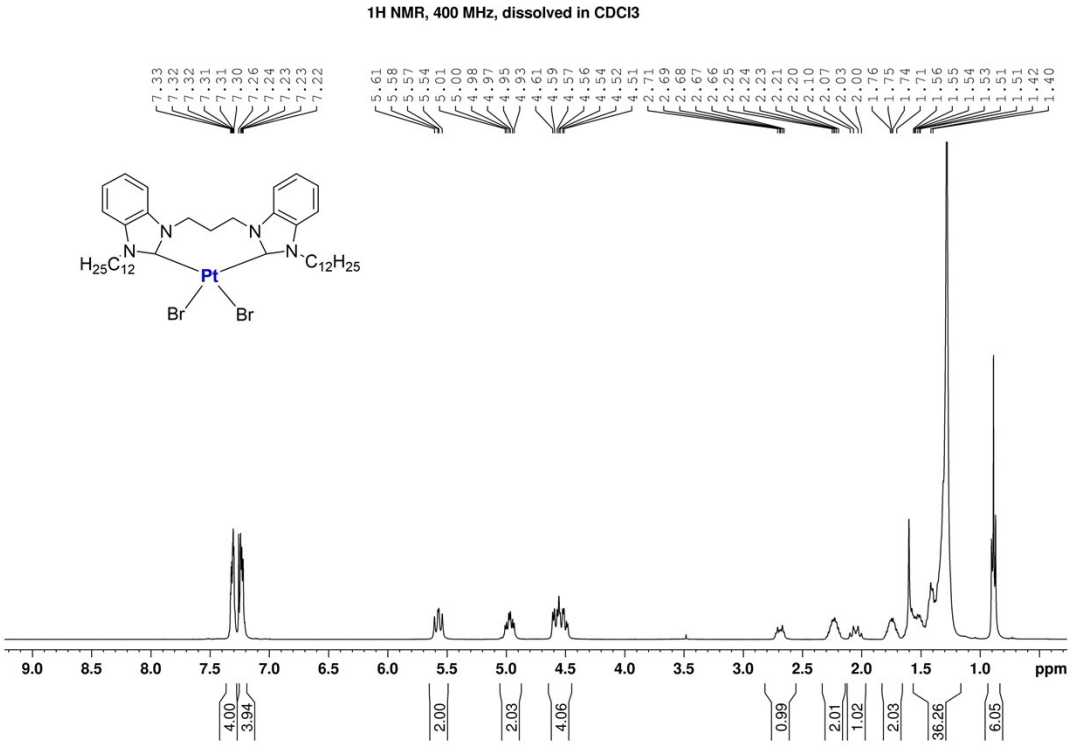


Figure S1. ^{1}H NMR spectrum of **Pt(*bis*-dpdb)Br$_2$** ($CDCl_3$)

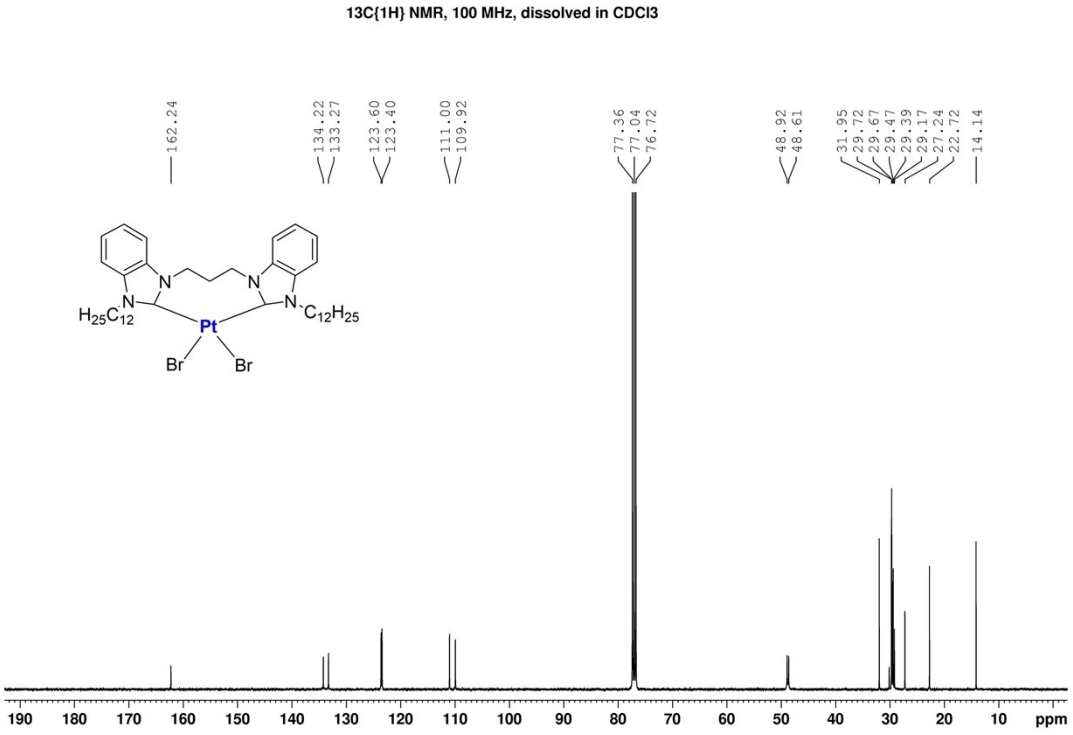


Figure S2. ^{13}C NMR spectrum of **Pt(*bis*-dpdb)Br$_2$** ($CDCl_3$)

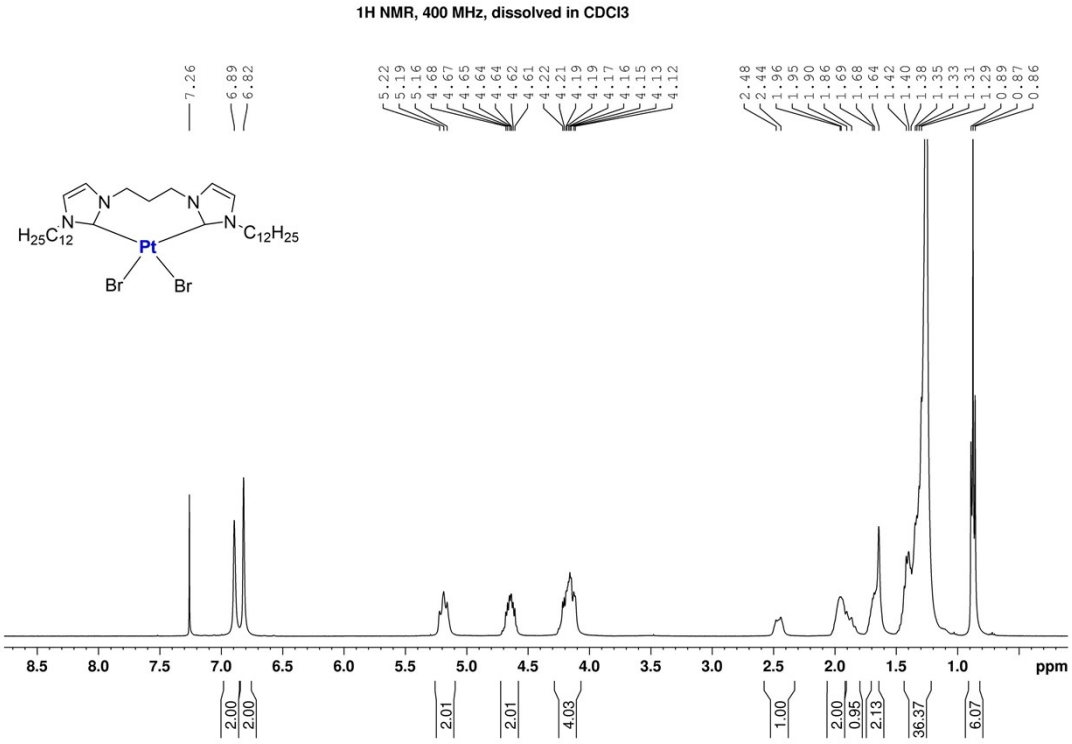


Figure S3. ^{1}H NMR spectrum of **Pt(*bis*-dpdi)Br$_2$** (CD_2Cl_3)

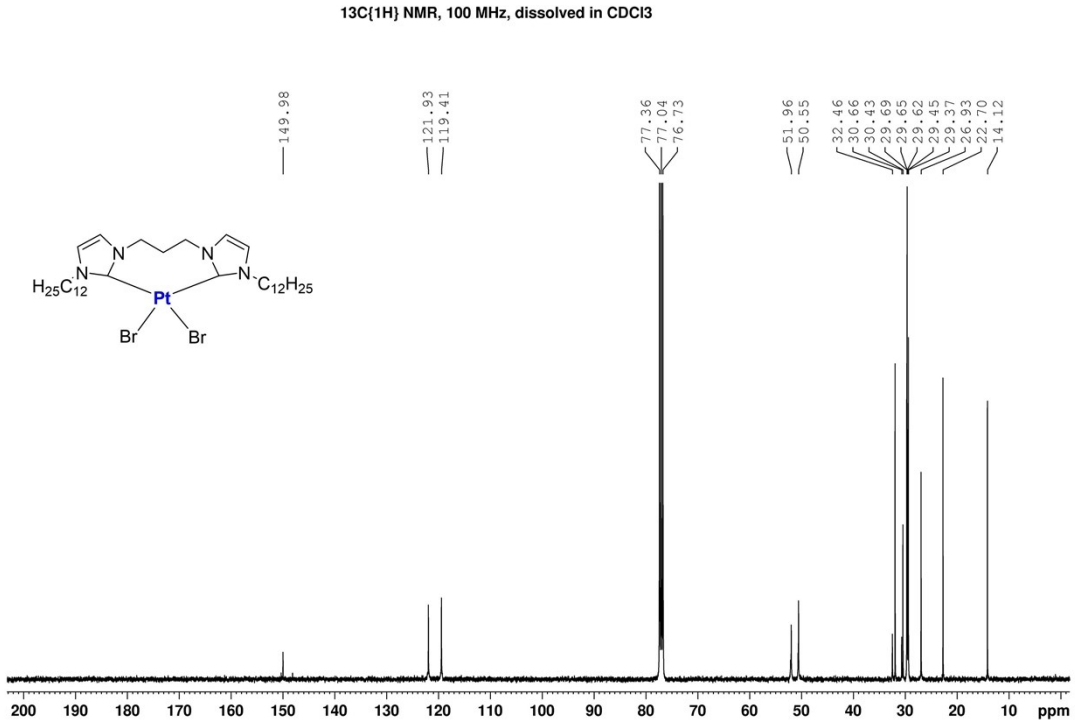


Figure S4. ^{13}C NMR spectrum of **Pt(*bis*-dpdi)Br$_2$** ($CDCl_3$)

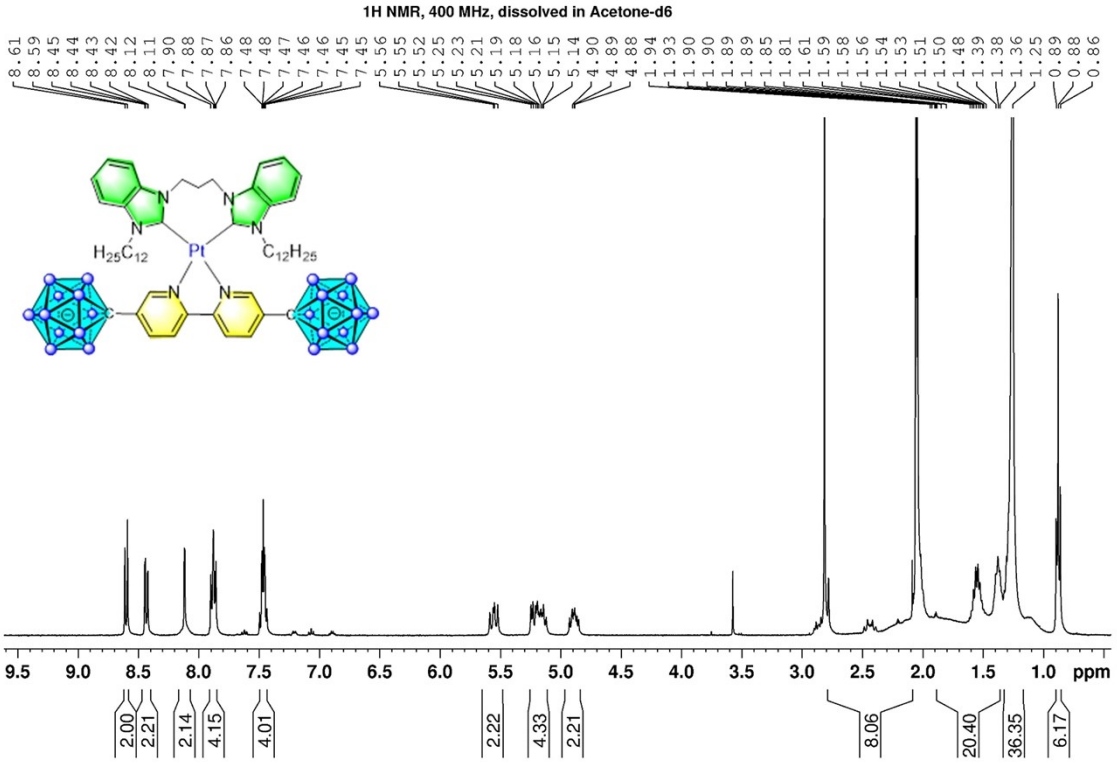


Figure S5. ^{1}H NMR spectrum of **1a** (acetone-d_6)

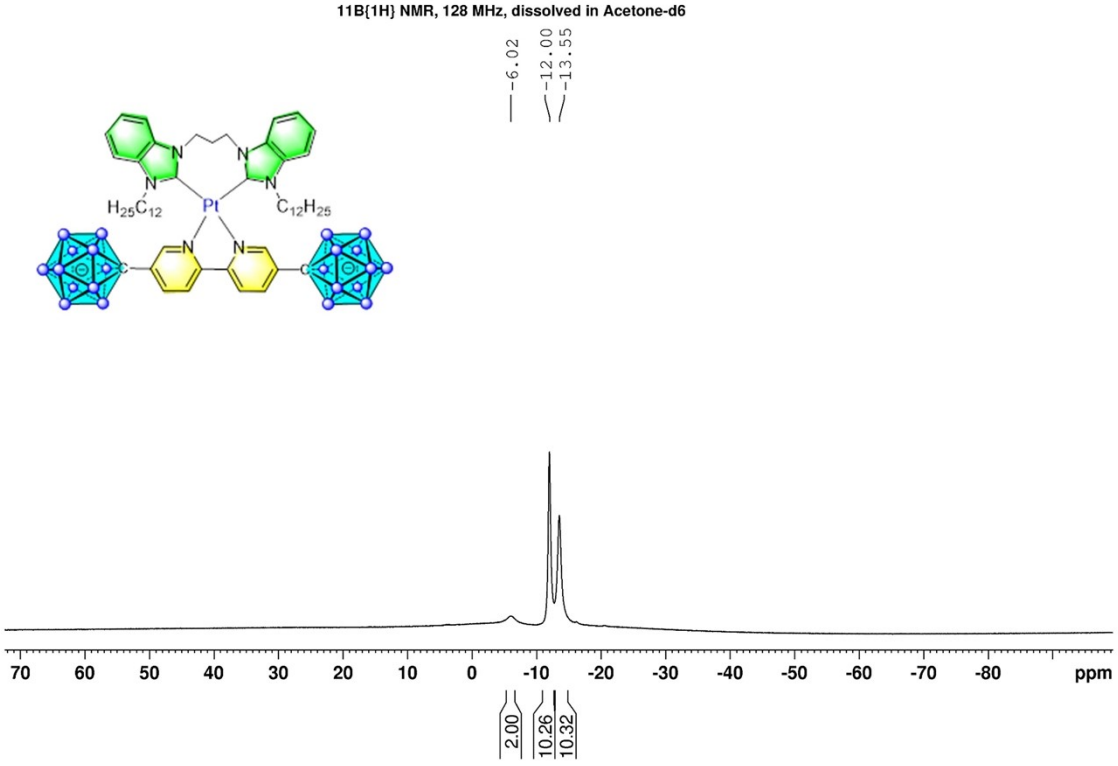


Figure S6. ^{11}B NMR spectrum of **1a** (acetone-d_6)

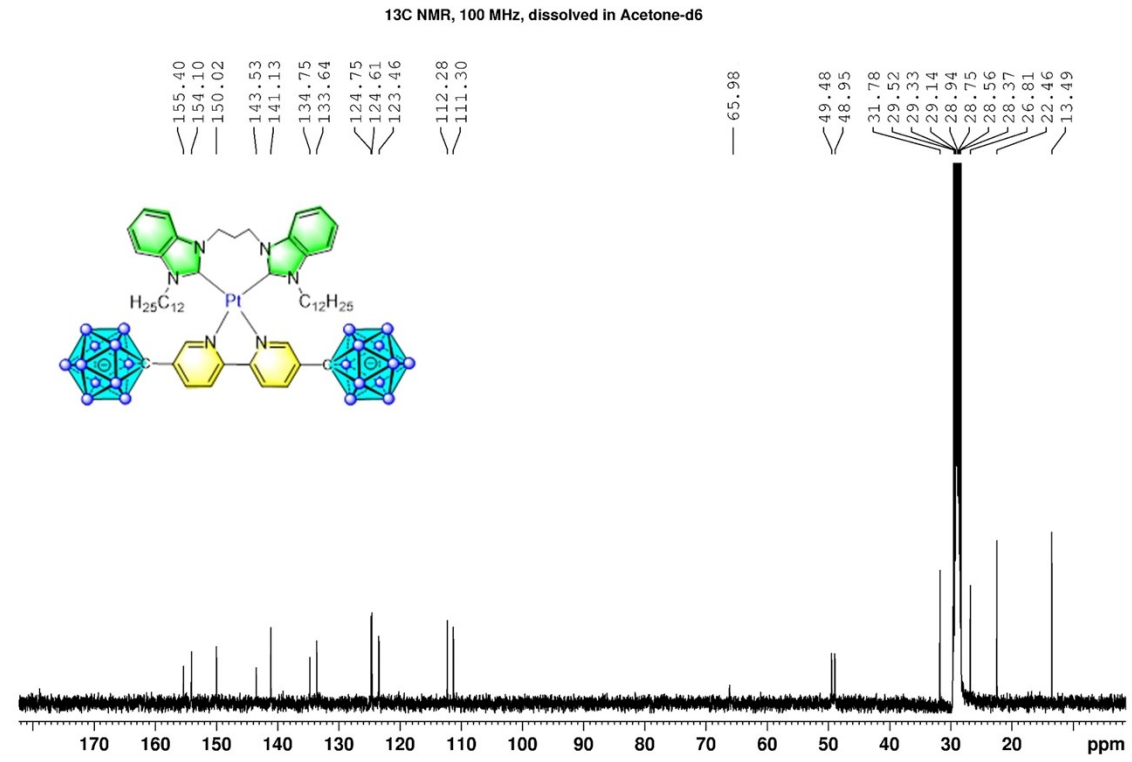


Figure S7. ^{13}C NMR spectrum of **1a** (acetone-d_6)

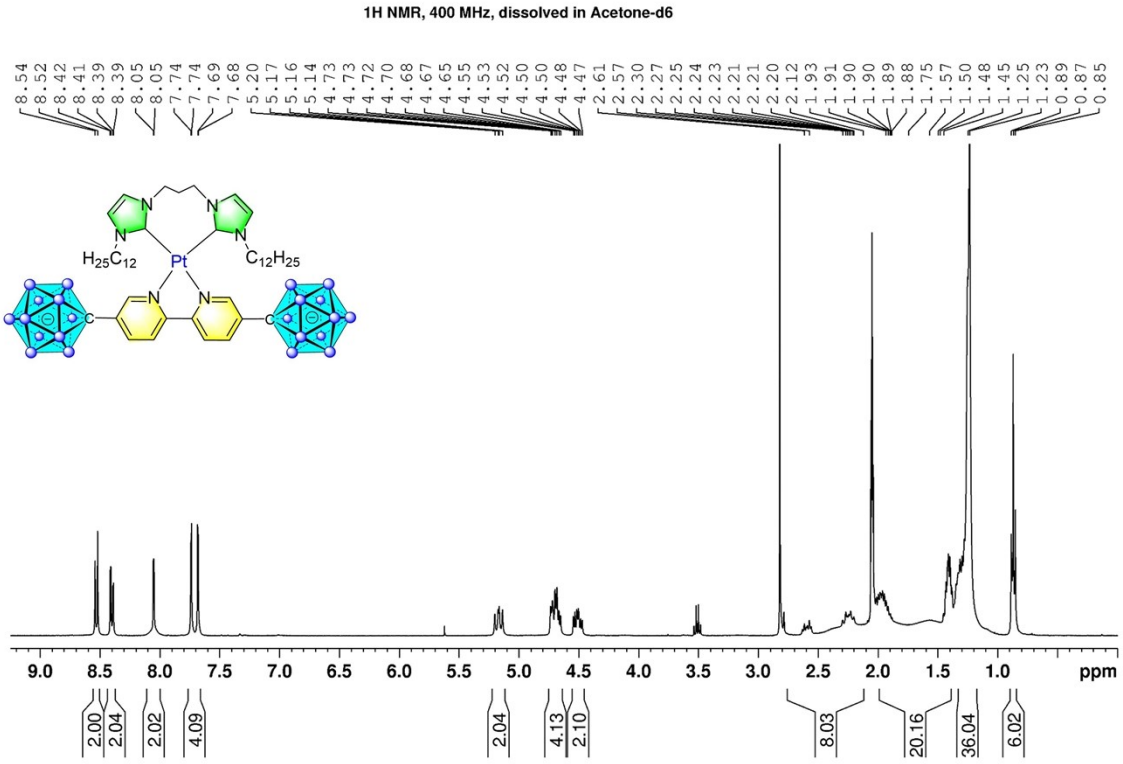


Figure S8. ^{1}H NMR spectrum of **1b** (acetone-d_6)

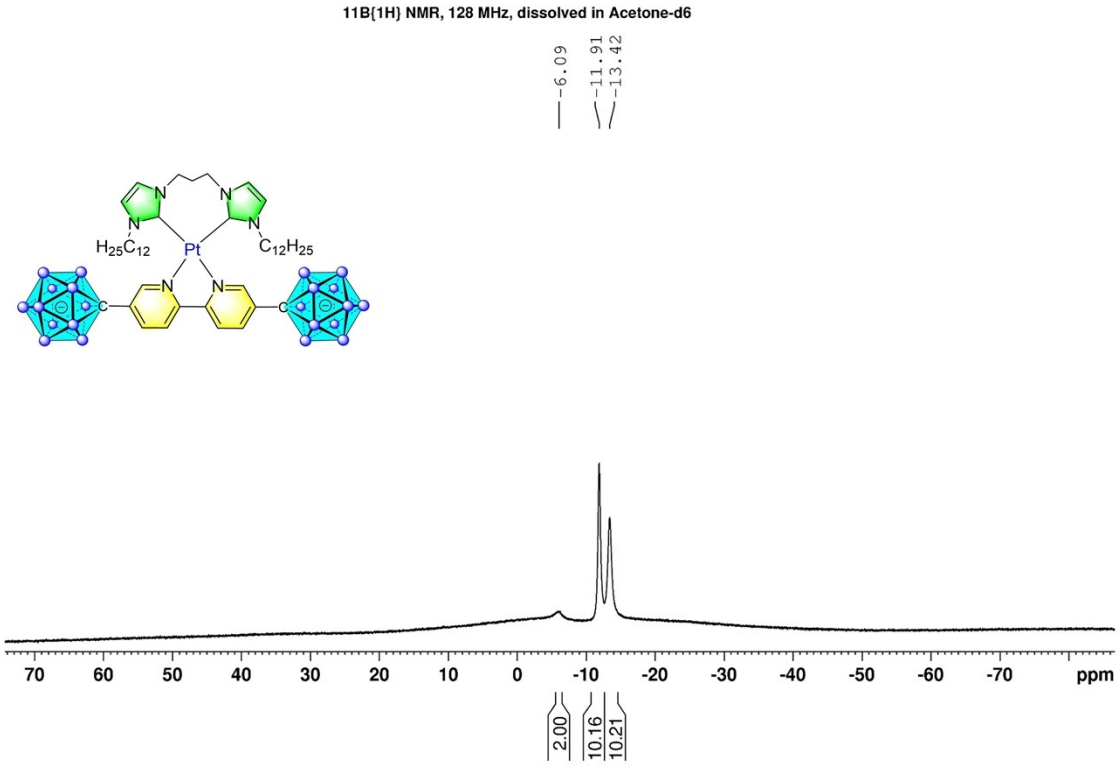


Figure S9. ^{11}B NMR spectrum of **1b** (acetone-d_6)

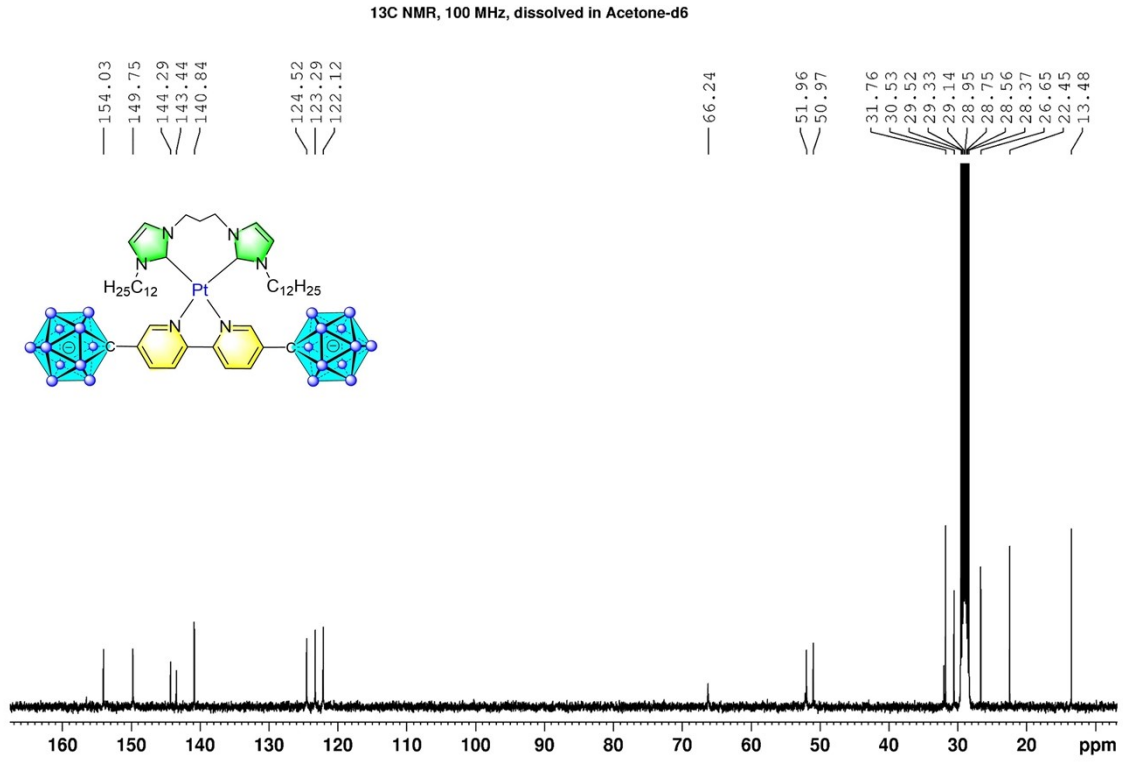


Figure S10. ^{13}C NMR spectrum of **1b** (acetone-d_6)

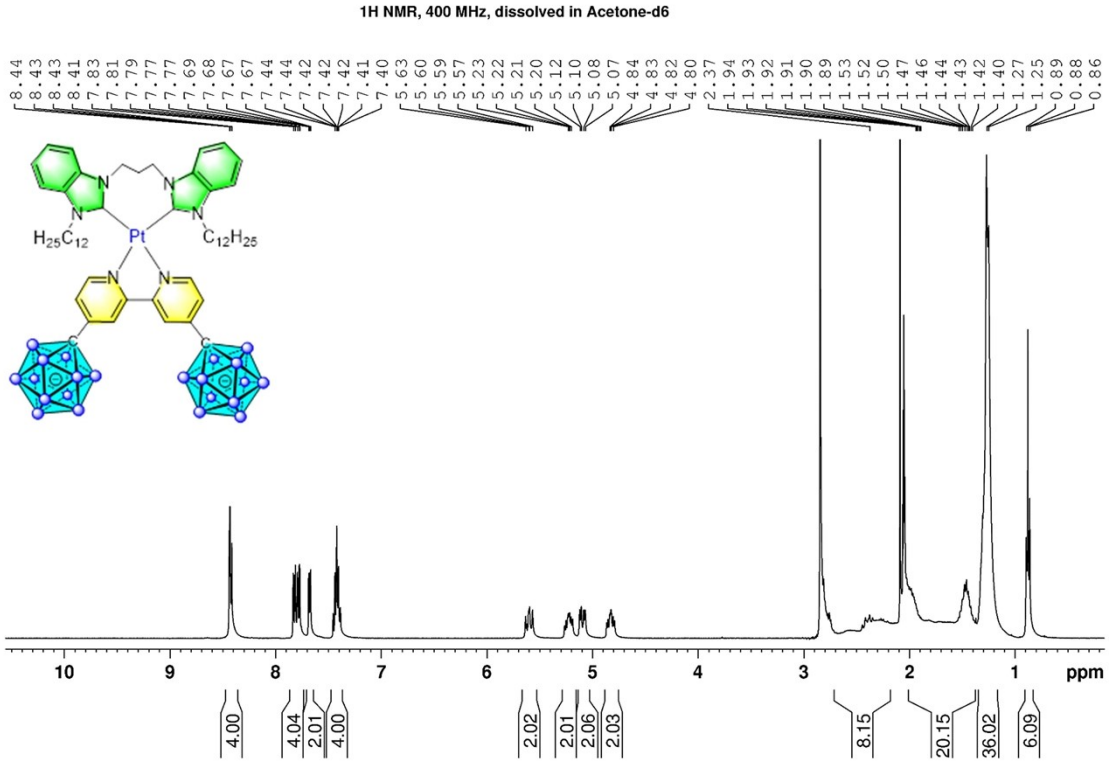


Figure S11. ^{1}H NMR spectrum of **2a** (acetone-d_6)

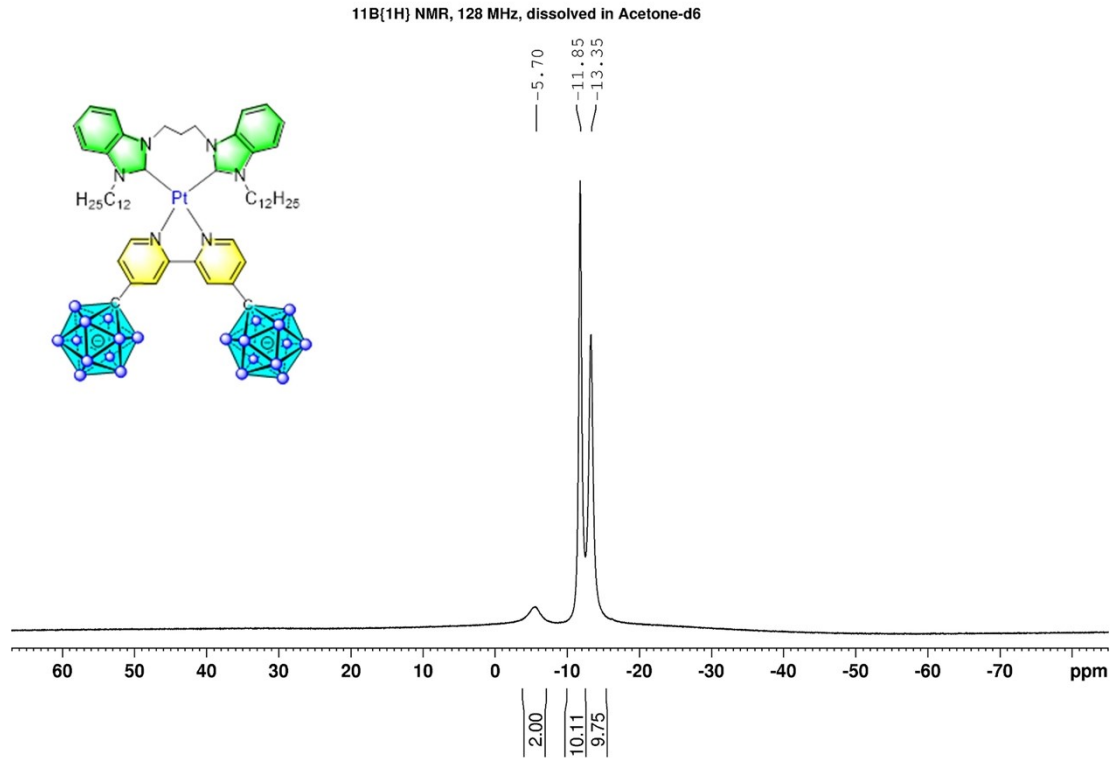


Figure S12. ^{11}B NMR spectrum of **2a** (acetone-d_6)

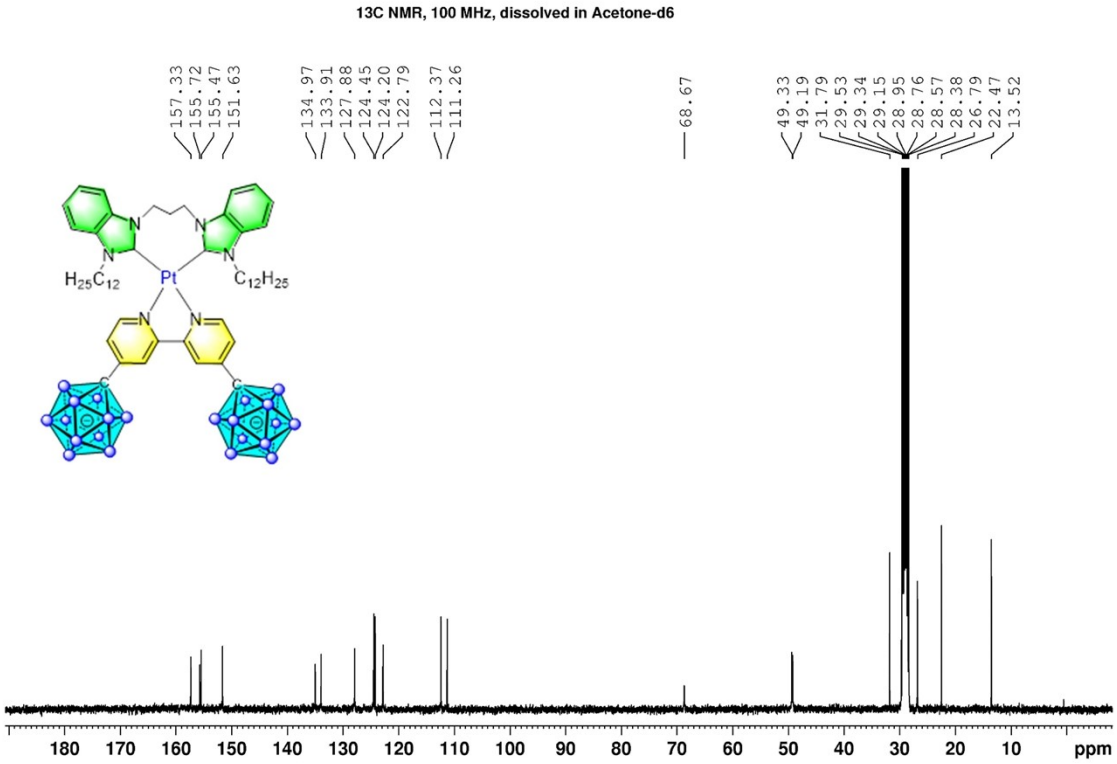


Figure S13. ^{13}C NMR spectrum of **2a** (acetone-d_6)

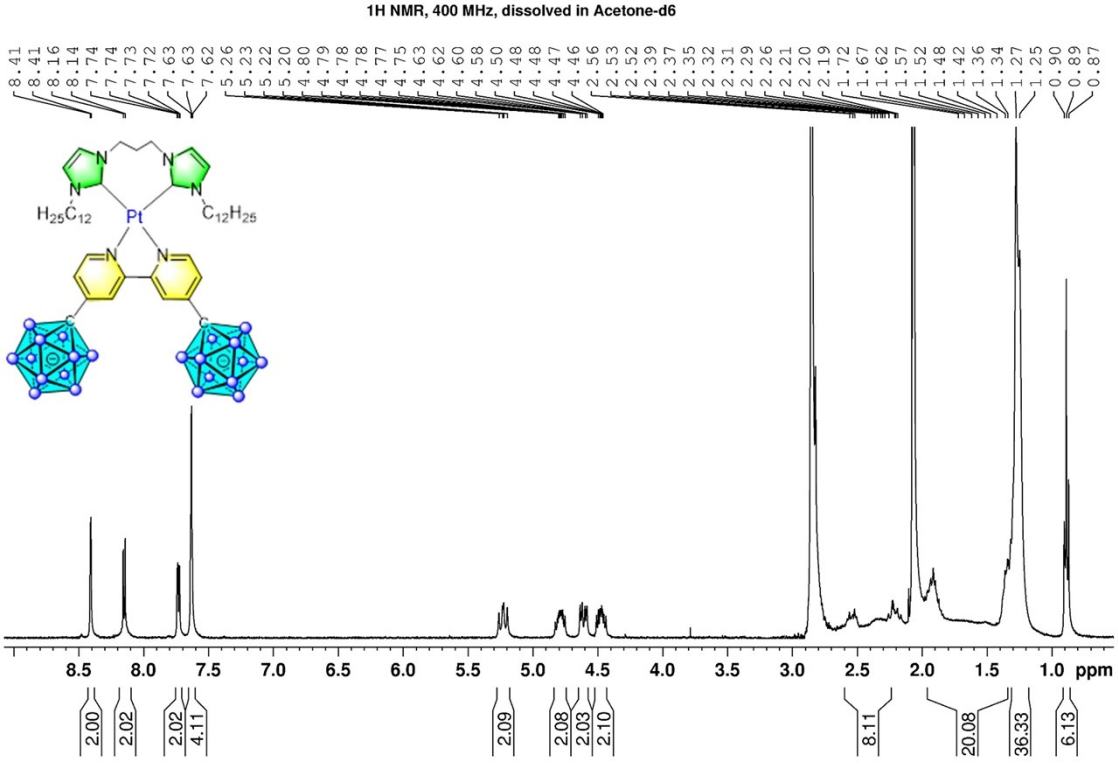


Figure S14. ^{1}H NMR spectrum of **2b** (acetone-d_6).

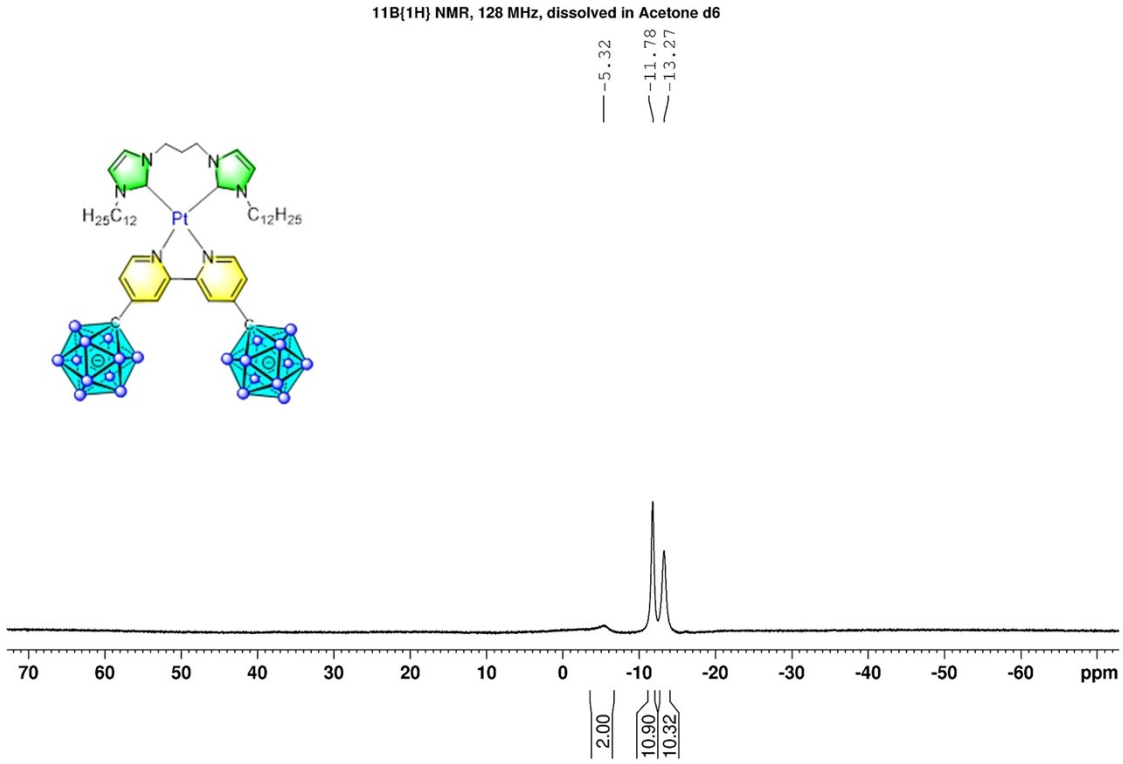


Figure S15. ^{11}B NMR spectrum of **2b** (acetone-d_6)

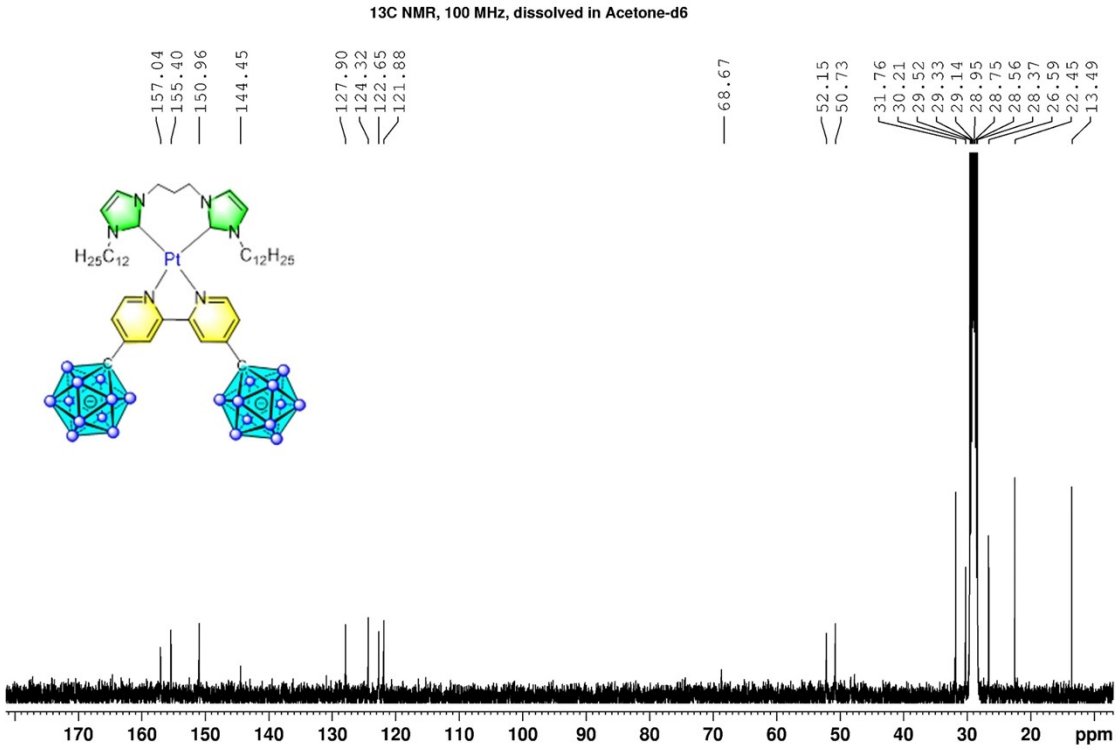


Figure S16. ^{13}C NMR spectrum of **2b** (acetone-d_6)

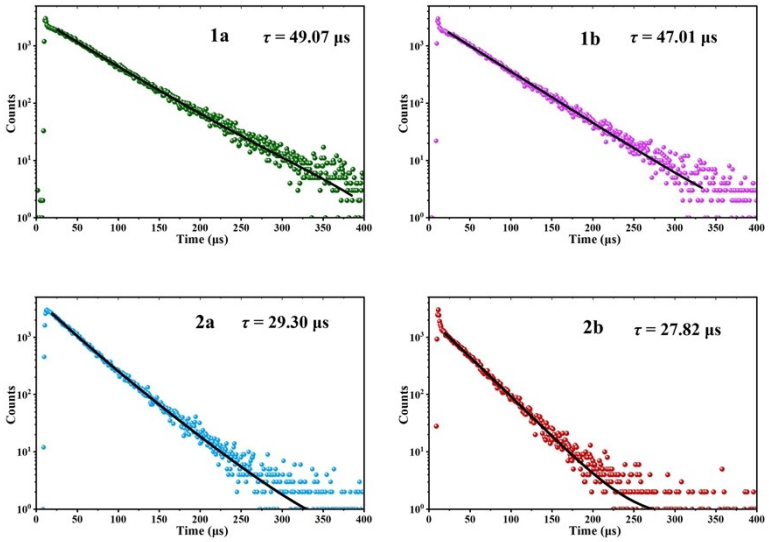


Figure S17. PL decay curves of all complexes in PMMA

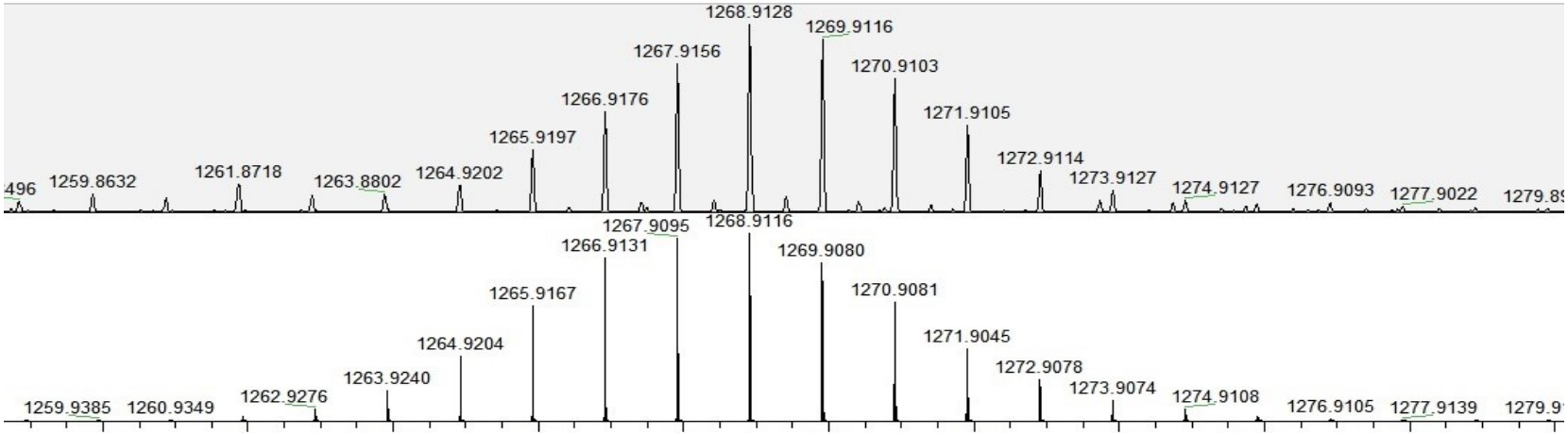


Figure S18. HRMS spectra for **1a** $[M + Na]^+$.

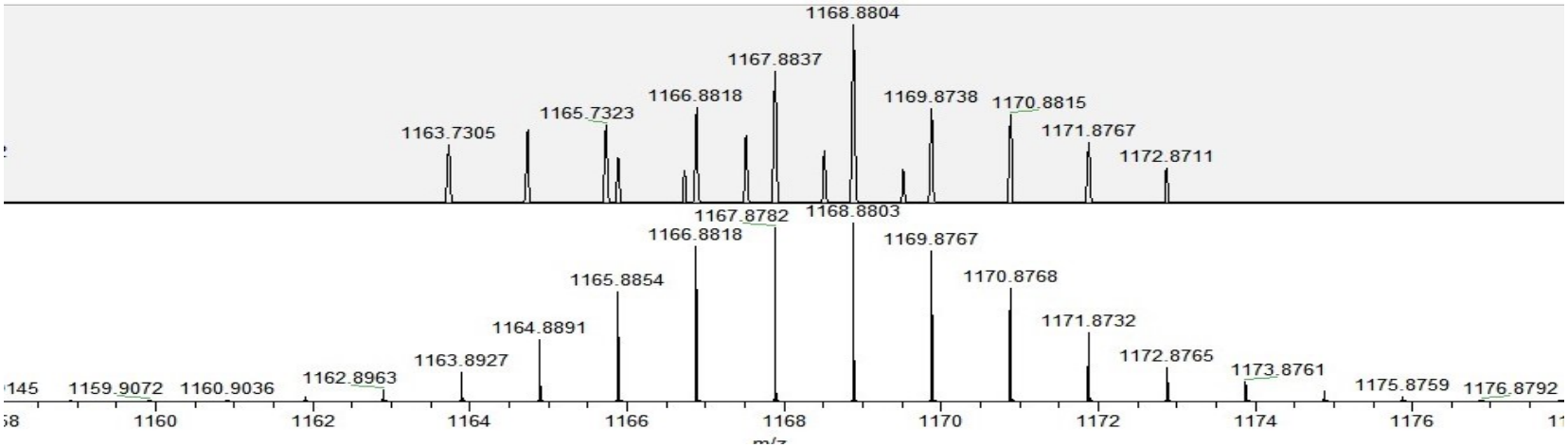


Figure S19. HRMS spectra for **1b** $[M + Na]^+$.

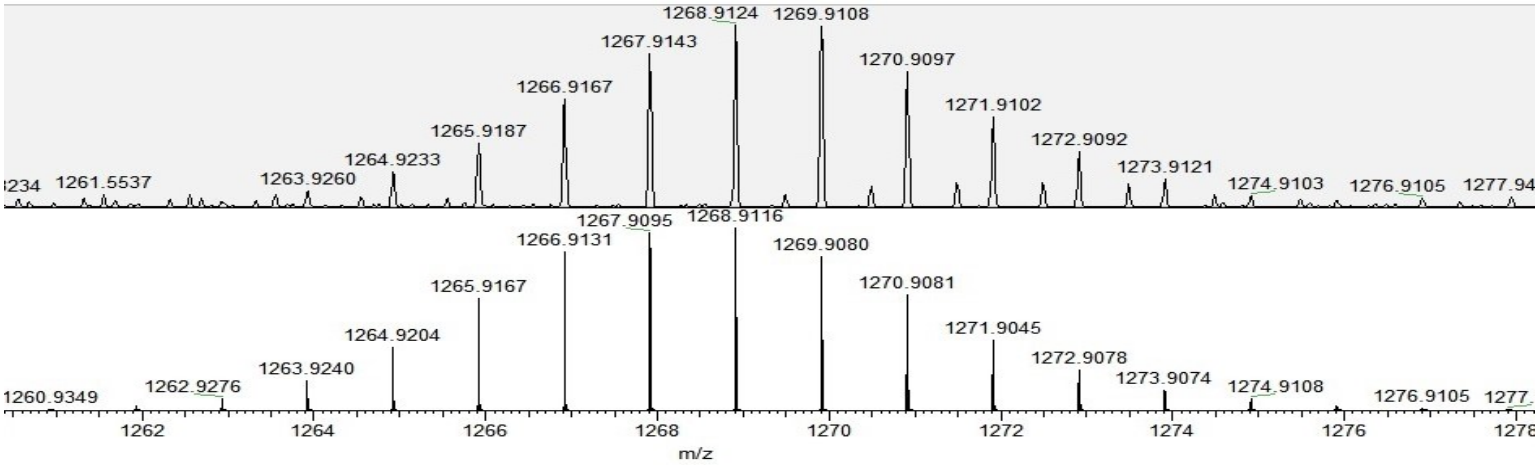


Figure S20. HRMS spectra for **2a** $[M + Na]^+$.

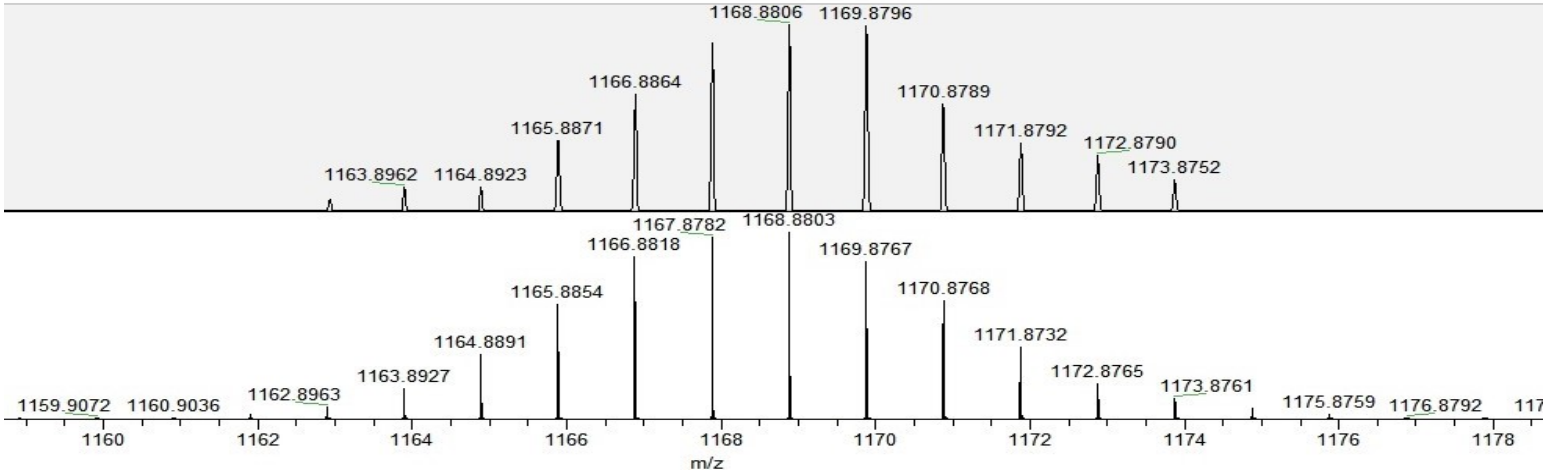


Figure S21. HRMS spectra for **2b** $[M + Na]^+$.