Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Triarylboryl-Functionalized Dibenzoylmethane and Its Phosphorescent Platinum(II) Complexes

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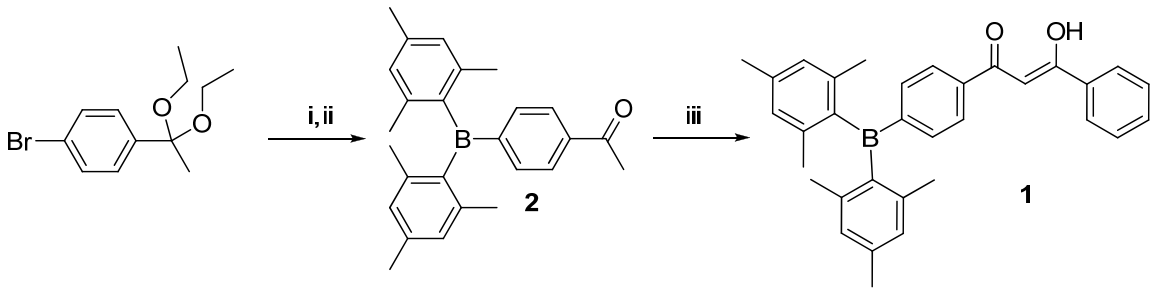
S1. General Experimental

Dry solvents were obtained from a solvent purification system (Innovative Technologies, Inc.). Reactions that required oxygen-free environments were conducted under an inert nitrogen atmosphere in oven-dried glassware using standard Schlenk techniques unless otherwise stated. ^{1}H and ^{13}C NMR spectra were recorded using a Bruker Avance 400 spectrometer as noted. All deuterated solvents were purchased from Cambridge Isotopes and used as is, without further drying. UV-Vis measurements were acquired using a Varian Cary 50 Bio Spectrometer. Excitation and emission spectra were recorded using a Photon Technologies International Quanta Master model C-60 spectrometer. High-resolution mass spectra were obtained using a Water/Micromass GC-TOF EI-MS spectrometer. Elemental analyses were conducted by the Elemental Analysis Service at the University of Montreal, Department of Chemistry. All reagents were obtained from the Sigma-Aldrich chemical company. Potassium tetrachloroplatinate was purchased from Pressure Chemicals. Crystal structures were obtained at 180 K using a Bruker AXS Apex II X-ray diffractometer (50 kV, 30 mA, Mo Kα radiation).

S2. Synthesis of Compound 2



Scheme S1. Reaction sequence for the synthesis of ligand **1;** i) *n*-BuLi, THF, -78°C, Mes_2BF, 18h; ii) hydrolysis of ketal with 2M HCl; iii) LHMDS, THF. 0°C, BzCl, 2h.

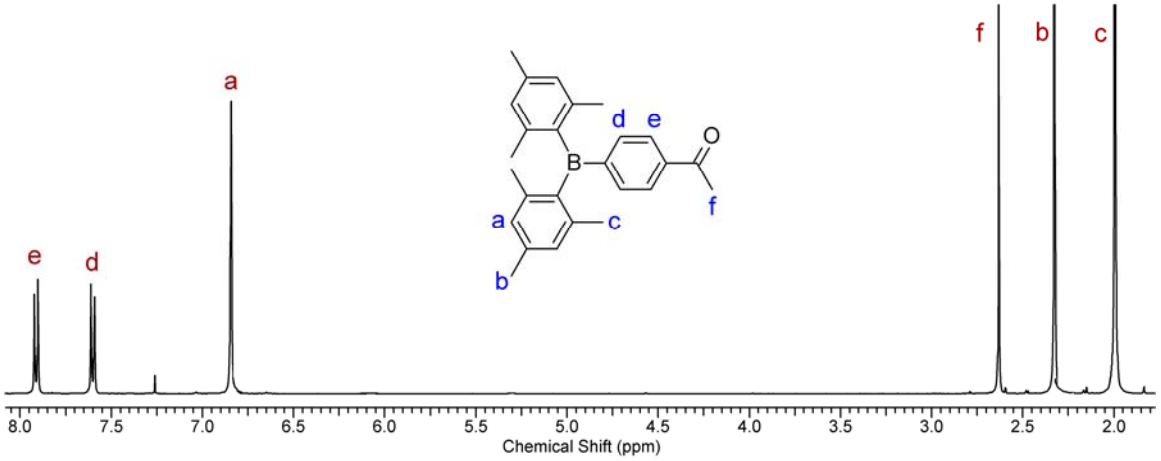


Figure S1: ^{1}H NMR (400 MHz, 298K, $CDCl_3$) of compound **2**.

1-(4-(dimesitylboryl)phenyl)ethanone (2): Under N_2**,** 4-bromoacetophenone diethylketal (3.05g, 0.011 mol, 1 eq.) was dissolved in anhydrous THF (125 mL) and cooled to -78^{o}C. 1.6 M *n*-BuLi (7.7 mL, 0.012 mol, 1.05 eq.) was added dropwise over 40 minutes and then allowed to stir for 60 min at -78^{o}C. In one portion, solid dimesitylboron fluoride (3.0 g, 0.011 mol 1 eq.) was added to the reaction mixture at -78^{o}C, and the reaction was allowed to warm to room temperature while stirring over night. The reaction was quenched and stirred with 2 M HCl and extracted with diethylether and washed with distilled water. The organic layer was dried with $MgSO_4$, filtered, and concentrated under reduced pressure to afford a pale yellow solid. The residue was purified by column chromatography (1:5 hexanes/DCM) to afford a colorless oil that solidified upon standing (3.36 g, 9.1 mmol, 83% yield). ^{1}H NMR (400MHz, 298 K, $CDCl_3$): δ 7.91 (d, J = 8.3 Hz, 2H), 7.59 (d, J = 8.3 Hz, 2H), 6.84 (s, 4H), 2.63 (s, 3H), 2.32 (s, 6H), 1.98 (s, 12H); ^{13}C NMR (100MHz, 298 K, $CDCl_3$): δ 198.5, 141.4, 140.8, 139.2, 138.8, 135.7, 128.3, 127.6, 26.8, 23.4, 21.2; ^{11}B NMR (128MHz, 298 K, $CDCl_3$): δ 78.7; Anal. Calcd for $C_{26}H_{29}BO$: C, 84.78; H, 7.94; Found: C, 84.46; H, 8.17.

S3. Synthesis of Compound 1

Compound **2** (0.6 g, 1.6 mmol, 1 eq.) was dissolved in anhydrous THF (10 mL) and cooled to 0^{o}C. Separately, lithium hexamethyldisilylamide (LHMDS, 0.57 g, 3.4 mmol 2.1 eq.) was dissolved in anhydrous THF (15 mL) and then quickly added dropwise to the cooled THF solution of **2**. The reaction was allowed to stir for 20 min allowing enolate to quantitatively form. Benzoyl chloride (0.18 mL, 1.55

mmol, 0.95 eq.) was added dropwise to the reaction mixture (still cooled at 0°C), the reaction was allowed to stir for 1h at 0°C, and then 1h room temperature. The reaction mixture was diluted with diethylether, and sequentially washed with a sat. NH_4Cl solution, water and brine. The organic layer was then dried with $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was recrystallized in DCM/MeOH to afford yellow crystals (0.67 g, 1.4 mmol, 87% yield). ^{1}H NMR (400 MHz, 298 K, $CDCl_3$): δ 16.87 (s, 1H), 8.02 (d, J = 7.1 Hz, 2H), 7.95 (d, J = 8.1 Hz, 2H), 7.64 (d, J = 8.1 Hz, 2H), 7.57 (t, J = 7.1 Hz, 1H), 7.50 (dd, J = 7.1 Hz, 7.1 Hz), 6.97 (s, 1H), 6.86 (s,4H), 2.34 (s, 6H), 2.03 (s, 12H); ^{13}C NMR (100MHz, 298 K, $CDCl_3$): δ 186.7, 184.8, 141.6, 140.9, 139.2 137.9, 136.1, 135.7, 132.6, 128.7, 128.4 (2C), 123.3, 126.5, 93.7, 23.5, 21.3; ^{11}B NMR (128 MHz, 298 K, $CDCl_3$): δ 83.5; Anal. Calcd for $C_{33}H_{33}BO_2$: C, 83.90; H, 7.04. Found: C, 83.70; H, 7.17.

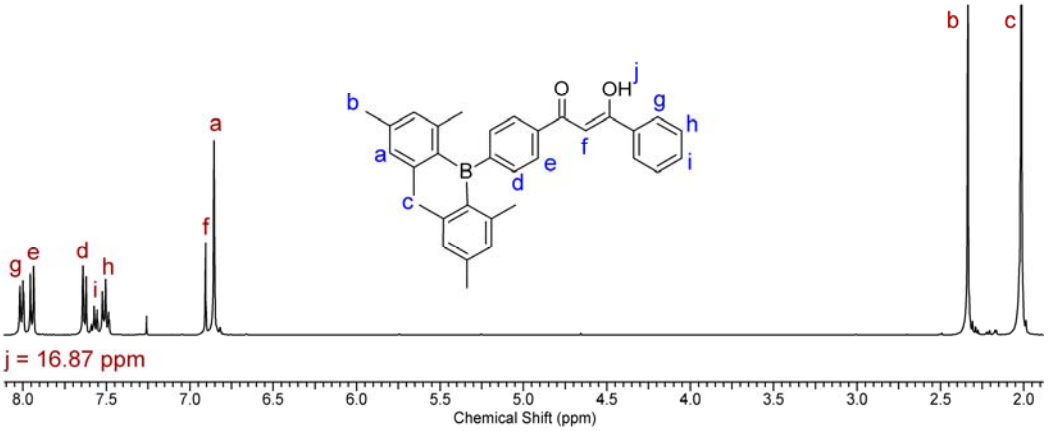
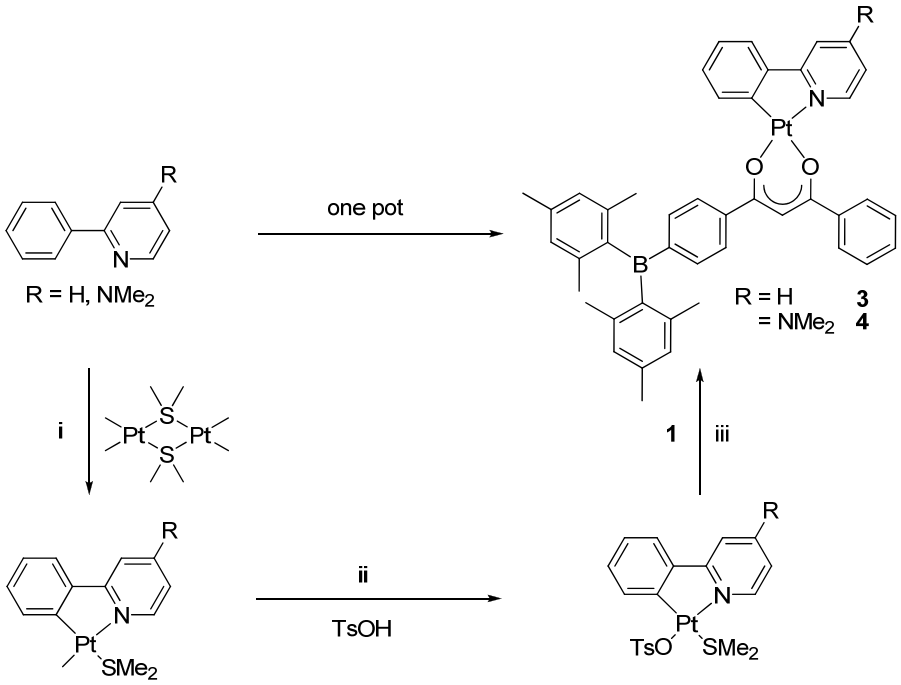


Figure S2: ^{1}H NMR (400 MHz, 298K, $CDCl_3$) of compound **1**.

S4. Synthesis of Compound 3



Scheme S2. Reaction sequence for the formation of platinum(II) complexes **3** and **4**; i) THF, rt, 1h; ii) THF, rt 1h; iii) KOMe, THF, rt, 1h.

Compound 3: In a 20 mL sample vial, 2-phenylpyridine (27 mg, 0.17 mmol, 1 eq.) was dissolved in THF (3ml), and $[Pt(SMe_2)Me_2]_2$ (50 mg, 0.087 mmol 0.5 eq.) was added in one portion to the reaction mixture. The mixture was stirred for 1h at room temperature. *p*-Toluenesulfonic acid (34 mg, 0.17 mmol, 1 eq.) dissolved in THF (2 mL) was then added dropwise to the reaction mixture which was allowed to stir for 1h at room temperature. In a separate vial, **1** (91 mg, 0.19 mmol, 1.1 eq.) was dissolved in THF (3 mL), and converted to the potassium salt by dropwise addition of KOMe (1 equivalent relative to **1**). The K·**1** solution was then added dropwise to the reaction mixture containing phenylpyridine and the mixture was allowed to stir for 1h at room temperature. The reaction was then diluted in DCM and washed with water and brine. The organic layer was then dried with $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by column

chromatography (3:1 hexanes EtOAc) to afford an orange powder (93 mg, 0.11 mmol, 67% yield). ^{1}H NMR (400MHz, 298 K, $CDCl_3$): δ 9.17 (d, J = 6.6 Hz, 1H, H_j), 8.08 (d, J = 8.1 Hz, 4H, $H_{e,g}$), 7.87 (dd, J = 6.6 Hz, 7.3 Hz, 1H, H_l), 7.77 (d, J = 7.1 Hz, 1H, H_q), 7.70, (d, J = 8.3 Hz, 1H, H_m), 7.63 (d, J = 7.8 Hz, 2H, H_d) 7.61, (t, J = 7.1 Hz, 1H, H_i) 7.52 (m, 3H, $H_{h,n}$), 7.27 (dd, J = 7.1 Hz, 7.1 Hz, 1H, H_p), 7.21 (dd, J = 6.6 Hz, 7.3, 1H, H_k), 7.15 (dd, J = 7.1 Hz, 7.1 Hz, 1H, H_o), 6.87 (s, 4H, H_d), 6.85 (s, 1H, H_f), 2.35 (s, 6H, H_a), 2.06 (s, 12H, H_c); ^{13}C NMR and ^{11}B NMR spectra were not successfully recorded due to poor solubility, and extremely broadened signals of the triarylboron moiety. Anal. Calcd for $C_{44}H_{40}BNO_2Pt$: C, 64.39; H, 4.91; N, 1.71. Found: C, 64.41; H, 4.93; N, 1.61.

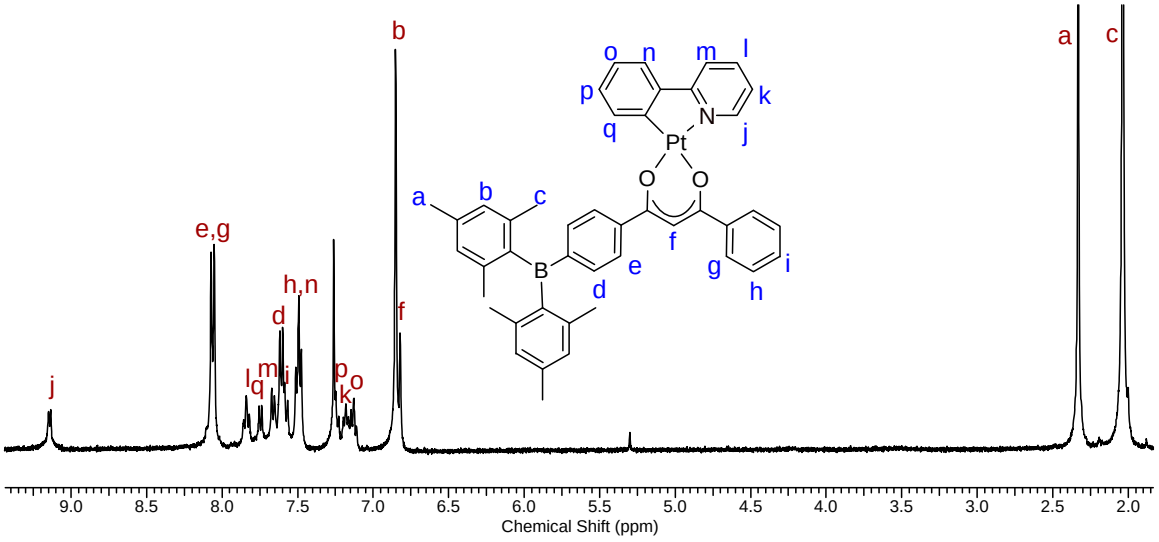


Figure S3: ^{1}H NMR (400 MHz, 298K, $CDCl_3$) of compound **3**.

S5. Synthesis of Compound 4

The same procedure and proportions for **3** were employed for the synthesis of **4**, which resulted in the isolation of an orange powder (90 mg, 0.10 mmol, 61% yield). ^{1}H NMR (400MHz, 298 K, $CDCl_3$): δ 8.61 (d, J = 6.8 Hz, 1H, H_j), 8.08 (d, J = 7.8 Hz, 4H, $H_{e,g}$), 7.73 (d, J = 6.8 Hz, 1H, H_q), 7.61 (d, J = 8.1 Hz, 2H, H_d), 7.58, (t, J = 7.6 Hz, 1H, H_i), 7.48 (dd, J = 7.6 Hz, 7.6 Hz, 2H, H_h) 7.45, (d, J = 7.1 Hz, 1H,

H_n) 7.21 (dd, J = 6.8 Hz, 7.6 Hz, 1H, H_p) 7.10 (dd, J = 7.1 Hz, 7.6 Hz, 1H, H_o) 6.86 (s, 4H, H_b), 6.84 (d, J = 2.8 Hz, 1H, H_m), 6.81 (s, 1H, H_f), 6.47 (dd, J = 2.8 Hz, 6.8 Hz, 1H, H_k) 3.18 (s, 6H, H_l), 2.35 (s, 6H, H_a), 2.05 (s, 12H, H_c); ^{13}C NMR and ^{11}B NMR spectra were not successfully recorded due to poor solubility, and extremely broadened signals of the triarylboron moiety. Anal. Calcd for $C_{46}H_{45}BN_2O_2Pt \cdot 2H_2O$: C, 61.40; H, 5.49; N, 3.11. Found: C, 61.14; H, 5.04; N, 3.12.

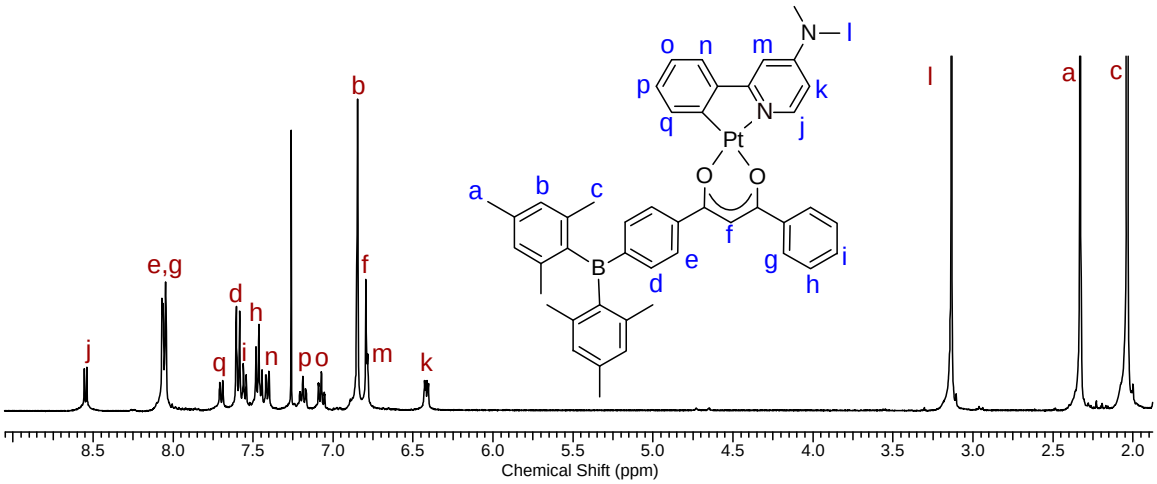


Figure S4: ^{1}H NMR (400 MHz, 298K, $CDCl_3$) of compound **4**.

S6. NMR Confirmation of Regiochemistry (^{1}H & NOESY).

Assignments for the ^{1}H NMR spectra above were determined/confirmed using ^{1}H NMR, COSY, and NOESY in $CDCl_3$, however, ambiguity associated with protons H_e and H_g and their respective NOEs with H_j and H_q remained. Thus, spectra taken in $CDCl_3/C_6D_6$ (50:50) were employed to separate the signal overlap of protons H_e and H_g. With this NOEs between H_e-H_q and H_g-H_j were visible in both compounds **3** and **4**.

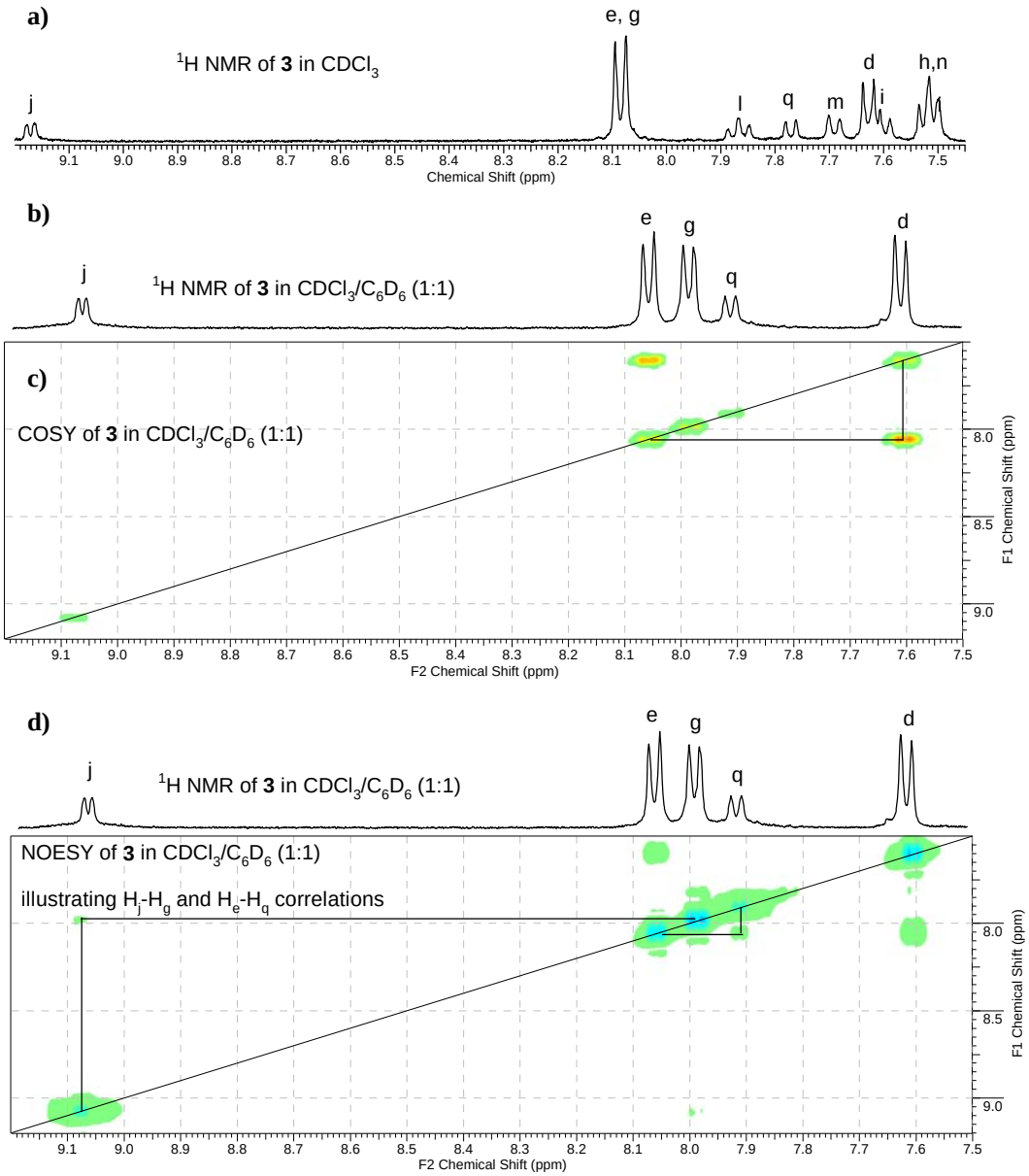


Figure S5: Illustration of isomer identification of platinum(II) complex **3**; a) ^{1}H NMR of **3** in $CDCl_3$; b) ^{1}H NMR of **3** in $CDCl_3/C_6D_6$ (1:1); c) COSY of **3** in $CDCl_3/C_6D_6$ illustrating H_e-H_d correlation; d) ^{1}H NMR and NOESY of **3** in $CDCl_3/C_6D_6$ illustrating H_j-H_g and H_e-H_q NOE correlations.

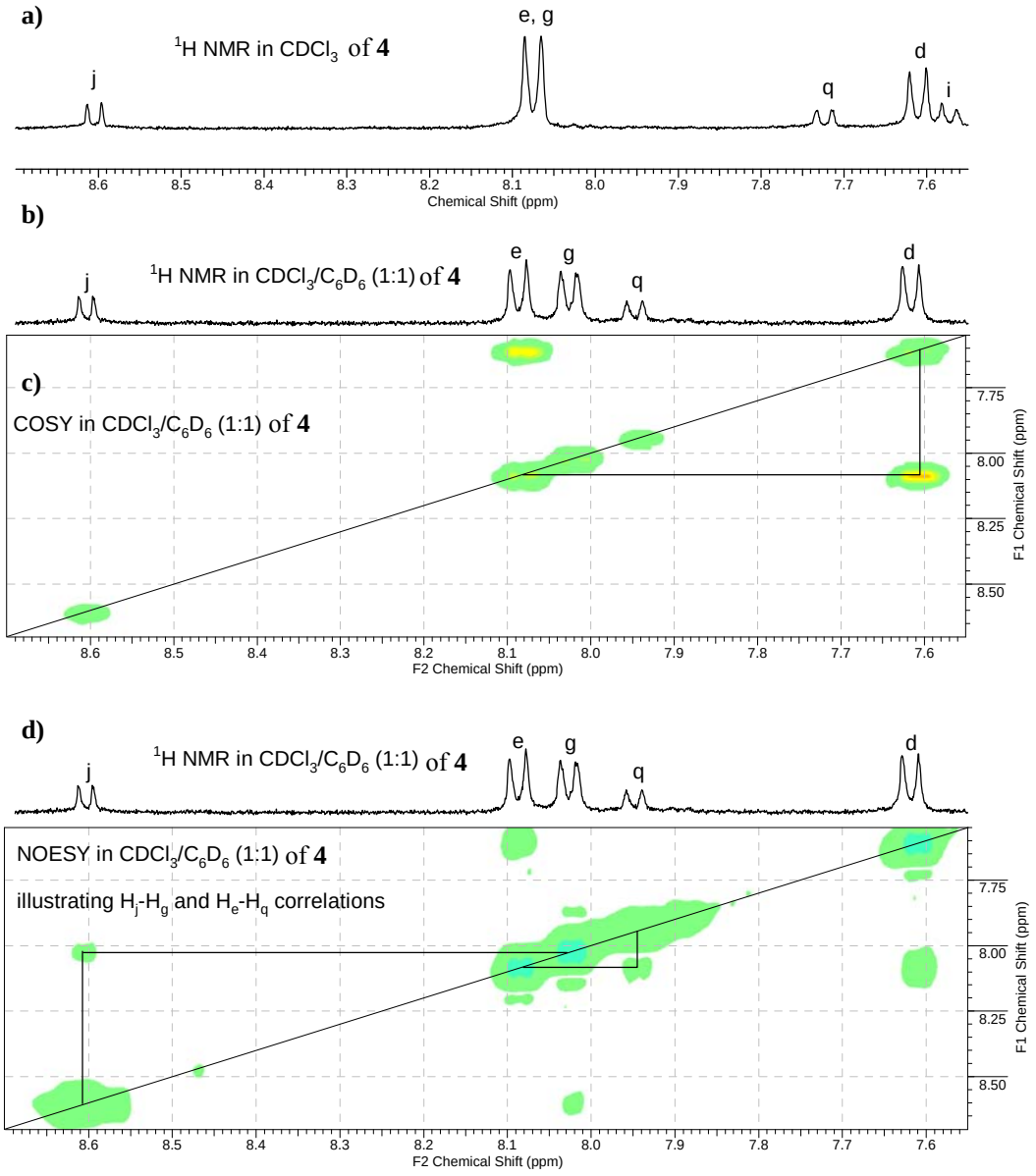


Figure S6: Illustration of isomer identification of platinum(II) complex **4**; a) ^{1}H NMR of **4** in $CDCl_3$; b) ^{1}H NMR of 4 in $CDCl_3/C_6D_6$ (1:1); c) COSY of **4** in $CDCl_3/C_6D_6$ illustrating H_e-H_d correlation; d) ^{1}H NMR and NOESY of **4** in $CDCl_3/C_6D_6$ illustrating H_j-H_g and H_e-H_q NOE correlations.

S7. UV-Vis and luminescent Spectra of Compounds 1, 3 and 4

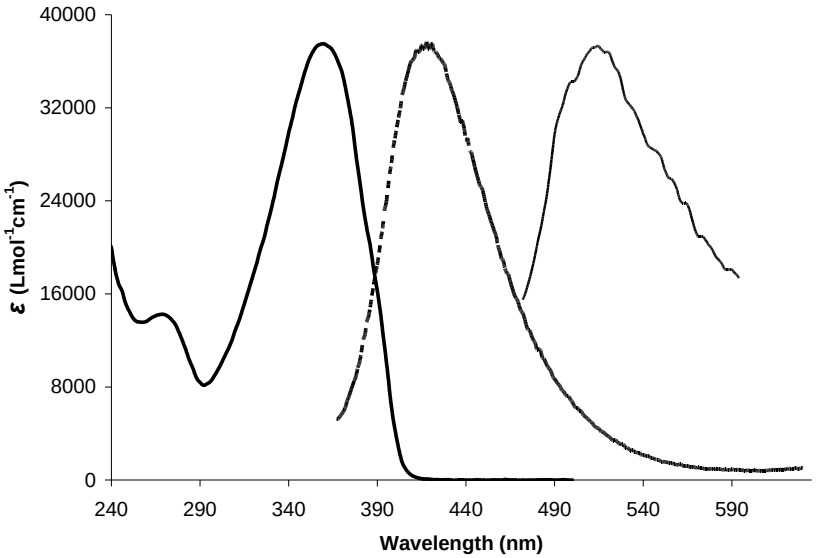


Figure S7: UV-vis (thick line; λ_{max} = 358 nm, 298K), normalized fluorescence (dashed line; λ_{ex} = 358 nm, λ_{em} = 420 nm), and normalized phosphorescent (thin line; λ_{ex} = 358 nm, λ_{em} = 516 nm, 77 K) spectra of ligand **1** in 2-methyltetrahydrofuran.

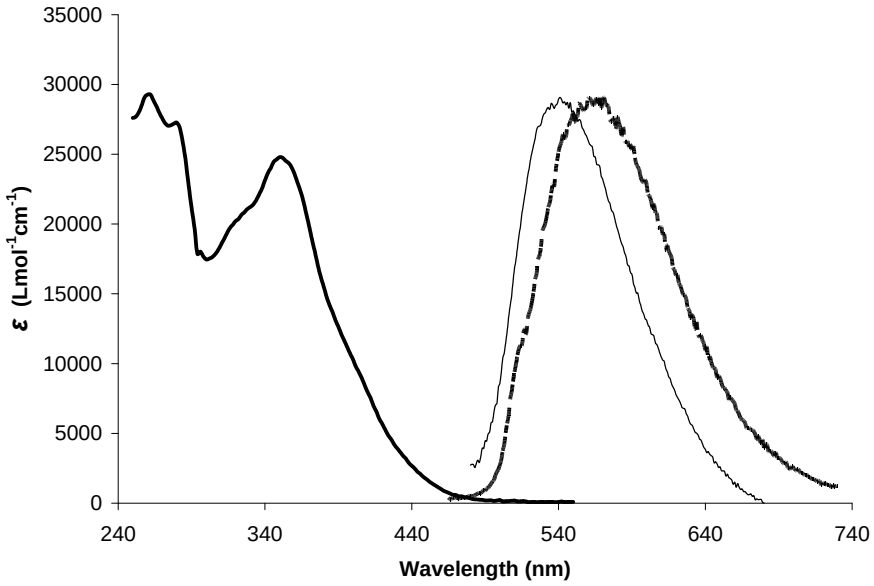


Figure S8: UV-vis (thick line; λ_{max} = 350 nm, 298K), normalized solid-state phosphorescent (thin line λ_{ex} = 350 nm, λ_{em} = 545 nm) in 5 wt% PMMA thin film, and normalized phosphorescent (dashed line; λ_{ex} = 350 nm, λ_{em} = 565 nm) spectra of compound **3** in CH_2Cl_2.

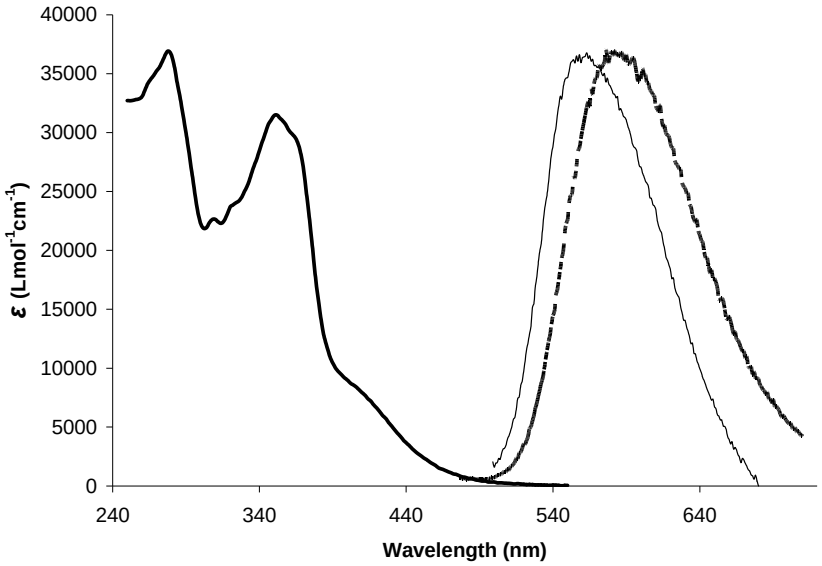


Figure S9: UV-vis (thick line; λ_{max} = 350 nm, 298K), normalized solid-state phosphorescent (thin line λ_{ex} = 350 nm, λ_{em} = 565 nm) 5% loading in PMMA thin film, and normalized phosphorescent (dashed line; λ_{ex} = 350 nm, λ_{em} = 587 nm) spectra of compound **4** in CH_2Cl_2.

S8. Solvent-Dependent Absorption and Luminescent Spectra in Solution

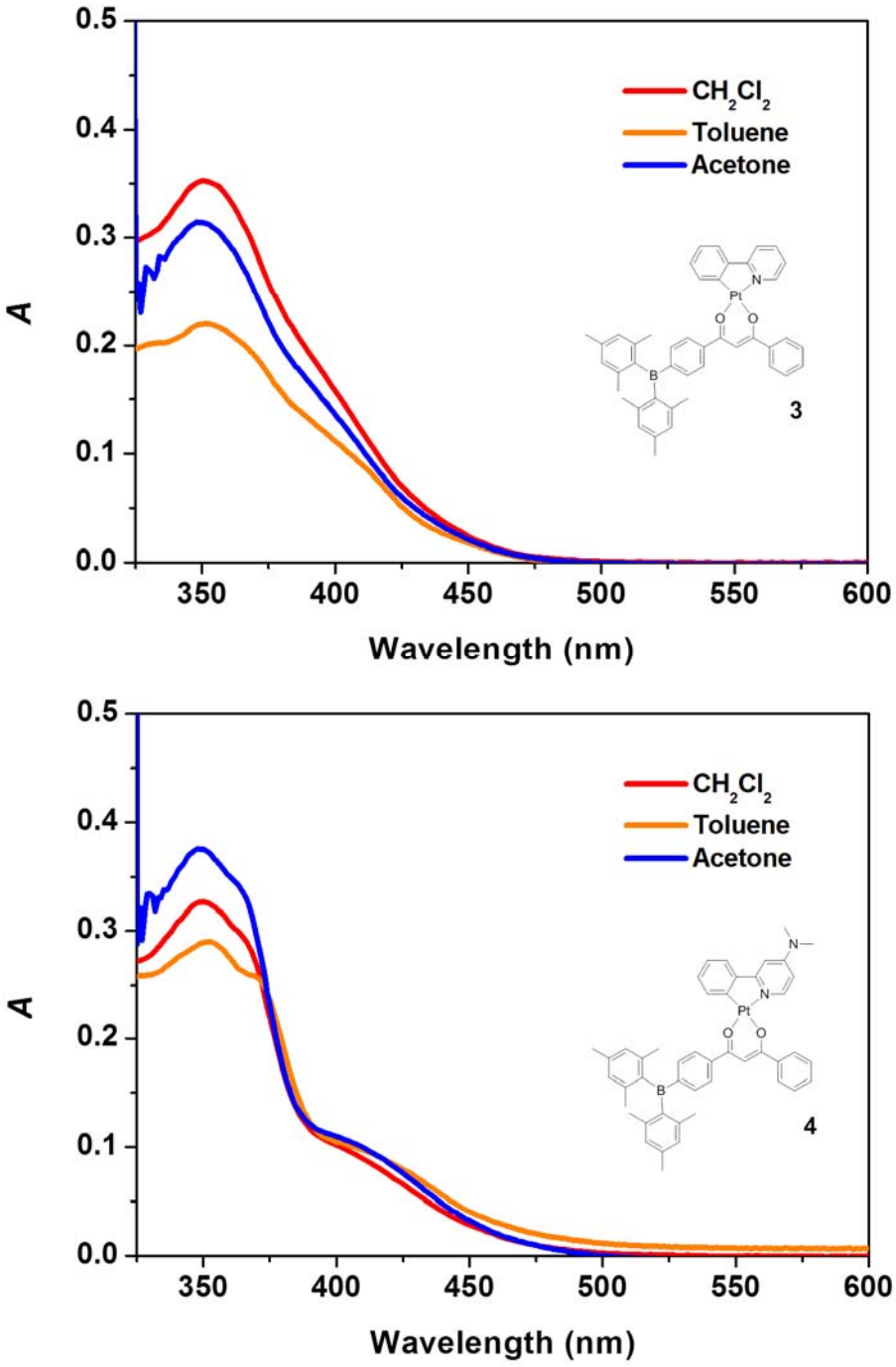


Figure S10: Normalized absorption spectra for **3** and **4** at 1.0×10^{-5} M in various solvents.

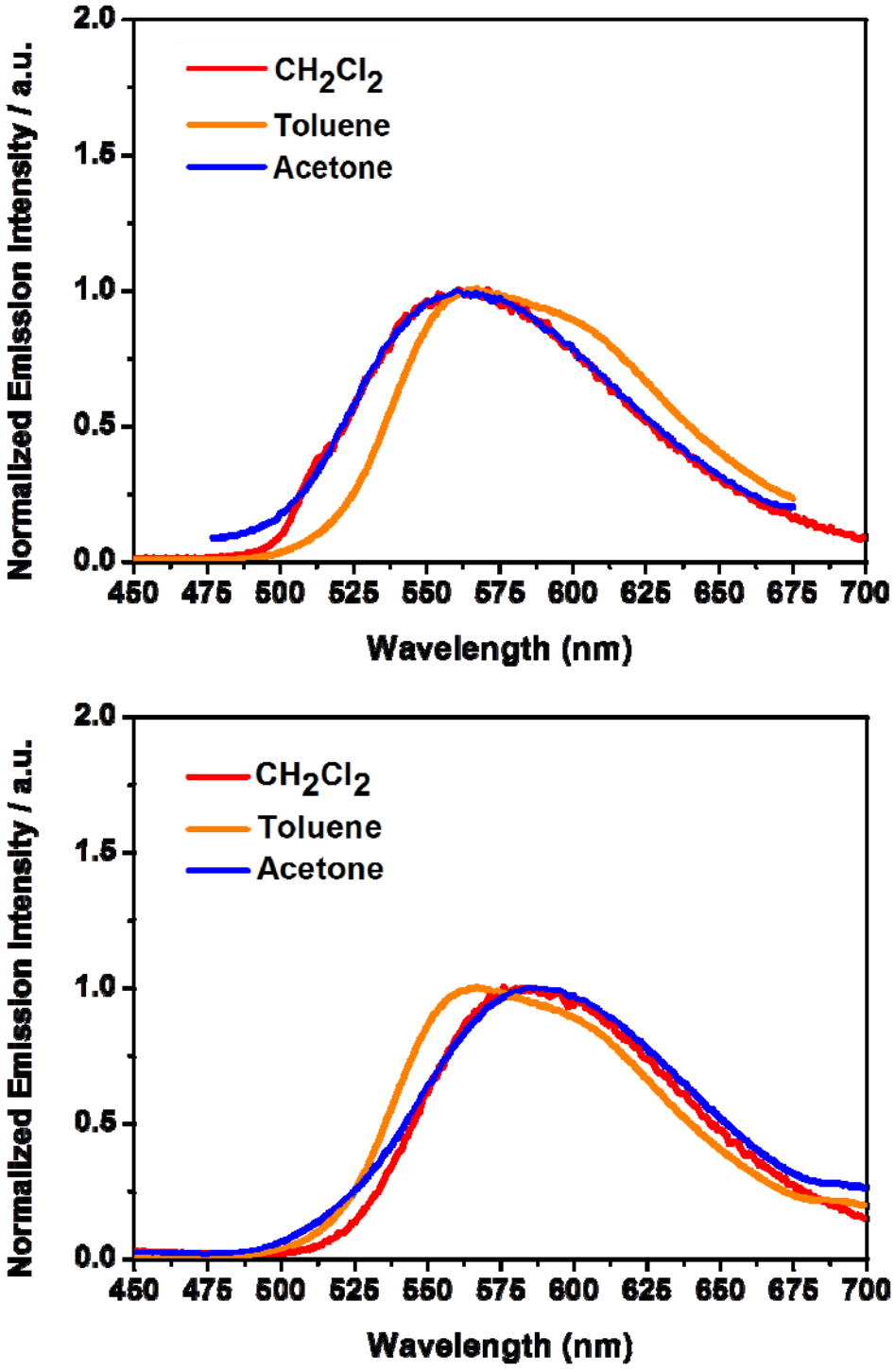


Figure S11: Normalized emission spectra for **3** (top) and **4** (bottom) at 1.0×10^{-5} M in various solvents.

S9. Cyclic Voltammetry Diagrams of Compound 3 and 4

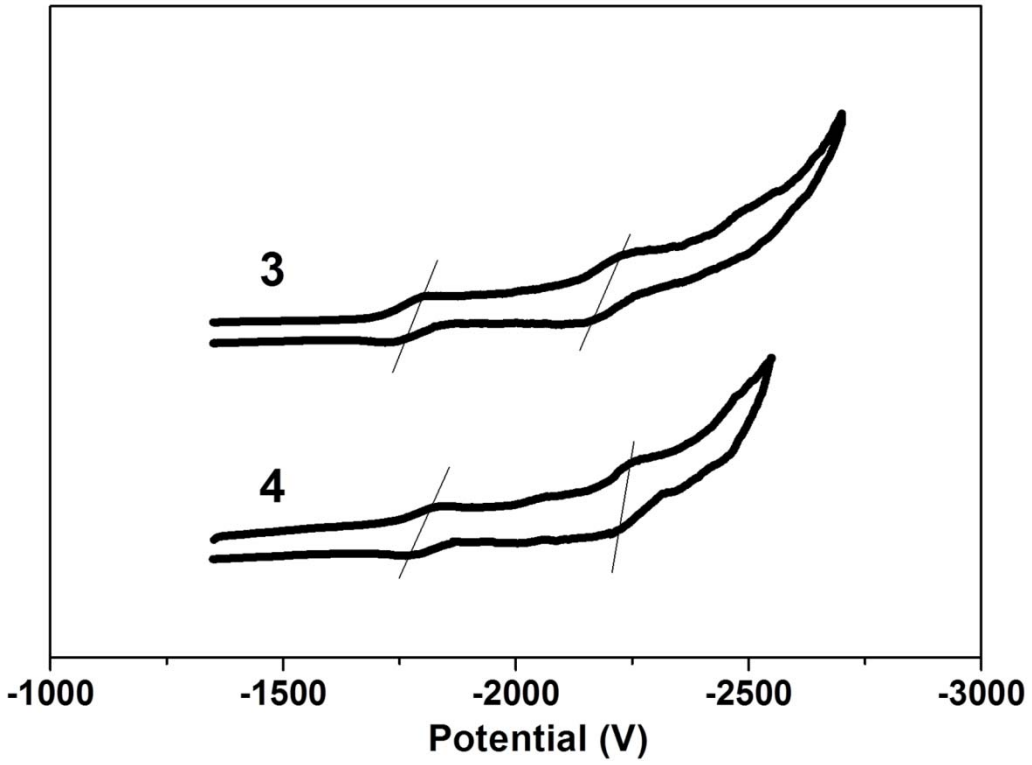


Figure S12: CV diagrams for Pt(II) complexes **3-4** recorded in DMF relative to $FeCp_2^{0/+}$.

Table S1. Electrochemical Data[a]

Complex	$E_{1/2}^{red1}$ (V)	$E_{1/2}^{red2}$ (V)	Optical energy gap (eV)	HOMO (eV)[b]	LUMO (eV)[c]
3	-1.77	-2.20	2.58	-5.61	-3.03
4	-1.83	-2.23	2.45	-5.42	-2.97

[a] The CV were recorded in DMF solution containing 0.10 M $(n\text{-Bu})_4PF_6$ as the electrolyte, relative to $E^o(Fc/Fc^+) = 0.55$ V. [b] Estimated from the optical energy gap and the LUMO energy. [c] Estimated from the reduction potentials.

S10. Fluoride Titration Resutls

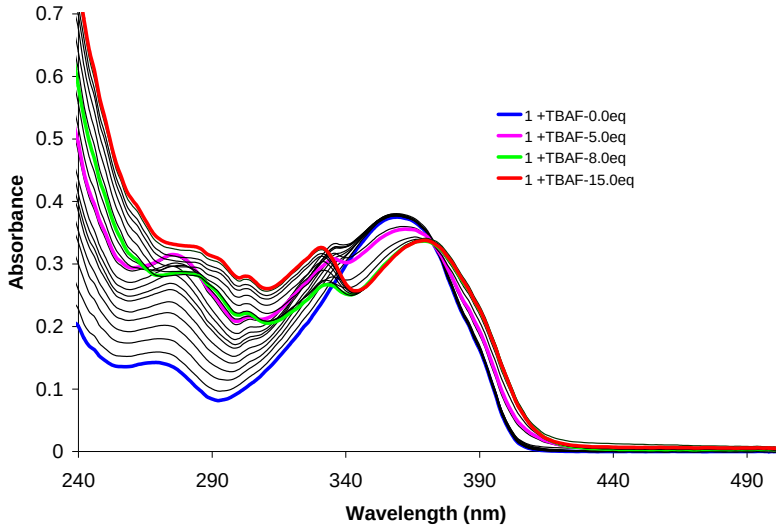


Figure S13: UV-Vis titration of ligand **1** (1 x 10^{-5} M) with aliquots of TBAF (3 x 10^{-3} M) in THF at 298 K.

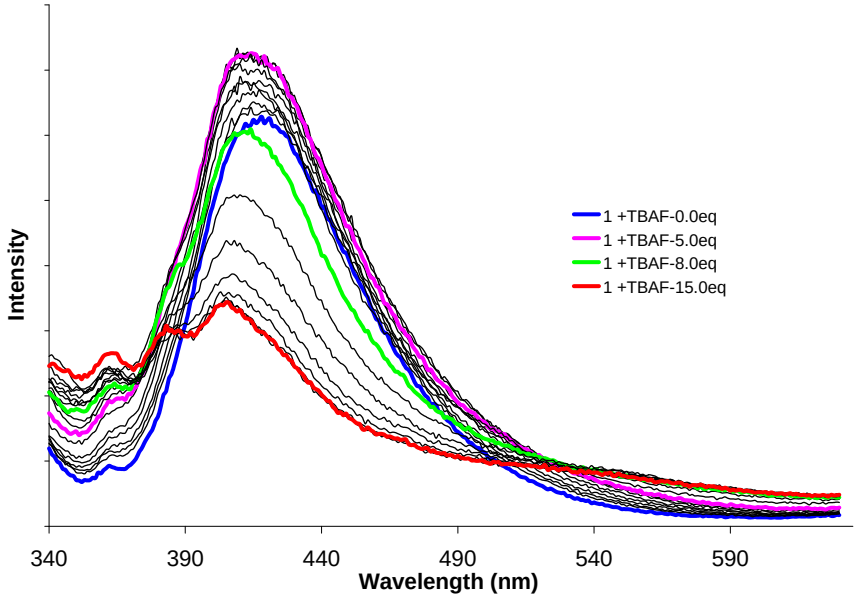


Figure S14: Fluorescence titration of ligand **1** (1 x 10^{-5} M) with aliquots of TBAF (3 x 10^{-3} M) in THF at 298 K (λ_{ex} = 358 nm).

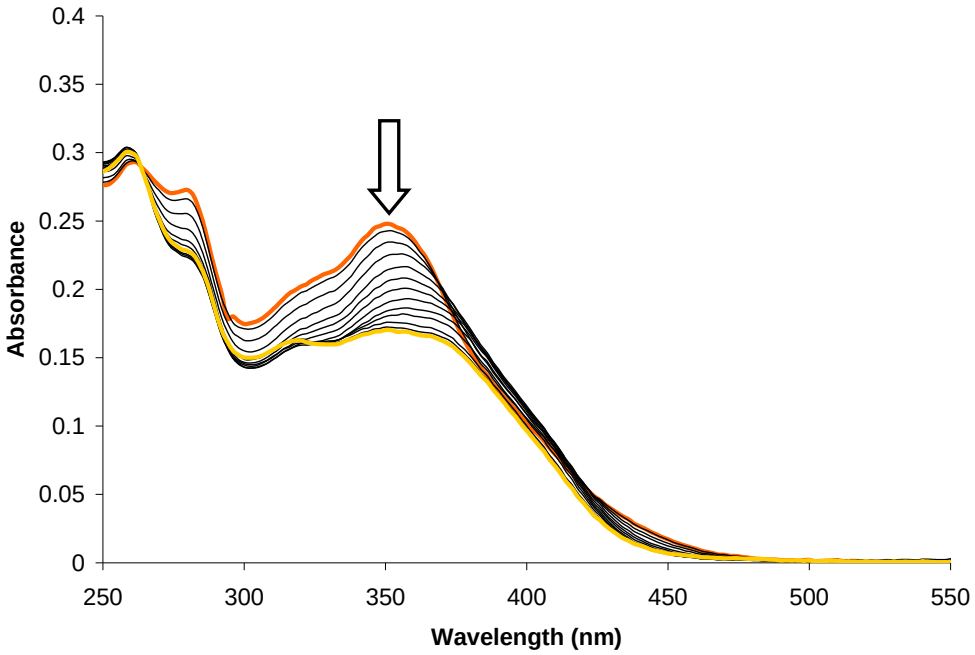


Figure S15: UV-Vis titration of compound **3** (1 x 10^{-5} M) with aliquots of TBAF (3 x 10^{-3}M) in DCM at 298 K.

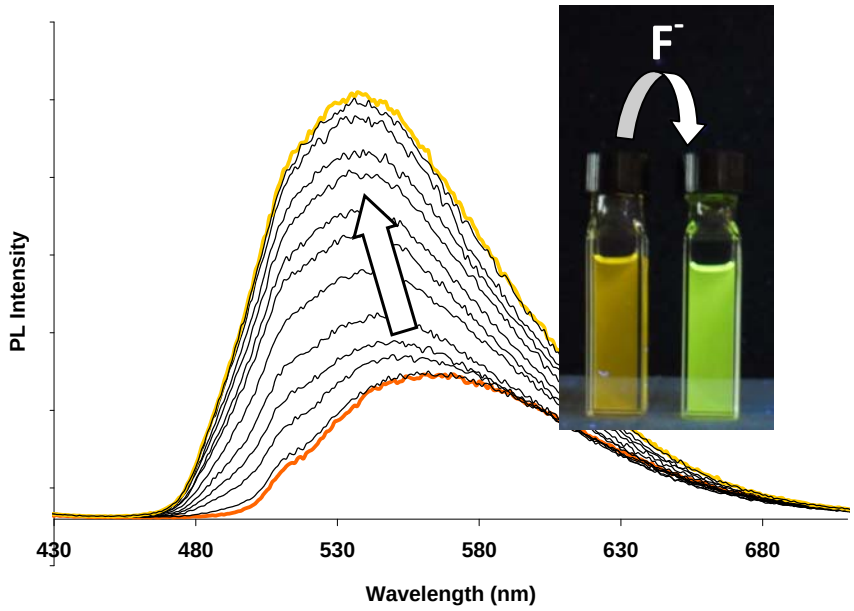


Figure S16: Phosphorescence titration of compound **3** (1 x 10^{-5} M) with aliquots of TBAF (3 x 10^{-3} M) in DCM at 298 K (λ_{ex} = 350 nm).

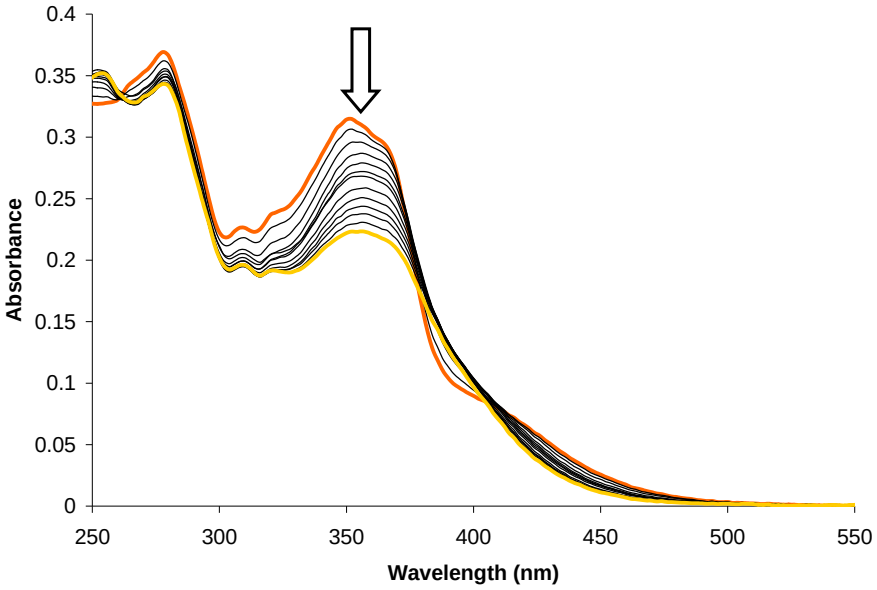


Figure S17: UV-Vis titration of compound **4** (1 x 10^{-5} M) with aliquots of TBAF (3 x 10^{-3} M) in DCM at 298 K.

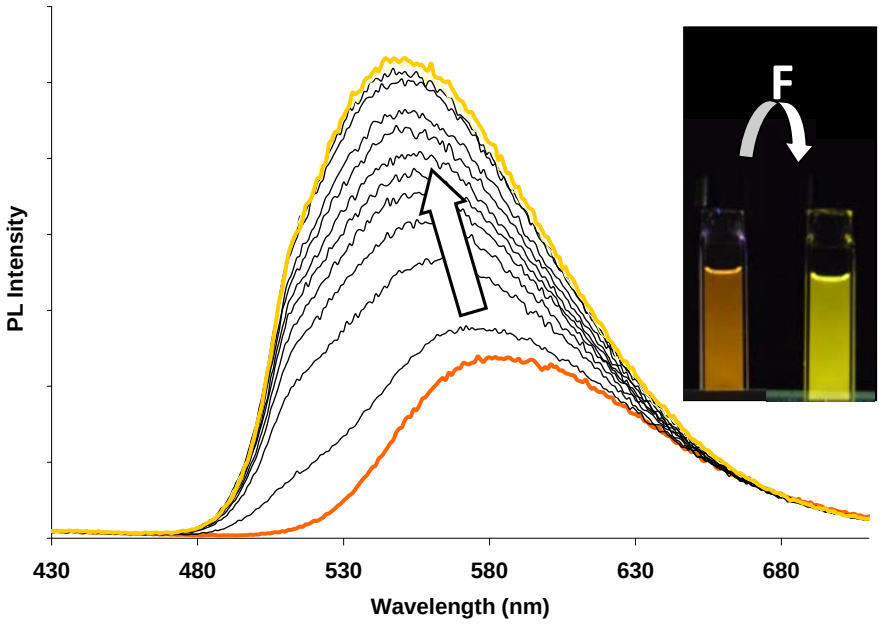


Figure S18: Phosphorescence titration of compound **4** (1 x 10^{-5} M) with aliquots of TBAF (3 x 10^{-3} M) in DCM at 298 K (λ_{ex} = 350 nm).

Table S2: Photophysical properties of compounds **1, 3** and **4**.

Compound	Absorbance data, 298 K	Emission data, 298 K [solid-state]			
	λ_{max} (nm), ε (10^4 $cm^{-1}M^{-1}$)	λ_{ex} (nm)	λ_{max} (nm)	τ (μs)[e]	Φ[e]
1[a]	266,1.42 / 358,3.75	358	420 [516][c]	-	<0.01
3[b]	262,2.96 / 279, 2.75 / 318,1.99 / 350,2.48	350	565 [545][d]	1.4	0.03 [0.16]
3·F$^-$ [b]	257,3.00 / 282,2.25 / 316,1.61 / 352,1.70	352	536	4	0.15
4[b]	278,3.69 / 308,2.26 / 320,2.36 / 350,3.14	350	587 [565][d]	1.1	0.04 [0.11]
4·F$^-$ [b]	288,3.43 / 308,1.95 / 320,1.91 / 355, 2.23	355	550	5.46	0.24

[a] Measurements performed in 2-methyltetrahydrofuran, 9,10-diphenylantracene was used as the QY reference (0.90).

[b] Measurements were performed in CH_2Cl_2, $IrPPy_3$ was used as the QY reference compound (0.98).

[c]Measured in a frozen glass of 2-methyltetrahydrofuran (77 K).

[d] Polymer film was comprised of 5% **3** or **4** in PMMA, and spin coated using THF as the solvent.

[e] Analyses were performed with samples in solution (either 2-MeTHF or DCM as noted); value for **1** corresponds to fluorescence quantum yield, while the values for **3** and **4** correspond to phosphorescent quantum yield.

S11. Computational Results of Compounds 3 and 4

The computational calculations were performed using Gaussian09, revision B.01[1] software package and the High Performance Computing Virtual Laboratory (HPCVL) at Queen's University. The ground-state geometries were fully optimized at the B3LYP[2] level using LANL2DZ basis set for platinum and 6-31G(d) basis set for all other atoms.[3] The initial geometric parameters in the calculations were employed from crystal structure data for geometry optimization. Time-dependent density function theory (TD-DFT) calculations were performed to obtain the vertical singlet and triplet excitation energies.

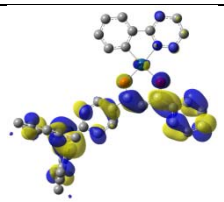
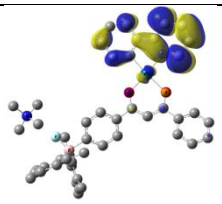
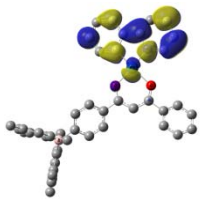
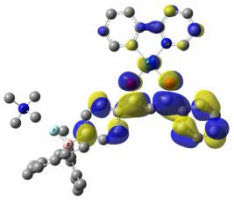
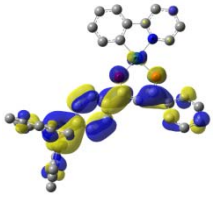
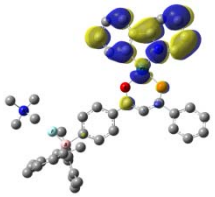
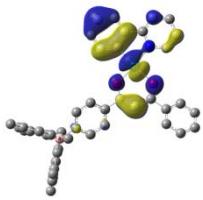
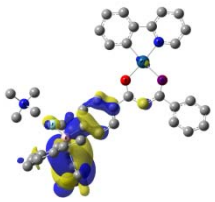
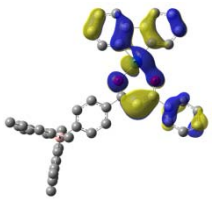
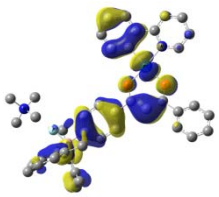
References

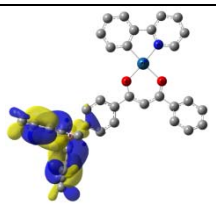
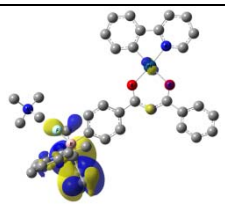
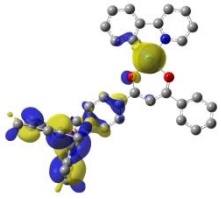
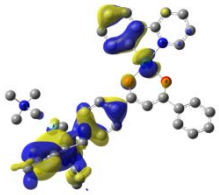
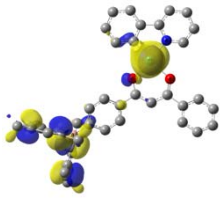
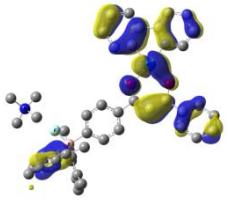
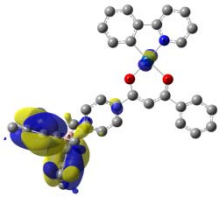
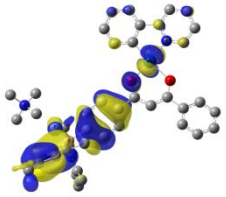
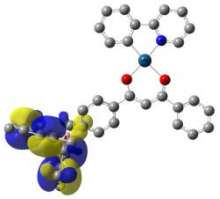
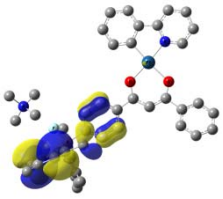
[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, 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, 2010.

[2] (a) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648; (b) C. Lee, C, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785.

[3] P. J. Hay, *J. Phys. Chem. A* **2002**, *106*, 1634.

DFT Calculation Results for 3 / 3F$^-$ in Ground States: Isodensity contour = 0.02 a.u.

	3	**3 + (NMe$_4^+$)F$^-$**
LUMO+2		
	-1.25 eV [B p orbital = 20%]	**-0.81 eV**
LUMO+1		
	-1.63 eV	**-1.21 eV**
LUMO		
	-2.03 eV [B p orbital = 20%]	**-1. 44 eV**
HOMO		
	-5.48 eV [Pt d orbital = 31%]	**-4.85 eV**
HOMO-1		
	-5.78 eV [Pt d orbital = 29%]	**-5.10 eV [Pt d orbital = 16%]**

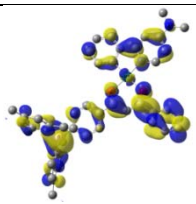
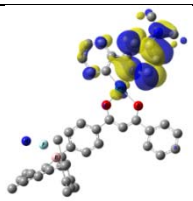
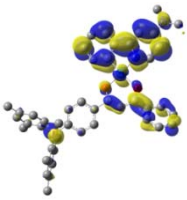
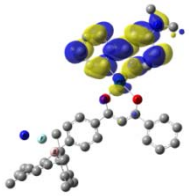
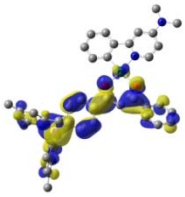
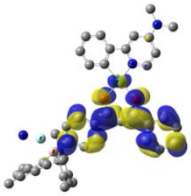
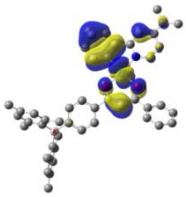
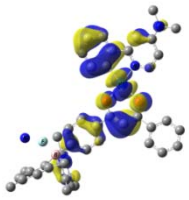
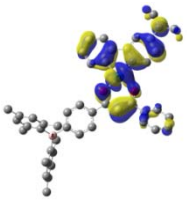
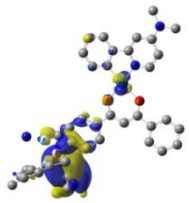
HOMO-2	 **-5.77 eV**	 **-5.14 eV**
HOMO-3	 **-5.97 eV [Pt d orbital = 30%]**	 **-5.35 eV [Pt d orbital = 10%]**
HOMO-4	 **-6.05 eV [Pt d orbital = 42%]**	 **-5.47 eV [Pt d orbital = 28%]**
HOMO-5	 **-6.06 eV**	 **-5.54 eV [Pt d orbital = 14%]**
HOMO-6	 **-6.12 eV**	 **-5.70 eV**

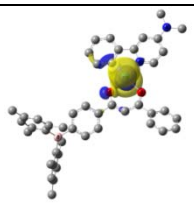
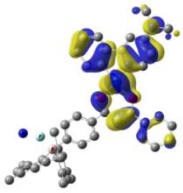
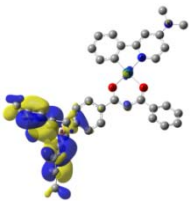
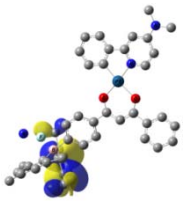
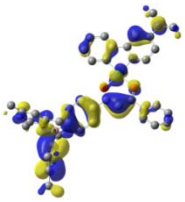
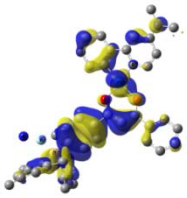
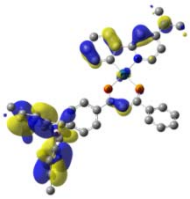
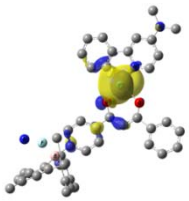
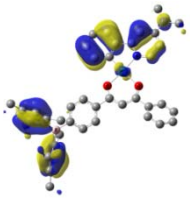
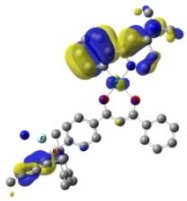
TD-DFT Calculation Results: The calculated electronic transition configurations, excitation energy and oscillator strengths for the transitions of **3** and **3F**$^{-}$.

Complex	Spin state	Transition configurations	Excitation energy (nm, eV)	Oscillator strength
3	S_1	HOMO → LUMO (97%)	421.6 (2.94)	0.0651
	S_2	HOMO-1 → LUMO (5%) HOMO-1 → LUMO+1 (11%) HOMO → LUMO+1 (82%)	396.7 (3.13)	0.0564
	S_3	HOMO-4 → LUMO (6%) HOMO-3 → LUMO (8%) HOMO-2 → LUMO (6%) HOMO-1 → LUMO (71%) HOMO → LUMO+1 (5%)	376.3 (3.29)	0.1431
	S_4	HOMO-4 → LUMO (10%) HOMO-3 → LUMO (8%) HOMO-2 → LUMO (75%) HOMO-2 → LUMO+2 (4%)	374.5 (3.31)	0.0399
	S_5	HOMO-4 → LUMO (33%) HOMO-4 → LUMO+2 (2%) HOMO-3 → LUMO (28%) HOMO-2 → LUMO (12%) HOMO-1 → LUMO (18%)	372.4 (3.33)	0.0272
	S_6	HOMO-4 → LUMO (41%) HOMO-3 → LUMO (49%) HOMO-3 → LUMO+2 (2%) HOMO-1 → LUMO+1 (4%)	362.0 (3.43)	0.2261
	S_7	HOMO-5 → LUMO (19%) HOMO-4 → LUMO+1 (34%) HOMO-3 → LUMO+1 (28%) HOMO-1 → LUMO+1 (13%)	352.1 (3.52)	0.0430
	S_8	HOMO-5 → LUMO (50%) HOMO-5 → LUMO+2 (2%) HOMO-4 → LUMO+1 (22%) HOMO-3 → LUMO+1 (12%) HOMO-1 → LUMO+1 (9%)	351.7 (3.53)	0.0820
	S_9	HOMO-5 → LUMO (25%) HOMO-1 → LUMO+1 (56%) HOMO → LUMO+1 (6%)	348.8 (3.55)	0.0158
	S_{10}	HOMO-6 → LUMO (94%) HOMO-6 → LUMO+2 (4%)	346.5 (3.58)	0.0062
	T_1	HOMO-8 → LUMO (2%) HOMO-7 → LUMO (2%) HOMO-1→ LUMO (31%) HOMO-1 → LUMO+2 (6%) HOMO → LUMO (47%) HOMO → LUMO+2 (6%)	513.4 (2.42)	0.0000
	T_2	HOMO-7 → LUMO+1 (7%) HOMO-1 → LUMO+1 (23%) HOMO → LUMO+1 (56%)	466.7 (2.66)	0.0000
	T_3	HOMO-8 → LUMO (7%) HOMO-3 → LUMO (5%) HOMO-1 → LUMO (34%) HOMO-1 → LUMO+1 (4%) HOMO-1 → LUMO+2 (8%) HOMO → LUMO (24%)	427.5 (2.90)	0.0000

Complex	Spin state	Transition configurations	Excitation energy (nm, eV)	Oscillator strength
3F$^-$	S_1	HOMO-4 → LUMO (14%) HOMO-3 → LUMO (7%) HOMO-2 → LUMO (2%) HOMO-1 → LUMO (58%) HOMO → LUMO (15%)	409.6 (3.03)	0.0227
	S_2	HOMO-4 → LUMO (3%) HOMO-1 → LUMO (7%) HOMO → LUMO (76%) HOMO → LUMO+1 (11%)	391.8 (3.16)	0.0366
	S_3	HOMO-1 → LUMO (3%) HOMO-1 → LUMO+1 (6%) HOMO → LUMO (8%) HOMO → LUMO+1 (81%)	380.0 (3.26)	0.0858
	S_4	HOMO-5 → LUMO (5%) HOMO-4 → LUMO (37%) HOMO-3 → LUMO+1 (4%) HOMO-1 → LUMO (15%) HOMO-1 → LUMO+1 (31%) HOMO → LUMO+1 (4%)	373.6 (3.32)	0.0434
	S_5	HOMO-5 → LUMO (3%) HOMO-4 → LUMO (32%) HOMO-1 → LUMO (5%) HOMO-1 → LUMO+1 (50%) HOMO → LUMO+1 (3%)	366.0 (3.39)	0.1728
	S_6	HOMO-7 → LUMO (93%)	362.6 (3.42)	0.0031
	S_7	HOMO-2 → LUMO (91%) HOMO-2 → LUMO+1 (4%) HOMO-1 → LUMO (4%)	358.7 (3.46)	0.0036
	S_8	HOMO-7 → LUMO (2%) HOMO-5 → LUMO (17%) HOMO-3 → LUMO (64%) HOMO-1 → LUMO (6%)	350.2 (3.54)	0.1449
	S_9	HOMO-2 → LUMO (4%) HOMO-2 → LUMO+1 (91%) HOMO-1 → LUMO+1 (3%)	345.8 (3.59)	0.0015
	S_{10}	HOMO-7 → LUMO+1 (3%) HOMO-4 → LUMO+2 (2%) HOMO-3 → LUMO+1 (3%) HOMO-3 → LUMO+2 (8%) HOMO-2 → LUMO+2 (2%) HOMO-1 → LUMO+2 (62%) HOMO → LUMO+2 (13%)	339.2 (3.66)	0.0232
	T_1 (T_A)	HOMO-4 → LUMO+1 (17%) HOMO-1 → LUMO (9%) HOMO-1 → LUMO+1 (55%) HOMO → LUMO+1 (6%)	486.6 (2.55)	0.0000
	T_2 (T_C)	HOMO-9 → LUMO (7%) HOMO-4 → LUMO (35%) HOMO-3 → LUMO (11%) HOMO-1 → LUMO (29%) HOMO-1 → LUMO+1 (5%)	470.7 (2.63)	0.0000
	T_3	HOMO-9 → LUMO (8%) HOMO-9 → LUMO+2 (3%) HOMO-5 → LUMO (15%) HOMO-4 → LUMO (20%) HOMO-4 → LUMO+1 (4%) HOMO-3 → LUMO (7%) HOMO-1 → LUMO (27%)	427.8 (2.90)	0.0000

DFT Calculation Results for 4 / 4F$^-$ in Ground States: Isodensity contour = 0.02 a.u.

	4	**4 + $(NMe_4^+)F^-$**
LUMO+2		
	-1.11 eV [B p orbital = 16%]	**-0.37 eV**
LUMO+1		
	-1.14 eV	**-0.96 eV**
LUMO		
	-1.89 eV [B p orbital = 23%]	**-1.05 eV**
HOMO		
	-5.22 eV [Pt d orbital = 33%]	**-4.62 eV [Pt d orbital = 28%]**
HOMO-1		
	-5.43 eV [Pt d orbital = 39%]	**-4.88 eV**

HOMO-2		
	-5.77 eV [Pt d orbital = 71%]	**-4.91eV [Pt d orbital = 40%]**
HOMO-3		
	-5.90 eV	**-5.14 eV**
HOMO-4		
	-5.93 eV	**-5.20 eV [Pt d orbital = 13%]**
HOMO-5		
	-6.02 eV	**-5.49 eV [Pt d orbital = 67%]**
HOMO-6		
	-6.05 eV	**-5.50 eV**

TD-DFT Calculation Results: The calculated electronic transition configurations, excitation energy and oscillator strengths for the transitions of **4** and **4F**$^{-}$.

Complex	Spin state	Transition configurations	Excitation energy (nm, eV)	Oscillator strength
4	S_1	HOMO → LUMO (96%)	439.0 (2.82)	0.0490
	S_2	HOMO-1 → LUMO (95%)	400.5 (3.10)	0.1074
	S_3	HOMO-2 → LUMO (91%) HOMO-2 → LUMO (5%)	389.0 (3.19)	0.0035
	S_4	HOMO-4 → LUMO (3%) HOMO-3 → LUMO (91%) HOMO-3 → LUMO+2 (4%)	370.0 (3.35)	0.0653
	S_5	HOMO-4 → LUMO (7%) HOMO-1 → LUMO+1 (11%) HOMO-1 → LUMO+2 (2%) HOMO → LUMO+1 (65%) HOMO → LUMO+2 (10%)	364.2 (3.40)	0.1924
	S_6	HOMO-5 → LUMO (12%) HOMO-4 → LUMO (69%) HOMO-1 → LUMO+1 (2%) HOMO → LUMO+1 (5%)	359.3 (3.45)	0.2382
	S_7	HOMO-6 → LUMO (24%) HOMO-5 → LUMO (62%) HOMO-4 → LUMO (4%)	348.1 (3.56)	0.1195
	S_8	HOMO-7 → LUMO (17%) HOMO-6 → LUMO (3%) HOMO-1 → LUMO+2 (2%) HOMO → LUMO+1 (8%) HOMO → LUMO+2 (66%)	341.2 (3.63)	0.0008
	S_9	HOMO-8 → LUMO (33%) HOMO-7 → LUMO (44%) HOMO-1 → LUMO+1 (5%) HOMO → LUMO+2 (9%)	340.6 (3.64)	0.0041
	S_{10}	HOMO-8 → LUMO (5%) HOMO-7 → LUMO (2%) HOMO-1 → LUMO+1 (60%) HOMO-1 → LUMO+2 (9%) HOMO → LUMO+1 (15%)	340.4 (3.64)	0.0801
	T_1	HOMO-8 → LUMO (2%) HOMO-4 → LUMO (6%) HOMO-1→ LUMO (19%) HOMO-1 → LUMO+2 (3%) HOMO → LUMO (52%) HOMO → LUMO+2 (6%)0	527.0 (2.35)	0.0000
	T_2	HOMO-9 → LUMO (4%) HOMO-4 → LUMO (3%) HOMO-1 → LUMO (55%) HOMO-1 → LUMO+2 (6%) HOMO → LUMO (22%)	444.8 (2.79)	0.0000
	T_3	HOMO-6 → LUMO+1(6%) HOMO-1 → LUMO+1 (26%) HOMO-1 → LUMO+2 (4%) HOMO → LUMO+1 (37%) HOMO → LUMO+2 (7%)	435.4 (2.85)	0.0000

Complex	Spin state	Transition configurations	Excitation energy (nm, eV)	Oscillator strength
4F$^-$	S_1	HOMO-1 → LUMO (5%) HOMO → LUMO (92%)	389.6 (3.18)	0.1235
	S_2	HOMO-4 → LUMO+1 (4%) HOMO-3 → LUMO (3%) HOMO-3 → LUMO+1 (3%) HOMO-1 → LUMO (55%) HOMO-1 → LUMO+1 (21%) HOMO → LUMO (6%) HOMO → LUMO+1 (3%)	379.0 (3.27)	0.0873
	S_3	HOMO-4 → LUMO (3%) HOMO-4 → LUMO+1 (7%) HOMO-3 → LUMO+1 (3%) HOMO-1 → LUMO (31%) HOMO-1 → LUMO+1 (41%) HOMO → LUMO+1 (12%)	375.5 (3.30)	0.0176
	S_4	HOMO-4 → LUMO+1 (3%) HOMO-1 → LUMO+1 (12%) HOMO → LUMO+1 (83%)	361.0 (3.44)	0.0128
	S_5	HOMO-4 → LUMO+1 (6%) HOMO-3 → LUMO (38%) HOMO-3 → LUMO+1 (39%) HOMO-1 → LUMO+1 (10%)	355.3 (3.49)	0.2851
	S_6	HOMO-2 → LUMO (97%)	353.3 (3.51)	0.0008
	S_7	HOMO-5 → LUMO (18%) HOMO-4 → LUMO+1 (6%) HOMO-3 → LUMO (41%) HOMO-3 → LUMO+1 (26%) HOMO-1 → LUMO+1 (3%)	348.1 (3.56)	0.0394
	S_8	HOMO-6 → LUMO (8%) HOMO-5 → LUMO (70%) HOMO-4 → LUMO (3%) HOMO-3 → LUMO (13%) HOMO-3 → LUMO+1(3%)	343.9 (3.61)	0.0330
	S_9	HOMO-6 → LUMO+1 (9%) HOMO-5 → LUMO+1 (88%)	337.6 (3.67)	0.0047
	S_{10}	HOMO-4 → LUMO (89%) HOMO-3 → LUMO (2%) HOMO-1 → LUMO (4%)	336.7 (3.68)	0.3570
	T_1 (T_A)	HOMO-10 → LUMO (2%) HOMO-8 → LUMO (2%) HOMO-4 → LUMO (7%) HOMO-3 → LUMO (6%) HOMO-1 → LUMO (67%) HOMO → LUMO (7%)	491.5 (2.52)	0.0000
	T_2 (T_C)	HOMO-10 → LUMO+1 (2%) HOMO-9 → LUMO+1 (8%) HOMO-4 → LUMO+1 (29%) HOMO-3 → LUMO+1 (13%) HOMO-1 → LUMO+1 (32%)	440.3 (2.82)	0.0000
	T_3	HOMO-11 → LUMO (2%) HOMO-4 → LUMO (3%) HOMO-3 → LUMO (47%) HOMO-3 → LUMO+1 (2%) HOMO → LUMO (26%)	417.1 (2.97)	0.0000

Figure S19. Energy level diagram for 3 with and without fluoride ions.

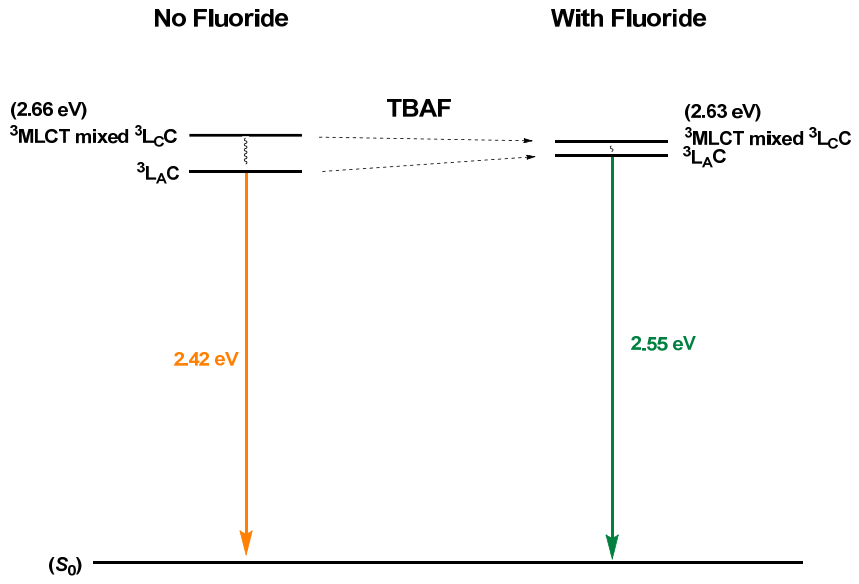
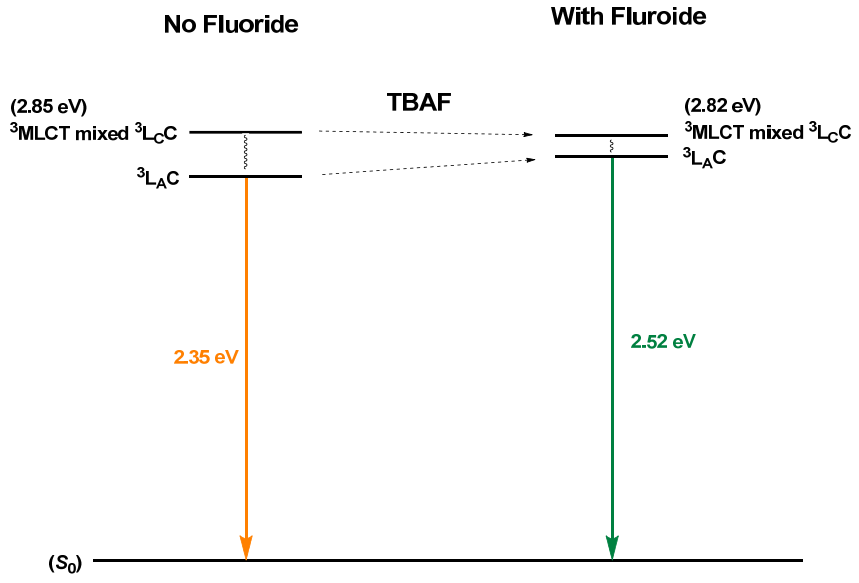


Figure S20. Energy level diagram for 4 with and without fluoride ions.



S12. X-ray Crystallographic Data

Table 1. Crystal data and structure refinement for Compd **3**.

Identification code	Compd 3	
Empirical formula	C44 H40 B N O2 Pt	
Formula weight	820.67	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.105(2) Å	α= 95.968(2)°.
	b = 11.650(3) Å	β= 93.914(3)°.
	c = 19.084(5) Å	γ = 97.898(2)°.
Volume	1769.0(8) $Å^3$	
Z	2	
Density (calculated)	1.541 Mg/m^3	
Absorption coefficient	4.005 mm^{-1}	
F(000)	820	
Crystal size	0.02 x 0.01 x 0.01 mm^3	
Theta range for data collection	1.78 to 26.00°.	
Index ranges	-9<=h<=9, -14<=k<=14, -23<=l<=23	
Reflections collected	15883	
Independent reflections	6869 [R(int) = 0.0715]	
Completeness to theta = 26.00°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9610 and 0.9242	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6869 / 0 / 443	
Goodness-of-fit on F^2	1.020	
Final R indices [I>2sigma(I)]	R1 = 0.0567, wR2 = 0.1362	
R indices (all data)	R1 = 0.0716, wR2 = 0.1451	
Largest diff. peak and hole	4.326 and -2.590 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Compd 3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	-836(1)	2258(1)	431(1)	31(1)
B(1)	2315(11)	8108(8)	3514(5)	33(2)
N(1)	-1753(8)	739(6)	-138(4)	39(2)
O(1)	591(6)	2884(4)	-341(3)	34(1)
O(2)	16(7)	3713(5)	1099(3)	38(1)
C(1)	-2199(9)	1544(6)	1150(4)	26(2)
C(2)	-2399(10)	2055(8)	1811(5)	42(2)
C(3)	-3373(10)	1457(8)	2277(4)	40(2)
C(4)	-4160(11)	323(8)	2069(5)	45(2)
C(5)	-3975(10)	-218(7)	1397(5)	39(2)
C(6)	-3013(10)	389(7)	941(4)	34(2)
C(7)	-2741(9)	-60(7)	202(5)	34(2)
C(8)	-3389(10)	-1162(7)	-135(5)	38(2)
C(9)	-3027(11)	-1467(7)	-822(5)	42(2)
C(10)	-2039(11)	-661(8)	-1167(5)	43(2)
C(11)	-1433(10)	422(7)	-819(4)	37(2)
C(12)	1139(9)	4571(6)	980(4)	29(2)
C(13)	1950(10)	4660(7)	358(4)	33(2)
C(14)	1641(9)	3849(6)	-265(4)	28(2)
C(15)	2584(9)	4078(6)	-905(4)	30(2)
C(16)	3404(10)	5173(7)	-1003(4)	38(2)
C(17)	4194(11)	5323(8)	-1615(5)	47(2)
C(18)	4174(11)	4419(8)	-2141(5)	44(2)
C(19)	3331(12)	3322(8)	-2053(5)	48(2)
C(20)	2525(9)	3162(7)	-1408(4)	32(2)
C(21)	1501(10)	5507(7)	1601(4)	34(2)
C(22)	2193(9)	6680(6)	1543(4)	31(2)
C(23)	2437(10)	7493(6)	2140(4)	32(2)
C(24)	2061(10)	7203(7)	2815(4)	35(2)

C(25)	1392(11)	6028(7)	2846(4)	42(2)
C(26)	1118(11)	5216(7)	2257(4)	42(2)
C(27)	2224(10)	7567(6)	4239(4)	34(2)
C(28)	3319(11)	6790(7)	4451(4)	38(2)
C(29)	3079(12)	6200(8)	5044(5)	47(2)
C(30)	1519(16)	5723(11)	6118(6)	79(4)
C(31)	1749(13)	6365(8)	5470(5)	51(2)
C(32)	714(13)	7149(8)	5279(5)	51(2)
C(33)	909(11)	7727(7)	4686(4)	43(2)
C(34)	-396(12)	8507(9)	4482(6)	60(3)
C(35)	4842(12)	6575(8)	4050(5)	47(2)
C(36)	2585(10)	9468(7)	3469(4)	35(2)
C(37)	1375(11)	10027(8)	3122(4)	41(2)
C(38)	1604(11)	11251(8)	3144(5)	43(2)
C(39)	3033(12)	11933(7)	3469(5)	43(2)
C(40)	4246(11)	11389(7)	3798(4)	38(2)
C(41)	4046(10)	10184(7)	3806(4)	35(2)
C(42)	-269(12)	9361(9)	2767(5)	50(2)
C(43)	5499(10)	9648(7)	4127(4)	40(2)
C(44)	3273(15)	13254(8)	3457(7)	68(3)

Table 3. Bond lengths [Å] and angles [°] for Compd 3.

Pt(1)-C(1)	1.996(7)	C(1)-C(2)	1.368(11)
Pt(1)-N(1)	1.998(7)	C(1)-C(6)	1.419(10)
Pt(1)-O(2)	2.021(5)	C(2)-C(3)	1.404(12)
Pt(1)-O(1)	2.065(5)	C(2)-H(2A)	0.9300
B(1)-C(27)	1.580(12)	C(3)-C(4)	1.391(12)
B(1)-C(36)	1.581(12)	C(3)-H(3A)	0.9300
B(1)-C(24)	1.595(12)	C(4)-C(5)	1.397(12)
N(1)-C(11)	1.365(11)	C(4)-H(4A)	0.9300
N(1)-C(7)	1.386(11)	C(5)-C(6)	1.392(11)
O(1)-C(14)	1.303(9)	C(5)-H(5A)	0.9300
O(2)-C(12)	1.306(9)	C(6)-C(7)	1.493(12)

C(7)-C(8)	1.391(11)	C(27)-C(28)	1.421(12)
C(8)-C(9)	1.385(12)	C(27)-C(33)	1.430(11)
C(8)-H(8A)	0.9300	C(28)-C(29)	1.395(12)
C(9)-C(10)	1.397(13)	C(28)-C(35)	1.531(12)
C(9)-H(9A)	0.9300	C(29)-C(31)	1.416(13)
C(10)-C(11)	1.373(12)	C(29)-H(29A)	0.9300
C(10)-H(10A)	0.9300	C(30)-C(31)	1.520(13)
C(11)-H(11A)	0.9300	C(30)-H(29B)	0.9600
C(12)-C(13)	1.403(11)	C(30)-H(29C)	0.9600
C(12)-C(21)	1.508(11)	C(30)-H(29D)	0.9600
C(13)-C(14)	1.423(11)	C(31)-C(32)	1.382(14)
C(13)-H(13A)	0.9300	C(32)-C(33)	1.382(12)
C(14)-C(15)	1.512(11)	C(32)-H(31A)	0.9300
C(15)-C(20)	1.354(11)	C(33)-C(34)	1.541(12)
C(15)-C(16)	1.393(11)	C(34)-H(33A)	0.9600
C(16)-C(17)	1.385(12)	C(34)-H(33B)	0.9600
C(16)-H(16A)	0.9300	C(34)-H(33C)	0.9600
C(17)-C(18)	1.374(12)	C(35)-H(34A)	0.9600
C(17)-H(17A)	0.9300	C(35)-H(34B)	0.9600
C(18)-C(19)	1.396(12)	C(35)-H(34C)	0.9600
C(18)-H(18A)	0.9300	C(36)-C(37)	1.414(12)
C(19)-C(20)	1.448(11)	C(36)-C(41)	1.423(11)
C(19)-H(19A)	0.9300	C(37)-C(38)	1.409(12)
C(20)-H(20A)	0.9300	C(37)-C(42)	1.523(12)
C(21)-C(26)	1.376(12)	C(38)-C(39)	1.380(12)
C(21)-C(22)	1.423(10)	C(38)-H(38A)	0.9300
C(22)-C(23)	1.388(11)	C(39)-C(40)	1.389(12)
C(22)-H(22A)	0.9300	C(39)-C(44)	1.527(12)
C(23)-C(24)	1.408(11)	C(40)-C(41)	1.393(11)
C(23)-H(23A)	0.9300	C(40)-H(40A)	0.9300
C(24)-C(25)	1.409(10)	C(41)-C(43)	1.528(11)
C(25)-C(26)	1.377(11)	C(42)-H(42A)	0.9600
C(25)-H(25A)	0.9300	C(42)-H(42B)	0.9600
C(26)-H(26A)	0.9300	C(42)-H(42C)	0.9600

C(43)-H(43A)	0.9600	C(6)-C(5)-H(5A)	120.3
C(43)-H(43B)	0.9600	C(4)-C(5)-H(5A)	120.3
C(43)-H(43C)	0.9600	C(5)-C(6)-C(1)	121.1(8)
C(44)-H(44A)	0.9600	C(5)-C(6)-C(7)	125.6(7)
C(44)-H(44B)	0.9600	C(1)-C(6)-C(7)	113.3(7)
C(44)-H(44C)	0.9600	N(1)-C(7)-C(8)	121.3(8)
		N(1)-C(7)-C(6)	113.4(7)
C(1)-Pt(1)-N(1)	81.4(3)	C(8)-C(7)-C(6)	125.3(8)
C(1)-Pt(1)-O(2)	92.7(3)	C(9)-C(8)-C(7)	119.2(8)
N(1)-Pt(1)-O(2)	173.9(2)	C(9)-C(8)-H(8A)	120.4
C(1)-Pt(1)-O(1)	176.1(2)	C(7)-C(8)-H(8A)	120.4
N(1)-Pt(1)-O(1)	95.2(3)	C(8)-C(9)-C(10)	119.6(8)
O(2)-Pt(1)-O(1)	90.7(2)	C(8)-C(9)-H(9A)	120.2
C(27)-B(1)-C(36)	122.8(7)	C(10)-C(9)-H(9A)	120.2
C(27)-B(1)-C(24)	116.3(7)	C(11)-C(10)-C(9)	119.5(8)
C(36)-B(1)-C(24)	120.9(7)	C(11)-C(10)-H(10A)	120.2
C(11)-N(1)-C(7)	118.3(7)	C(9)-C(10)-H(10A)	120.2
C(11)-N(1)-Pt(1)	125.2(6)	N(1)-C(11)-C(10)	122.1(8)
C(7)-N(1)-Pt(1)	116.4(6)	N(1)-C(11)-H(11A)	119.0
C(14)-O(1)-Pt(1)	125.5(5)	C(10)-C(11)-H(11A)	119.0
C(12)-O(2)-Pt(1)	126.4(5)	O(2)-C(12)-C(13)	126.0(7)
C(2)-C(1)-C(6)	118.3(7)	O(2)-C(12)-C(21)	112.2(7)
C(2)-C(1)-Pt(1)	126.4(6)	C(13)-C(12)-C(21)	121.7(7)
C(6)-C(1)-Pt(1)	115.3(5)	C(12)-C(13)-C(14)	125.8(7)
C(1)-C(2)-C(3)	121.3(8)	C(12)-C(13)-H(13A)	117.1
C(1)-C(2)-H(2A)	119.3	C(14)-C(13)-H(13A)	117.1
C(3)-C(2)-H(2A)	119.3	O(1)-C(14)-C(13)	125.4(7)
C(4)-C(3)-C(2)	120.1(8)	O(1)-C(14)-C(15)	114.7(6)
C(4)-C(3)-H(3A)	120.0	C(13)-C(14)-C(15)	119.8(6)
C(2)-C(3)-H(3A)	120.0	C(20)-C(15)-C(16)	120.5(8)
C(3)-C(4)-C(5)	119.7(8)	C(20)-C(15)-C(14)	116.3(7)
C(3)-C(4)-H(4A)	120.1	C(16)-C(15)-C(14)	123.1(7)
C(5)-C(4)-H(4A)	120.1	C(17)-C(16)-C(15)	119.8(8)
C(6)-C(5)-C(4)	119.5(8)	C(17)-C(16)-H(16A)	120.1

C(15)-C(16)-H(16A)	120.1	C(29)-C(28)-C(27)	121.6(8)
C(18)-C(17)-C(16)	121.8(8)	C(29)-C(28)-C(35)	116.5(8)
C(18)-C(17)-H(17A)	119.1	C(27)-C(28)-C(35)	121.8(7)
C(16)-C(17)-H(17A)	119.1	C(28)-C(29)-C(31)	121.4(9)
C(17)-C(18)-C(19)	118.8(8)	C(28)-C(29)-H(29A)	119.3
C(17)-C(18)-H(18A)	120.6	C(31)-C(29)-H(29A)	119.3
C(19)-C(18)-H(18A)	120.6	C(31)-C(30)-H(29B)	109.5
C(18)-C(19)-C(20)	119.4(8)	C(31)-C(30)-H(29C)	109.5
C(18)-C(19)-H(19A)	120.3	H(29B)-C(30)-H(29C)	109.5
C(20)-C(19)-H(19A)	120.3	C(31)-C(30)-H(29D)	109.5
C(15)-C(20)-C(19)	119.7(8)	H(29B)-C(30)-H(29D)	109.5
C(15)-C(20)-H(20A)	120.2	H(29C)-C(30)-H(29D)	109.5
C(19)-C(20)-H(20A)	120.2	C(32)-C(31)-C(29)	117.1(8)
C(26)-C(21)-C(22)	118.2(7)	C(32)-C(31)-C(30)	122.2(9)
C(26)-C(21)-C(12)	118.3(7)	C(29)-C(31)-C(30)	120.6(10)
C(22)-C(21)-C(12)	123.5(7)	C(31)-C(32)-C(33)	122.4(9)
C(23)-C(22)-C(21)	119.6(7)	C(31)-C(32)-H(31A)	118.8
C(23)-C(22)-H(22A)	120.2	C(33)-C(32)-H(31A)	118.8
C(21)-C(22)-H(22A)	120.2	C(32)-C(33)-C(27)	121.9(9)
C(22)-C(23)-C(24)	122.7(7)	C(32)-C(33)-C(34)	118.5(8)
C(22)-C(23)-H(23A)	118.7	C(27)-C(33)-C(34)	119.5(8)
C(24)-C(23)-H(23A)	118.7	C(33)-C(34)-H(33A)	109.5
C(23)-C(24)-C(25)	115.5(7)	C(33)-C(34)-H(33B)	109.5
C(23)-C(24)-B(1)	124.4(7)	H(33A)-C(34)-H(33B)	109.5
C(25)-C(24)-B(1)	120.1(7)	C(33)-C(34)-H(33C)	109.5
C(26)-C(25)-C(24)	122.5(7)	H(33A)-C(34)-H(33C)	109.5
C(26)-C(25)-H(25A)	118.8	H(33B)-C(34)-H(33C)	109.5
C(24)-C(25)-H(25A)	118.8	C(28)-C(35)-H(34A)	109.5
C(21)-C(26)-C(25)	121.5(7)	C(28)-C(35)-H(34B)	109.5
C(21)-C(26)-H(26A)	119.3	H(34A)-C(35)-H(34B)	109.5
C(25)-C(26)-H(26A)	119.3	C(28)-C(35)-H(34C)	109.5
C(28)-C(27)-C(33)	115.5(7)	H(34A)-C(35)-H(34C)	109.5
C(28)-C(27)-B(1)	122.5(7)	H(34B)-C(35)-H(34C)	109.5
C(33)-C(27)-B(1)	121.6(8)	C(37)-C(36)-C(41)	117.4(8)

C(37)-C(36)-B(1)	122.0(7)	H(44B)-C(44)-H(44C)	109.5
C(41)-C(36)-B(1)	120.5(7)		
C(38)-C(37)-C(36)	120.2(8)		
C(38)-C(37)-C(42)	117.3(8)		
C(36)-C(37)-C(42)	122.3(8)		
C(39)-C(38)-C(37)	121.6(8)		
C(39)-C(38)-H(38A)	119.2		
C(37)-C(38)-H(38A)	119.2		
C(38)-C(39)-C(40)	118.6(8)		
C(38)-C(39)-C(44)	120.3(9)		
C(40)-C(39)-C(44)	121.1(9)		
C(39)-C(40)-C(41)	121.6(8)		
C(39)-C(40)-H(40A)	119.2		
C(41)-C(40)-H(40A)	119.2		
C(40)-C(41)-C(36)	120.6(8)		
C(40)-C(41)-C(43)	118.2(7)		
C(36)-C(41)-C(43)	121.0(7)		
C(37)-C(42)-H(42A)	109.5		
C(37)-C(42)-H(42B)	109.5		
H(42A)-C(42)-H(42B)	109.5		
C(37)-C(42)-H(42C)	109.5		
H(42A)-C(42)-H(42C)	109.5		
H(42B)-C(42)-H(42C)	109.5		
C(41)-C(43)-H(43A)	109.5		
C(41)-C(43)-H(43B)	109.5		
H(43A)-C(43)-H(43B)	109.5		
C(41)-C(43)-H(43C)	109.5		
H(43A)-C(43)-H(43C)	109.5		
H(43B)-C(43)-H(43C)	109.5		
C(39)-C(44)-H(44A)	109.5		
C(39)-C(44)-H(44B)	109.5		
H(44A)-C(44)-H(44B)	109.5		
C(39)-C(44)-H(44C)	109.5		
H(44A)-C(44)-H(44C)	109.5		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Compd 3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	31(1)	19(1)	44(1)	10(1)	4(1)	-3(1)
B(1)	29(5)	28(5)	41(5)	6(4)	6(4)	-3(4)
N(1)	30(4)	35(4)	55(4)	12(3)	0(3)	10(3)
O(1)	32(3)	26(3)	43(3)	6(2)	-1(2)	-1(2)
O(2)	41(3)	28(3)	45(3)	7(2)	3(3)	0(3)
C(1)	19(3)	22(4)	37(4)	8(3)	0(3)	-2(3)
C(2)	32(4)	34(5)	59(5)	11(4)	9(4)	-4(4)
C(3)	36(5)	43(5)	38(4)	8(4)	7(3)	-4(4)
C(4)	37(5)	48(5)	51(5)	24(4)	11(4)	-6(4)
C(5)	36(4)	24(4)	55(5)	15(4)	1(4)	-6(3)
C(6)	27(4)	26(4)	51(5)	16(4)	0(3)	4(3)
C(7)	23(4)	23(4)	58(5)	14(4)	-2(3)	2(3)
C(8)	39(5)	18(4)	57(5)	13(4)	0(4)	-1(3)
C(9)	39(5)	26(4)	58(5)	6(4)	-5(4)	-6(4)
C(10)	42(5)	35(5)	53(5)	1(4)	2(4)	9(4)
C(11)	39(5)	31(4)	43(5)	10(4)	0(4)	6(4)
C(12)	29(4)	13(3)	45(4)	12(3)	-6(3)	0(3)
C(13)	29(4)	23(4)	44(4)	9(3)	0(3)	-4(3)
C(14)	23(4)	17(3)	45(4)	15(3)	-1(3)	-1(3)
C(15)	27(4)	16(3)	45(4)	9(3)	-2(3)	-1(3)
C(16)	35(4)	30(4)	48(5)	7(4)	11(4)	-4(4)
C(17)	49(5)	34(5)	55(5)	10(4)	14(4)	-11(4)
C(18)	38(5)	42(5)	49(5)	14(4)	10(4)	-11(4)
C(19)	57(6)	26(4)	56(5)	-2(4)	19(4)	-12(4)
C(20)	23(4)	32(4)	42(4)	-1(3)	6(3)	12(3)
C(21)	32(4)	20(4)	51(5)	9(3)	4(4)	0(3)
C(22)	25(4)	25(4)	41(4)	12(3)	2(3)	-3(3)
C(23)	34(4)	19(4)	44(4)	16(3)	4(3)	-4(3)

C(24)	34(4)	23(4)	45(4)	8(3)	4(3)	-7(3)
C(25)	53(5)	29(4)	39(4)	10(4)	8(4)	-16(4)
C(26)	55(6)	21(4)	47(5)	10(4)	7(4)	-14(4)
C(27)	43(5)	18(4)	37(4)	0(3)	4(3)	-12(3)
C(28)	47(5)	23(4)	42(4)	6(3)	7(4)	-7(4)
C(29)	57(6)	38(5)	45(5)	16(4)	2(4)	-10(4)
C(30)	86(9)	75(8)	77(8)	42(7)	28(7)	-16(7)
C(31)	67(6)	38(5)	46(5)	14(4)	13(5)	-15(5)
C(32)	57(6)	45(6)	48(5)	3(4)	20(4)	-14(5)
C(33)	51(6)	28(5)	46(5)	7(4)	9(4)	-12(4)
C(34)	52(6)	61(7)	75(7)	17(6)	35(5)	8(5)
C(35)	62(6)	29(5)	52(5)	18(4)	12(4)	2(4)
C(36)	36(4)	32(4)	36(4)	13(3)	5(3)	-7(4)
C(37)	41(5)	39(5)	43(5)	4(4)	10(4)	0(4)
C(38)	45(5)	35(5)	51(5)	5(4)	3(4)	14(4)
C(39)	55(6)	24(4)	51(5)	11(4)	12(4)	-2(4)
C(40)	41(5)	26(4)	43(4)	3(4)	6(4)	-10(4)
C(41)	41(5)	25(4)	37(4)	7(3)	4(3)	-5(4)
C(42)	43(5)	49(6)	59(6)	9(5)	0(4)	4(4)
C(43)	41(5)	27(4)	50(5)	6(4)	0(4)	-7(4)
C(44)	76(8)	26(5)	108(9)	24(5)	19(7)	9(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for Compd 3.

	x	y	z	U(eq)
H(2A)	-1879	2814	1955	50
H(3A)	-3491	1820	2725	47
H(4A)	-4808	-73	2377	54
H(5A)	-4489	-979	1256	46
H(8A)	-4057	-1687	99	45
H(9A)	-3438	-2205	-1053	51
H(10A)	-1794	-856	-1630	52

H(11A)	-784	956	-1054	45
H(13A)	2761	5305	351	39
H(16A)	3422	5803	-659	46
H(17A)	4752	6055	-1673	56
H(18A)	4713	4536	-2548	53
H(19A)	3288	2700	-2404	57
H(20A)	1970	2433	-1341	38
H(22A)	2479	6901	1108	37
H(23A)	2867	8261	2092	39
H(25A)	1125	5794	3281	50
H(26A)	663	4453	2304	51
H(29A)	3809	5687	5162	57
H(29B)	562	5936	6342	118
H(29C)	2496	5930	6444	118
H(29D)	1352	4897	5978	118
H(31A)	-146	7294	5559	62
H(33A)	-1192	8523	4832	91
H(33B)	-962	8198	4030	91
H(33C)	155	9284	4458	91
H(34A)	5421	6025	4272	70
H(34B)	5579	7297	4059	70
H(34C)	4482	6270	3569	70
H(38A)	771	11609	2934	52
H(40A)	5215	11841	4017	46
H(42A)	-913	9895	2564	76
H(42B)	-887	8982	3111	76
H(42C)	-44	8786	2402	76
H(43A)	6371	10258	4329	60
H(43B)	5922	9160	3765	60
H(43C)	5115	9188	4489	60
H(44A)	2314	13471	3208	102
H(44B)	4254	13488	3222	102
H(44C)	3401	13633	3933	102

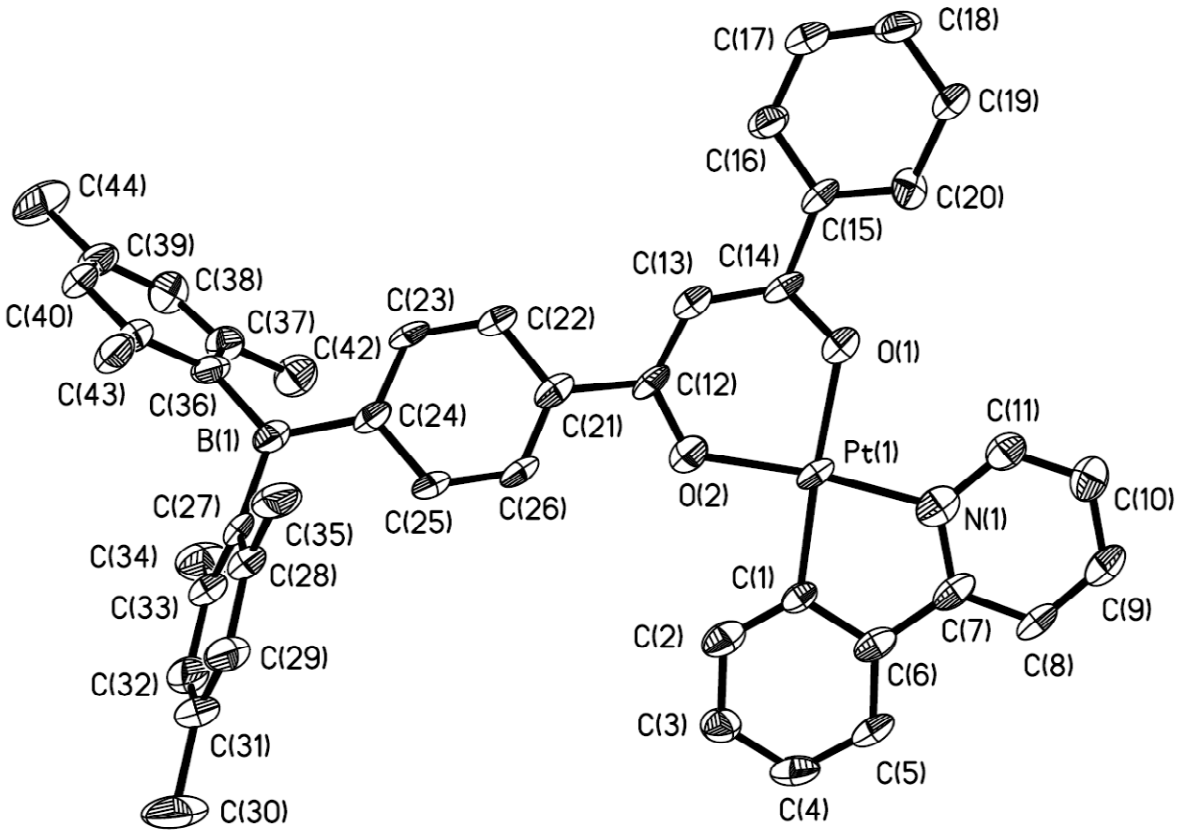


Figure S21. A diagram showing the structure of compound **3** with labeling schemes and 50% thermal ellipsoids. H atoms are omitted for clarity.

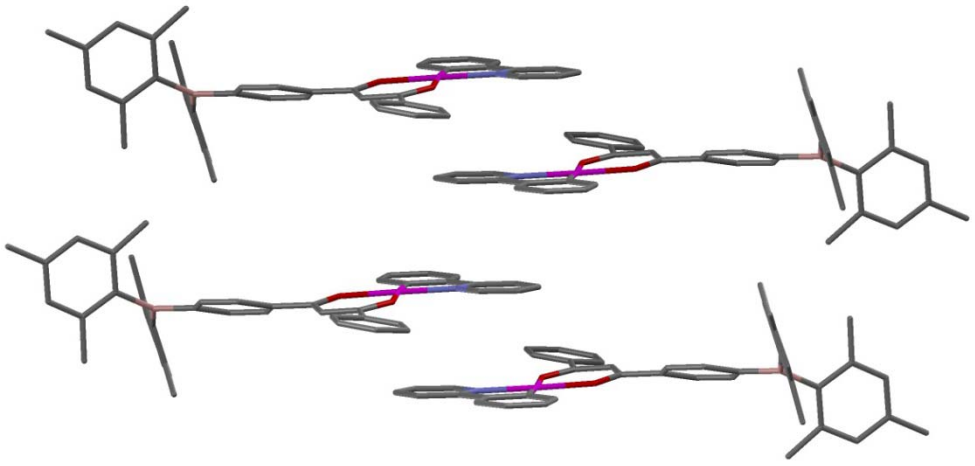


Figure S22. Unit cell packing diagram showing the π-stacking of compound **3**

Table 1. Crystal data and structure refinement for Compd 4.

Identification code	Compd 4/2 benzene	
Empirical formula	C58 H57 B1 N2 O2 Pt1	
Formula weight	1019.96	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 51.501(4) Å	α= 90°.
	b = 8.4801(6) Å	β= 118.5670(10)°.
	c = 25.3881(18) Å	γ = 90°.
Volume	9738.1(12) $Å^3$	
Z	8	
Density (calculated)	1.391 Mg/m^3	
Absorption coefficient	2.926 mm^{-1}	
F(000)	4144	
Crystal size	0.03 x 0.03 x 0.01 mm^3	
Theta range for data collection	1.60 to 26.00°.	
Index ranges	-63<=h<=63, -10<=k<=10, -31<=l<=31	
Reflections collected	44074	
Independent reflections	9570 [R(int) = 0.0782]	
Completeness to theta = 26.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9713 and 0.9174	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9570 / 0 / 585	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.0733	
R indices (all data)	R1 = 0.0710, wR2 = 0.0847	
Largest diff. peak and hole	0.751 and -1.451 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for Compd 4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	1980(1)	2633(1)	221(1)	28(1)
B(1)	752(1)	-3336(7)	628(3)	31(1)
O(1)	2297(1)	2152(3)	1091(1)	22(1)
O(2)	1678(1)	1361(4)	321(2)	31(1)
N(1)	2259(1)	3907(4)	62(2)	29(1)
N(2)	2800(1)	6763(5)	-343(2)	43(1)
C(1)	1714(1)	3145(6)	-624(2)	33(1)
C(2)	1422(1)	2653(6)	-986(2)	42(1)
C(3)	1265(1)	3094(7)	-1580(3)	48(2)
C(4)	1390(1)	4058(7)	-1839(3)	49(2)
C(5)	1676(1)	4557(6)	-1500(2)	42(1)
C(6)	1840(1)	4104(5)	-898(2)	31(1)
C(7)	2147(1)	4555(5)	-503(2)	31(1)
C(8)	2325(1)	5502(6)	-650(2)	35(1)
C(9)	2623(1)	5824(6)	-221(2)	35(1)
C(10)	2727(1)	5105(5)	344(2)	31(1)
C(11)	2542(1)	4195(6)	460(2)	32(1)
C(12)	3107(1)	7036(6)	112(3)	50(2)
C(13)	2695(1)	7552(6)	-917(3)	51(2)
C(14)	1730(1)	621(6)	802(2)	31(1)
C(15)	1995(1)	551(6)	1337(2)	31(1)
C(16)	2266(1)	1262(5)	1461(2)	28(1)
C(17)	2538(1)	1003(5)	2053(2)	29(1)
C(18)	2805(1)	1618(6)	2130(2)	38(1)
C(19)	3060(1)	1476(6)	2677(2)	41(1)
C(20)	3054(1)	720(6)	3151(2)	41(1)
C(21)	2790(1)	78(6)	3070(2)	38(1)
C(22)	2539(1)	230(6)	2531(2)	36(1)
C(23)	1472(1)	-309(5)	756(2)	28(1)

C(24)	1433(1)	-573(6)	1256(2)	35(1)
C(25)	1197(1)	-1464(6)	1204(2)	34(1)
C(26)	1000(1)	-2200(5)	664(2)	28(1)
C(27)	1045(1)	-1923(6)	170(2)	34(1)
C(28)	1272(1)	-967(6)	210(2)	32(1)
C(29)	659(1)	-4772(6)	179(2)	32(1)
C(30)	362(1)	-4983(6)	-268(2)	34(1)
C(31)	280(1)	-6318(6)	-633(2)	38(1)
C(32)	482(1)	-7475(6)	-573(2)	43(1)
C(33)	775(1)	-7254(6)	-142(3)	42(1)
C(34)	865(1)	-5937(6)	220(2)	39(1)
C(35)	134(1)	-3716(6)	-376(3)	47(2)
C(36)	1193(1)	-5820(7)	677(3)	59(2)
C(37)	387(1)	-8937(7)	-962(3)	64(2)
C(38)	626(1)	-3049(6)	1071(2)	34(1)
C(39)	635(1)	-4254(6)	1470(3)	39(1)
C(40)	555(1)	-3938(7)	1912(3)	45(2)
C(41)	456(1)	-2484(8)	1974(3)	48(2)
C(42)	443(1)	-1299(7)	1583(3)	48(2)
C(43)	524(1)	-1546(6)	1139(3)	39(1)
C(44)	730(1)	-5925(6)	1427(3)	53(2)
C(45)	366(2)	-2193(8)	2451(3)	74(2)
C(46)	488(1)	-193(6)	715(3)	54(2)
C(47)	1878(2)	1991(7)	2668(3)	48(2)
C(48)	1592(2)	2515(7)	2391(3)	53(2)
C(49)	1379(2)	1673(8)	2444(3)	62(2)
C(50)	1450(1)	295(7)	2771(3)	54(2)
C(51)	1734(1)	-233(7)	3050(3)	46(2)
C(52)	1948(1)	621(7)	2997(3)	50(2)
C(53)	482(3)	7776(11)	7900(5)	125(4)
C(54)	459(3)	6577(13)	8251(6)	121(4)
C(55)	702(3)	5851(12)	8684(5)	118(5)
C(56)	974(3)	6333(11)	8768(4)	110(4)
C(57)	997(3)	7523(11)	8433(5)	114(3)

C(58)	754(3)	8217(11)	8003(5)	125(4)

Table 3. Bond lengths [Å] and angles [°] for Compd 4.

Pt(1)-C(1)	1.964(5)	C(19)-C(20)	1.377(7)
Pt(1)-N(1)	1.987(4)	C(20)-C(21)	1.383(7)
Pt(1)-O(2)	2.007(3)	C(21)-C(22)	1.367(7)
Pt(1)-O(1)	2.065(3)	C(23)-C(28)	1.389(6)
B(1)-C(38)	1.562(8)	C(23)-C(24)	1.396(7)
B(1)-C(26)	1.566(7)	C(24)-C(25)	1.382(6)
B(1)-C(29)	1.577(7)	C(25)-C(26)	1.402(6)
O(1)-C(16)	1.273(5)	C(26)-C(27)	1.403(7)
O(2)-C(14)	1.284(6)	C(27)-C(28)	1.385(6)
N(1)-C(11)	1.340(6)	C(29)-C(34)	1.417(7)
N(1)-C(7)	1.378(6)	C(29)-C(30)	1.418(7)
N(2)-C(9)	1.353(6)	C(30)-C(31)	1.394(7)
N(2)-C(13)	1.453(7)	C(30)-C(35)	1.516(7)
N(2)-C(12)	1.464(7)	C(31)-C(32)	1.386(7)
C(1)-C(2)	1.397(7)	C(32)-C(33)	1.389(7)
C(1)-C(6)	1.415(7)	C(32)-C(37)	1.514(7)
C(2)-C(3)	1.380(7)	C(33)-C(34)	1.379(7)
C(3)-C(4)	1.382(8)	C(34)-C(36)	1.526(7)
C(4)-C(5)	1.372(7)	C(38)-C(43)	1.422(7)
C(5)-C(6)	1.402(7)	C(38)-C(39)	1.425(7)
C(6)-C(7)	1.460(7)	C(39)-C(40)	1.394(7)
C(7)-C(8)	1.398(7)	C(39)-C(44)	1.520(7)
C(8)-C(9)	1.421(7)	C(40)-C(41)	1.371(8)
C(9)-C(10)	1.407(7)	C(41)-C(42)	1.393(8)
C(10)-C(11)	1.361(7)	C(41)-C(45)	1.509(8)
C(14)-C(15)	1.392(7)	C(42)-C(43)	1.389(7)
C(14)-C(23)	1.497(6)	C(43)-C(46)	1.523(7)
C(15)-C(16)	1.412(6)	C(47)-C(48)	1.367(8)
C(16)-C(17)	1.500(7)	C(47)-C(52)	1.375(7)
C(17)-C(22)	1.377(7)	C(48)-C(49)	1.368(8)
C(17)-C(18)	1.395(7)	C(49)-C(50)	1.378(8)
C(18)-C(19)	1.386(7)	C(50)-C(51)	1.360(7)

C(51)-C(52)	1.379(8)	C(1)-C(6)-C(7)	114.5(5)
C(53)-C(58)	1.346(12)	N(1)-C(7)-C(8)	120.3(5)
C(53)-C(54)	1.396(13)	N(1)-C(7)-C(6)	112.8(4)
C(54)-C(55)	1.358(13)	C(8)-C(7)-C(6)	126.9(5)
C(55)-C(56)	1.374(13)	C(7)-C(8)-C(9)	120.7(5)
C(56)-C(57)	1.360(11)	N(2)-C(9)-C(10)	121.4(5)
C(57)-C(58)	1.342(12)	N(2)-C(9)-C(8)	122.3(5)
		C(10)-C(9)-C(8)	116.3(5)
C(1)-Pt(1)-N(1)	81.63(19)	C(11)-C(10)-C(9)	120.2(5)
C(1)-Pt(1)-O(2)	94.41(18)	N(1)-C(11)-C(10)	124.0(5)
N(1)-Pt(1)-O(2)	176.03(15)	O(2)-C(14)-C(15)	127.5(5)
C(1)-Pt(1)-O(1)	174.04(17)	O(2)-C(14)-C(23)	114.3(4)
N(1)-Pt(1)-O(1)	92.73(14)	C(15)-C(14)-C(23)	118.2(5)
O(2)-Pt(1)-O(1)	91.21(12)	C(14)-C(15)-C(16)	127.2(5)
C(38)-B(1)-C(26)	117.9(4)	O(1)-C(16)-C(15)	123.2(5)
C(38)-B(1)-C(29)	123.6(5)	O(1)-C(16)-C(17)	116.1(4)
C(26)-B(1)-C(29)	118.3(5)	C(15)-C(16)-C(17)	120.7(4)
C(16)-O(1)-Pt(1)	126.4(3)	C(22)-C(17)-C(18)	117.7(5)
C(14)-O(2)-Pt(1)	124.4(3)	C(22)-C(17)-C(16)	124.2(5)
C(11)-N(1)-C(7)	118.5(4)	C(18)-C(17)-C(16)	118.1(5)
C(11)-N(1)-Pt(1)	125.2(3)	C(19)-C(18)-C(17)	120.4(5)
C(7)-N(1)-Pt(1)	116.3(3)	C(20)-C(19)-C(18)	120.7(5)
C(9)-N(2)-C(13)	122.3(5)	C(19)-C(20)-C(21)	118.9(5)
C(9)-N(2)-C(12)	120.2(5)	C(22)-C(21)-C(20)	120.3(5)
C(13)-N(2)-C(12)	117.4(4)	C(21)-C(22)-C(17)	122.1(5)
C(2)-C(1)-C(6)	116.8(5)	C(28)-C(23)-C(24)	118.8(5)
C(2)-C(1)-Pt(1)	128.5(4)	C(28)-C(23)-C(14)	119.7(5)
C(6)-C(1)-Pt(1)	114.6(4)	C(24)-C(23)-C(14)	121.4(5)
C(3)-C(2)-C(1)	121.4(5)	C(25)-C(24)-C(23)	120.3(5)
C(2)-C(3)-C(4)	121.2(6)	C(24)-C(25)-C(26)	122.0(5)
C(5)-C(4)-C(3)	119.3(6)	C(25)-C(26)-C(27)	116.5(4)
C(4)-C(5)-C(6)	120.3(5)	C(25)-C(26)-B(1)	121.4(5)
C(5)-C(6)-C(1)	121.0(5)	C(27)-C(26)-B(1)	122.0(4)
C(5)-C(6)-C(7)	124.5(5)	C(28)-C(27)-C(26)	121.9(5)

C(27)-C(28)-C(23)	120.4(5)	C(47)-C(52)-C(51)	120.9(6)
C(34)-C(29)-C(30)	117.1(5)	C(58)-C(53)-C(54)	118.6(11)
C(34)-C(29)-B(1)	121.9(5)	C(55)-C(54)-C(53)	121.2(12)
C(30)-C(29)-B(1)	120.9(5)	C(54)-C(55)-C(56)	118.0(11)
C(31)-C(30)-C(29)	120.1(5)	C(57)-C(56)-C(55)	120.7(11)
C(31)-C(30)-C(35)	119.6(5)	C(58)-C(57)-C(56)	120.6(11)
C(29)-C(30)-C(35)	120.2(5)	C(57)-C(58)-C(53)	121.0(10)
C(32)-C(31)-C(30)	122.0(5)		
C(31)-C(32)-C(33)	117.9(5)		
C(31)-C(32)-C(37)	121.1(5)		
C(33)-C(32)-C(37)	121.0(5)		
C(34)-C(33)-C(32)	121.8(5)		
C(33)-C(34)-C(29)	121.0(5)		
C(33)-C(34)-C(36)	117.2(5)		
C(29)-C(34)-C(36)	121.8(5)		
C(43)-C(38)-C(39)	116.3(5)		
C(43)-C(38)-B(1)	122.3(5)		
C(39)-C(38)-B(1)	121.2(5)		
C(40)-C(39)-C(38)	120.9(5)		
C(40)-C(39)-C(44)	117.7(5)		
C(38)-C(39)-C(44)	121.3(5)		
C(41)-C(40)-C(39)	122.3(6)		
C(40)-C(41)-C(42)	117.4(5)		
C(40)-C(41)-C(45)	120.9(6)		
C(42)-C(41)-C(45)	121.7(6)		
C(43)-C(42)-C(41)	122.6(6)		
C(42)-C(43)-C(38)	120.5(5)		
C(42)-C(43)-C(46)	118.5(5)		
C(38)-C(43)-C(46)	121.0(5)		
C(48)-C(47)-C(52)	119.5(6)		
C(47)-C(48)-C(49)	119.8(6)		
C(48)-C(49)-C(50)	120.6(6)		
C(51)-C(50)-C(49)	120.1(6)		
C(50)-C(51)-C(52)	119.2(6)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Compd 4. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	28(1)	27(1)	29(1)	-2(1)	15(1)	-2(1)
B(1)	20(3)	29(3)	33(4)	0(3)	4(3)	-1(2)
O(1)	23(2)	20(2)	28(2)	-2(1)	16(2)	-6(1)
O(2)	28(2)	33(2)	33(2)	0(2)	16(2)	0(2)
N(1)	33(3)	28(2)	26(2)	-1(2)	14(2)	1(2)
N(2)	46(3)	36(3)	59(3)	6(2)	34(3)	-1(2)
C(1)	34(3)	26(3)	40(3)	-6(2)	19(3)	2(2)
C(2)	41(3)	43(3)	44(3)	1(3)	21(3)	-3(3)
C(3)	33(3)	55(4)	40(4)	4(3)	5(3)	5(3)
C(4)	46(4)	55(4)	37(4)	11(3)	12(3)	8(3)
C(5)	48(4)	43(3)	38(4)	8(3)	23(3)	8(3)
C(6)	33(3)	26(3)	34(3)	-2(2)	16(3)	3(2)
C(7)	35(3)	21(3)	38(3)	1(2)	18(3)	4(2)
C(8)	50(4)	27(3)	37(3)	4(2)	29(3)	6(3)
C(9)	47(4)	26(3)	46(4)	-2(2)	34(3)	1(2)
C(10)	29(3)	26(3)	44(4)	-4(2)	22(3)	-2(2)
C(11)	40(3)	29(3)	31(3)	-5(2)	19(3)	1(2)
C(12)	44(4)	46(4)	70(4)	-5(3)	37(4)	-12(3)
C(13)	72(4)	39(3)	62(4)	1(3)	48(4)	-2(3)
C(14)	32(3)	27(3)	36(3)	-10(2)	17(3)	-1(2)
C(15)	29(3)	31(3)	33(3)	0(2)	16(3)	-4(2)
C(16)	30(3)	22(3)	34(3)	-8(2)	18(3)	-3(2)
C(17)	29(3)	25(3)	32(3)	-7(2)	14(3)	-3(2)
C(18)	35(3)	47(3)	31(3)	-1(3)	15(3)	-5(3)
C(19)	25(3)	52(4)	40(4)	-6(3)	12(3)	-9(3)
C(20)	43(4)	39(3)	31(3)	3(3)	11(3)	11(3)
C(21)	38(3)	41(3)	34(3)	4(3)	16(3)	0(3)
C(22)	35(4)	40(3)	39(3)	1(3)	22(3)	-6(3)

C(23)	23(3)	24(3)	38(3)	-4(2)	15(3)	-1(2)
C(24)	31(3)	37(3)	34(3)	-6(2)	12(3)	-5(2)
C(25)	30(3)	40(3)	32(3)	-3(2)	15(3)	-7(2)
C(26)	22(3)	27(3)	34(3)	-7(2)	13(2)	-2(2)
C(27)	23(3)	38(3)	35(3)	-12(2)	10(3)	-6(2)
C(28)	29(3)	36(3)	32(3)	-5(2)	16(3)	-4(2)
C(29)	28(3)	31(3)	38(3)	2(2)	17(3)	-1(2)
C(30)	26(3)	38(3)	37(3)	2(2)	14(3)	-5(2)
C(31)	26(3)	39(3)	40(3)	-2(3)	10(3)	-8(2)
C(32)	46(3)	34(3)	44(3)	-3(3)	17(3)	-6(3)
C(33)	41(3)	29(3)	56(4)	-4(3)	24(3)	3(3)
C(34)	31(3)	41(3)	42(4)	-4(3)	16(3)	-3(3)
C(35)	29(3)	43(3)	49(4)	-3(3)	3(3)	0(3)
C(36)	34(4)	58(4)	66(5)	-11(3)	9(3)	8(3)
C(37)	69(5)	44(4)	69(5)	-15(3)	24(4)	-5(3)
C(38)	24(3)	39(3)	37(3)	-4(2)	13(3)	-11(2)
C(39)	21(3)	45(3)	42(4)	1(3)	9(3)	-4(2)
C(40)	30(3)	61(4)	37(4)	10(3)	12(3)	-1(3)
C(41)	29(3)	71(4)	43(3)	-13(4)	16(3)	-11(3)
C(42)	32(4)	53(4)	59(4)	-18(3)	22(3)	-11(3)
C(43)	34(3)	41(3)	47(4)	-13(3)	23(3)	-12(3)
C(44)	50(4)	47(4)	66(5)	22(3)	31(4)	10(3)
C(45)	70(5)	101(6)	69(5)	-11(4)	48(4)	-8(4)
C(46)	58(4)	35(3)	76(5)	2(3)	39(4)	3(3)
C(47)	61(4)	40(3)	42(4)	-6(3)	24(4)	-5(3)
C(48)	77(5)	37(3)	43(4)	4(3)	28(4)	9(4)
C(49)	52(5)	66(5)	66(5)	14(4)	26(4)	29(4)
C(50)	50(4)	54(4)	64(5)	2(3)	32(4)	2(3)
C(51)	52(4)	44(3)	38(4)	6(3)	19(3)	8(3)
C(52)	42(4)	52(4)	42(4)	-1(3)	7(3)	1(3)
C(53)	140(10)	77(7)	186(12)	33(7)	100(10)	17(7)
C(54)	171(13)	88(8)	158(12)	-26(7)	123(11)	-28(8)
C(55)	240(17)	67(7)	90(8)	-16(5)	113(11)	-26(8)
C(56)	211(13)	73(7)	70(6)	12(5)	86(8)	50(7)

C(57)	152(10)	106(8)	126(9)	34(7)	102(8)	48(7)
C(58)	145(11)	95(7)	177(12)	55(8)	111(10)	24(7)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Compd 4.

	x	y	z	U(eq)
H(2A)	1330	2000	-819	51
H(3A)	1068	2730	-1816	57
H(4A)	1278	4371	-2246	59
H(5A)	1764	5212	-1675	51
H(8A)	2246	5936	-1042	41
H(10A)	2926	5255	645	38
H(11A)	2619	3737	847	39
H(12A)	3112	7493	471	74
H(12B)	3200	7765	-47	74
H(12C)	3215	6033	216	74
H(13A)	2506	8065	-1028	77
H(13B)	2670	6776	-1225	77
H(13C)	2840	8347	-886	77
H(15A)	1993	-41	1653	37
H(18A)	2812	2137	1806	46
H(19A)	3240	1904	2725	49
H(20A)	3228	641	3528	49
H(21A)	2784	-470	3390	46
H(22A)	2360	-211	2485	43
H(24A)	1569	-138	1633	42
H(25A)	1168	-1581	1544	41
H(27A)	917	-2404	-203	40
H(28A)	1291	-760	-138	38
H(31A)	79	-6438	-932	45
H(33A)	917	-8032	-96	50
H(35A)	-65	-4151	-618	70

H(35B)	163	-2829	-589	70
H(35C)	156	-3351	9	70
H(36A)	1269	-6871	838	88
H(36B)	1218	-5120	1005	88
H(36C)	1302	-5394	482	88
H(37A)	216	-8688	-1350	96
H(37B)	334	-9766	-763	96
H(37C)	550	-9305	-1026	96
H(40A)	569	-4759	2179	54
H(42A)	376	-281	1620	58
H(44A)	713	-6591	1726	80
H(44B)	935	-5918	1505	80
H(44C)	602	-6344	1025	80
H(45A)	278	-3154	2512	110
H(45B)	221	-1336	2323	110
H(45C)	540	-1900	2827	110
H(46A)	330	509	682	80
H(46B)	437	-617	319	80
H(46C)	674	398	873	80
H(47A)	2027	2569	2633	58
H(48A)	1542	3461	2163	64
H(49A)	1181	2043	2254	75
H(50A)	1300	-289	2801	64
H(51A)	1784	-1177	3279	55
H(52A)	2147	257	3191	60
H(53A)	311	8270	7594	150
H(54A)	268	6264	8186	145
H(55A)	685	5034	8922	141
H(56A)	1148	5830	9063	132
H(57A)	1187	7865	8505	136
H(58A)	773	9031	7767	150

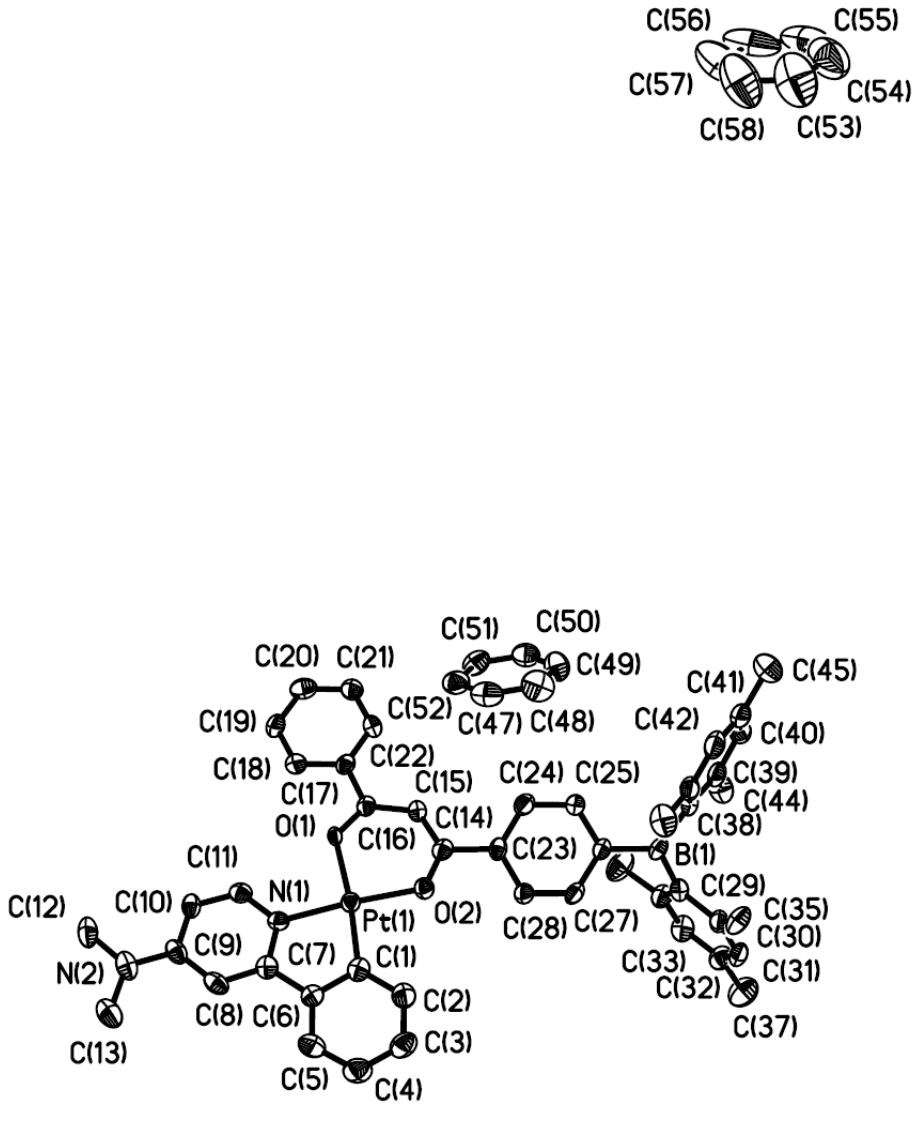


Figure S23. A diagram showing the structure of compound **4** and the two benzene solvent molecules with labeling schemes and 50% thermal ellipsoids. H atoms are omitted for clarity.

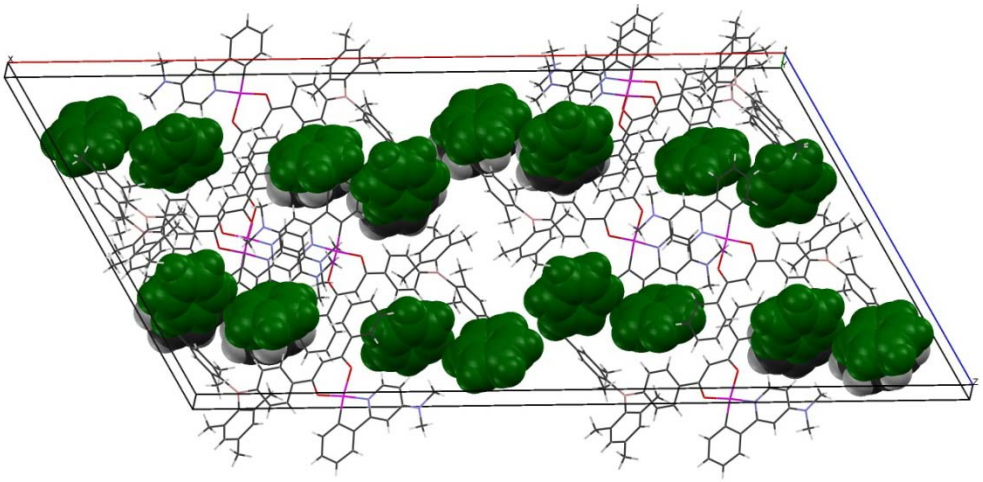


Figure S24. Unit cell packing diagram showing the benzene solvent molecules in the crystal lattice of compound **4**.