Supporting Information for

Columnar Mesophases from Half-Discoid Platinum Cyclometalated Metallomesogens

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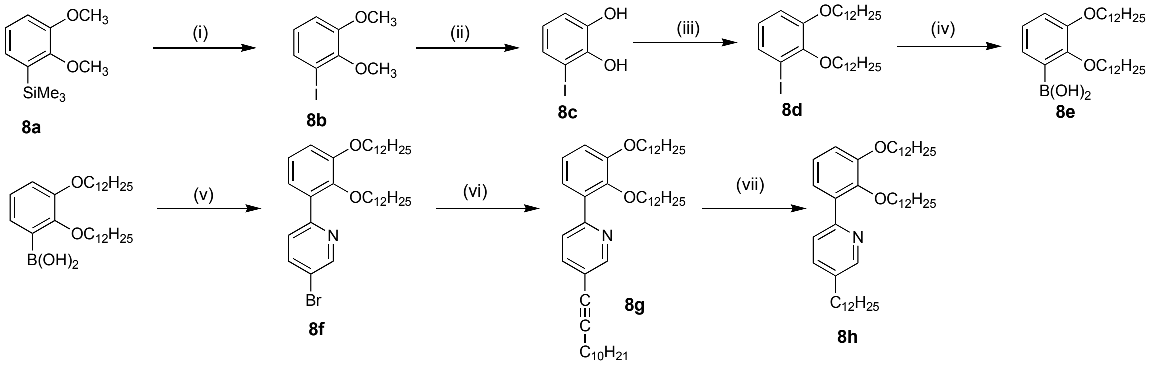
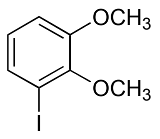
General Experimental Methods: All synthetic manipulations were performed under an argon atmosphere using standard Schlenk techniques unless otherwise noted. NMR (^{1}H and ^{13}C) spectra were recorded on either a Varian Mercury 300 MHz or a Varian INOVA 500 MHz spectrometer. NMR chemical shifts are referenced to residual protonated solvent. High-resolution mass spectra (HRMS) were obtained at the MIT Department of Chemistry Instrumentation Facility using a peak-matching protocol to determine the mass and error range of the molecular ion, using either electron impact or electrospray as the ionization technique. UV/vis spectra were recorded on an Agilent 8453 diode-array spectrophotometer and corrected for background signal with either a solvent-filled cuvette (for solution measurements) or a clean glass cover slip (for thin film measurements). Emission spectra were acquired on a SPEX Fluorolog-τ3 fluorimeter (model FL-321, 450 W Xenon lamp) using either right angle detection (solution measurements) or front face detection (thin film measurements). All room temperature solution samples for emission spectra were degassed by at least three freeze-pump-thaw cycles in an anaerobic cuvette and were repressurized with Ar following each cycle. 77K emission spectra were acquired in frozen 2-methyltetrahydrofuran glass. Quantum yields of phosphorescence were determined by comparison to Ru(bpy)3 in deoxygenated water and are corrected for solvent refractive index and absorption differences at the excitation wavelength. Phosphorescence lifetimes were determined by time-resolved phosphorescence spectroscopy. The irradiation source was an Oriel nitrogen laser (Model 79111) with a 5 ns pulsewidth operating at approximately 25 Hz. The emitted light was dispersed in an Oriel MS-260i spectrograph with a 300 lines/mm grating. The detector was an Andor Technologies Intensified CCD camera (1024 x 128 pixels) with an onboard delay generator and a minimum gate width of 5 ns operating in full vertical binning mode and triggered by a TTL prepulse from the nitrogen laser. Data taken of 77K glasses were subjected to no horizontal binning, while solution data was acquired with a horizontal binning of 2 or 3. 10-15 spectra at different delay times after the laser pulse were taken per lifetime measurement, the integrated intensities of which were fit to a single-exponential function. The detector was calibrated with a Hg(Ar)pencil-style calibration lamp.

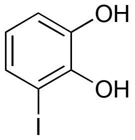


(i) ICl/ CH_2Cl_2, 80%; (ii) BBr_3/ CH_2Cl_2, 87%; (iii) $C_{12}H_{25}Br$/ K_2CO_3/ DMF/ 80°C/ 24 h, 61%; (iv) *t*-BuLi/ $B(OMe)_3$, 63%; (v) 2-iodo-5-bromopyridine/ $Pd(PPh_3)_4$ / 2M Na_2CO_3(aq)/ DME, 86%; (vi) 1-dodecyne/ $PdCl_2(PPh_3)_2$/ CuI/ Et_3N, 57%; (vii) Pd(C)/ EtOAc/ H_2(45psi), 52%.

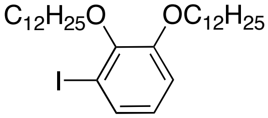


Compound **8b**: To 2,3-dimethoxy-trimethylsilyl benzene[1] **8a** (5.0 g, 2.37 mol) in CH_2Cl_2 (mL) at 0 ^oC, ICl (3.85 g, 0.0237 mol) was added and the reaction mixture was stirred for 24h. After the reaction mixture was poured into aq 2M NaOH solution, the organic layer was separated and the aqueous layer was washed with CH_2Cl_2. The combined organic layer was washed with water and sat.brine solution and was dried over anhydrous Na_2SO_4. The organic layer was filtered and evaporated in vacuo to yield a white solid. The white solid was chromatographed on silica gel using CH_2Cl_2:Hexane (1:2) as the eluent to afford a white solid. yield (5.0 g, 80%). ^1H NMR (300 MHz, $CDCl_3$): δ 7.35 (dd, 1H), 6.89 (m, 1H), 6.79 (m, 1H), 3.85 (s, 1H), 3.82 (s, 1H). ^{13}C NMR (125.78 MHz,

$CDCl_3$): 56.1, 60.6, 92.8, 112.9, 126.2, 130.3, 130.7, 149.1, 153.1. HRMS calcd for $C_8H_9IO_2$ ($M+Na^+$). (289.9539); found 286.9544.

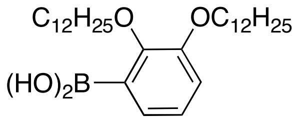


Compound 8c: To **8b** (15.0 g, 5.6 mmol) in CH_2Cl_2 at -80 °C, BBr_3 (42.6 g, 17.0 mmol) was added dropwise. The temperature of the reaction was raised to room temperature and was stirred at that temperature for 24h. The reaction mixture was poured into ice water to give a white precipitate. The white precipitate was dissolved in Et_2O was washed with water and sat.brine solution. The organic layer was dried over sodium sulfate, filtered and evaporated under vacuo to yield a white solid. Yield (11.5g, 87%). ^1H NMR (300 MHz, $CDCl_3$): δ 7.20 (dd, 1H), 6.88 (dd, 1H), 6.63 (t, 1H), 5.56 (br, 1H), 5.35 (br, 1H). ^{13}C NMR (125.78 MHz, $CDCl_3$): 85.0, 116.6, 123.7, 130.2, 143.7, 144.1. HRMS calcd for $C_8H_9IO_2$ ($M+H^+$). (235.9325); found 234.0141 .

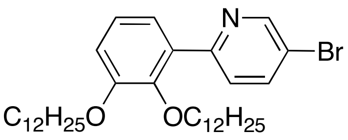


Compound 8d: **8c** (10.0 g, 4.2 mmol), K_2CO_3 (25.0 g, 18.1 mmol), and $C_{12}H_{25}I$ (22.5 g, 9.0 mmol) were added to 250 mL RBF containing DMF (100 mL). The reaction mixture was sparged with N_2 for 15 min. The temperature of the reaction mixture was raised to 120 °C and stirred at that temperature under N_2 for 24h. After, the reaction mixture was cooled down to room temperature and was poured into ice-cold water to yield a precipitate. The precipitate was filtered and dried under vacuo to yield a white solid (14.7 g, 61%). ^1H NMR (300 MHz, $CDCl_3$): δ 7.33 (d, 1H), 6.86 (d, 1H), 6.75 (d, 1H), 3.98 (m, 4H), 1.85 (m, 4H), 1.46-1.27 (m, 40H), 0.90 (t, 6H). ^{13}C NMR (125.78 MHz, $CDCl_3$): 14.8, 23.4, 26.86, 26.89, 30.03, 30.09, 30.11, 30.27, 30.35, 30.38, 30.40, 30.42, 30.44,

31.0, 32.65, 32.66, 69.5, 73.8, 93.7, 114.4, 126.2, 131.1, 149.2, 153.0. HRMS calcd for $C_{30}H_{53}IO_2$ (M+Na$^+$). (595.2982); found 595.2976.

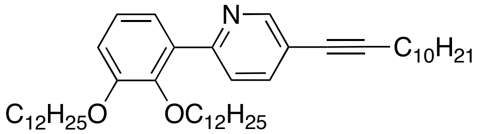


Compound 8e: To **8d** (14.7 g, 2.56 mmol) in Tetrahydrofuran at -78 ^oC, 1.7M *t*BuLi (45.3 mL, 7.7 mmol) was added dropwise. The reaction mixture was stirred at that temperature for 1h. $B(OMe)_3$ (25.7 mL, 23.1 mol) was added to the reaction mixture dropwise at -78 ^oC. The temperature was the reaction was raised to room temperature and was stirred at that temperature for 24h. The reaction was quenched with 3N HCl and allowed to stir for 1h at room temperature. The reaction mixture was extracted with Et_2O (3 times) and was washed with water and saturated brine solution. The organic layer was dried over Na_2SO_4, filtered and evaporated under vacuo to yield a pink solid. The pink solid was chromatographed on silica gel using DCM:EtOAc (4:1) to yield a white solid. (7.9 g, 63%). ^1H NMR (300 MHz, $CDCl_3$): δ 7.36 (d, 1H), 7.08 (m, 1H), 7.01 (m, 1H), 4.10 (t, 2H), 3.98 (t, 2H), 1.82 (m, 4H), 1.5-1.2 (m, 40H), 0.81 (t, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): 14.8, 23.4, 26.6, 26.9, 30.0, 30.12, 30.13, 30.19, 30.32, 30.35, 30.37, 30.40, 30.41, 31.1, 32.6, 69.2, 74.9, 117.3, 125.0, 127.8, 152.3, 154.6. HRMS calcd for $C_{30}H_{55}BO_4$ (M+Na$^+$). (512.4122); found 512.4091.



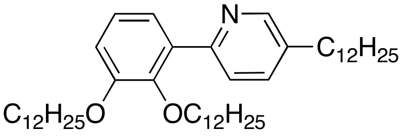
Compound 8f: **8e** (4.25 g, 0.866 mmol), 2-iodo-5-bromo pyridine (2.45 g, 0.866 mmol), $Pd(PPh_3)_4$ (603 mg, 0.0433 mmol), and 2M aq Na_2CO_3 (20 mL) in DME (50 mL) was sparged with N_2 for 15 min. Then the reaction mixture was heated at 100 ^oC for 24h. The reaction mixture was allowed to cool to room temperature and evaporated under vacuo to

yield a solid residue. The solid residue was extracted with dichloromethane and washed with water, followed by saturated brine solution. The organic layer was dried over Na_2SO_4, filtered and evaporated under vacuo to yield a solid residue. The solid residue was chromatographed on silica gel using DCM:Hexane (1:1) as the eluent to yield a white solid. (4.48 g, 86%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.74 (d, 1H), 7.82 (m, 2H), 7.31 (d, 1H), 7.11 (t, 1H), 6.94 (d, 1H), 4.01 (t, 2H), 3.78 (t, 2H), 1.83 (m, 4H), 1.56 - 1.28 (m, 40H), 0.89 (t, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): 14.8, 23.40, 23.41, 26.7, 26.9, 30.08, 30.09, 30.11, 30.14, 30.35, 30.38, 30.41, 30.43, 30.87, 32.64, 69.42, 74.51, 114.6, 119.7, 122.7, 124.8, 127.3, 134.1, 139.3, 148.2, 151.4, 153.3, 155.8. HRMS calcd for $C_{35}H_{56}BrNO_2$ (M+Na$^+$). (602.3567); found 604.3551.

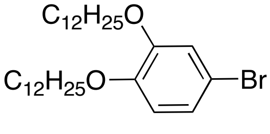


Compound 8g: **8f** (3.35 g, 5.5 mmol), 1-dodecyne (2.97 mL, 1.38 mmol), $PdCl_2(PPh_3)_2$ (194 mg, 0.027 mmol), and CuI (0.052 g, 0.027 mmol) in Et_3N (75 mL). After sparging with N_2 for 15 min, the reaction mixture was heated at 100 ^{o}C for 36h. The reaction mixture was allowed to cool to room temperature and evaporated under vacuo to yield a oily residue. The oily residue was extracted with dichloromethane and washed with water, followed by saturated brine solution. The organic layer was dried over Na_2SO_4, filtered and evaporated under vacuo to yield a brown solid. The brown solid was chromatographed on silica gel using DCM:Hexane (1:2) as the eluent to yield a white solid. Yield (2.15 g, 57%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.67 (s, 1H), 7.84 (m, 1H), 7.81 (m, 1H), 7.66 (m, 1H), 7.10 (m, 1H), 6.91 (m, 1H), 4.00 (t, 2H), 3.73 (t, 2H), 2.40 (t, 2H), 1.82 (m, 4H), 1.6-1.18 (m, 52H), 0.85 (m, 9H). ^{13}C NMR (125.78 MHz, $CDCl_3$): 14.8, 20.1, 20.2, 23.4, 26.7, 26.9, 29.9, 29.2, 29.3, 29.64, 29.68, 29.84, 29.87, 30.04, 30.08, 30.11, 30.12, 30.14, 30.16, 30.22, 30.25, 30.30, 30.35, 30.36, 30.37, 30.39, 30.41, 30.43, 30.8, 32.61, 32.64, 32.65, 69.4, 74.4, 78.4, 94.6, 114.4, 119.7, 122.9, 124.7, 125.1,

134.9, 138.7, 147.1, 152.4, 153.3, 155.0. HRMS calcd for $C_{47}H_{77}NO_2$ (M+H$^+$). (688.6027); found 688.6006.

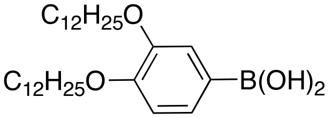


Compound 8h: **8g** (2.15 g, 0.31 mmol) and Pd/C (1.1 g) in ethylacetate (35 ml) pressurized in a parr bomb with 45 psi H_2 and the reaction mixture was shaken for 12h. After the reaction mixture was filtered over celite. The residue was washed with DCM and EtOAc and the filtrate was evaporated under vacuo to yield a off-white solid. The solid was chromatographed on silica gel using DCM:Hexane (1:1) as the eluent to yield a white solid. Yield (1.11 g, 52%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.50 (d, 1H), 7.80 (m, 2H), 7.51 (d, 1H), 7.12 (m, 1H), 6.91 (m, 1H), 4.02 (t, 2H), 3.77 (t, 2H), 2.64 (t, 2H), 1.82 (m, 4H), 1.6-1.18 (m, 56H), 0.85 (m, 9H). ^{13}C NMR (75 MHz, $CDCl_3$): 14.8, 23.40, 23.41, 26.74, 26.90, 29.98, 30.07, 30.08, 30.11, 30.12, 30.16, 30.17, 30.31, 30.36, 30.38, 30.39, 30.41, 30.45, 30.85, 31.88, 32.64, 32.65, 33.49, 69.38, 74.38, 114.2, 122.97, 124.69, 125.3, 13.8.4, 138.6, 147.9, 151.4, 153.29, 154.7. HRMS calcd for $C_{47}H_{81}NO_2$ (M+H$^+$). (692.6340); found 692.6342.

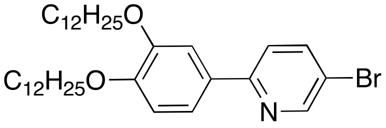


Compound **9b**: To **9a** (10.0 g, 2.2 mmol) in CH_2Cl_2 (250 mL) at 0 °C, Br_2 (3.57 g, 2.2 mmol) was added dropwise. The reaction mixture was allowed to stir at that temperature for 1h. The reaction mixture was poured into 10% NaOH solution (200 mL) and the organic layer was washed with water and sat.brine solution. The organic layer was dried over sodium sulfate, filtered and evaporated to yield a white solid. Yield (11.0 g, 96%).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.06 (s, 1H), 6.98 (m, 1H), 6.74 (d, 1H), 3.97 (m, 4H), 1.84 (m, 4H), 1.45 (m, 4H), 1.30 (m, 32H), 0.88 (m, 6H). ^{13}C NMR (125.78 MHz, $CDCl_3$): 14.8, 23.4, 26.6, 26.70, 26.71, 29.7, 29.8, 29.9, 30.0, 30.1, 30.13, 30.2, 30.32, 30.34, 30.38, 30.4, 32.6, 70.0, 70.2, 70.29, 77.4, 77.7, 78.0, 113.4, 115.3, 115.8, 117.5, 118.6, 124.1, 149.0, 149.7, 150.7. HRMS calcd for $C_{30}H_{53}BrO_2$ ($M+H^+$). (524.3222); found 524.5637.

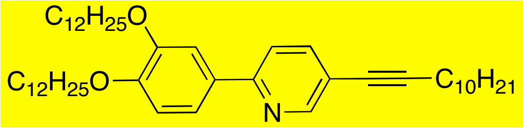


Compound 9c: To **9b** (11 g, 2.09 mmol) in Tetrahydrofuran at -78 °C, 1.7M *t*BuLi (41.3 mL, 6.2 mmol) was added dropwise. The reaction mixture was stirred at that temperature for 1h. $B(OMe)_3$ (20.9 mL, 23.9 mmol) was added to the reaction mixture dropwise at -78 °C. The temperature was the reaction was raised to room temperature and was stirred at that temperature for 24h. The reaction was quenched with 3N HCl and allowed to stir for 1h at room temperature. The reaction mixture was extracted with Et_2O (3 times) and was washed with water and saturated brine solution. The organic layer was dried over Na_2SO_4, filtered and evaporated under vacuo to yield a pink solid. The pink solid was directly used in the next step without any further purification.

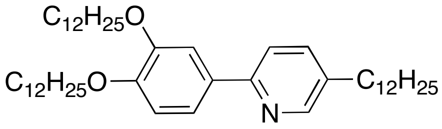


Compound 9d: **9c** (4.25 g, 0.866 mmol), 2-iodo-5-bromo pyridine (2.45 g, 0.866 mmol), $Pd(PPh_3)_4$ (603 mg, 0.0433 mmol), and 2M aq Na_2CO_3 (20 mL) in DME (50 mL) was sparged with N_2 for 15 min. Then the reaction mixture was heated at 100 °C for 24h. The reaction mixture was allowed to cool to room temperature and evaporated under vacuo to yield a solid residue. The solid residue was extracted with dichloromethane and washed with water, followed by saturated brine solution. The organic layer was dried over

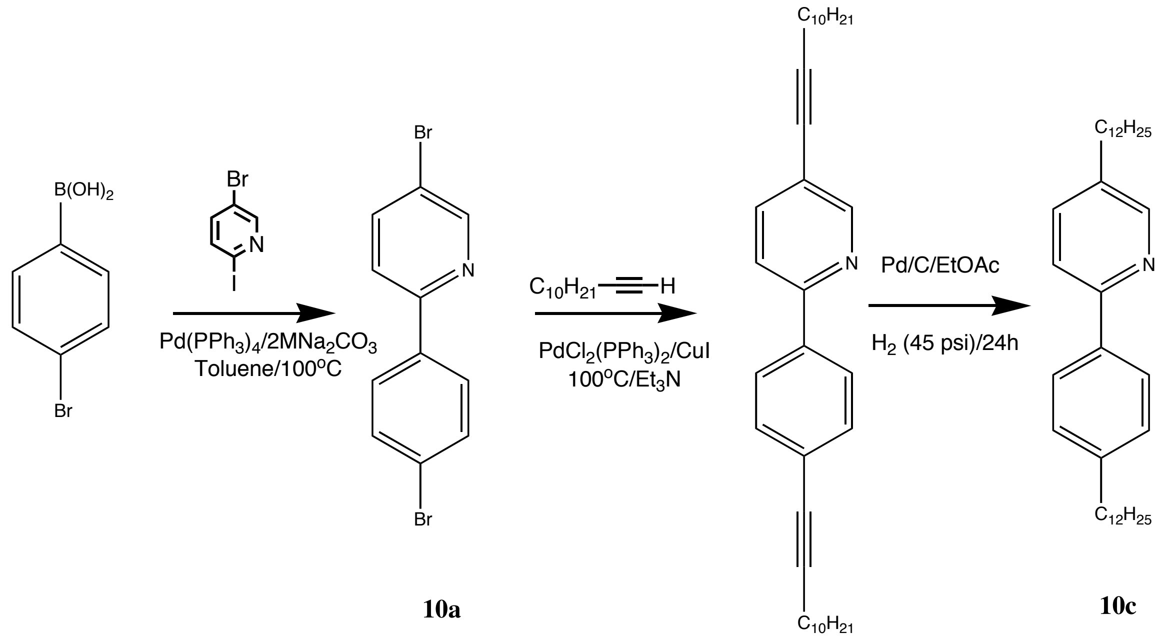
Na_2SO_4, filtered and evaporated under vacuo to yield a solid residue. The solid residue was chromatographed on silica gel using DCM:Hexane (1:1) as the eluent to yield a white solid. (2.75 g, 53%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.67 (s, 1H), 7.80 (m, 1H), 7.50 (s, 1H), 7.45 (dd, 2H), 6.93 (d, 1H), 4.05 (t, 4H), 1.85 (m, 4H), 1.48-1.27 (m, 36H), 0.87 (t, 6H). ^{13}C NMR (125.78 MHz, $CDCl_3$): 14.8, 23.4, 26.75, 26.79, 29.9, 30.0, 30.11, 30.17, 30.3, 30.40, 30.44, 32.6, 69.8, 70.2, 112.8, 114.0, 119.0, 120.1, 121.6, 131.7, 139.7, 150.1, 151.0, 151.1, 156.3. HRMS calcd for $C_{35}H_{56}BrNO_2$ ($M+H^+$). (601.3490); found 600.9622.



Compound 9e: **9d** (3.35 g, 0.55 mmol), 1-dodecyne (2.97 mL, 1.38 mmol), $PdCl_2(PPh_3)_2$ (194 mg, 0.0277 mmol), and CuI (0.052 g, 0.0277 mmol) in Et_3N (75 mL). After sparging with N_2 for 15 min, the reaction mixture was heated at 100 °C for 36h. The reaction mixture was allowed to cool to room temperature and evaporated under vacuo to yield a oily residue. The oily residue was extracted with dichloromethane and washed with water, followed by saturated brine solution. The organic layer was dried over Na_2SO_4, filtered and evaporated under vacuo to yield a brown solid. The brown solid was chromatographed on silica gel using DCM:Hexane (1:2) as the eluent to yield a white solid. Yield (2.55 g, 67%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.68 (m, 1H), 7.82 (m, 1H), 7.59 (dd, 2H), 7.69 (dd, 1H), 6.9 (d, 1H), 4.08 (m, 4H), 1.86 (m, 4H), 1.48 (m, 6H), 1.26 (m, 48H), 0.86 (m, 9H). ^{13}C NMR (75 MHz, $CDCl_3$): 14.8, 17.4, 20.2, 23.4, 26.73, 26.76, 29.3, 29.6, 29.8, 29.9, 30.02, 30.04, 30.08, 30.14, 30.15, 30.25, 30.29, 30.34, 30.35, 30.38, 30.41, 30.42, 32.61, 32.64, 69.9, 70.0, 94.7, 112.8, 114.0, 119.0, 119.3, 120.1, 120.2, 121.7, 131.7, 139.7, 150.1, 151.0, 155.9, 156.3. HRMS calcd for $C_{47}H_{77}NO_2$ ($M+H^+$). (687.5947); found 687.3605.



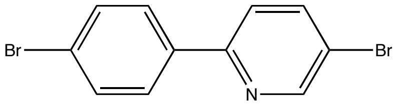
Compound 9f: **9e** (2.55 g, 0.37 mmol) and Pd/C (1.4 g) in ethylacetate (35 ml) pressurized in a parr bomb with 45 psi H_2 and the reaction mixture was shaken for 12h. After the reaction mixture was filtered over celite. The residue was washed with DCM and EtOAc and the filtrate was evaporated under vacuo to yield a off-white solid. The solid was chromatographed on silica gel using DCM:Hexane (1:1) as the eluent to yield a white solid. Yield (2.49 g, 95%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.46 (d, 1H), 7.6-7.5 (m, 2H), 7.46-7.25 (m, 2H), 6.92 (d, 1H), 4.10 (t, 2H), 4.03 (t, 2H), 2.61 (t, 2H), 1.87 (m, 4H), 1.61 (m, 4H), 1.48 (m, 4H), 1.29-1.25 (m, 46H), 0.87 (t, 9H). ^{13}C NMR (125.78 MHz, $CDCl_3$): 14.8, 23.4, 26.75, 26.78, 29.8, 30.0, 30.06, 30.09, 30.16, 30.28, 30.35, 30.38, 30.4, 31.9, 32.63, 32.64, 33.3, 69.94, 69.98, 112.8, 114.2, 119.9, 120.1, 133.1, 136.4, 137.2, 150.0, 150.2, 150.5, 155.4. HRMS calcd for $C_{47}H_{81}NO_2$ (M+H$^+$). (691.6260); found 692.4498.



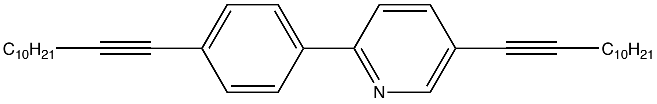
10a

10b

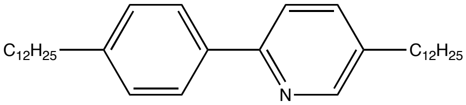
10c



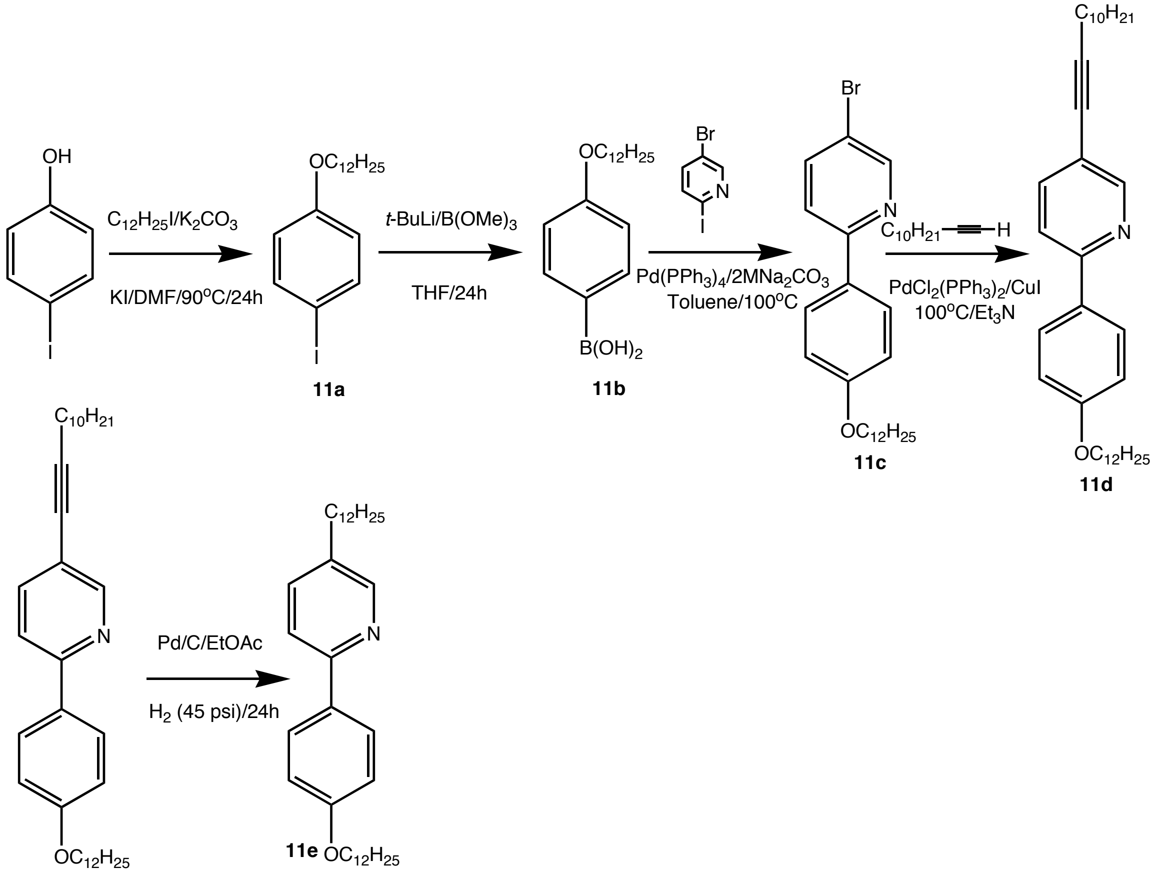
Compound 10a: 4-bromophenyl-boronic acid (2.5 g, 1.2 mmol), 2-iodo-5-bromo pyridine (3.53 g, 1.2 mmol), $Pd(PPh_3)_4$ (0.716 g, 0.062 mmol), and 2M aq Na_2CO_3 (20 mL) in toluene (50 mL) was sparged with N_2 for 15 min. Then the reaction mixture was heated at 100 ^oC for 24h. The reaction mixture was cooled to room temperature and evaporated under vacuo to yield a solid residue. The solid residue was extracted with dichloromethane and washed with water, followed by saturated brine solution. The organic layer was dried over Na_2SO_4, filtered and evaporated under vacuo to yield a solid residue. The solid residue was chromatographed on silica gel using DCM:Hexane as the eluent. The yellow solid was dissolved in hot hexane, filtered and evaporated under vacuo to yield a white solid. Yield (2.2 g, 57%). ^1H NMR (300 MHz, $CDCl_3$): δ 8.72 (dd, 1H, C*H*), 7.83 (m, 3H), 7.60 (m, 3H), ^{13}C NMR (75 MHz, $CDCl_3$): 119.9, 121.6, 124.1, 128.5, 132.2, 137.3, 139.6, 151.0, 154.9. MS calcd for $C_{11}H_7NBr_2$ (M^+). (310.89); found 310.90.

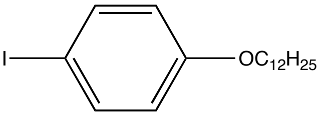


Compound 10b: **10a** (2.0 g, 0.75 mmol), 1-dodecyne (4.25 g, 2.55 mmol), $PdCl_2(PPh_3)_2$ (223 mg, 0.032 mmol), and CuI (0.060 g, 0.032 mmol) in Et_3N (50 mL) was sparged with N_2 for 15 min, the reaction mixture then was heated at 100 ^{o}C for 36h. The reaction mixture was allowed to cool to room temperature and evaporated under vacuo to yield a oily residue. The oily residue was extracted with dichloromethane and washed with water, followed by saturated brine solution. The organic layer was dried over Na_2SO_4, filtered and evaporated under vacuo to yield a oily residue. The oily residue was chromatographed on silica gel using DCM:Hexane (1:1) as the eluent to yield a white solid. Yield (1.42 g, 46%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.67 (m, 1H), 7.91 (m, 2H), 7.71 (dd, 1H), 7.63 (dd, 1H), 7.48 (m, 2H), 2.43 (m, 4H), 1.61 (m, 4H), 1.46 (m, 4H), 1.28 (m, 28H), 0.88 (t, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): 119.9, 121.6, 124.1, 128.5, 132.2, 137.3, 139.6, 151.0, 154.9. HRMS calcd for $C_{35}H_{49}N$ ($M+H^+$). (484.3938); found 484.3938.



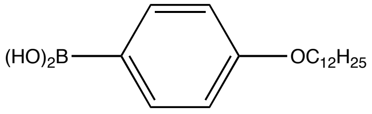
Compound 10c: **10b** (1.3 g, 0.26 mmol) and Pd/C (0.7 g) in ethylacetate in a parr apparatus was hydrogenated under 45 psi H_2 for 12h. The reaction mixture was filtered over celite. The solid residue was washed with DCM and EtOAc and evaporated under vacuo to yield an off-white solid. The solid was chromatographed on silica gel using DCM:Hexane (2:1) as the eluent to yield a white solid. Yield (1.0 g, 79%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.48 (d, 1H), 7.88 (m, 2H), 7.61 (d, 1H), 7.51 (dd, 1H), 7.26 (d, 2H), 2.63 (q, 4H), 1.64 (m, 4H), 1.4-1.2 (m, 36H), 0.88 (t, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): 14.3, 22.9, 29.4, 29.52, 29.57, 29.6, 29.74, 29.79, 29.82, 29.86, 29.9, 31.4, 31.6, 32.1, 32.9, 120.0, 126.7, 129.0, 136.3, 136.7, 137.0, 143.7, 149.9, 155.3. HRMS calcd for $C_{35}H_{57}N$ ($M+H^+$). (492.4564); found 492.4554.



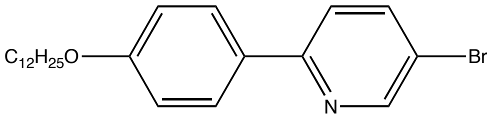


Compound 11a: 4-iodophenol (10.0 g, 4.54 mmol), K_2CO_3 (25.0 g, 18.1 mmol), and $C_{12}H_{25}I$ (22.5 g, 9.0 mmol) were added to 250 mL RBF containing DMF (100 mL). The reaction mixture was sparged with N_2 for 15 min. The temperature of the reaction mixture was raised to 120 °C and stirred at that temperature under N_2 for 24h. After, the reaction mixture was cooled down to room temperature and was poured into ice-cold water to yield a precipitate. The precipitate was filtered and chromatographed on silicagel using Hexane as the eluent to yield a white solid (14.8 g, 84%). ^1H NMR (300 MHz, $CDCl_3$): δ 7.56 (m, 2H), 6.69 (m, 2H), 3.91 (t, 2H), 1.80 (m, 2H), 1.4 (m, 2H), 1.4 (m, 16H), 0.88 (t, 3H). ^{13}C NMR (125.78 MHz, $CDCl_3$): 15.0, 23.5, 26.8, 30.0, 30.2, 30.26,

30.44, 30.48, 30.52, 30.54, 32.8, 68.8, 83.2, 117.6, 138.8, 159.7. HRMS calcd for $C_{18}H_{29}IO$ ($M+H^+$). (388.1257); found 388.0980.

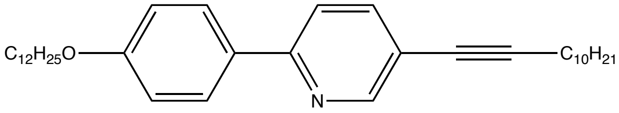


Compound 11b: To **11a** (10 g, 2.57 mmol) in Tetrahydrofuran at -78 °C, 1.7M *t*BuLi (45.4 mL, 7.72 mmol) was added dropwise. The reaction mixture was stirred at that temperature for 1h. $B(OMe)_3$ (25.8 mL, 93.2 mmol) was added to the reaction mixture dropwise at -78 °C. The temperature was the reaction was raised to room temperature and was stirred at that temperature for 24h. The reaction was quenched with 3N HCl and allowed to stir for 1h at room temperature. The reaction mixture was extracted with Et_2O (3 times) and was washed with water and saturated brine solution. The organic layer was dried over Na_2SO_4, filtered and evaporated under vacuo to yield a pink solid. The pink solid was chromatographed on silica gel using DCM:EtOAc (4:1) to yield a white solid. (4.4 g, 56%). ^1H NMR (300 MHz, $CDCl_3$): δ 8.16 (d, 2H), 7.01 (m, 2H), 4.03 (t, 2H), 1.82 (m, 2H), 1.4-1.3 (m, 20H), 0.88 (t, 3H). ^{13}C NMR (125.78 MHz, $CDCl_3$): 14.8, 23.4, 26.7, 29.9, 30.0, 30.1, 30.3, 30.32, 30.36, 30.38, 32.6, 68.6, 114.7, 114.8, 116.2, 116.6, 117.6, 135.9, 138.1, 138.8, 163.4. HRMS calcd for $C_{18}H_{31}BO_3$ ($M+H^+$). (306.2364); found 306.4239.

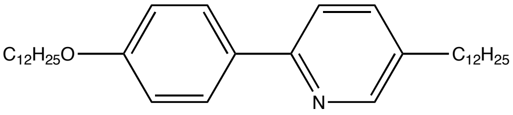


Compound 11c: **11b** (3.2 g, 1.04 mmol), 2-iodo-5-bromo pyridine (2.96 g, 1.04 mmol), $Pd(PPh_3)_4$ (603 mg, 0.0522 mmol), and 2M aq Na_2CO_3 (20 mL) in DME (50 mL) was sparged with N_2 for 15 min. Then the reaction mixture was heated at 100 °C for 24h. The reaction mixture was allowed to cool to room temperature and evaporated under vacuo to yield a solid residue. The solid residue was extracted with dichloromethane and washed with water, followed by saturated brine solution. The organic layer was dried over Na_2SO_4, filtered and evaporated under vacuo to yield a solid residue. The solid residue was chromatographed on silica gel using DCM:Hexane (1:1) as the eluent to yield a

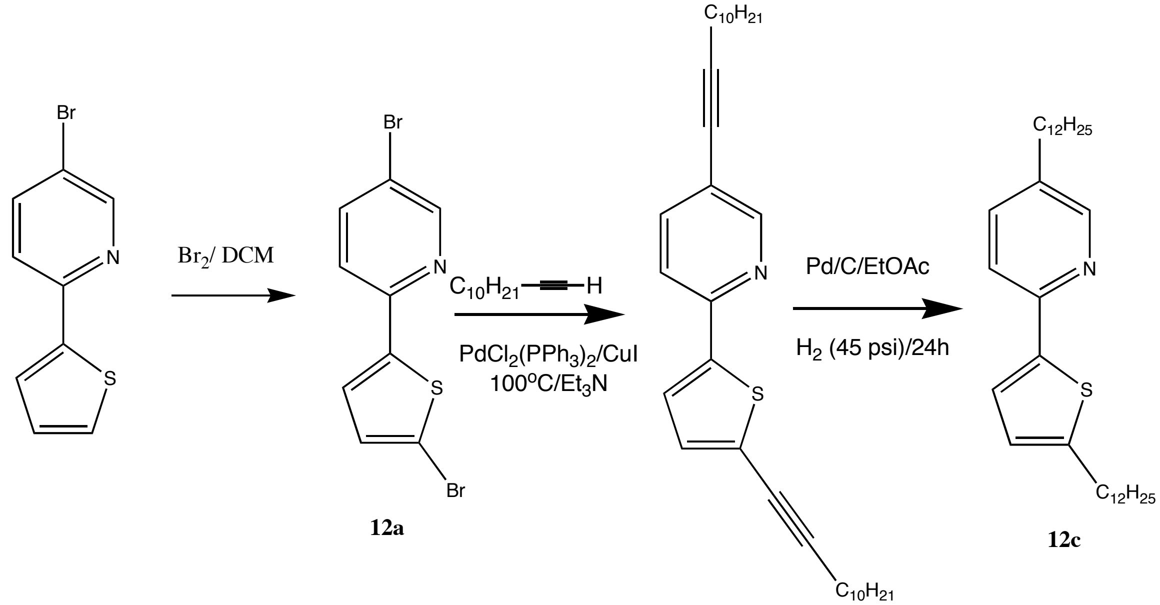
white solid. (3.2 g, 74%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.68 (d, 1H), 7.91 (m, 2H), 7.82 (dd, 1H), 7.56 (d, 1H), 6.98 (d, 2H), 4.02 (t, 2H), 1.80 (m, 2H), 1.46 (m, 2H), 1.28 (m, 17H), 0.88 (t, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): 14.8, 23.4, 26.7, 29.9, 30.0, 30.1, 30.2, 30.31, 30.35, 30.4, 32.6, 68.8, 115.5, 119.0, 121.6, 128.7, 139.9, 151.1, 156.3, 161.0. HRMS calcd for $C_{23}H_{32}BrNO$ (M+H$^+$). (418.1740); found 418.1752.



Compound 11d: **11c** (3.2 g, 0.764 mmol), 1-dodecyne (3.26 mL, 1.52 mmol), $PdCl_2(PPh_3)_2$ (268 mg, 0.0382 mmol), and CuI (43 mg, 0.0382 mmol) in Et_3N (75 mL). After sparging with N_2 for 15 min, the reaction mixture was heated at 100 °C for 36h. The reaction mixture was allowed to cool to room temperature and evaporated under vacuo to yield a solid residue. The solid residue was extracted with dichloromethane and washed with water, followed by saturated brine solution. The organic layer was dried over Na_2SO_4, filtered and evaporated under vacuo to yield a solid residue. The solid residue was chromatographed on silica gel using DCM:Hexane (1:2) as the eluent to yield a white solid. Yield (3.9 g, 99%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.68 (m, 1H), 7.92 (m, 2H), 7.80 (dd, 1H), 7.69 (dd, 1H), 7.57 (m, 2H), 4.00 (m, 4H), 2.43 (m, 4H), 1.82 (m, 4H), 1.6-1.4 (m, 28H), 0.86 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): 14.85, 20.14, 20.24, 20.27, 23.40, 23.41, 26.74, 29.07, 29.24, 29.35, 29.65, 29.67, 29.71, 29.84, 29.87, 29.94, 29.95, 30.04, 30.05, 30.07, 30.12, 30.22, 30.23, 30.26, 30.30, 30.32, 30.36, 30.38, 32.61, 32.62, 32.64, 68.80, 81.2, 92.3, 94.3, 95.1, 115.39, 115.44, 119.47, 121.53, 126.63, 128.72, 128.8, 132.1 133.2, 136.9, 151.17, 152.8, 153.01, 156.2, 156.8, 161.3. HRMS calcd for $C_{35}H_{53}NO$ (M+H$^+$). (504.4200); found 504.4215.



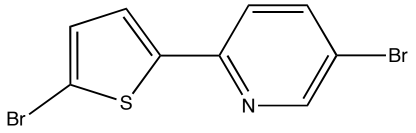
Compound 11e: **11d** (3.9 g, 0.77 mmol) and Pd/C (1.9 g) in ethylacetate (35 ml) pressurized in a parr bomb with 45 psi H_2 and the reaction mixture was shaken for 12h. After the reaction mixture was filtered over celite. The residue was washed with DCM and EtOAc and the filtrate was evaporated under vacuo to yield a off-white solid. The solid was chromatographed on silica gel using DCM:Hexane (1:1) as the eluent to yield a white solid. Yield (3.7 g, 95%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.48 (d, 1H), 7.89 (m, 2H), 7.75 (dd, 1H), 7.68 (dd, 1H), 6.98 (m, 2H), 4.00 (m, 4H), 2.41 (m, 4H), 1.79 (m, 4H), 1.6-1.25 (m, 28H), 0.87 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): 14.84, 23.40, 26.75, 29.87, 29.98, 30.06, 30.13, 30.15, 30.28, 30.29, 30.32, 30.35, 30.38, 31.90, 32.63, 33.36, 68.78, 115.32, 123.4, 128.58, 136.2, 138.6, 151.3, 156.7, 162.3. HRMS calcd for $C_{34}H_{56}N_2O$ (M+H$^+$). (509.4465); found 508.4518.



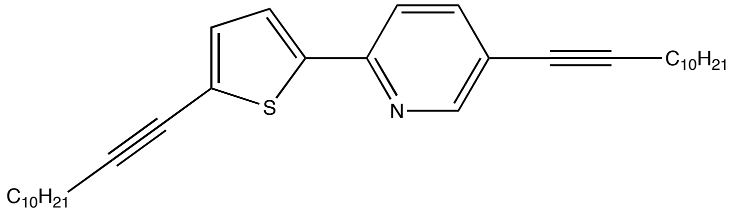
12a

12c

12b

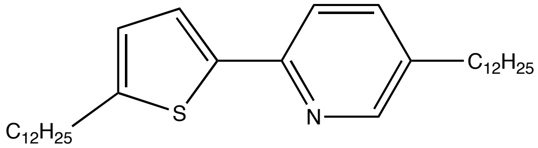


Compound 12a: To 2-thienyl-5-bromo-pyridine (3.0g, 1.24 mmol) in CH_2Cl_2 (85 mL), Br_2 (3.96g, 2.48 mmol) was added dropwise during 10 min. The reaction mixture was stirred at room temperature for 2h. After the reaction mixture was poured into 10% NaOH solution (200 mL) and the organic layer was washed with water and sat.brine solution. The organic layer was dried over Na2SO4, filtered and evaporated under vacuo to yield a white solid. The solid was chromatographed on silicagel using DCM: Hexane (2:1) as the eluent to yield a white solid. (2.55g, 64%). HRMS calcd for $C_9H_4Br_2NS$ ($M+H^+$). (317.8582); found 319.8562.



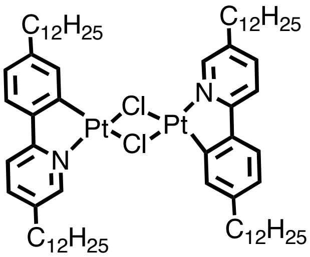
Compound 12b: **12a** (1.8 g, 0.564 mmol), 1-dodecyne (2.8 g, 1.6 mmol), $PdCl_2(PPh_3)_2$ (0.396 g, 0.0564 mmol), and CuI (0.107 g, 0.0564 mmol) in Et_3N (75 mL). After sparging with N_2 for 15 min, the reaction mixture was heated at 100 ^oC for 36h. The reaction mixture was allowed to cool to room temperature and evaporated under vacuo to yield a solid residue. The solid residue was extracted with dichloromethane and washed with water, followed by saturated brine solution. The organic layer was dried over Na_2SO_4, filtered and evaporated under vacuo to yield a solid residue. The solid residue was chromatographed on silica gel using DCM:Hexane (1:1) as the eluent to yield a white solid. Yield (2.0 g, 72%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.52 (m, 1H), 7.61 (m, 1H), 7.49 (dd, 1H), 7.37 (d, 1H), 7.07 (d, 1H), 2.43 (m, 4H), 1.63 (m, 4H), 1.43 (m, 4H),

1.26 (m, 28H), 0.86 (t, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): 14.8, 20.3, 20.5, 29.2, 29.6, 29.8, 30.0, 30.2, 32.6, 74.7, 78.3, 95.5, 97.2, 118.5, 120.0, 125.1, 127.2, 132.7, 139.6, 144.7, 150.8, 152.8. HRMS calcd for $C_{33}H_{47}NS$ (M+H$^+$). (489.3425); found 488.1155.

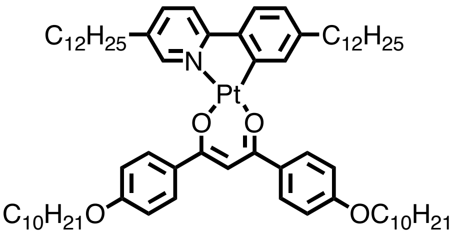


Compound 12c: **12b** (2.0 g, 0.4 mmol) and Pd/C (2.0 g) in ethylacetate (35 ml) pressurized in a parr bomb with 45 psi H_2 and the reaction mixture was shaken for 12h. After the reaction mixture was filtered over celite. The residue was washed with DCM and EtOAc and the filtrate was evaporated under vacuo to yield a off-white solid. The solid was chromatographed on silica gel using DCM:Hexane (1:1) as the eluent to yield a white solid. Yield (1.9 g, 95%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.35 (d, 1H), 7.51 (m, 2H), 7.33 (d, 1H), 6.75 (d, 2H), 2.82 (t, 2H), 2.59 (t, 2H), 1.69 (m, 6H), 1.4-1.2 (m, 44H), 0.87 (t, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): 14.8, 23.4, 29.7, 29.8, 30.07, 30.1, 30.14, 30.3, 30.4, 31.1, 31.8, 32.3, 32.6, 33.4, 118.6, 124.4, 125.7, 136.5, 137.1, 142.8, 148.6, 151.2 HRMS calcd for $C_{33}H_{55}NS$ (M+H$^+$). (497.4051); found 497.9369.

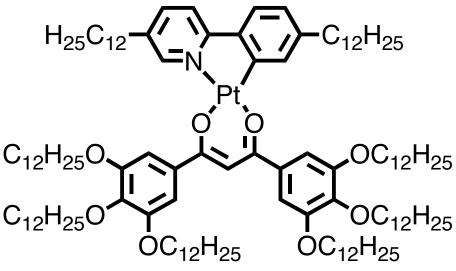
Synthesis of Metal Complexes



Compound **13**: To di-μ-chlorobis(η^3-2-methallyl)diplatinum (580 mg, 0.1 mmol) and ligand (1.00 g, 0.2 mmol) under argon, dry MeOH (20 mL) and dry CH_2Cl_2 (20 mL) was added. The reaction mixture was allowed to stir at room temperature for 96 h during which a precipitate formed. The precipitate was filtered and washed with MeOH and Hexane. Yield (0.840 g, 59%). The crude product was used in the next step without further purification.



Compound **1**: To **13** (218 mg, 0.151mmol), Ag_2O (60 mg, 0.225 mmol) and (*Z*)-1,3,-bis(4-(decyloxy)phenyl)-3-hydroxyprop-2-en-1-one[2] (161 mg, 0. 300mmol) under argon, dry THF was added and the reaction mixture was stirred at 65 °C for 24h. After the reaction mixture was allowed to cool to room temperature, it was evaporated under vacuo to yield a brown oily residue. The oily residue was dissolved in CH_2Cl_2 (25 mL) and passed through a short activated alumina column. CH_2Cl_2 was passed through the column until there was no elution of the target compound. The organic fractions were evaporated under vacuo to yield a yellow oily residue. The yellow oily residue wad chromatographed on a silica gel column using CH_2Cl_2:Hexane (1:2) as the eluent to afford a yellow solid. Further recrystallization from a mixture of CH_2Cl_2 and EtOH gave yellow crystals of **1**. Yield (0.147g, 40%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.97 (s, 1H), 8.08 (dd, 4H), 7.60 (m, 2H), 7.48 (d, 1H), 7.32 (d, 1H), 6.91 (m, 5H), 6.69 (s, 1H), 4.03 (m, 4H), 2.69 (m, 4H), 1.84 (m, 8H), 1.4-1.2 (m, 64H), 0.87 (m, 12H). ^{13}C NMR (125.78 MHz, $CDCl_3$): 14.8, 23.4, 26.7, 29.8, 30.05, 30.09, 30.14, 30.19, 30.26, 30.29, 30.31, 30.32, 30.36, 30.39, 30.42, 30.45, 30.49, 31.07, 31.86, 32.61, 32.63, 32.65, 33.42, 37.11, 68.85, 68.88, 96.24, 114.93, 114.99, 118.34, 123.23, 124.52, 129.42, 129.56, 131.27, 132.35, 133.22, 136.13, 138.82, 139.30, 143.24, 144.57, 147.19, 161.97, 162.10, 166.63, 178.37, 179.15. MS (MALDI-TOF) calcd for $C_{70}H_{107}NO_4Pt$ (M+H$^+$). (1221.7665); found 1222.1370.



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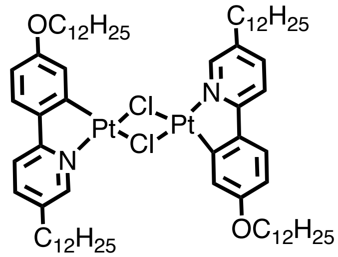
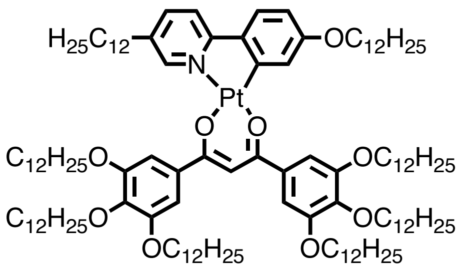
Compound **2**: To **13** (400 mg, 0. 27 mmol), Ag_2O (128 mg, 0. 50 mmol) and (*Z*)-3-hydroxy-1,3,-bis(3,4,5-tris(dodecyloxy)phenyl)prop-2-en-1-one[2] (1.10 g, 0. 80 mmol) under argon, dry THF was added and the reaction mixture was stirred at 65°C for 24h. After the reaction mixture was allowed to cool to room temperature, it was evaporated under vacuo to yield a brown oily residue. The oily residue was dissolved in CH_2Cl_2 (25 mL) and passed through a short activated alumina column. CH_2Cl_2 was passed through the column until there was no elution of the target compound. The organic fractions were evaporated under vacuo to yield a yellow oily residue. The yellow oily residue was chromatographed on a silica gel column with CH_2Cl_2:Hexane (1:1) as the eluent to afford a yellow solid. Further recrystallization of the solid from a CH_2Cl_2/EtOH mixture gave yellow crystals of **2**. Recrytsallization was repeated using EtOAc/EtOH mixture to afford yellow crystals of the title compound. Yield (0.150 g, 28%). ^1H NMR (300 MHz, $CDCl_3$): δ 8.85 (s, 1H), 7.64 (m, 4H), 7.32 (m, 4H), 6.89 (d, 1H), 6.60 (s, 1H), 4.06 (m, 12H), 2.63 (t, 4H), 1.86 (m, 12H), 1.4-1.2 (m, 148H), 0.87 (m, 24H). ^{13}C NMR (125.78 MHz, $CDCl_3$): 14.83, 23.41, 26.85, 26.95, 26.97, 29.97, 30.10, 30.12, 30.22, 30.23, 30.36, 30.37, 30.38, 30.40, 30.42, 30.46, 30.49, 31.11, 31.71, 32.42, 32.65, 32.66, 69.99, 74.18, 74.22, 97.47, 106.50, 106.70, 118.50, 123.38, 124.57, 131.53, 135.03, 136.14, 138.82, 138.92, 141.44, 141.58, 143.30, 144.62, 147.43, 153.69, 153.79, 166.76, 178.85, 179.84. MS (MALDI-TOF) calcd for $C_{122}H_{211}NO_8Pt$ ($M+H^+$). (2014.5807); found 2014.2601.



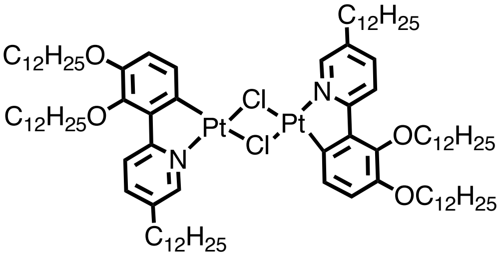
Compound **14**: To di-μ-chlorobis(η^3-2-methallyl)diplatinum (134 mg, 0.2 mmol) and ligand (240 mg, 0.5 mmol) under argon, dry MeOH (10 mL) and dry CH_2Cl_2 (10 mL) was added. The reaction mixture was allowed to stir at room temperature for 96 h during which a precipitate formed. The precipitate was filtered and washed with MeOH and Hexane. Yield (0.230 g, 78%). The crude product was used in the next step without further purification.



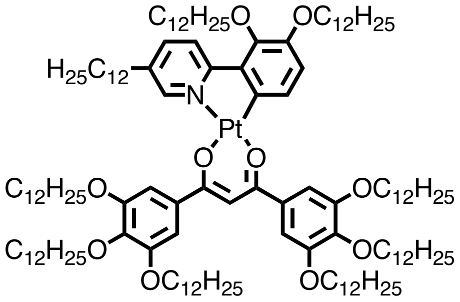
3

Compound **3**: To **14** (100 mg, 0.7 mmol), Ag_2O (23 mg, 0.9 mmol) and (*Z*)-3-hydroxy-1,3,-bis(3,4,5-tris(dodecyloxy)phenyl)prop-2-en-1-one (176 mg, 0. 14 mmol) under argon, dry THF was added and the reaction mixture was stirred at 65 ^oC for 24h. After the reaction mixture was allowed to cool to room temperature, it was evaporated under vacuo to yield a brown oily residue. The oily residue was dissolved in CH_2Cl_2 (25 mL) and passed through a short activated alumina column. CH_2Cl_2 was passed through the column until there was no elution of the target compound. The organic fractions were evaporated under vacuo to yield a yellow oily residue. The yellow oily residue was chromatographed on a silica gel column with CH_2Cl_2:Hexane (1:1) as the eluent to afford a yellow solid. Further recrystallization of the solid from a CH_2Cl_2/EtOH mixture gave yellow crystals of **3**. Recrytsallization was repeated using EtOAc/EtOH mixture to afford yellow crystals of the title compound. Yield (0.125 g, 88%). ^1H NMR (300 MHz,

$CDCl_3$): δ 8.86 (s, 1H), 7.58 (m, 1H), 7.43 (d, 1H), 7.37 (d, 1H), 7.25 (m, 4H), 6.67 (d, 1H), 6.56 (s, 1H), 4.03 (m, 14H), 2.63 (t, 2H), 1.86 (m, 20H), 1.4-1.2 (m, 150H), 0.86 (m, 24H). ^{13}C NMR (125.78 MHz, $CDCl_3$): 14.83, 23.41, 26.85, 26.95, 26.97, 29.97, 30.10, 30.12, 30.22, 30.23, 30.36, 30.37, 30.38, 30.40, 30.42, 30.46, 30.49, 31.11, 31.71, 32.42, 32.65, 32.66, 69.99, 74.18, 74.22, 97.47, 106.50, 106.79, 118.50, 123.38, 124.57, 131.26, 135.83, 136.23, 138.91, 138.92, 141.44, 141.58, 143.30, 144.62, 147.43, 153.70, 153.79, 160.64, 166.76, 179.34, 179.86. MS (MALDI-TOF) calcd for $C_{122}H_{211}NO_9Pt$ (M+H$^+$). (2030.5756); found 2030.6500.

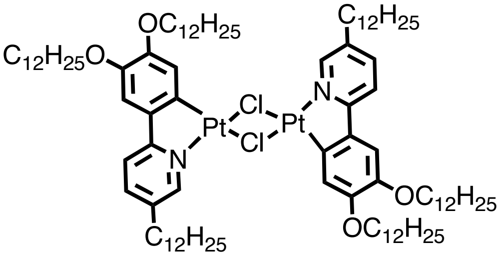


Compound **15**: To di-μ-chlorobis(η^3-2-methallyl)diplatinum (580 mg, 0.072 mmol) and ligand (1.00 g, 0.14 mmol) under argon, dry MeOH (20 mL) and dry CH_2Cl_2 (20 mL) was added. The reaction mixture was allowed to stir at room temperature for 96 h during which a precipitate formed. The precipitate was filtered and washed with MeOH and Hexane. Yield (0.480 g, 36%). The crude product was used in the next step without further purification.

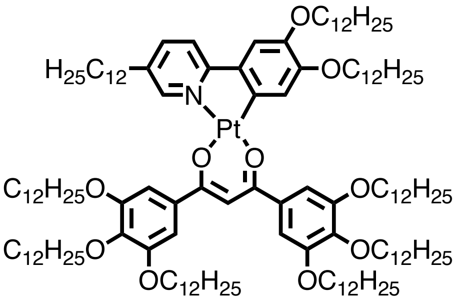


4

Compound **4**: To **15** (100 mg, 0.5 mmol), Ag_2O (25 mg, 0.10 mmol) and (*Z*)-3-hydroxy-1,3,-bis(3,4,5-tris(dodecyloxy)phenyl)prop-2-en-1-one (216 mg, 0.16 mmol) under argon, dry THF was added and the reaction mixture was stirred at 65°C for 24h. After the reaction mixture was allowed to cool to room temperature, it was evaporated under vacuo to yield a brown oily residue. The oily residue was dissolved in CH_2Cl_2 (25 mL) and passed through a short activated alumina column. CH_2Cl_2 was passed through the column until there was no elution of the target compound. The organic fractions were evaporated under vacuo to yield a yellow oily residue. The yellow oily residue was chromatographed on a silica gel column with CH_2Cl_2:Hexane (1:1) as the eluent to afford a yellow solid. Further recrystallization of the solid from a CH_2Cl_2/EtOH mixture gave yellow crystals of **4**. Recrytsallization was repeated using EtOAc/EtOH mixture to afford yellow crystals of the title compound. Yield (50 mg, 42%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.0 (s, 1H), 8.41 (d, 2H), 7.62 (d, 2H), 7.37 (d, 2H), 6.88 (d, 2H), 6.56 (s, 1H), 4.03 (m, 16H), 2.64 (t, 2H), 1.86 (m, 18H), 1.4-1.2 (m, 172H), 0.86 (m, 27H). ^{13}C NMR (125.78 MHz, $CDCl_3$): 14.8, 23.4, 26.8, 26.9, 27.0, 30.0, 30.1, 30.2, 30.23, 30.26, 30.27, 30.32, 30.34, 30.37, 30.40, 30.42, 30.44, 30.46, 30.48, 31.0, 31.1, 31.14, 31.6, 32.65, 32.66, 33.66, 70.0, 70.03, 70.07, 73.7, 74.1, 74.2, 97.5, 106.4, 106.7, 116.5, 122.4, 125.6, 128.9, 135.2, 136.1, 136.5, 138.2, 138.8, 141.4, 141.5, 147.4, 147.5, 150.0, 153.6, 153.7, 165.6, 179.0, 179.8. MS (MALDI-TOF) calcd for $C_{134}H_{235}NO_{10}Pt$ (M+H$^+$). (2214.7584); found 2214.9632.

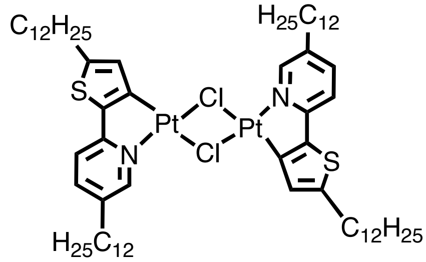


Compound **16**: To di-μ-chlorobis(η^3-2-methallyl)diplatinum (288 mg, 0.5 mmol) and ligand (700 mg, 0.10 mmol) under argon, dry MeOH (15 mL) and dry CH_2Cl_2 (15 mL) was added. The reaction mixture was allowed to stir at room temperature for 96 h during which precipitate formed. The precipitate was filtered and washed with MeOH and Hexane. Yield (250 mg, 27%). The crude product was used in the next step without further purification.

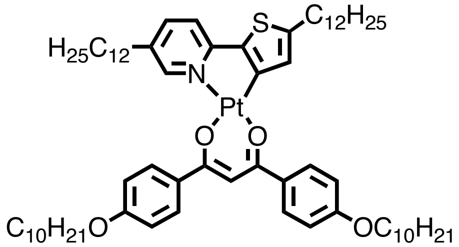


5

Compound **5**: To **16** (250 mg, 0.13 mmol), Ag_2O (62 mg, 0.26 mmol) and (*Z*)-3-hydroxy-1,3,-bis(3,4,5-tris(dodecyloxy)phenyl)prop-2-en-1-one (541 mg, 0.40 mmol) under argon, dry THF was added and the reaction mixture was stirred at 65°C for 24h. After the reaction mixture was allowed to cool to room temperature, it was evaporated under vacuo to yield a brown oily residue. The oily residue was dissolved in CH_2Cl_2 (25 mL) and passed through a short activated alumina column. CH_2Cl_2 was passed through the column until there was no elution of the target compound. The organic fractions were evaporated under vacuo to yield a yellow oily residue. The yellow oily residue was chromatographed on a silica gel column starting with CH_2Cl_2:Hexane (1:1) as the eluent and was later ramped to CH_2Cl_2:Hexane (2:1) to afford a yellow solid. Further recrystallization of the solid from a CH_2Cl_2/EtOH mixture gave yellow crystals of **7**. Recrytsallization was repeated using EtOAc/EtOH mixture to afford yellow crystals of the title compound. Yield (200 mg, 70%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.85 (s, 1H), 7.57 (d, 1H), 7.38 (d, 1H), 7.20 (m, 4H), 7.05 (s, 1H), 6.52 (s, 1H), 4.03 (m, 16H), 2.63 (t, 2H), 1.83 (m, 18H), 1.4-1.2 (m, 172H), 0.86 (m, 27H). ^{13}C NMR (125.78 MHz, $CDCl_3$): 14.8, 23.4, 26.83, 26.84, 26.86, 26.92, 26.94, 27.0, 29.9, 30.0, 30.10, 30.11, 30.13, 30.21, 30.24, 30.25, 30.32, 30.33, 30.35, 30.37, 30.40, 30.41, 30.43, 30.45, 30.46, 30.47, 30.49, 31.1, 31.7, 32.63, 32.65, 32.67, 33.6, 69.3, 69.9, 70.2, 71.3, 74.2, 77.4, 77.7, 77.9, 98.2, 106.4, 106.8, 111.7, 115.1, 118.0, 132.5, 135.1, 135.9, 137.2, 138.8, 141.5, 141.6, 146.7, 147.2, 151.2, 153.7, 153.8, 166.8, 179.61, 179.65. MS (MALDI-TOF) calcd for $C_{134}H_{235}NO_{10}Pt$ ($M+H^+$). (2214.7584); found 2214.0121.

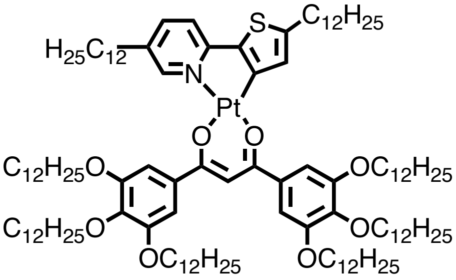


Compound **17**: To di-μ-chlorobis(η^3-2-methallyl)diplatinum (946 mg, 0.16 mmol) and ligand (1.65, 0.33 mmol) under argon, dry MeOH (20 mL) and dry CH_2Cl_2 (20 mL) was added. The reaction mixture was allowed to stir at room temperature for 96 h during which a yellow precipitate formed. The precipitate was filtered and washed with MeOH and Hexane. Yield (686 mg, 35%). The crude product was used in the next step without further purification.



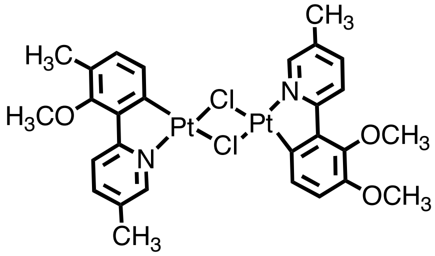
Compound **6**: To **17** (169 mg, 0.12 mmol), Ag_2O (60 mg, 0.26 mmol) and (*Z*)-1,3,-bis(4-(decyloxy)phenyl)-3-hydroxyprop-2-en-1-one (207 mg, 0.35 mmol) under argon, dry THF was added and the reaction mixture was stirred at 65 °C for 24h. After the reaction mixture was allowed to cool to room temperature, it was evaporated under vacuo to yield a brown oily residue. The oily residue was dissolved in CH_2Cl_2 (25 mL) and passed through a short activated alumina column. CH_2Cl_2 was passed through the column until there was no elution of the target compound. The organic fractions were evaporated under vacuo to yield a yellow oily residue. The yellow oily residue wad chromatographed on a silica gel column using CH_2Cl_2:Hexane (1:1) as the eluent to afford a yellow solid. Further recrystallization from a mixture of CH_2Cl_2 and EtOH gave yellow crystals of **6**. Yield (35 mg, 24%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.70 (s, 1H), 7.49 (d, 1H), 7.14 (d, 1H), 6.94 (s, 1H), 6.59 (s, 1H), 4.03 (t, 4H), 2.94 (t, 2H), 2.64 (t, 2H), 1.83 (m, 18H), 1.56-1.26 (m, 72

H), 0.86 (m, 12H). ^{13}C NMR (125.78 MHz, CDCl$_3$): 14.8, 23.4, 26.83, 26.84, 26.86, 26.92, 26.94, 27.0, 29.9, 30.0, 30.10, 30.11, 30.13, 30.21, 30.24, 30.25, 30.32, 30.33, 30.35, 30.37, 30.40, 30.41, 30.43, 30.45, 30.46, 30.47, 30.49, 31.1, 31.7, 32.63, 32.65, 32.67, 33.6, 69.3, 69.9, 70.2, 71.3, 74.2, 77.4, 77.7, 77.9, 98.2, 106.4, 106.8, 111.7, 115.1, 118.0, 132.5, 135.1, 135.9, 137.2, 138.8, 141.5, 141.6, 146.7, 147.2, 151.2, 153.7, 153.8, 166.8, 179.61, 179.65. MS (MALDI-TOF) calcd for $C_{68}H_{101}NO_4PtS$ (M+H$^+$). (1226.7483); found 1226.8975.

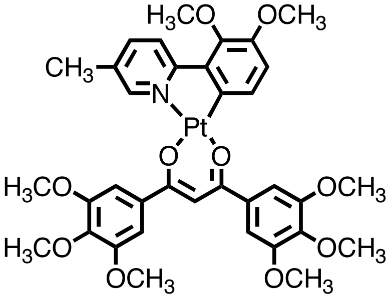


7

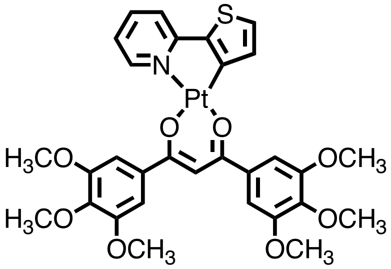
Compound **6**: To **17** (600 mg, 0.4 mmol), Ag$_2$O (143 mg, 0.6 mmol) and (*Z*)-3-hydroxy-1,3,-bis(3,4,5-tris(dodecyloxy)phenyl)prop-2-en-1-one (1.64 g, 0.12 mmol) under argon, dry THF was added and the reaction mixture was stirred at 65°C for 24h. After the reaction mixture was allowed to cool to room temperature, it was evaporated under vacuo to yield a brown oily residue. The oily residue was dissolved in CH$_2$Cl$_2$ (25 mL) and passed through a short activated alumina column. CH$_2$Cl$_2$ was passed through the column until there was no elution of the target compound. The organic fractions were evaporated under vacuo to yield a yellow oily residue. The yellow oily residue wad chromatographed on a silica gel column using CH$_2$Cl$_2$:Hexane (1:1) as the eluent to afford a yellow solid. Further recrystallization from a mixture of CH$_2$Cl$_2$ and EtOH gave yellow crystals of **7**.Yield (170 mg, 21%). ^{1}H NMR (300 MHz, CDCl$_3$): δ 8.68 (s, 1H), 7.47 (d, 1H), 7.10 (d, 1H), 6.93 (s, 1H), 6.54 (s, 1H), 4.09 (m, 12H), 2.89 (t, 2H), 2.59 (t, 2H), 1.89-1.77 (m, 16H), 1.56-1.26 (m, 144H), 0.86 (m, 24H). ^{13}C NMR (125.78 MHz, CDCl$_3$): 14.8, 23.4, 26.82, 26.85, 30.0, 30.1, 30.32, 30.39, 30.41, 30.44, 30.45, 30.47, 31.0, 32.64, 32.65, 70.0, 70.1, 74.1, 97.8, 106.7, 118.0, 119.1, 128.6, 130.6, 134.7, 136.0, 139.5, 139.6, 141.8, 144.2, 147.7, 153.6, 153.7, 165.0, 178.7, 179.9. MS (MALDI-TOF) calcd for $C_{120}H_{209}NO_8PtS$ (M+H$^+$). (2020.5369); found 2020.7283.



Compound **18**: To K_2PtCl_4 (400 mg, 0.20 mmol) and (2-(3,4-dimethoxyphenyl)-5-methyl pyridine (440 mg, 0.20 mmol) under argon, 2-Ethoxyethanol (60 mL) and H_2O (20 mL) were added. The reaction mixture was heated at 100°C for 20h after sparging with argon for 15 min. The reaction mixture was allowed to cool down before pouring into H_2O (200 mL) to precipitate the product. The precipitate was filtered, dissolved in CH_2Cl_2 and dried over Na_2SO_4. After filtration, the solvent was evaporated under vacuo to afford a yellow solid. Yield (360 mg, 42%). The crude product was directly used in the next without further purification.



Compound **4a**: To **18** (240 mg, 0.26 mmol), Na_2CO_3 (277 mg, 2.6 mmol) and (Z)-3-hydroxy-1,3,-bis(3,4,5-trimethoxyphenyl)prop-2-en-1-one (317 mg, 0.78 mmol) under argon, 2-Ethoxyethanol (25 mL) was added and the reaction mixture was heated at 100°C for 20h after sparging with argon for 15 min. After the reaction mixture was allowed to cool to room temperature, it was evaporated under vacuo to yield a brown oily residue. The oily residue was dissolved in CH_2Cl_2 (25 mL) and passed through a short activated alumina column. The column was washed with CH_2Cl_2 till there was no elution of the target compound. The organic fractions were evaporated under vacuo to yield a yellow oily residue. The yellow oily residue was chromatographed on a silica gel column with CH_2Cl_2:Hexane (4:1) as the eluent to afford a yellow solid. Yellow colored X-ray quality single crystals were obtained by slow evaporation of the title compound from a CH_2Cl_2/MeOH mixture. Yield (154mg, 72%). ^1H NMR (300 MHz, $CDCl_3$): δ 8.89 (s, 1H), 8.15 (d, 1H), 7.50 (d, 1H), 7.32 (m, 5H), 6.85 (d, 1H), 6.49 (s, 1H), 4.03 (m, 24H), 2.26 (s, 3H). ^{13}C NMR (125.78 MHz, $CDCl_3$): 18.9, 56.70, 56.72, 56.92, 56.93, 56.97, 56.98, 60.67, 60.68, 61.43, 61.44, 61.49, 61.5, 97.1, 104.9, 105.1, 113.9, 123.4, 125.7, 129.4, 131.9, 135.6, 135.8, 138.0, 139.7, 140.9, 141.3, 147.8, 150.5, 153.72, 153.73, 164.7, 178.4, 178.8. MS (MALDI-TOF) calcd for $C_{35}H_{37}NO_{10}Pt$ ($M+H^+$). (826.2062); found 826.0698.



Compound **8a**: To di-μ-chlorobis(2-(thiophen-2-yl)pyridine)diplatinum (450 mg, 0.6 mmol), Na_2CO_3 (610 mg, 6.0 mmol) and (Z)-3-hydroxy-1,3,-bis(3,4,5-trimethoxyphenyl)prop-2-en-1-one (698 mg, 0.17 mmol) under argon, 2-Ethoxyethanol (25 mL) was added and the reaction mixture was heated at 100°C for 20h after sparging with argon for 15 min. After the reaction mixture was allowed to cool to room temperature, it was evaporated under vacuo to yield a brown oily residue. The oily residue was dissolved in CH_2Cl_2 (25 mL) and passed through a short activated alumina column. The column was washed with CH_2Cl_2 till there was no elution of the target compound. The organic fractions were evaporated under vacuo to yield a yellow oily residue. The yellow oily residue was chromatographed on a silica gel column with CH_2Cl_2:Hexane (3:1) as the eluent to afford a orange solid. Orange colored X-ray quality single crystals were obtained by slow evaporation of the title compound from a CH_2Cl_2/MeOH mixture. Yield (286 mg, 63%). ^1H NMR (300 MHz, $CDCl_3$): δ 8.81 (s, 1H), 7.16 (t, 1H), 7.50 (d, 1H), 7.23 (m, 3H), 6.86 (t, 1H), 6.53 (s, 1H), 4.03 (m, 18H), ^{13}C NMR (125.78 MHz, $CDCl_3$): 56.9, 61.5, 97.6, 105.1, 118.0, 119.2, 128.5, 130.5, 135.1, 136.3, 139.4, 139.6, 141.2, 141.3, 144.0, 147.5, 153.8, 164.8, 178.1, 179.4. MS (MALDI-TOF) calcd for $C_{30}H_{29}NO_8PtS$ ($M+H^+$). (758.1258); found 757.9170.

References:

1 Z. G. Zhu, T. M. Swager, *Org. Lett.*, 2001, **22**, 3471.

2 T. Hegemann, J. Kain, S. Diele, B. Schubert, H. Bögel, and C. Tschierske, *J. Mat. Chem.,* 2003, **13**, 991.

Fitting procedure of the XRD results.

Lattice parameters were obtained after fitting the experimental XRD data to a theoretical lattice. First the lattice was estimated and corresponding reflections were calculated. Then the error of the experimental spacings with those of the theoretical lattice was calculated and weighed by the intensity of the experimental spacing. A summation of the weighed errors was minimized by variation of the lattice parameters of the theoretical lattice in several iterations. It is noted that this procedure is solely used for optimization of the experimentally observed lattice parameters and not to find appropriate lattices.

Crystallographic Details

Low temperature (100 K) diffraction data were collected on a Siemens Platform three-circle diffractometer coupled to a Bruker-AXS Smart Apex CCD detector with graphite-monochromated Mo Kα radiation ($\lambda = 0.71073$ Å), performing φ- and ω-scans. Data reduction for all datasets was performed with the program SAINT version 7.12[1], and semi-empirical absorption correction was performed using SADABS[2]. All structures were solved by direct methods using SHELXS[3] and refined against F^2 on all data by full-matrix least squares with SHELXL-97[4]. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model.

The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). Details of the data quality and a summary of the residual values of the refinements are listed in Tables 1 and 6, all bond lengths and angles are given in Tables 3 and 8.

The C_9H_6NS ligand in the structure of compound **7a** is disordered over two coplanar positions. This disorder was refined with the help of planarity restraints, similarity restraints on 1-2 and 1-3 distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters. In addition equal anisotropic displacement parameter constraints were used for the following four almost overlapping pairs of atoms: C(9)/C(7A), C(8)/C(8A), N(1)/C(3A), C(3)/N(1A). The occupancy ratio was refined freely, while constraining the total occupancy of both components to unity.

Table 1. Crystal data and structure refinement for **4a**.

Identification code	07062	
Empirical formula	C35 H37 N O10 Pt	
Formula weight	826.75	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.484(3) Å	α= 93.617(4)°.
	b = 10.860(3) Å	β= 104.214(4)°.
	c = 14.752(3) Å	γ = 98.912(4)°.
Volume	1599.5(6) Å^3	
Z	2	
Density (calculated)	1.717 Mg/m^3	
Absorption coefficient	4.448 mm^{-1}	
F(000)	824	
Crystal size	0.20 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.43 to 29.57°.	
Index ranges	-14<=h<=14, -15<=k<=14, -20<=l<=20	
Reflections collected	35584	
Independent reflections	8951 [R(int) = 0.0312]	
Completeness to theta = 29.57°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6647 and 0.4699	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8951 / 81 / 433	
Goodness-of-fit on F^2	1.077	
Final R indices [I>2sigma(I)]	R1 = 0.0203, wR2 = 0.0505	
R indices (all data)	R1 = 0.0225, wR2 = 0.0516	
Largest diff. peak and hole	1.905 and -1.205 e.Å^{-3}	

$R1 = \sum(F_o - F_c) / \sum F_o$; $I > 2\sigma(I)$; $wR2 = \{\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2\}^{1/2}$

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

	x	y	z	U(eq)
Pt(1)	5446(1)	7114(1)	5606(1)	13(1)
O(1)	4778(2)	7208(1)	4161(1)	18(1)
O(2)	4258(2)	8291(1)	5867(1)	16(1)
O(6)	718(2)	12166(1)	5026(1)	20(1)
O(7)	1268(2)	12529(1)	6920(1)	21(1)
O(8)	2736(2)	11100(2)	8010(1)	22(1)
O(9)	9110(2)	5672(1)	8255(1)	19(1)
O(10)	8377(2)	6710(2)	9709(1)	23(1)
N(1)	6708(2)	5968(2)	5479(1)	14(1)
C(7)	4091(2)	8016(2)	3794(1)	16(1)
C(6)	3826(2)	7996(2)	2750(1)	18(1)
C(1)	4403(2)	7176(2)	2277(2)	21(1)
C(2)	4190(2)	7129(2)	1307(2)	24(1)
O(3)	4717(2)	6351(2)	793(1)	30(1)
C(16)	5524(3)	5546(2)	1308(2)	32(1)
C(3)	3386(3)	7904(2)	796(2)	26(1)
O(4)	3241(2)	7903(2)	-160(1)	34(1)
C(17)	2081(3)	7048(3)	-709(2)	46(1)
C(4)	2781(2)	8704(2)	1265(2)	25(1)
O(5)	1996(2)	9422(2)	721(1)	32(1)
C(18)	1183(3)	10070(2)	1169(2)	31(1)
C(5)	3006(2)	8756(2)	2244(2)	22(1)
C(8)	3597(2)	8881(2)	4305(1)	16(1)
C(9)	3649(2)	8955(2)	5262(1)	15(1)
C(10)	2972(2)	9876(2)	5673(1)	15(1)
C(11)	2130(2)	10569(2)	5108(1)	17(1)
C(12)	1556(2)	11448(2)	5525(2)	16(1)
C(13)	1809(2)	11638(2)	6502(2)	16(1)
C(14)	2607(2)	10904(2)	7067(1)	17(1)
C(15)	3194(2)	10039(2)	6650(1)	17(1)
C(19)	270(2)	11833(2)	4030(2)	22(1)
C(20)	-94(2)	12072(2)	6919(2)	24(1)
C(21)	3356(3)	10215(2)	8576(2)	26(1)
C(22)	6791(2)	5485(2)	4636(1)	16(1)
C(23)	7686(2)	4702(2)	4532(2)	18(1)
C(24)	8517(2)	4409(2)	5352(2)	19(1)
C(25)	8430(2)	4895(2)	6228(2)	18(1)
C(26)	7517(2)	5680(2)	6292(1)	15(1)
C(27)	7262(2)	6277(2)	7142(1)	15(1)
C(28)	6202(2)	6974(2)	6949(1)	15(1)
C(29)	5828(2)	7507(2)	7708(1)	17(1)
C(30)	6499(2)	7402(2)	8634(1)	19(1)
C(31)	7587(2)	6788(2)	8820(1)	17(1)
C(32)	7970(2)	6208(2)	8073(1)	16(1)
C(33)	8062(2)	7383(2)	10468(2)	24(1)
C(34)	9007(2)	4548(2)	8717(2)	23(1)
C(35)	7717(2)	4208(2)	3564(2)	23(1)

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

Pt(1)-C(28)	1.970(2)
Pt(1)-N(1)	1.9844(17)
Pt(1)-O(2)	1.9989(15)
Pt(1)-O(1)	2.0890(15)
O(1)-C(7)	1.283(2)
O(2)-C(9)	1.292(2)
O(6)-C(12)	1.374(2)
O(6)-C(19)	1.432(3)
O(7)-C(13)	1.380(2)
O(7)-C(20)	1.438(3)
O(8)-C(14)	1.364(2)
O(8)-C(21)	1.440(3)
O(9)-C(32)	1.385(2)
O(9)-C(34)	1.438(3)
O(10)-C(31)	1.383(2)
O(10)-C(33)	1.433(3)
N(1)-C(22)	1.347(3)
N(1)-C(26)	1.373(3)
C(7)-C(8)	1.404(3)
C(7)-C(6)	1.495(3)
C(6)-C(1)	1.394(3)
C(6)-C(5)	1.400(3)
C(1)-C(2)	1.389(3)
C(2)-O(3)	1.365(3)
C(2)-C(3)	1.406(4)
O(3)-C(16)	1.433(3)
C(3)-O(4)	1.381(3)
C(3)-C(4)	1.395(4)
O(4)-C(17)	1.438(3)
C(4)-O(5)	1.372(3)
C(4)-C(5)	1.401(3)
O(5)-C(18)	1.436(3)
C(8)-C(9)	1.396(3)
C(9)-C(10)	1.492(3)
C(10)-C(15)	1.397(3)
C(10)-C(11)	1.402(3)
C(11)-C(12)	1.392(3)
C(12)-C(13)	1.396(3)
C(13)-C(14)	1.406(3)
C(14)-C(15)	1.389(3)
C(22)-C(23)	1.390(3)
C(23)-C(24)	1.393(3)
C(23)-C(35)	1.502(3)
C(24)-C(25)	1.394(3)
C(25)-C(26)	1.393(3)
C(26)-C(27)	1.477(3)
C(27)-C(32)	1.404(3)
C(27)-C(28)	1.421(3)
C(28)-C(29)	1.395(3)
C(29)-C(30)	1.394(3)
C(30)-C(31)	1.388(3)
C(31)-C(32)	1.408(3)
C(28)-Pt(1)-N(1)	81.22(8)
C(28)-Pt(1)-O(2)	93.38(7)

N(1)-Pt(1)-O(2)	174.51(6)
C(28)-Pt(1)-O(1)	175.31(7)
N(1)-Pt(1)-O(1)	94.32(6)
O(2)-Pt(1)-O(1)	91.06(6)
C(7)-O(1)-Pt(1)	124.14(13)
C(9)-O(2)-Pt(1)	125.00(13)
C(12)-O(6)-C(19)	116.34(16)
C(13)-O(7)-C(20)	111.72(16)
C(14)-O(8)-C(21)	116.18(17)
C(32)-O(9)-C(34)	114.71(16)
C(31)-O(10)-C(33)	115.69(17)
C(22)-N(1)-C(26)	120.22(18)
C(22)-N(1)-Pt(1)	122.37(14)
C(26)-N(1)-Pt(1)	117.41(13)
O(1)-C(7)-C(8)	124.52(18)
O(1)-C(7)-C(6)	115.46(18)
C(8)-C(7)-C(6)	120.02(18)
C(1)-C(6)-C(5)	119.89(19)
C(1)-C(6)-C(7)	118.18(19)
C(5)-C(6)-C(7)	121.9(2)
C(2)-C(1)-C(6)	120.2(2)
O(3)-C(2)-C(1)	123.8(2)
O(3)-C(2)-C(3)	116.0(2)
C(1)-C(2)-C(3)	120.2(2)
C(2)-O(3)-C(16)	116.37(18)
O(4)-C(3)-C(4)	120.4(2)
O(4)-C(3)-C(2)	119.8(2)
C(4)-C(3)-C(2)	119.7(2)
C(3)-O(4)-C(17)	112.88(19)
O(5)-C(4)-C(3)	116.6(2)
O(5)-C(4)-C(5)	123.5(2)
C(3)-C(4)-C(5)	119.9(2)
C(4)-O(5)-C(18)	116.63(18)
C(6)-C(5)-C(4)	120.0(2)
C(9)-C(8)-C(7)	127.41(19)
O(2)-C(9)-C(8)	126.04(19)
O(2)-C(9)-C(10)	113.86(17)
C(8)-C(9)-C(10)	120.09(18)
C(15)-C(10)-C(11)	119.87(19)
C(15)-C(10)-C(9)	118.30(18)
C(11)-C(10)-C(9)	121.83(18)
C(12)-C(11)-C(10)	119.78(19)
O(6)-C(12)-C(11)	123.68(19)
O(6)-C(12)-C(13)	115.97(18)
C(11)-C(12)-C(13)	120.35(19)
O(7)-C(13)-C(12)	120.57(18)
O(7)-C(13)-C(14)	119.60(18)
C(12)-C(13)-C(14)	119.82(18)
O(8)-C(14)-C(15)	124.45(19)
O(8)-C(14)-C(13)	115.86(18)
C(15)-C(14)-C(13)	119.69(19)
C(14)-C(15)-C(10)	120.40(19)
N(1)-C(22)-C(23)	123.23(19)
C(22)-C(23)-C(24)	116.99(19)
C(22)-C(23)-C(35)	119.75(19)
C(24)-C(23)-C(35)	123.25(19)
C(23)-C(24)-C(25)	120.23(19)
C(26)-C(25)-C(24)	120.39(19)

N(1)-C(26)-C(25)	118.93(18)
N(1)-C(26)-C(27)	112.28(17)
C(25)-C(26)-C(27)	128.79(19)
C(32)-C(27)-C(28)	120.51(18)
C(32)-C(27)-C(26)	125.62(18)
C(28)-C(27)-C(26)	113.86(17)
C(29)-C(28)-C(27)	118.12(18)
C(29)-C(28)-Pt(1)	126.91(16)
C(27)-C(28)-Pt(1)	114.95(14)
C(30)-C(29)-C(28)	121.42(19)
C(31)-C(30)-C(29)	120.29(19)
O(10)-C(31)-C(30)	124.80(19)
O(10)-C(31)-C(32)	115.32(18)
C(30)-C(31)-C(32)	119.87(19)
O(9)-C(32)-C(27)	120.27(18)
O(9)-C(32)-C(31)	119.88(18)
C(27)-C(32)-C(31)	119.60(18)

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	15(1)	16(1)	10(1)	2(1)	4(1)	5(1)
O(1)	21(1)	21(1)	12(1)	2(1)	5(1)	7(1)
O(2)	19(1)	20(1)	12(1)	4(1)	4(1)	9(1)
O(6)	21(1)	19(1)	21(1)	3(1)	3(1)	8(1)
O(7)	19(1)	20(1)	25(1)	-3(1)	6(1)	7(1)
O(8)	28(1)	25(1)	15(1)	1(1)	7(1)	12(1)
O(9)	17(1)	21(1)	19(1)	5(1)	4(1)	7(1)
O(10)	28(1)	31(1)	11(1)	0(1)	1(1)	14(1)
N(1)	14(1)	14(1)	15(1)	1(1)	5(1)	2(1)
C(7)	14(1)	20(1)	12(1)	2(1)	3(1)	-1(1)
C(6)	16(1)	24(1)	11(1)	1(1)	3(1)	-1(1)
C(1)	22(1)	26(1)	13(1)	-1(1)	6(1)	-1(1)
C(2)	27(1)	28(1)	14(1)	-2(1)	8(1)	-5(1)
O(3)	39(1)	36(1)	15(1)	-4(1)	12(1)	1(1)
C(16)	43(2)	30(1)	24(1)	-4(1)	18(1)	1(1)
C(3)	34(1)	28(1)	12(1)	3(1)	4(1)	-7(1)
O(4)	48(1)	36(1)	12(1)	3(1)	7(1)	-9(1)
C(17)	66(2)	42(2)	14(1)	1(1)	-1(1)	-17(1)
C(4)	30(1)	26(1)	15(1)	7(1)	1(1)	-3(1)
O(5)	43(1)	33(1)	17(1)	10(1)	1(1)	4(1)
C(18)	31(1)	34(1)	26(1)	15(1)	0(1)	3(1)
C(5)	24(1)	24(1)	15(1)	4(1)	4(1)	0(1)
C(8)	16(1)	21(1)	13(1)	3(1)	3(1)	5(1)
C(9)	13(1)	16(1)	15(1)	2(1)	4(1)	2(1)
C(10)	13(1)	18(1)	14(1)	2(1)	4(1)	2(1)
C(11)	16(1)	18(1)	15(1)	2(1)	3(1)	3(1)
C(12)	14(1)	14(1)	20(1)	4(1)	4(1)	3(1)
C(13)	15(1)	15(1)	20(1)	0(1)	6(1)	3(1)
C(14)	15(1)	20(1)	16(1)	1(1)	4(1)	2(1)
C(15)	15(1)	20(1)	16(1)	3(1)	4(1)	4(1)
C(19)	23(1)	23(1)	21(1)	6(1)	2(1)	9(1)
C(20)	22(1)	28(1)	27(1)	4(1)	12(1)	11(1)
C(21)	34(1)	33(1)	15(1)	5(1)	7(1)	15(1)
C(22)	16(1)	18(1)	15(1)	1(1)	5(1)	3(1)
C(23)	18(1)	20(1)	18(1)	0(1)	8(1)	2(1)
C(24)	18(1)	21(1)	20(1)	4(1)	9(1)	9(1)
C(25)	18(1)	20(1)	17(1)	5(1)	6(1)	6(1)
C(26)	16(1)	16(1)	14(1)	2(1)	6(1)	2(1)
C(27)	16(1)	15(1)	14(1)	2(1)	5(1)	2(1)
C(28)	16(1)	15(1)	14(1)	2(1)	4(1)	2(1)
C(29)	18(1)	20(1)	15(1)	3(1)	4(1)	6(1)
C(30)	22(1)	22(1)	13(1)	1(1)	6(1)	8(1)
C(31)	20(1)	19(1)	12(1)	1(1)	2(1)	5(1)
C(32)	16(1)	17(1)	16(1)	3(1)	3(1)	5(1)
C(33)	29(1)	31(1)	12(1)	-1(1)	4(1)	8(1)
C(34)	26(1)	21(1)	21(1)	4(1)	3(1)	10(1)
C(35)	23(1)	28(1)	20(1)	-1(1)	9(1)	9(1)

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

	x	y	z	U(eq)
H(1)	4945	6648	2619	25
H(16A)	6322	6055	1739	47
H(16B)	5794	4989	868	47
H(16C)	5008	5043	1669	47
H(17A)	2172	6189	-575	69
H(17B)	1998	7119	-1379	69
H(17C)	1281	7254	-547	69
H(18A)	561	9460	1384	47
H(18B)	677	10558	718	47
H(18C)	1756	10636	1708	47
H(5)	2603	9308	2564	26
H(8)	3180	9485	3959	20
H(11)	1953	10440	4443	20
H(15)	3750	9556	7032	20
H(19A)	1039	11948	3758	33
H(19B)	-359	12370	3751	33
H(19C)	-175	10954	3900	33
H(20A)	-652	11923	6270	36
H(20B)	-415	12695	7276	36
H(20C)	-144	11286	7211	36
H(21A)	2865	9365	8343	39
H(21B)	3342	10407	9231	39
H(21C)	4283	10270	8538	39
H(22)	6209	5690	4086	19
H(24)	9144	3875	5314	22
H(25)	8998	4690	6785	21
H(29)	5101	7950	7592	21
H(30)	6211	7754	9139	22
H(33A)	8199	8281	10396	36
H(33B)	8644	7237	11067	36
H(33C)	7126	7092	10461	36
H(34A)	8644	4690	9260	34
H(34B)	9894	4324	8931	34
H(34C)	8411	3864	8277	34
H(35A)	8619	4448	3483	34
H(35B)	7081	4562	3093	34
H(35C)	7470	3293	3485	34

Table 6. Crystal data and structure refinement for **7a**.

Identification code	07132	
Empirical formula	C31 H31 Cl2 N O8 Pt S	
Formula weight	843.62	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 20.9960(19) Å	α= 90°.
	b = 10.4617(10) Å	β= 112.4730(10)°.
	c = 15.1265(14) Å	γ = 90°.
Volume	3070.3(5) $Å^3$	
Z	4	
Density (calculated)	1.825 Mg/m^3	
Absorption coefficient	4.865 mm^{-1}	
F(000)	1664	
Crystal size	0.25 x 0.05 x 0.05 mm^3	
Theta range for data collection	2.10 to 26.02°.	
Index ranges	-25<=h<=25, -12<=k<=12, -18<=l<=18	
Reflections collected	35378	
Independent reflections	6033 [R(int) = 0.0314]	
Completeness to theta = 26.02°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7930 and 0.3759	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6033 / 429 / 489	
Goodness-of-fit on F^2	0.988	
Final R indices [I>2sigma(I)]	R1 = 0.0142, wR2 = 0.0248	
R indices (all data)	R1 = 0.0150, wR2 = 0.0250	
Absolute structure parameter	0.004(3)	
Largest diff. peak and hole	0.788 and -0.704 e.$Å^{-3}$	

$R1 = \sum(F_o - F_c) / \sum F_o \, ; I > 2\sigma(I); wR2 = \{\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2\}^{1/2}$

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	9501(1)	1771(1)	5650(1)	14(1)
S(1)	8564(1)	2548(2)	2535(1)	21(1)
C(1)	7885(2)	2326(3)	2889(3)	21(1)
C(2)	8093(3)	2121(5)	3860(4)	17(1)
C(3)	8827(5)	2053(6)	4331(7)	14(1)
C(4)	9141(4)	2266(5)	3688(5)	14(1)
C(5)	9876(4)	2305(6)	4046(6)	15(1)
C(6)	10305(4)	2546(9)	3569(7)	18(2)
C(7)	11021(2)	2602(4)	4063(3)	19(1)
C(8)	11292(2)	2366(5)	5040(3)	18(1)
C(9)	10843(3)	2098(6)	5486(4)	17(1)
N(1)	10163(3)	2077(5)	5022(5)	14(1)
S(1A)	10447(4)	2712(9)	3540(6)	20(1)
C(1A)	11131(7)	2483(10)	4602(9)	16(3)
C(2A)	10934(9)	2205(14)	5349(13)	14(3)
C(3A)	10198(11)	2121(14)	5079(17)	14(1)
C(4A)	9894(12)	2391(14)	4112(16)	12(3)
C(5A)	9160(12)	2384(14)	3672(15)	14(3)
C(6A)	8729(9)	2582(15)	2740(12)	18(3)
C(7A)	8016(6)	2564(10)	2460(9)	17(1)
C(8A)	7747(8)	2354(12)	3144(10)	18(1)
C(9A)	8194(10)	2073(15)	4060(12)	18(3)
N(1A)	8865(11)	2102(14)	4322(14)	14(1)
O(1)	10258(1)	1500(2)	6976(2)	14(1)
C(10)	9488(1)	948(3)	7739(2)	16(1)
O(2)	8750(1)	1475(2)	6143(2)	16(1)
C(11)	10136(1)	1156(3)	7707(2)	14(1)
C(12)	10764(1)	926(3)	8602(2)	14(1)
C(13)	11373(1)	545(3)	8506(2)	15(1)
C(14)	11944(1)	224(3)	9326(2)	16(1)
C(15)	11918(1)	342(3)	10227(2)	15(1)
C(16)	11319(1)	787(3)	10317(2)	15(1)
C(17)	10737(1)	1051(3)	9499(2)	16(1)
O(3)	12545(1)	-261(2)	9311(1)	21(1)
C(18)	12542(2)	-624(4)	8403(2)	22(1)
O(4)	12454(1)	-93(2)	11029(1)	19(1)
C(19)	13019(2)	775(3)	11384(2)	25(1)
O(5)	11336(1)	882(2)	11226(1)	20(1)
C(20)	10747(2)	1436(4)	11336(3)	21(1)
C(21)	8848(1)	1147(3)	6996(2)	14(1)
C(22)	8194(1)	970(3)	7161(2)	14(1)
C(23)	7579(1)	837(3)	6358(2)	15(1)
C(24)	6961(1)	728(3)	6477(2)	17(1)
C(25)	6939(2)	741(3)	7383(2)	17(1)
C(26)	7556(1)	907(3)	8188(2)	15(1)
C(27)	8179(1)	1016(2)	8072(2)	15(1)
O(6)	6333(1)	621(2)	5728(1)	19(1)
C(28)	6336(2)	759(3)	4791(2)	21(1)
O(7)	6323(1)	687(2)	7508(2)	21(1)
C(29)	6040(2)	-581(3)	7414(2)	23(1)
O(8)	7487(1)	958(2)	9049(1)	20(1)
C(30)	8084(2)	1328(4)	9863(3)	23(1)
C(1S)	9629(8)	4683(9)	113(6)	30(2)

C(1T)	9390(20)	4762(17)	-28(15)	37(6)
Cl(1S)	9379(1)	3892(1)	953(1)	38(1)
Cl(2S)	9445(1)	3770(1)	-938(1)	32(1)

Table 8. Bond lengths [Å] and angles [°] for **7a**.

Pt(1)-N(1A)	1.972(19)
Pt(1)-C(3)	1.978(9)
Pt(1)-N(1)	1.986(6)
Pt(1)-C(3A)	1.997(19)
Pt(1)-O(2)	2.008(2)
Pt(1)-O(1)	2.047(2)
S(1)-C(1)	1.718(5)
S(1)-C(4)	1.727(8)
C(1)-C(2)	1.381(7)
C(2)-C(3)	1.432(9)
C(3)-C(4)	1.385(10)
C(4)-C(5)	1.428(6)
C(5)-C(6)	1.376(10)
C(5)-N(1)	1.385(8)
C(6)-C(7)	1.401(9)
C(7)-C(8)	1.388(6)
C(8)-C(9)	1.382(6)
C(9)-N(1)	1.329(8)
S(1A)-C(1A)	1.714(14)
S(1A)-C(4A)	1.726(19)
C(1A)-C(2A)	1.376(15)
C(2A)-C(3A)	1.442(19)
C(3A)-C(4A)	1.38(2)
C(4A)-C(5A)	1.425(13)
C(5A)-C(6A)	1.370(19)
C(5A)-N(1A)	1.38(2)
C(6A)-C(7A)	1.392(16)
C(7A)-C(8A)	1.372(13)
C(8A)-C(9A)	1.376(15)
C(9A)-N(1A)	1.310(19)
O(1)-C(11)	1.278(3)
C(10)-C(11)	1.396(4)
C(10)-C(21)	1.400(4)
O(2)-C(21)	1.274(3)
C(11)-C(12)	1.505(4)
C(12)-C(17)	1.387(4)
C(12)-C(13)	1.398(4)
C(13)-C(14)	1.396(4)
C(14)-O(3)	1.368(3)
C(14)-C(15)	1.391(4)
C(15)-O(4)	1.379(3)
C(15)-C(16)	1.395(4)
C(16)-O(5)	1.365(3)
C(16)-C(17)	1.395(4)
O(3)-C(18)	1.422(4)
O(4)-C(19)	1.427(3)
O(5)-C(20)	1.432(4)
C(21)-C(22)	1.497(4)
C(22)-C(27)	1.391(4)
C(22)-C(23)	1.401(4)
C(23)-C(24)	1.383(4)
C(24)-O(6)	1.376(3)
C(24)-C(25)	1.388(4)
C(25)-O(7)	1.379(4)
C(25)-C(26)	1.408(4)
C(26)-O(8)	1.365(3)

C(26)-C(27)	1.391(4)
O(6)-C(28)	1.427(3)
O(7)-C(29)	1.439(4)
O(8)-C(30)	1.434(4)
C(1S)-Cl(1S)	1.755(6)
C(1S)-Cl(2S)	1.768(7)
C(1T)-Cl(1S)	1.747(14)
C(1T)-Cl(2S)	1.765(14)

N(1A)-Pt(1)-N(1)	79.0(8)
C(3)-Pt(1)-N(1)	81.6(3)
N(1A)-Pt(1)-C(3A)	81.3(7)
C(3)-Pt(1)-C(3A)	84.0(9)
N(1A)-Pt(1)-O(2)	94.8(7)
C(3)-Pt(1)-O(2)	92.1(3)
N(1)-Pt(1)-O(2)	173.7(2)
C(3A)-Pt(1)-O(2)	175.9(7)
N(1A)-Pt(1)-O(1)	172.8(7)
C(3)-Pt(1)-O(1)	175.5(3)
N(1)-Pt(1)-O(1)	93.9(2)
C(3A)-Pt(1)-O(1)	91.5(7)
O(2)-Pt(1)-O(1)	92.35(9)
C(1)-S(1)-C(4)	90.4(3)
C(2)-C(1)-S(1)	112.9(4)
C(1)-C(2)-C(3)	112.4(6)
C(4)-C(3)-C(2)	110.7(7)
C(4)-C(3)-Pt(1)	112.6(6)
C(2)-C(3)-Pt(1)	136.8(7)
C(3)-C(4)-C(5)	118.3(8)
C(3)-C(4)-S(1)	113.5(6)
C(5)-C(4)-S(1)	128.1(8)
C(6)-C(5)-N(1)	119.1(8)
C(6)-C(5)-C(4)	129.5(9)
N(1)-C(5)-C(4)	111.4(7)
C(5)-C(6)-C(7)	120.8(8)
C(8)-C(7)-C(6)	118.7(5)
C(9)-C(8)-C(7)	118.4(5)
N(1)-C(9)-C(8)	122.8(6)
C(9)-N(1)-C(5)	120.1(6)
C(9)-N(1)-Pt(1)	123.8(5)
C(5)-N(1)-Pt(1)	116.1(5)
C(1A)-S(1A)-C(4A)	89.3(10)
C(2A)-C(1A)-S(1A)	113.0(12)
C(1A)-C(2A)-C(3A)	114.0(15)
C(4A)-C(3A)-C(2A)	107.4(17)
C(4A)-C(3A)-Pt(1)	112.1(14)
C(2A)-C(3A)-Pt(1)	140.5(16)
C(3A)-C(4A)-C(5A)	118(2)
C(3A)-C(4A)-S(1A)	116.2(15)
C(5A)-C(4A)-S(1A)	126(2)
C(6A)-C(5A)-N(1A)	117.8(19)
C(6A)-C(5A)-C(4A)	131(2)
N(1A)-C(5A)-C(4A)	112(2)
C(5A)-C(6A)-C(7A)	121.5(18)
C(8A)-C(7A)-C(6A)	118.5(13)
C(7A)-C(8A)-C(9A)	118.3(15)
N(1A)-C(9A)-C(8A)	122.8(18)
C(9A)-N(1A)-C(5A)	120.9(18)

C(9A)-N(1A)-Pt(1)	122.4(15)
C(5A)-N(1A)-Pt(1)	116.7(14)
C(11)-O(1)-Pt(1)	123.33(19)
C(11)-C(10)-C(21)	126.8(3)
C(21)-O(2)-Pt(1)	124.90(19)
O(1)-C(11)-C(10)	126.4(3)
O(1)-C(11)-C(12)	115.3(2)
C(10)-C(11)-C(12)	118.3(3)
C(17)-C(12)-C(13)	120.7(3)
C(17)-C(12)-C(11)	121.0(3)
C(13)-C(12)-C(11)	118.3(2)
C(14)-C(13)-C(12)	119.0(3)
O(3)-C(14)-C(15)	115.5(2)
O(3)-C(14)-C(13)	124.0(3)
C(15)-C(14)-C(13)	120.4(3)
O(4)-C(15)-C(14)	120.5(2)
O(4)-C(15)-C(16)	119.2(2)
C(14)-C(15)-C(16)	120.0(3)
O(5)-C(16)-C(17)	123.7(3)
O(5)-C(16)-C(15)	116.4(2)
C(17)-C(16)-C(15)	119.8(3)
C(12)-C(17)-C(16)	119.9(3)
C(14)-O(3)-C(18)	116.8(2)
C(15)-O(4)-C(19)	113.8(2)
C(16)-O(5)-C(20)	117.1(2)
O(2)-C(21)-C(10)	125.9(3)
O(2)-C(21)-C(22)	113.6(2)
C(10)-C(21)-C(22)	120.5(3)
C(27)-C(22)-C(23)	120.0(3)
C(27)-C(22)-C(21)	122.0(2)
C(23)-C(22)-C(21)	117.8(2)
C(24)-C(23)-C(22)	119.7(3)
O(6)-C(24)-C(23)	123.4(3)
O(6)-C(24)-C(25)	115.6(2)
C(23)-C(24)-C(25)	121.0(3)
O(7)-C(25)-C(24)	121.5(3)
O(7)-C(25)-C(26)	119.1(3)
C(24)-C(25)-C(26)	119.3(3)
O(8)-C(26)-C(27)	124.4(3)
O(8)-C(26)-C(25)	115.7(2)
C(27)-C(26)-C(25)	119.9(3)
C(22)-C(27)-C(26)	120.1(3)
C(24)-O(6)-C(28)	116.3(2)
C(25)-O(7)-C(29)	113.5(2)
C(26)-O(8)-C(30)	117.0(2)
Cl(1S)-C(1S)-Cl(2S)	111.9(4)
Cl(1S)-C(1T)-Cl(2S)	112.4(10)

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters ($Å^2$x 10^3)for **7a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$[$h^2a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	14(1)	15(1)	12(1)	1(1)	5(1)	1(1)
S(1)	25(1)	23(1)	12(1)	1(1)	3(1)	0(1)
C(1)	18(2)	19(2)	21(2)	0(2)	3(2)	0(2)
C(2)	14(2)	15(3)	21(3)	1(2)	4(2)	3(2)
C(3)	16(2)	12(2)	14(1)	-1(1)	6(1)	-1(2)
C(4)	19(2)	11(3)	12(2)	-1(2)	5(2)	-2(2)
C(5)	22(2)	11(3)	13(2)	-1(2)	10(2)	2(3)
C(6)	25(3)	12(3)	17(3)	-1(2)	7(2)	-7(3)
C(7)	24(2)	16(2)	25(2)	1(2)	18(2)	-1(2)
C(8)	17(2)	19(2)	19(2)	-4(2)	8(2)	-1(2)
C(9)	20(2)	15(3)	18(2)	2(2)	8(2)	1(2)
N(1)	15(1)	13(2)	15(2)	-2(1)	8(1)	0(1)
S(1A)	26(3)	18(3)	25(2)	1(2)	21(2)	-6(2)
C(1A)	16(4)	16(7)	20(6)	-14(8)	13(4)	-6(5)
C(2A)	12(3)	11(7)	19(4)	-5(5)	7(4)	2(5)
C(3A)	15(1)	13(2)	15(2)	-2(1)	8(1)	0(1)
C(4A)	17(3)	9(7)	13(4)	-6(6)	10(3)	-6(6)
C(5A)	18(3)	12(7)	13(4)	0(6)	9(3)	2(7)
C(6A)	18(4)	20(8)	19(4)	7(6)	10(4)	6(6)
C(7A)	20(2)	15(3)	18(2)	2(2)	8(2)	1(2)
C(8A)	17(2)	19(2)	19(2)	-4(2)	8(2)	-1(2)
C(9A)	21(4)	17(7)	17(4)	5(5)	7(3)	-6(6)
N(1A)	16(2)	12(2)	14(1)	-1(1)	6(1)	-1(2)
O(1)	15(1)	18(1)	12(1)	2(1)	7(1)	1(1)
C(10)	15(2)	20(2)	12(2)	1(1)	5(1)	1(1)
O(2)	13(1)	23(1)	12(1)	4(1)	6(1)	1(1)
C(11)	14(2)	12(2)	18(2)	-3(1)	5(1)	2(1)
C(12)	14(2)	11(2)	15(2)	4(1)	4(1)	-2(1)
C(13)	15(2)	14(2)	16(2)	0(1)	6(1)	-4(1)
C(14)	12(2)	13(2)	21(2)	0(1)	6(1)	-2(1)
C(15)	15(2)	11(2)	16(2)	4(1)	1(1)	-2(1)
C(16)	20(2)	10(2)	15(2)	0(1)	7(1)	-2(1)
C(17)	15(2)	14(2)	19(2)	0(1)	7(1)	1(1)
O(3)	12(1)	27(1)	21(1)	0(1)	4(1)	3(1)
C(18)	14(2)	27(2)	27(2)	1(2)	11(2)	5(2)
O(4)	15(1)	17(1)	20(1)	4(1)	1(1)	-2(1)
C(19)	17(2)	21(2)	30(2)	-1(2)	1(1)	-4(1)
O(5)	21(1)	25(1)	14(1)	2(1)	6(1)	5(1)
C(20)	29(2)	25(2)	13(2)	0(2)	12(2)	5(2)
C(21)	13(2)	11(2)	18(2)	-2(1)	7(1)	1(1)
C(22)	13(2)	10(2)	19(2)	1(1)	8(1)	1(1)
C(23)	16(2)	14(2)	16(2)	-2(1)	7(1)	0(1)
C(24)	13(2)	14(2)	22(2)	-3(1)	5(1)	0(1)
C(25)	14(2)	15(2)	25(2)	0(1)	11(1)	1(1)
C(26)	19(2)	10(2)	18(2)	-1(1)	10(1)	-2(1)
C(27)	14(2)	10(2)	19(2)	1(1)	5(1)	-1(1)
O(6)	10(1)	28(1)	18(1)	-4(1)	3(1)	0(1)
C(28)	17(2)	22(2)	21(2)	-4(1)	5(1)	2(1)
O(7)	15(1)	20(1)	32(2)	-2(1)	13(1)	-4(1)
C(29)	24(2)	23(2)	24(2)	-2(1)	11(1)	-8(1)
O(8)	19(1)	28(1)	17(1)	-3(1)	10(1)	-4(1)
C(30)	24(2)	25(2)	21(2)	-1(2)	10(2)	0(2)
C(1S)	34(5)	22(4)	44(4)	-6(3)	25(4)	-6(3)

C(1T)	53(16)	28(9)	28(8)	-8(7)	11(9)	6(9)
Cl(1S)	38(1)	42(1)	34(1)	3(1)	14(1)	-5(1)
Cl(2S)	20(1)	41(1)	34(1)	-6(1)	8(1)	-1(1)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **7a**.

	x	y	z	U(eq)
H(1)	7416	2343	2460	25
H(2)	7784	2035	4180	21
H(6)	10113	2675	2896	22
H(7)	11315	2799	3736	23
H(8)	11776	2388	5394	21
H(9)	11028	1921	6152	21
H(1A)	11599	2541	4667	19
H(2A)	11254	2080	5986	17
H(6A)	8921	2736	2274	22
H(7A)	7721	2693	1810	21
H(8A)	7264	2401	2988	21
H(9A)	8008	1849	4521	22
H(10)	9482	640	8326	19
H(13)	11398	504	7893	18
H(17)	10322	1318	9557	19
H(18A)	12183	-1265	8113	33
H(18B)	12992	-984	8485	33
H(18C)	12450	129	7987	33
H(19A)	13185	973	10876	37
H(19B)	13392	385	11925	37
H(19C)	12869	1565	11594	37
H(20A)	10664	2291	11050	32
H(20B)	10831	1499	12018	32
H(20C)	10342	896	11016	32
H(23)	7588	822	5734	18
H(27)	8596	1121	8615	18
H(28A)	6516	1605	4730	31
H(28B)	5865	669	4315	31
H(28C)	6630	97	4685	31
H(29A)	5990	-937	6792	34
H(29B)	5587	-545	7461	34
H(29C)	6349	-1125	7926	34
H(30A)	8445	682	9982	35
H(30B)	7962	1398	10426	35
H(30C)	8251	2155	9738	35
H(1S1)	10130	4862	403	36
H(1S2)	9384	5512	-54	36
H(1T1)	9786	5356	189	45
H(1T2)	8963	5281	-292	45

References

[1] Chambers, J. L. (2005). SAINT 7.12, Bruker-AXS, Inc., Madison, Wisconsin, USA.
[2] Sheldrick, G. M. (2005). SADABS, Bruker AXS, Inc., Madison, Wisconsin, USA.
[3] Sheldrick, G. M., Acta Cryst. Sect. A (1990), 46, 467.
[4] Sheldrick, G. M. SHELXL 97, Universität Göttingen, Göttingen, Germany, 1997.