Electronic Supporting Information

Helical donor-acceptor platinum complexes displaying dual luminescence and near-infrared circularly polarized luminescence

Pablo Vázquez-Domínguez,[b] Océane Journaud,[a] Nicolas Vanthuyne,[c] Denis Jacquemin,*[,d] Ludovic Favereau,*[,a] Jeanne Crassous,*[,a] and Abel Ros,*[,b]

[a] *Univ Rennes, CNRS, ISCR-UMR 6226, F-35000 Rennes, France.*
[b] *Institute for Chemical Research (CSIC-US) C/Américo Vespucio 49, E-41092 Seville (Spain).*
[c] *Aix Marseille University, CNRS, Centrale Marseille, iSm2, Marseille, France*
[d] *Laboratoire CEISAM, UMR 6230, CNRS, Université de Nantes, Nantes, France*

Table of Contents

1. General Information

^{1}H and ^{13}C NMR spectra were recorded at room temperature on an *AVANCE III 400 BRUKER* or an *AVANCE I 500 BRUKER* at Centre Régional de Mesures Physiques de l'Ouest (CRMPO), Université de Rennes 1. Chemical shifts δ are given in ppm and coupling constants *J* in Hz. Chemical shifts for ^{1}H NMR spectra are referenced relative to residual protium in the deuterated solvent (δ = 7.26 ppm, $CDCl_3$). ^{13}C shifts are referenced to $CDCl_3$ peaks at δ = 77.16 ppm.

High-resolution mass (HR-MS) determinations were performed at CRMPO on a Bruker MaXis 4G by ASAP (+ or -) or ESI and MALDI with CH_2Cl_2 as solvent techniques. Experimental and calculated masses are given with consideration of the mass of the electron.

UV-Visible (UV-vis, in M^{-1} cm^{-1}) absorption spectra were recorded on a UV-2401PC Shimadzu spectrophotometer.

Steady-state luminescence spectra were measured using an Edinburgh FS920 Fluorimeter combined with a FL920 Fluorescence Lifetime Spectrometer. The spectra were corrected for the wavelength dependence of the detector, and the quoted emission maxima refer to the values after correction. Life-times measurements were conducted with 375 nm diode laser excitation (EPL-series) plugged to a TCSPC pulsed source interface. Absolute fluorescence quantum yields ϕ were recorded with a Hamamatsu C9920-03 integrating sphere.

Electronic circular dichroism (ECD, in M^{-1} cm^{-1}) was measured on a Jasco J-815 Circular Dichroism Spectrometer (IFR140 facility - Biosit - Université de Rennes 1). The absorption and ECD spectra of the complexes have been measured in both dichloromethane and toluene, which afforded similar responses. The data in dichloromethane are shown to have the full spectra in the UV region, specially to see the complete ECD couplet signal from the binaphtyl unit around 250 nm (UV cut off of toluene is around 290 nm). The circularly polarized luminescence (CPL) measurements were performed using a home-built CPL spectrofluoropolarimeter (constructed with the help of the JASCO Company). The samples were excited using a 90° geometry with a Xenon ozone-free lamp 150 W LS. The following parameters were used: emission slit width ≈ 2 mm, integration time = 4 sec, scan

speed = 50 nm/min, accumulations = 10. The concentration of all the samples was ca. 10^{-6} M.

Thin-layer chromatography (TLC) was performed on aluminum sheets precoated with Merck 5735 Kieselgel 60F254. Column chromatography was carried out with Merck 5735 Kieselgel 60F (0.040-0.063 mm mesh). Chemicals were purchased from Sigma-Aldrich, Alfa Aesar or TCI Europe and used as received.

2. Synthesis of Pt-complexes: PtH, PtOMe and $PtNMe_2$

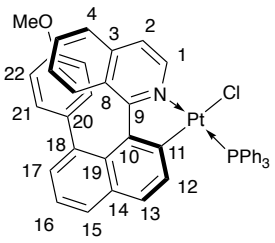
Synthesis of **PtH**.

A dried Schlenk tube was charged with the substrated **1** (0.1 mmol, 33.1 mg), $[Pt(DMSO)_2Cl_2]$ (0.12 mmol, 51.2 mg) and Na_2CO_3 (0.2 mmol, 21.2 mg). After cycles of vacuum-Ar, dried and deoxygented toluene (4 mL) was added and the resulting reaction mixture was stirred at 110°C for 16 h. Then, reaction was cooled to rt, filtered through a pad of celite, washed with CH_2Cl_2 and concentrated to dryness in the rotavap. Reaction crude was analyzed by NMR to corroborate the total consumption of the starting **1**, and used in the next step without purification. This reaction crude was placed in a Schlenk tube, and after cycles of vacuum-Ar, deoxygenated DCM (3 mL) was added. Then, a solution of PPh_3 (1.1 equiv.) in DCM (1.5 mL) was dropwise added at rt and the resulting solution was heated at 40°C overnight. Then, the reaction crude was concentrated in the rovatavapor and purified by column chromatography (Cyclohexane/EtOAc 4:1) to give the complex (±)-**7** (~6:1 *trans/cis*-N,P isomers) as a yelow-orange solid (58 mg, 71%).

^{1}H-RMN (400 MHz, $CDCl_3$) for *trans*-N,P isomer: δ 9.45 (dd, $^3J_{H,H}$ = 6.4 Hz, $^4J_{P,H}$= 3.4 Hz, 1H, H_1) 7.85 (ddd, $^3J_{P,H}$ = 11.7 Hz, $^3J_{H,H}$ = 7.1 Hz, $^3J_{H,H}$ = 1.4 Hz, 6H$_o$ phenyl rings of PPh_3), 7.63 (dd, $^3J_{H,H}$ = 8.2 Hz, $^4J_{H,H}$ = 1.1 Hz, 1H), 7.49-7.42 (m, 5H, 3H$_p$ phenyl rings of PPh_3 and 2H of C^N ligand) 7.41-7.36 (m, 6H$_m$ phenyl rings of PPh_3 and 2H of C^N ligand) 7.28-7.24 (m, 2H, H_2 and another H of C^N ligand), 7.18-7.14 (m, 1H), 7.11 (d, $^3J_{H,H}$ = 8.5 Hz, 1H, H_{13}), 6.92 (dd, $^3J_{H,H}$ = 8.5 Hz, $^4J_{P,H}$ = 2.9 Hz, 1H, H_{12}. $^4J_{Pt,H}$ could not be measured accurately), 6.70-6.62 (m, 5H, Ph susbtituent).

^{13}C-RMN (100 MHz, $CDCl_3$) for *trans*-N,P isomer: δ 169.9 (d, $^3J_{P,C}$ = 2 Hz, C_9), 139.2 (s, C_1), 137.8 (s, C_q), 136.4 (s, C_q), 135.4 (d, $^2J_{P,C}$ = 11 Hz, C$_o$ phenyl rings of PPh_3), 135.0 (d, $^3J_{P,C}$= 8 Hz, C_{12}), 133.1 (s, C_q), 132.1 (s), 132.0 (s, C_q), 131.9 (s, C_q), 130.8 (d, $^4J_{P,C}$ = 3 Hz, C$_p$ phenyl rings of PPh_3), 130.7 (s, C_q), 130.6 (s, C_q), 130.5 (d, $^1J_{P,C}$ = 51 Hz, C$_{ipso}$ phenyl rings of PPh_3), 130.1 (s, C_q), 129.3 (s), 128.0 (d, $^3J_{P,C}$ = 11 Hz, C$_m$ phenyl rings of PPh_3), 127.4 (s, C_{21}), 126.5 (s), 126.4 (s), 126.3 (s), 126.0 (s, C_q), 125.3 (s), 124.0 (s), 118.3, (d, $^4J_{P,C}$ = 3 Hz, C_2). ^{31}P-RMN (162 MHz, $CDCl_3$): δ 22.6 (s+d, $^1J_{Pt,P}$ = 4.374 Hz). For *cis*-N,P isomer: δ 20.2 (s+d, $^1J_{Pt,P}$ = 2.624 Hz).

Synthesis of **PtOMe**.

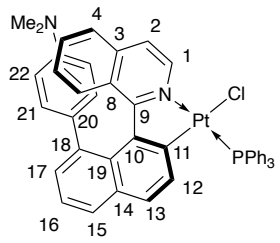


A dried Schlenk tube was charged with the substrated **2** (0.15 mmol, 54 mg), $[Pt(DMSO)_2Cl_2]$ (0.23 mmol, 96 mg) and Na_2CO_3 (0.3 mmol, 32 mg). After cycles of vacuum-Ar, dried and deoxygented toluene (6 mL) was added and the resulting reaction mixture was stirred at 110°C for 16 h. Then, reaction was cooled to rt, filtered through a pad of celite, washed with CH_2Cl_2 and concentrated to dryness in the rotavap. Reaction crude was purified by cloumn chromatography (silicagel, $CHCl_3$), to afford **5** as a yellow solid (92 mg, 91%). The complex **5** (0.067 mmol, 45 mg) was placed in a Schlenk tube, and after cycles of vacuum-Ar, deoxygenated DCM (3 mL) was added. Then, a solution of PPh_3 (0.074 mmol, 19.4 mg) in DCM (1 mL) was dropwise added at rt and the resulting solution was heated at 40°C for 4 hours. Then, the solvent was evaporated and the reaction crude was washed with a pentane/DCM mixture to give (±)-**8** as a yellow solid (45 mg, 79%).

^{1}H-RMN (400 MHz, $CDCl_3$): δ 9.47 (dd, $^3J_{H,H}$ = 6.4 Hz, $^4J_{P,H}$ = 3.3 Hz, 1H, H_1) 7.85 (ddd, $^3J_{P,H}$ = 11.8 Hz, $^3J_{H,H}$ = 8.5 Hz, $^3J_{H,H}$ = 1.4 Hz, 6H$_o$ phenyl rings of PPh_3), 7.60 (dd, $^3J_{H,H}$ = 8.0 Hz, $^4J_{H,H}$ = 0.9 Hz, 1H), 7.52-7.48 (m, 1H), 7.49-7.44 (m, 3H$_p$ phenyl rings of PPh_3 and 1H of C^N ligand), 7.42-7.36 (m, 6H$_m$ phenyl rings of PPh_3 and 2H of C^N ligand), 7.29 (d, $^3J_{H,H}$ = 6.3 Hz, 1H, H_2) 7.23 (dd, $^3J_{H,H}$ = 7.0 Hz, $^4J_{H,H}$ = 1.1 Hz, 1H), 7.17-7.13 (m, 1H), 7.11 (d, $^3J_{H,H}$ = 8.4 Hz, 1H, H_{13}), 6.91 (dd, $^3J_{H,H}$ = 8.4 Hz, $^4J_{P,H}$ = 2.8 Hz, 1H, H_{12}. ^{195}Pt satellites signals with $^4J_{Pt,H}$ = 52.0 Hz), 6.63 (br s, 2H, H_{21}), 6.19 (d, $^3J_{H,H}$ = 8.2 Hz, 2H, H_{22}), 3.60 (s, 6H, *Me*O).

^{13}C-RMN (100 MHz, $CDCl_3$): δ 170.0 (d, $^3J_{P,C}$ = 3 Hz, C_9) 157.5 (s, C_{23}), 157.3 (s, C_q), 143.7 (d, $^2J_{P,C}$ = 6 Hz, C_{11}), 141.4 (s, C_q), 139.2 (s, C_1), 137.5 (s, C_q), 136.4 (s, C_q), 135.4 (d, $^2J_{P,C}$ = 11 Hz, C_o phenyl rings of PPh_3), 135.4 (s), 135.0 (d, $^3J_{P,C}$ = 7 Hz, C_{12}), 132.1 (s, C_q), 130.8 (d, $^4J_{P,C}$ = 2 Hz, C_p phenyl rings of PPh_3), 130.8 (s), 130.7 (s, C_q), 130.3 (d, $^1J_{P,C}$ = 43 Hz, C_{ipso} phenyl rings of PPh_3), 128.7 (s), 128.6 (s, C_q), 128.6 (s), 128.5 (s, C_q), 128.3 (br s, C_{21}), 128.0 (d, ^3J (PC) = 11.2 Hz, C_m phenyl rings of PPh_3), 127.9 (s), 127.8 (s), 126.9 (s), 126.5 (s), 126.2 (s), 125.8 (C_q), 125.8 (C_q), 124.1 (s) 121.3 (s, C_q) 118.2, (d, $^4J_{P,C}$ = 3 Hz, C_2), 114.0 (br s, C_{22}), 111.2 (br s, C_{22}), 55.2 (C_{MeO}). ^{31}P-RMN (162 MHz, $CDCl_3$): δ 22.6 (s+d, $^1J_{PtP}$ = 4.378 Hz).

Synthesis of **PtNMe$_2$**.

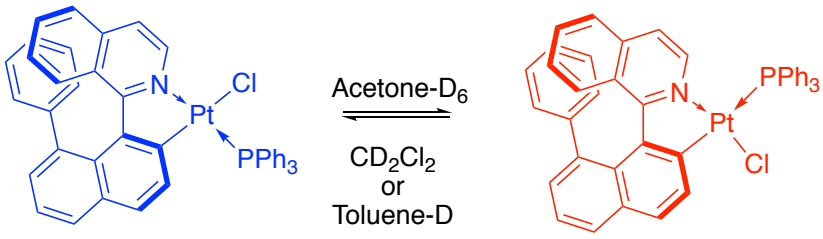


A dried Schlenk tube was charged with the substrated **3** (0.18 mmol, 68 mg), [Pt(DMSO)$_2$Cl$_2$] (0.27 mmol, 115 mg) and Na_2CO_3 (0.36 mmol, 38.4 mg). After cycles of vacuum-Ar, dried and deoxygented toluene (6 mL) was added and the resulting reaction mixture was stirred at 110°C for 16 h. Then, reaction was cooled to rt, filtered through a pad of celite, washed with CH_2Cl_2 and concentrated to dryness in the rotavap. Reaction crude was purified by cloumn chromatography (silicagel, heptane/EtOAc 6:4→EtOAc→EtOAc/MeOH 95:5), to afford **6** as a red solid (50 mg, 41%). The complex **6** (0.037 mmol, 25 mg) was placed in a Schlenk tube, and after cycles of vacuum-Ar, deoxygenated DCM (2 mL) was added. Then, a solution of PPh_3 (0.05 mmol, 13 mg) in DCM (0.5 mL) was dropwise added at rt and the resulting solution was heated at 40°C for 5 hours. Then, the solvent was evaporated and the reaction crude was purified by cloumn chromatography (silica gel, $CHCl_3$) to give (±)-**9** as a red solid (29 mg, 92%).

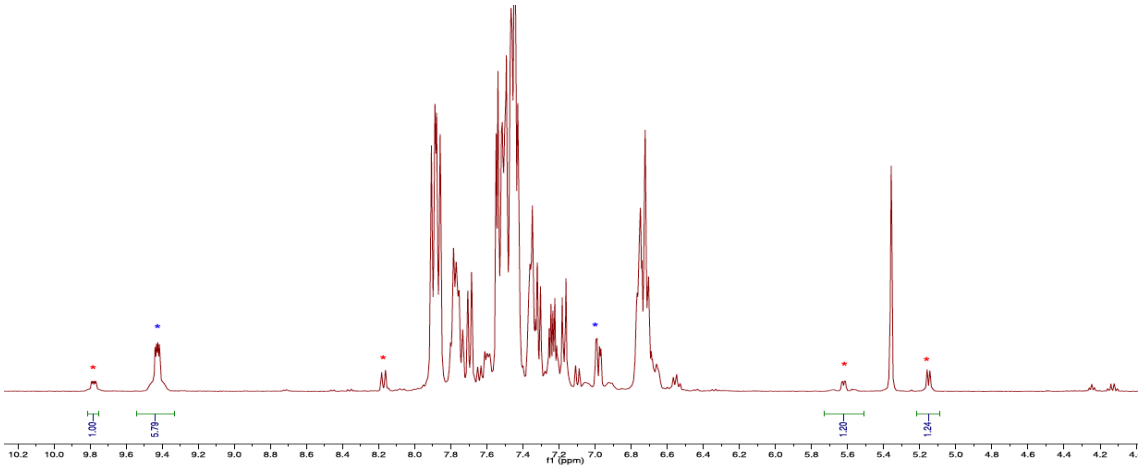
^{1}H-RMN (400 MHz, $CDCl_3$): δ 9.45 (dd, $^3J_{H,H}$ = 6.4 Hz, $^4J_{P,H}$ = 3.4 Hz 1H, H_1), 7.85 (ddd, $^3J_{P,H}$ = 11.7 Hz, $^3J_{H,H}$ = 7.1 Hz, $^3J_{H,H}$ = 1.4 Hz, 6H$_o$ phenyl rings of PPh_3), 7.57 (dd, $^3J_{H,H}$ = 8.0 Hz, $^4J_{H,H}$ = 0.9 Hz, 1H), 7.44 (td, $^3J_{H,H}$ = 7.6 Hz, $^4J_{H,H}$ = 1.4 Hz, 3H$_p$ phenyl rings of PPh_3 and 2H of C^N ligand), 7.38 (td, $^3J_{H,H}$ = 7.6 Hz, $^4J_{P,H}$ = 2.6 Hz, 6H$_m$ phenyl rings of PPh_3 and 2H of C^N ligand), 7.27-7.23 (m, 2H, H_2 and another H of C^N ligand), 7.16-7.11 (m, 1H), 7.08 (d, $^3J_{H,H}$ = 8.4 Hz, 1H, H_{13}), 6.89 (dd, $^3J_{H,H}$ = 8.4 Hz, $^4J_{P,H}$ = 2.9 Hz, 1H, H_{12}. ^{195}Pt satellites signals with $^4J_{Pt,H}$ = 52.0 Hz), 6.57 (d, $^3J_{H,H}$ = 7.8 Hz, 2H, H_{21}), 6.03 (d, $^3J_{H,H}$ = 7.8 Hz, 2H, H_{22}), 2.74 (s, 6H, *Me$_2$*N).

^{13}C-RMN (100 MHz, $CDCl_3$): δ 170.2 (d, $^3J_{P,C}$ = 2.5 Hz, C_9), 148.4 (C_{23}), 143.2 (s, C_q), 141.6 (s, C_q), 139.1 (s, C_1), 138.1 (s, C_q), 136.5 (s, C_q), 135.4 (d, $^2J_{P,C}$ = 11 Hz, C_o phenyl rings of PPh_3), 134.9 (d, $^3J_{P,C}$ = 7 Hz, C_{12}), 132.1 (s, C_q), 131.5 (s, C_q), 130.8 (s, C_q), 130.8 (d, $^4J_{P,C}$ = 3 Hz, C_p phenyl rings of PPh_3), 130.6 (s), 130.4 (d, $^1J_{P,C}$ = 51 Hz, C_{ipso} phenyl rings of PPh_3), 128.4 (s), 128.4 (s), 128.3 (s), 128.0 (d, $^3J_{P,C}$ = 11 Hz, C_m phenyl rings of PPh_3), 127.9 (s, C_{21}), 126.3 (s), 126.2 (s), 126.1 (s), 126.0 (C_q), 125.9 (C_q), 124.1 (s), 118.2, (d, $^4J_{P,C}$ = 3 Hz), 112.5 (br s, C_{22}), 40.7 (C_{Me2N}). ^{31}P-RMN (162 MHz, $CDCl_3$): δ 22.8 (s+d, $^1J_{PtP}$ = 4.377 Hz).

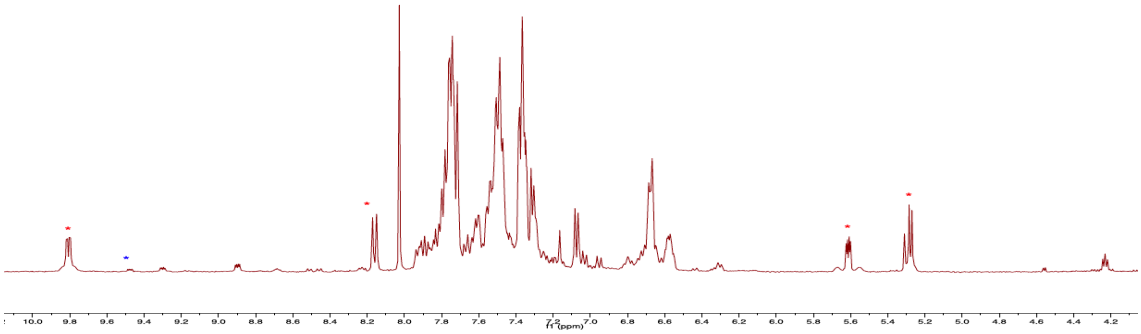
trans/cis-N,P-**PtH isomers interconversion studies.**



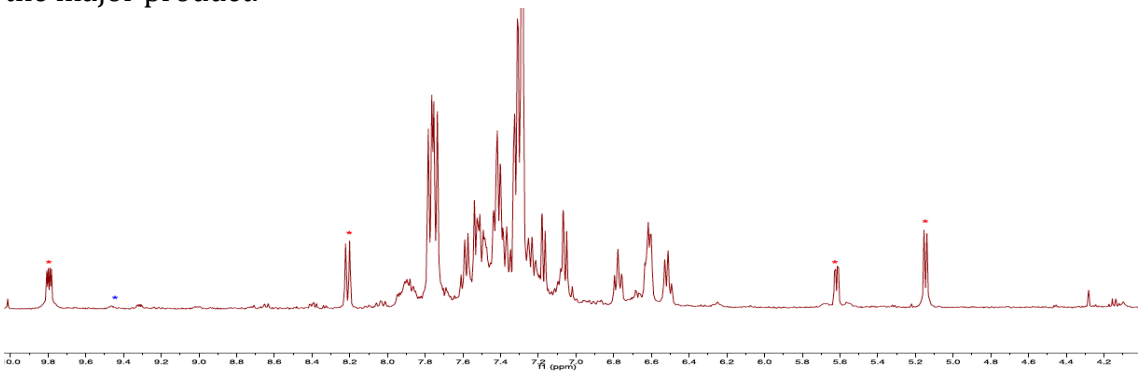
^{1}H in CD_2Cl_2 of *trans*-N,P/*cis*-N,P 6:1 mixture.



^{1}H in acetone-D_6 of the previous *trans*-N,P/*cis*-N,P 6:1 mixture converted to *cis*-N,P as the major product.

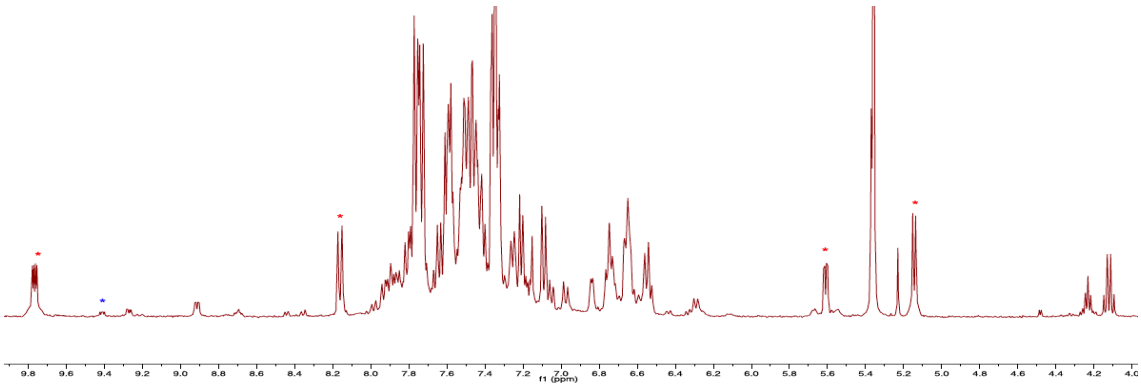


^{1}H in $CDCl_3$ of the previous *trans*-N,P/*cis*-N,P 6:1 mixture converted to *cis*-N,P as the major product.

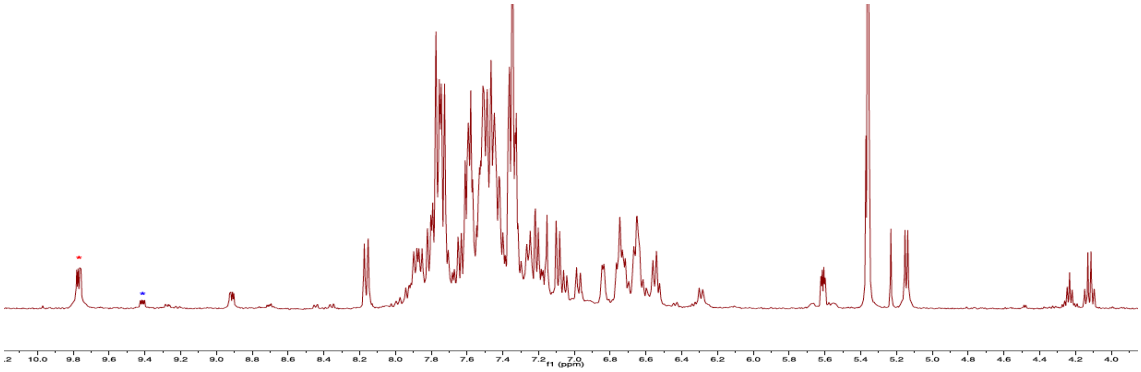


cis-N,P to _trans_-N,P isomerization studies in CD_2Cl_2.

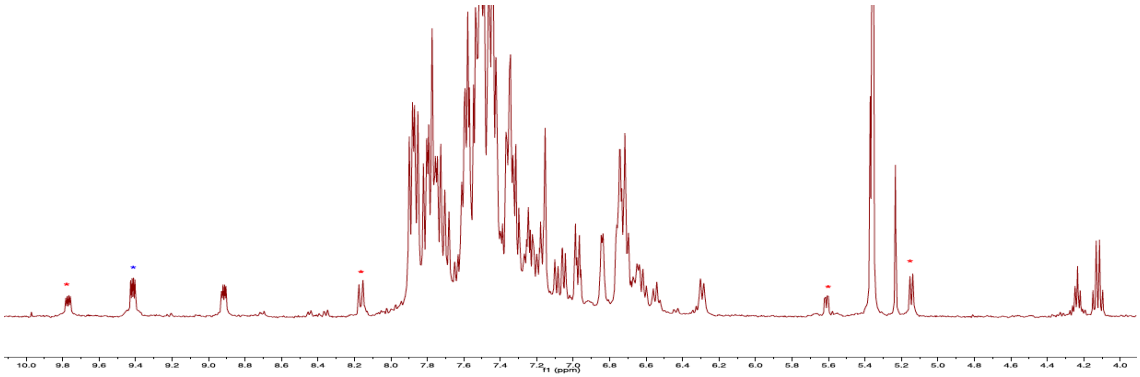
^1H in CD_2Cl_2 of the conversion of *cis*-N,P to *trans*-N,P after overnight at rt.



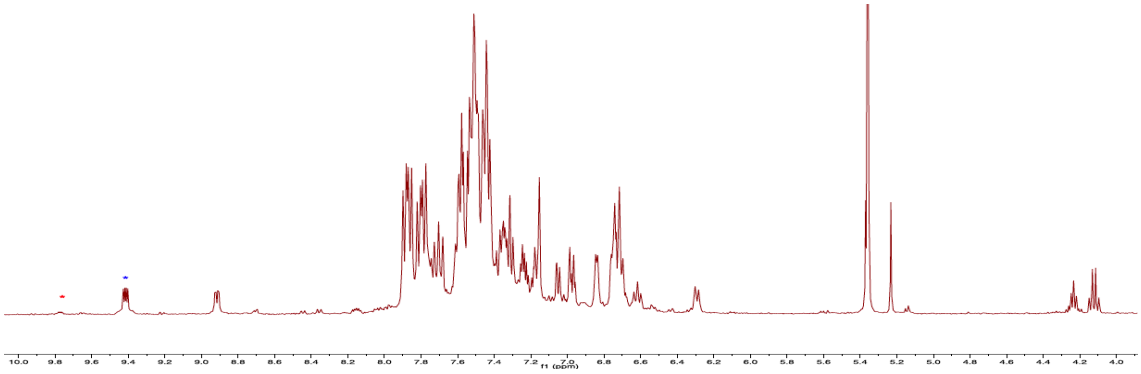
^1H in CD_2Cl_2 of the conversion of *cis*-N,P to *trans*-N,P after 5h at 40°C.



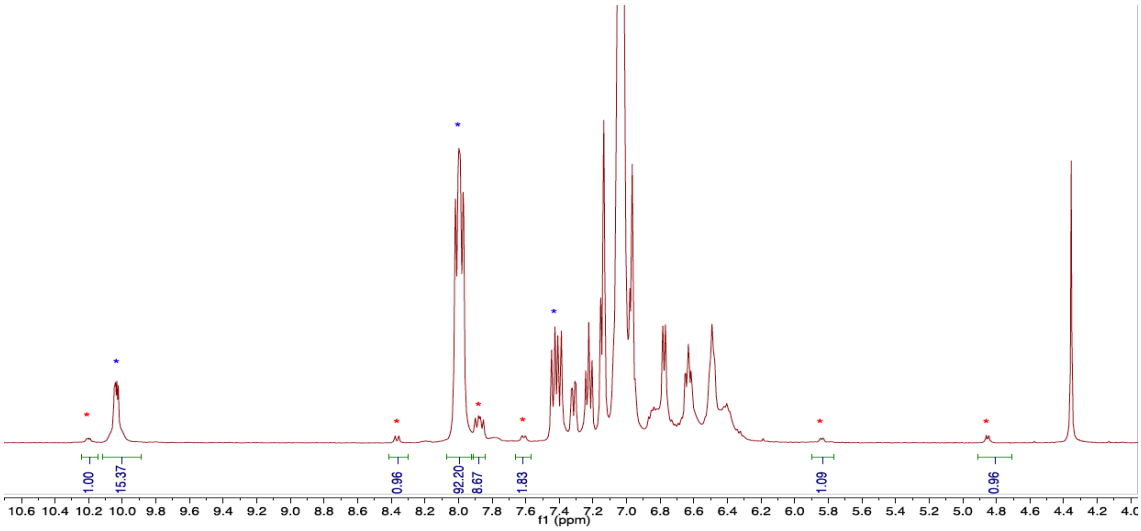
^1H in CD_2Cl_2 of the conversion of *cis*-N,P to *trans*-N,P after 24h at 40°C.



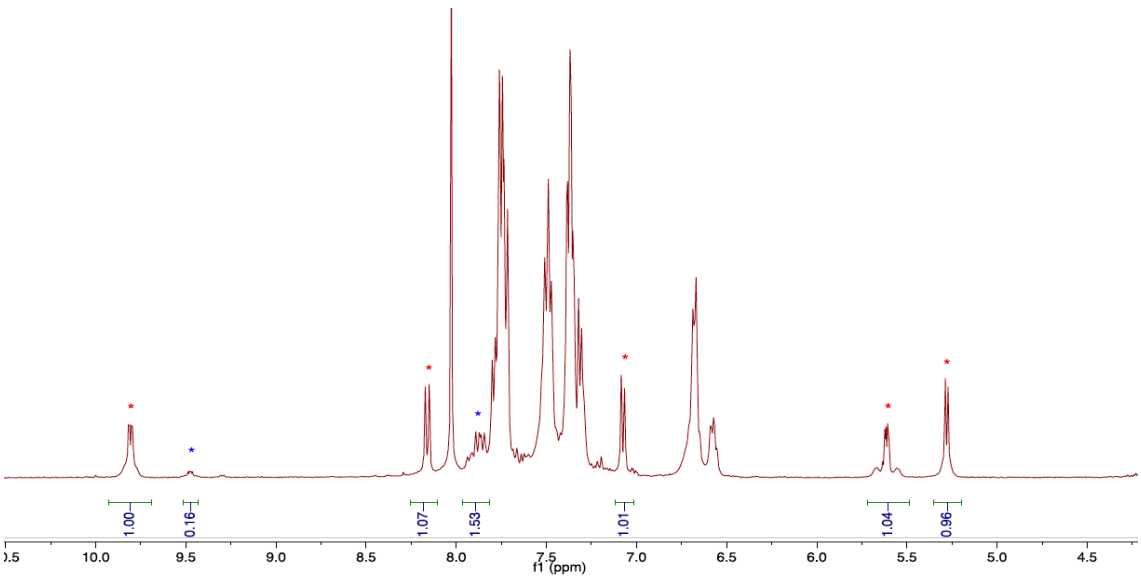
^1H in CD_2Cl_2 of the conversion of *cis*-N,P to *trans*-N,P after 72h at 40°C.



^{1}H in Toluene-D_8 of *trans*-N,P/*cis*-N,P 15:1 mixture.

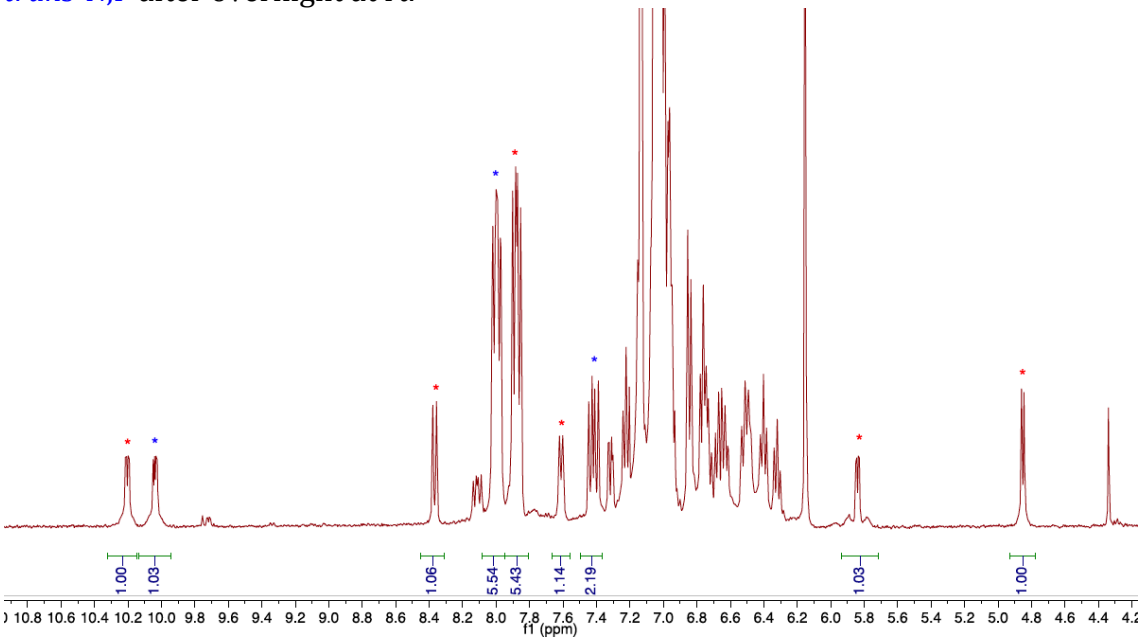


^{1}H in acetone-D_6 of the previous *trans*-N,P/*cis*-N,P 15:1 mixture converted to *cis*-N,P as the major product after 24 at rt.

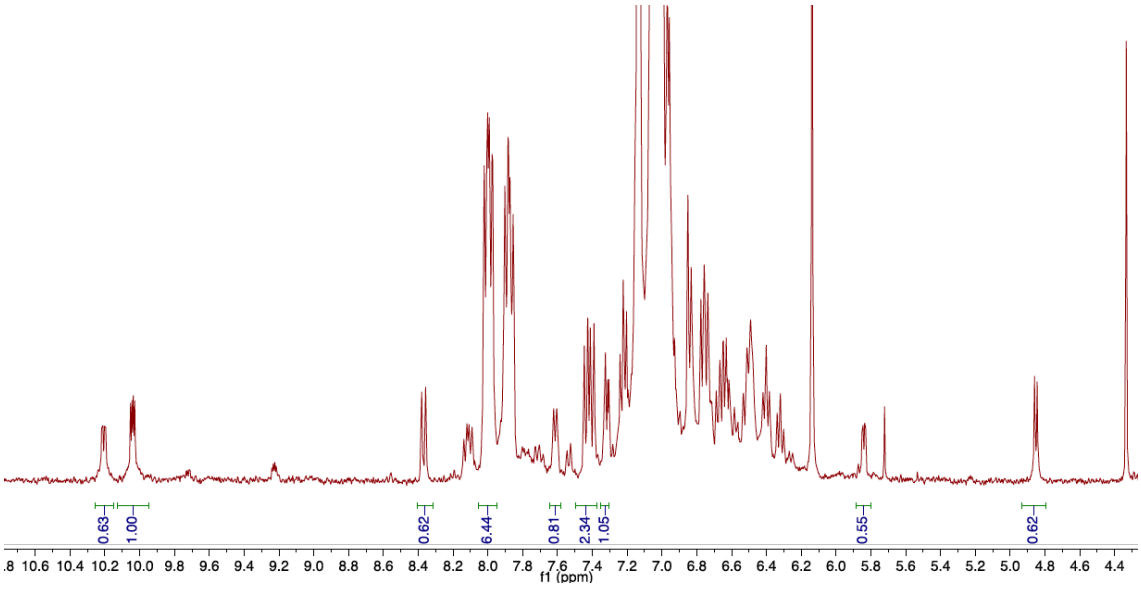


***cis*-N,P to *trans*-N,P isomerization studies in Toluene-D_8.**

^{1}H in Toluene-D_8 of the conversion of *cis*-N,P (previous sample in acetone-D_6) to *trans*-N,P after overnight at rt.

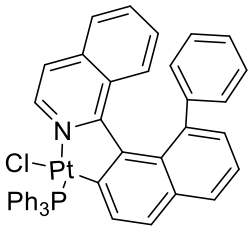


^{1}H in Toluene-D_8 of the conversion of *cis*-N,P to *trans*-N,P after 48 h at rt.



Complementary to this nmr study, we also evaluate the DFT-computed differences of free energies between the two forms, that amount to ca. 7 kcal.mol^{-1} for all the three complexes, indicating small, yet non-negligible differences.

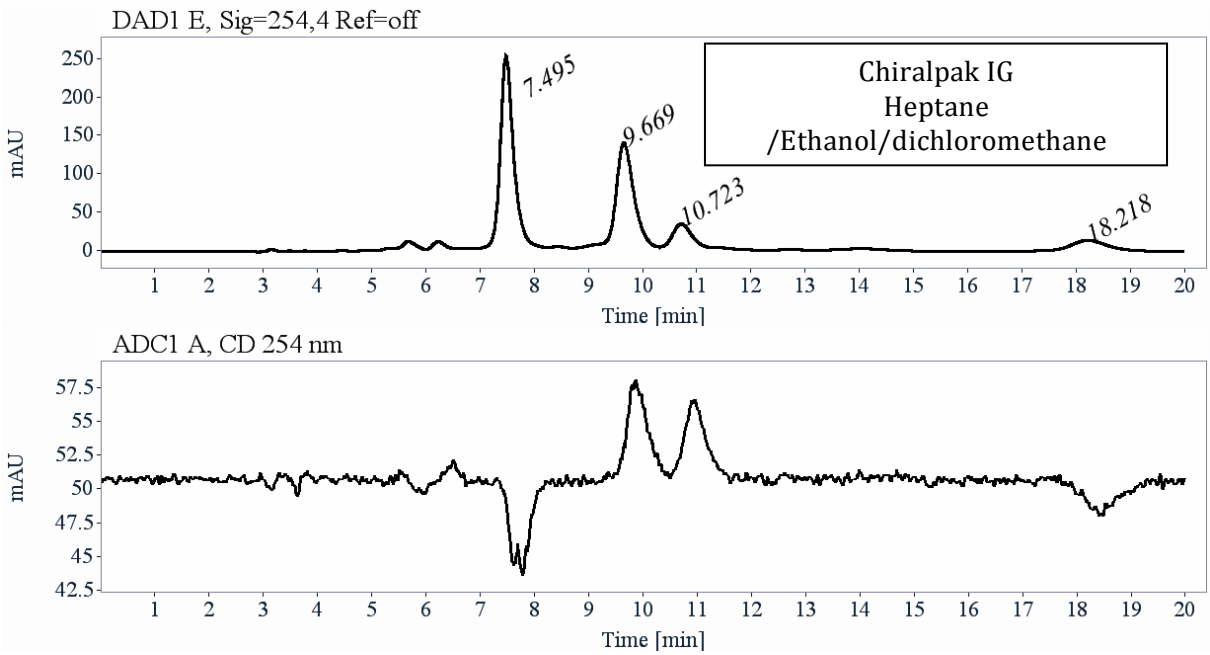
3. Chiral HPLC separation.



Analytical chiral HPLC separation for compound **PtH**

• The sample is dissolved in dichloromethane, injected on the chiral column, and detected with an UV and CD detectors at 254 nm. The flow-rate is 1 mL/min.

Column	Mobile Phase	t1	k1	t2	k2	α	Rs
Chiralpak IG	Heptane / ethanol / dichloromethane (70/20/10)	7.49 (-)	1.54	9.67 (+)	2.28	1.48	4.33

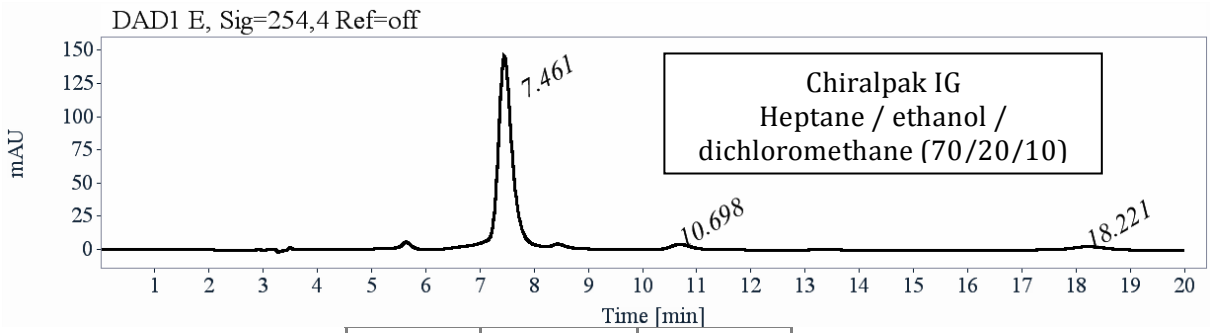


RT [min]	Area	Area%	Capacity Factor
7.49	4291	48.76	1.54
9.67	3093	35.15	2.28
10.72	750	8.53	2.64
18.22	665	7.56	5.18
Sum	8799	100.00	

Preparative separation for compound **PtH**:

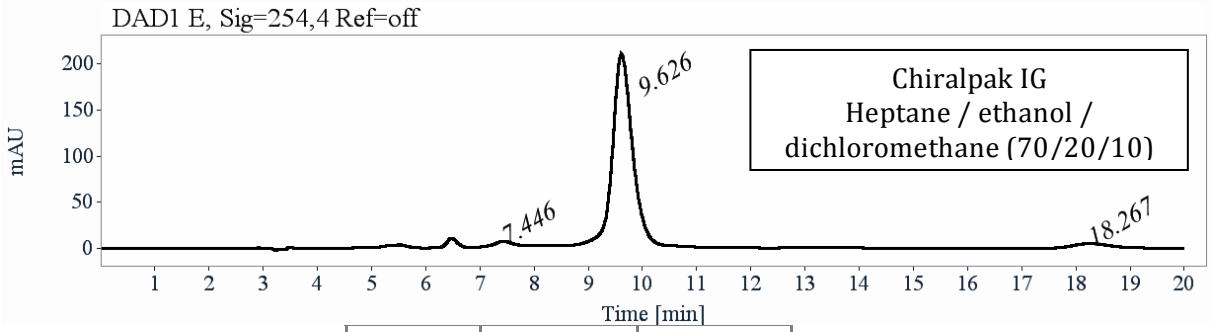
• Sample preparation: About 27 mg of compound **PtH** are dissolved in 2.6 mL of mixture of dichloromethane / hexane (50/50).
• Chromatographic conditions: Chiralpak IG (250 x 4.6 mm), hexane / ethanol / dichloromethane (70/20/10) as mobile phase, flow-rate = 5 mL/min, UV detection at 254 nm.
• Injections (stacked):17 times 150 μL, every 11.8 minutes.

• First fraction: 10.4 mg of the first eluted with ee > 99.5 %



RT [min]	Area	Area%
7.46	2456	91.40
10.70	102	3.81
18.22	129	4.79
Sum	2687	100.00

• Second fraction: 6 mg of the second eluted with ee > 95 %



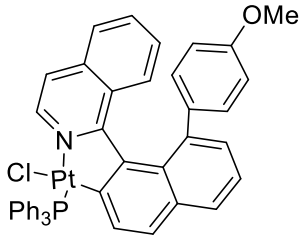
RT [min]	Area	Area%
7.45	131	2.37
9.63	5183	93.31
18.27	240	4.32
Sum	5555	100.00

Optical rotations

Optical rotations were measured on a Jasco P-2000 polarimeter with a halogen lamp (589, 578 and 546 nm), in a 10 cm cell, thermostated at 25°C with a Peltier controlled cell holder.

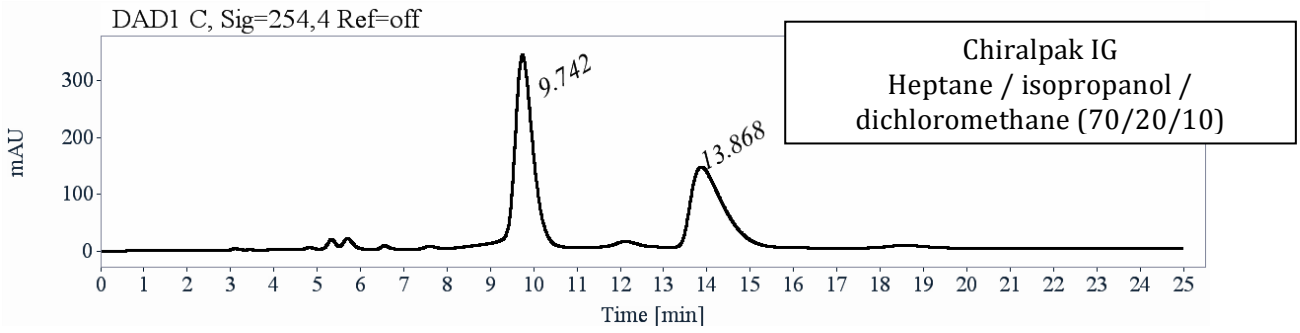
λ (nm)	PtH first eluted on Chiralpak IG $[\alpha]_{\lambda}^{25}$ (CH_2Cl_2, c = 0.021)	PtH second eluted on on Chiralpak IG $[\alpha]_{\lambda}^{25}$ (CH_2Cl_2, c = 0.027)
589	+ 540	- 500
578	+ 570	- 540
546	+ 750	- 700

Analytical chiral HPLC separation for compound **PtOMe**



• The sample is dissolved in dichloromethane, injected on the chiral column, and detected with an UV detector at 254 nm. The flow-rate is 1 mL/min.

Column	Mobile Phase	t1	k1	t2	k2	α	Rs
Chiralpak IG	Heptane / isopropanol / dichloromethane (70/20/10)	9.74	2.30	13.87	3.70	1.61	3.89

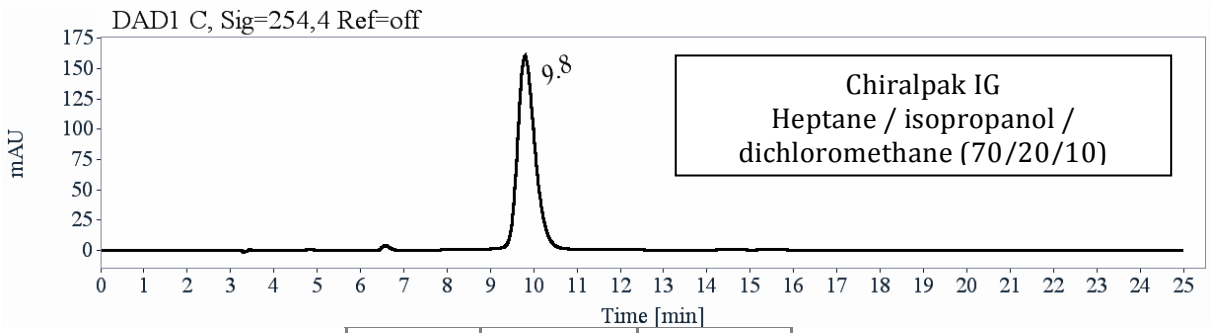


RT [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
9.74	9922	57.36	2.30		
13.87	7375	42.64	3.70	1.61	3.89
Sum	17298	100.00			

Preparative separation for compound **PtOMe**:

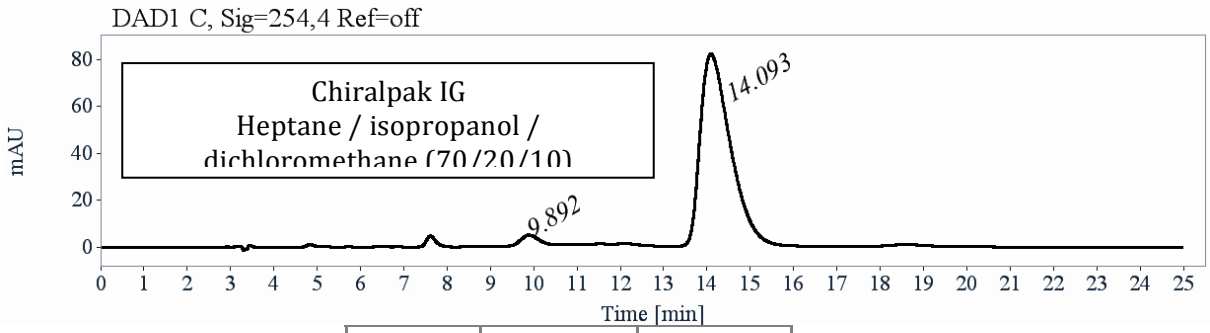
• Sample preparation: About 54 mg of compound **PtOMe** are dissolved in 3 mL of mixture of dichloromethane / hexane (50/50).
• Chromatographic conditions: Chiralpak IG (250 x 4.6 mm), Hexane / isopropanol / dichloromethane (70/20/10) as mobile phase, flow-rate = 5 mL/min, UV detection at 254 nm.
• Injections (stacked): 30 times 100 µL, every 14.5 minutes.

• First fraction: 22 mg of the first eluted with ee > 99.5 %



RT [min]	Area	Area%
9.80	4465	100.00
Sum	4465	100.00

• Second fraction: 15 mg of the second eluted with ee > 93.5 %



RT [min]	Area	Area%
9.89	130	3.15
14.09	3983	96.85
Sum	4113	100.00

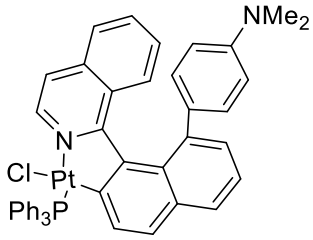
Optical rotations

Optical rotations were measured on a Jasco P-2000 polarimeter with a halogen lamp (589, 578 and 546 nm), in a 10 cm cell, thermostated at 25°C with a Peltier controlled cell holder.

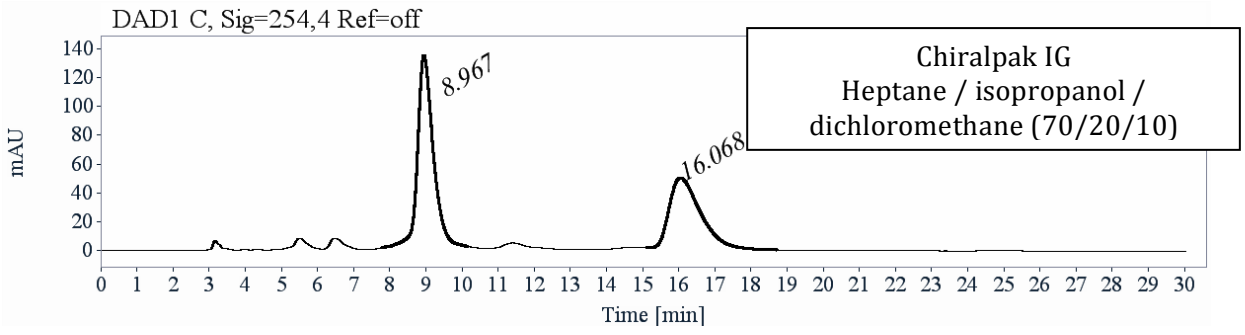
λ (nm)	PtOMe first eluted on Chiralpak IG $[\alpha]_{\lambda}^{25}$ (CH_2Cl_2, c = 0.026)	PtOMe second eluted on on Chiralpak IG $[\alpha]_{\lambda}^{25}$ (CH_2Cl_2, c = 0.027)
589	+ 590	- 550
578	+ 630	- 600
546	+ 850	-800

Analytical chiral HPLC separation for compound **$PtNMe_2$**

• The sample is dissolved in dichloromethane, injected on the chiral column, and detected with an UV detector at 254 nm. The flow-rate is 1 mL/min.



Column	Mobile Phase	t1	k1	t2	k2	α	Rs
Chiralpak IG	Heptane / isopropanol / dichloromethane (70/20/10)	8.97	2.04	16.07	4.45	2.18	6.19

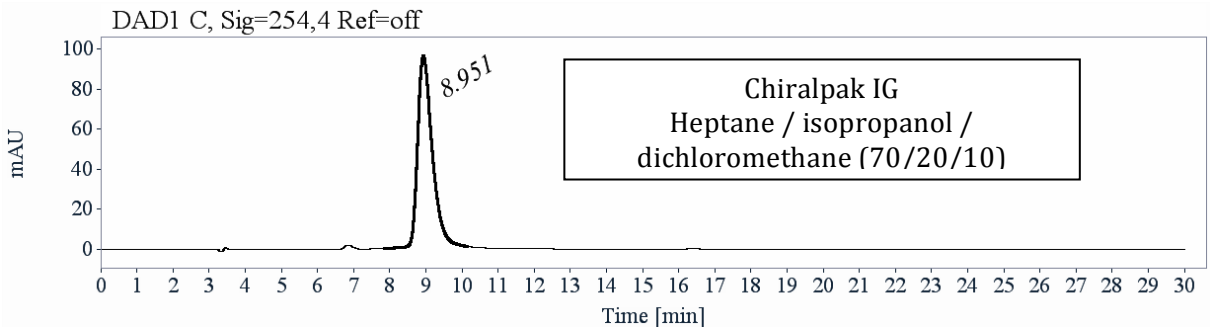


RT [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
8.97	4062	58.17	2.04		
16.07	2921	41.83	4.45	2.18	6.19
Sum	6983	100.00			

Preparative separation for compound **$PtNMe_2$**:

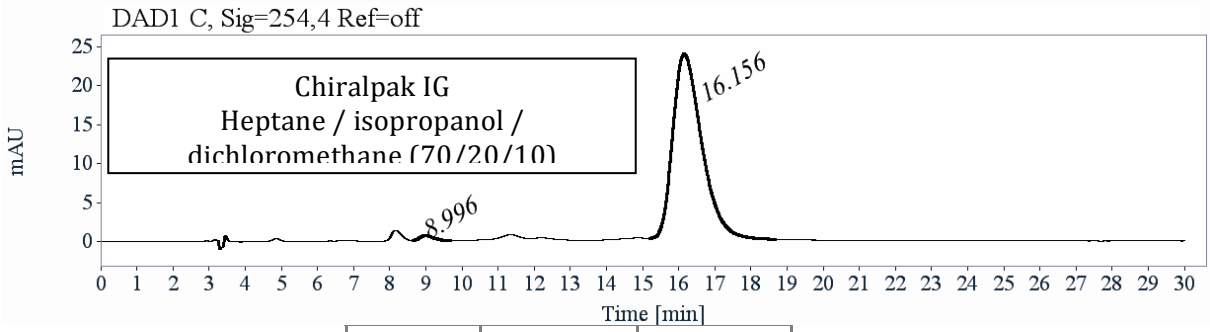
• Sample preparation: About 26 mg of compound **$PtNMe_2$** are dissolved in 3 mL of mixture of dichloromethane / hexane (50/50).
• Chromatographic conditions: Chiralpak IG (250 x 4.6 mm), hexane / isopropanol / dichloromethane (70/20/10) as mobile phase, flow-rate = 5 mL/min, UV detection at 254 nm.
• Injections (stacked): 15 times 200 µL, every 16.8 minutes.

• First fraction: 10 mg of the first eluted with ee > 99.5 %



RT [min]	Area	Area%
8.95	2711	100.00
Sum	2711	100.00

• Second fraction: 8 mg of the second eluted with ee > 97 %



RT [min]	Area	Area%
9.00	20	1.48
16.16	1323	98.52
Sum	1343	100.00

Optical rotations

Optical rotations were measured on a Jasco P-2000 polarimeter with a halogen lamp (589, 578 and 546 nm), in a 10 cm cell, thermostated at 25°C with a Peltier controlled cell holder.

λ (nm)	$PtNMe_2$ first eluted on Chiralpak IG $[\alpha]_\lambda^{25}$ (CH_2Cl_2, c = 0.030)	$PtNMe_2$ second eluted on on Chiralpak IG $[\alpha]_\lambda^{25}$ (CH_2Cl_2, c = 0.027)
589	+ 660	- 640
578	+ 740	- 710
546	+ 1100	- 1050

4. UV-vis spectra of ligands and lifetimecharacterizations.

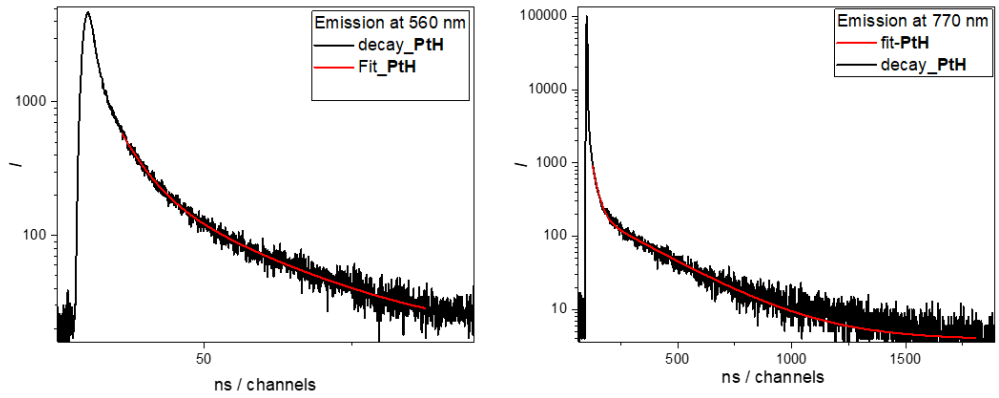


Figure S1. Luminescence decay of complex **PtH** with corresponding fit (red) at 560 (left) and 770 nm (right).

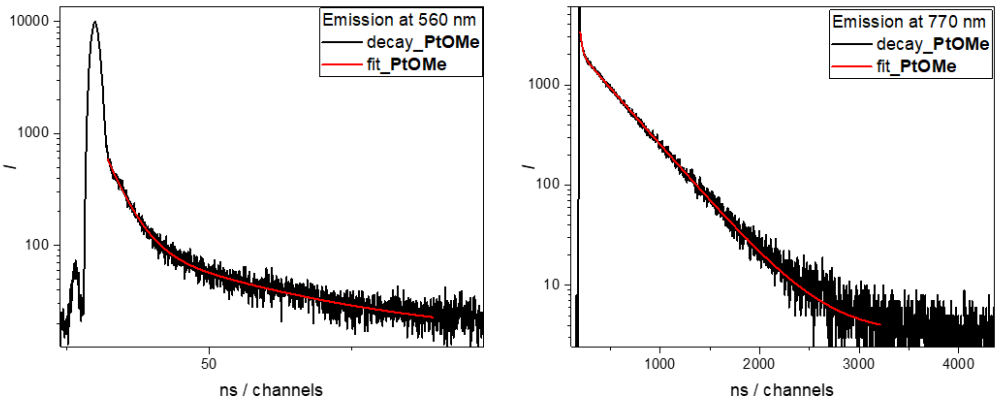
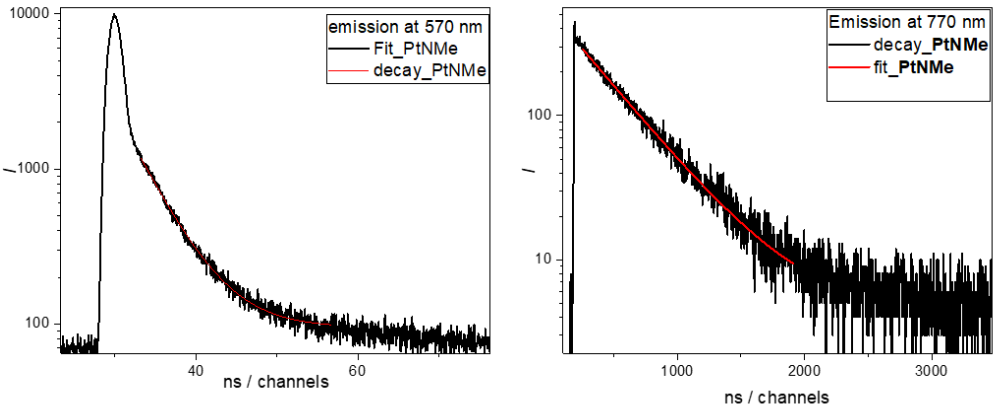
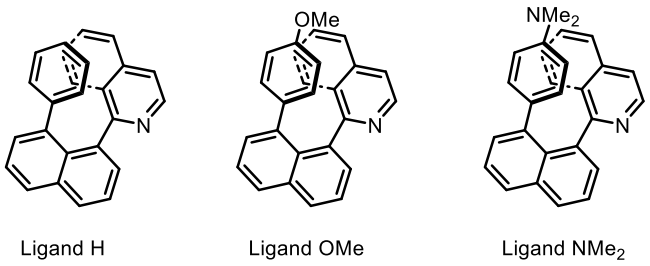


Figure S2. Luminescence decay of complex **PtOMe** with corresponding fit (red) at 560 (left) and 770 nm (right).



S3. Luminescence decay of complex **PtNMe$_2$** with corresponding fit (red) at 560 (left) and 770 nm (right).



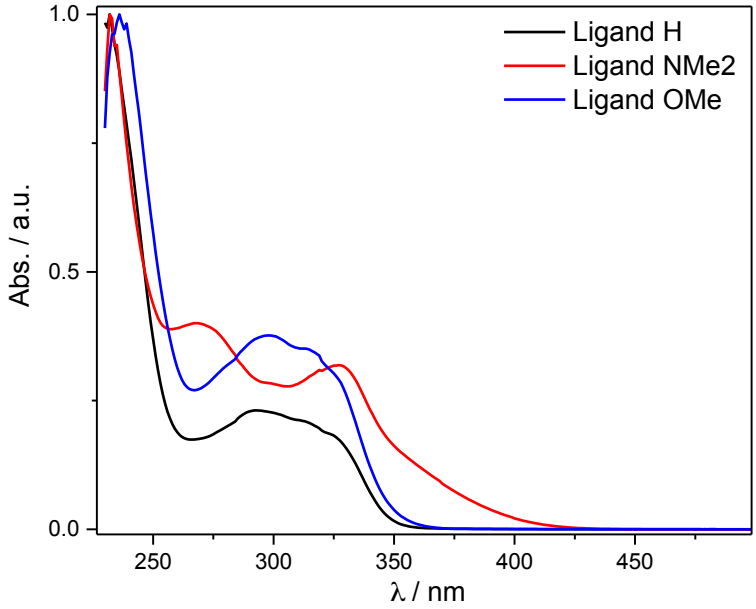
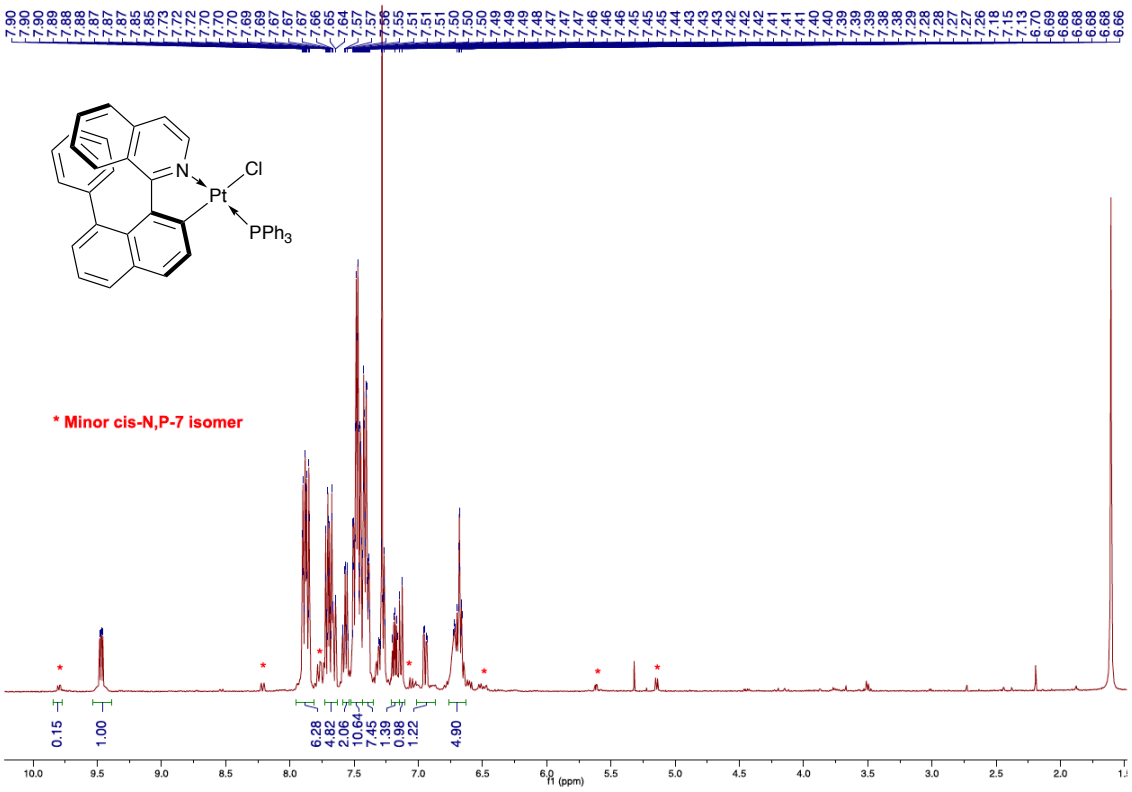


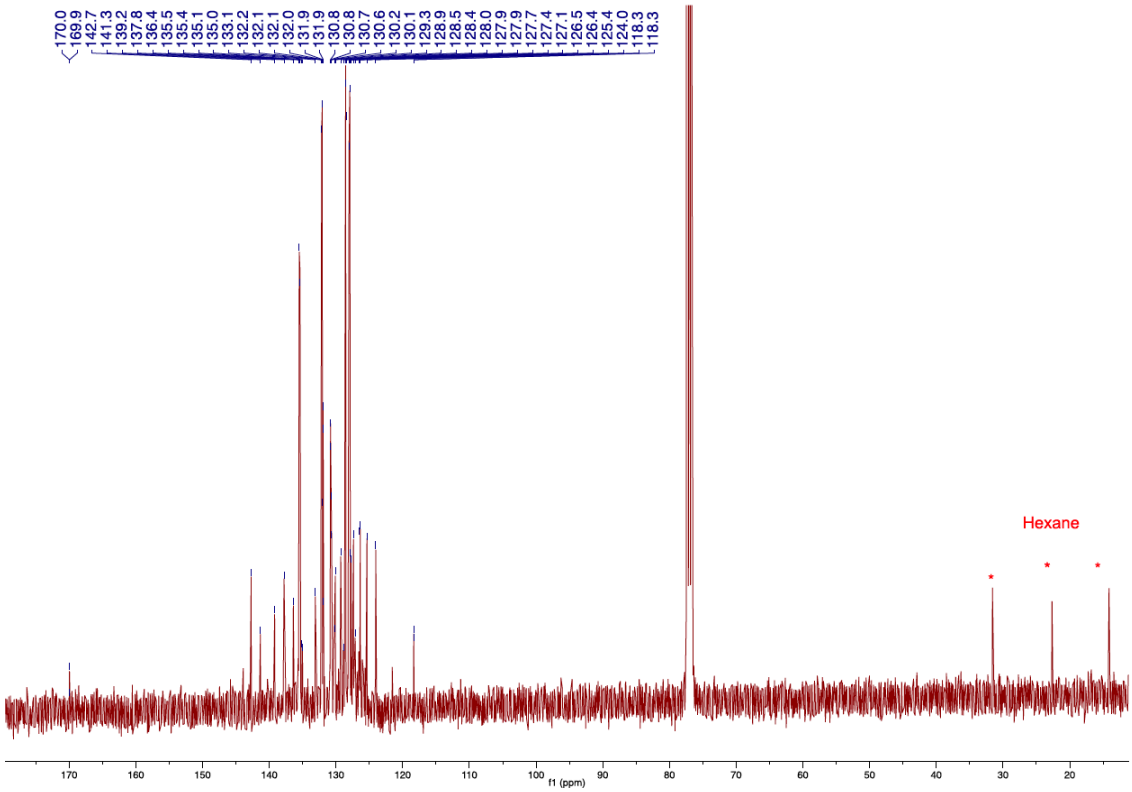
Figure S4. Chemical structures of organic helical **ligands H**, **OMe** and **NMe_2**, precursors of corresponding complexes **PtH, PtOMe** and **$PtNMe_2$**, respectively, with their UV-vis spectra measured in dichloromethane (~10^{-5} M) at 298 K.

5. NMR spectra.

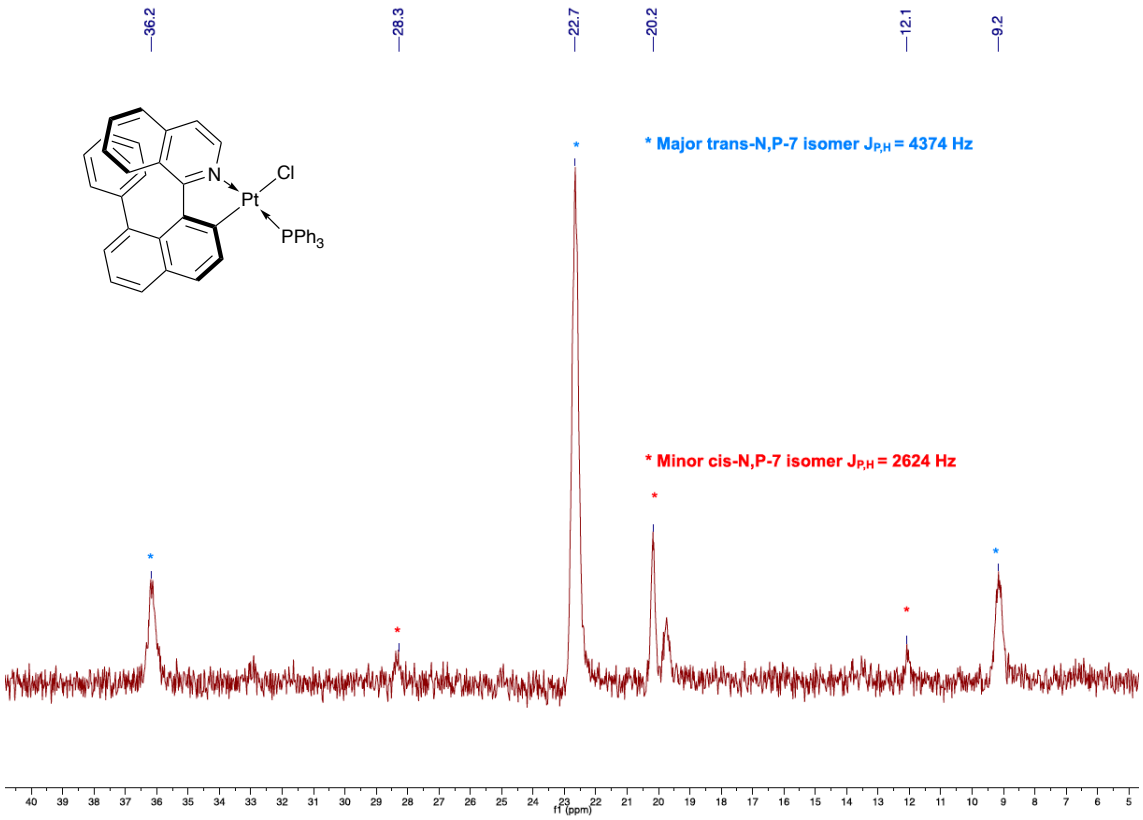
^{1}H-NMR (400 MHz, $CDCl_3$):



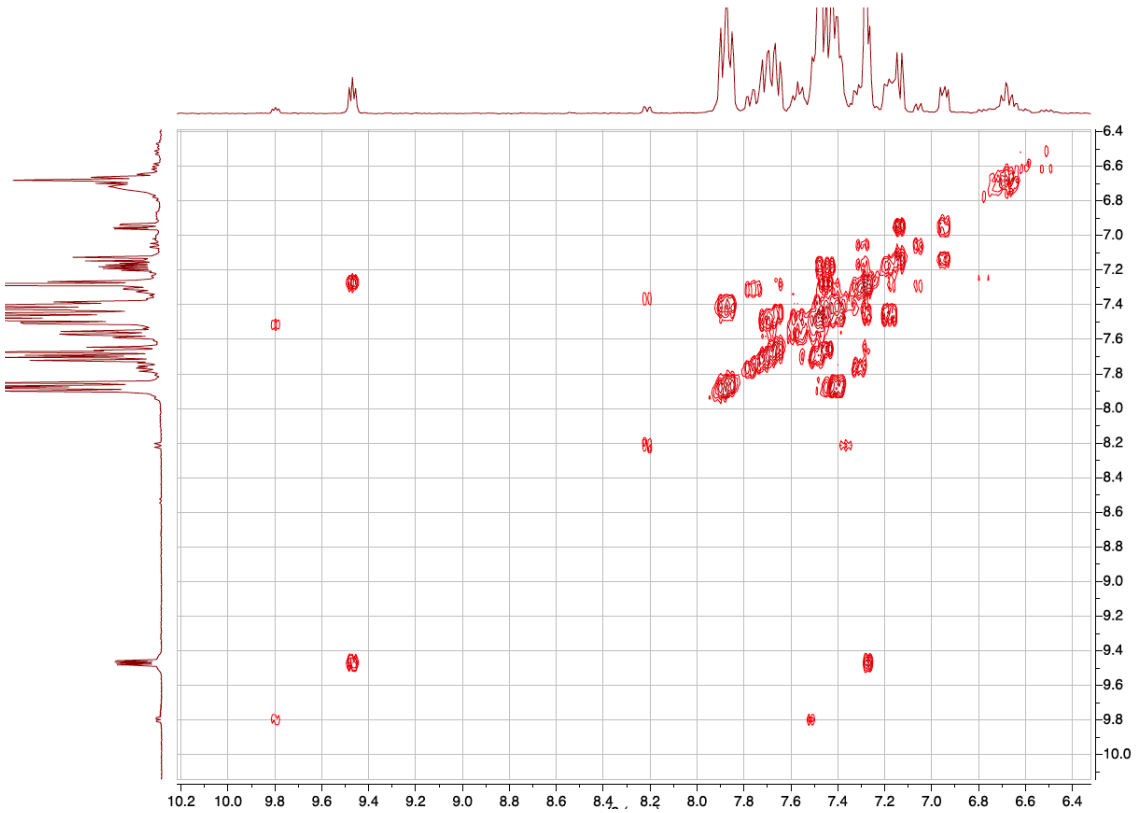
^{13}C-NMR (100 MHz, $CDCl_3$):



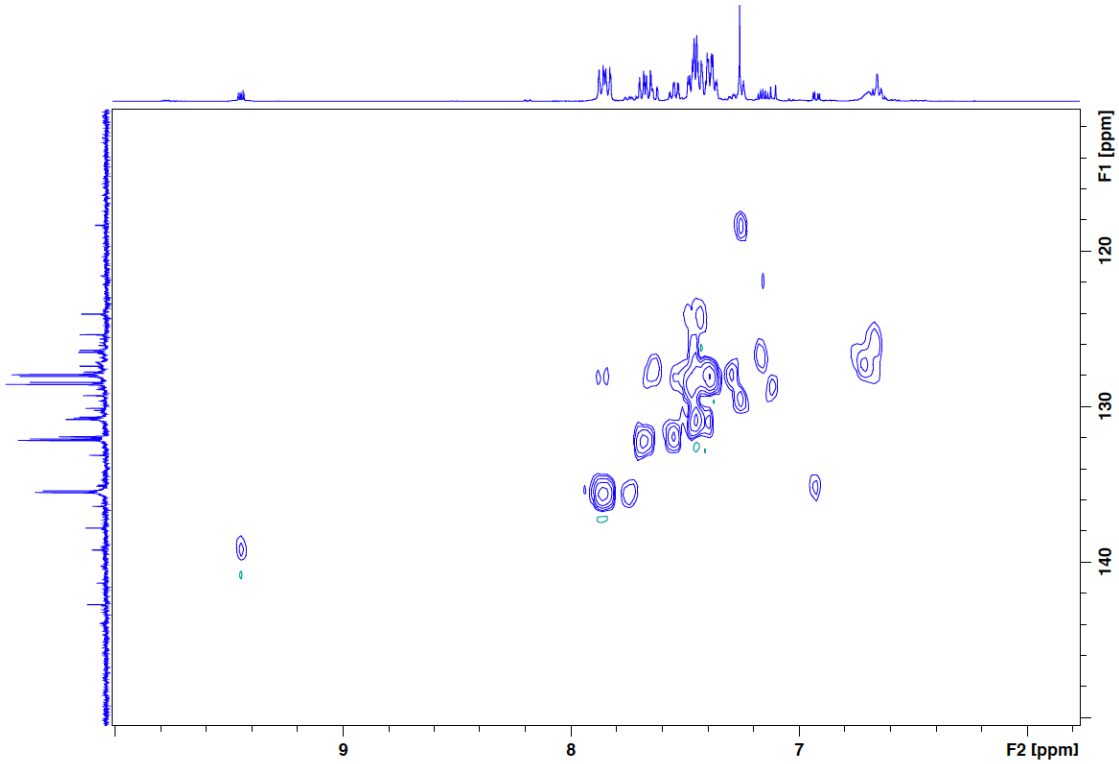
^{31}P-NMR (162 MHz, $CDCl_3$):



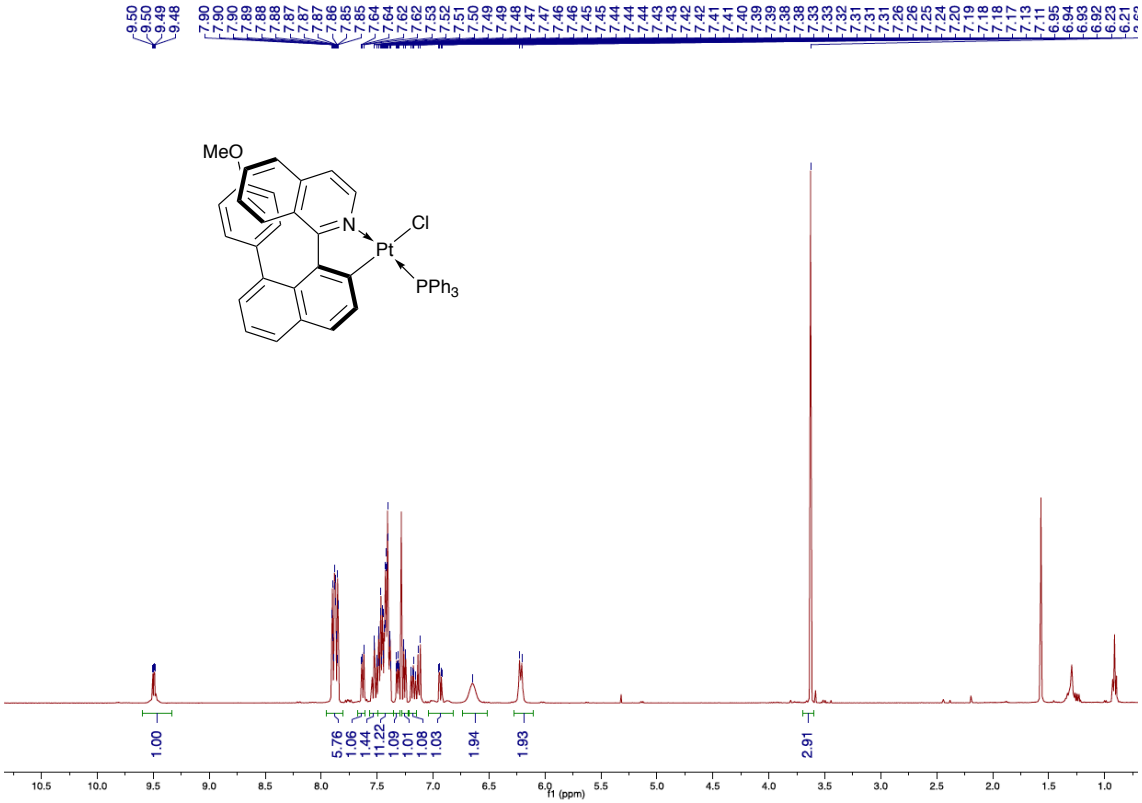
COSY



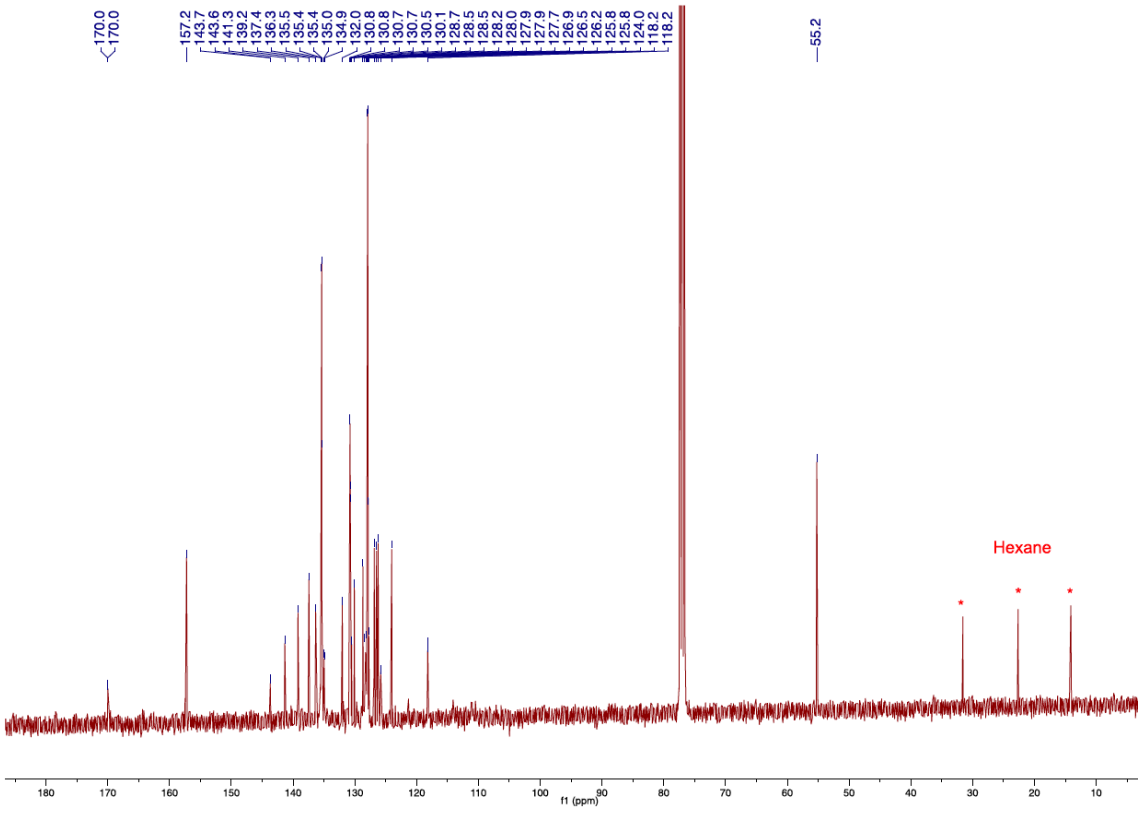
HSQC



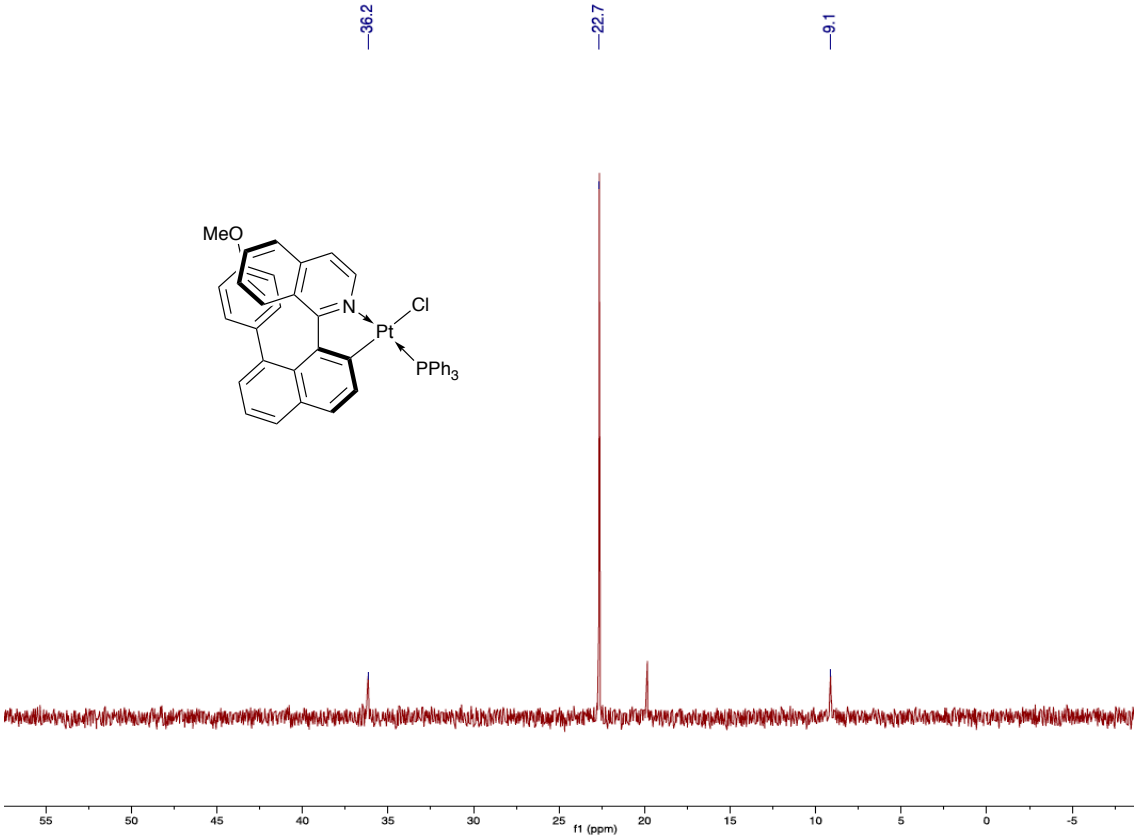
^{1}H-NMR (400 MHz, $CDCl_3$):



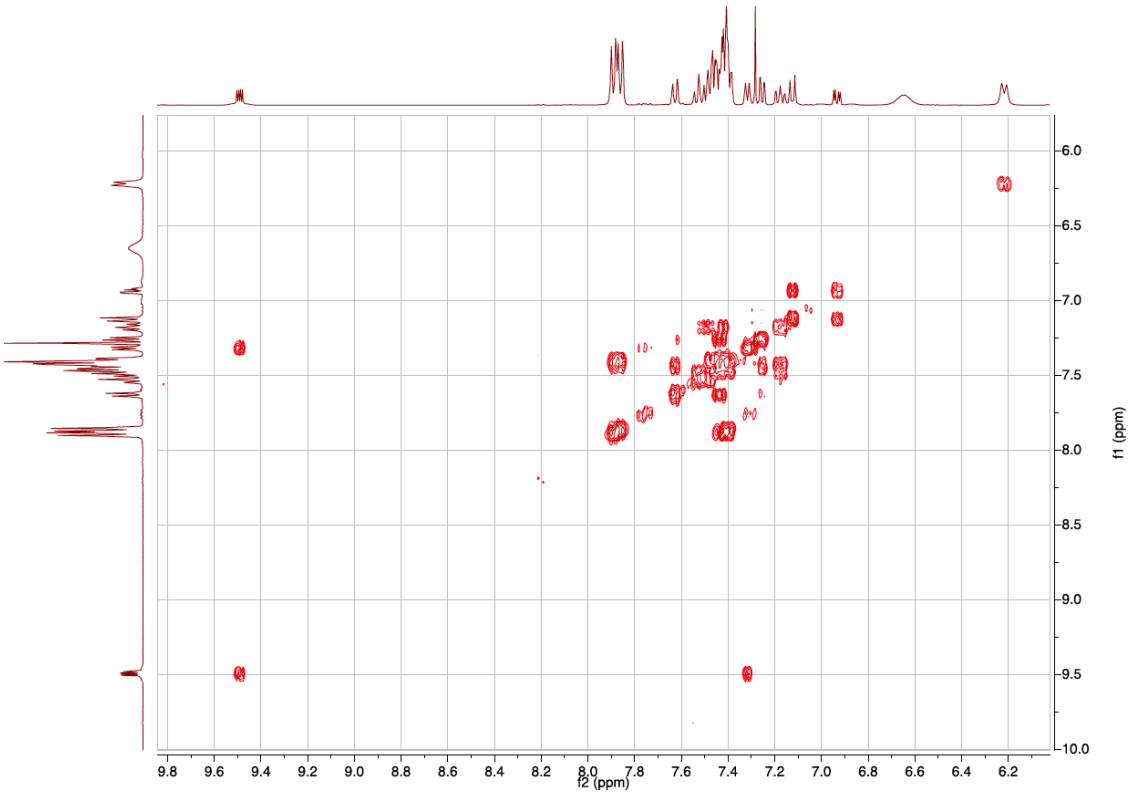
^{13}C-NMR (100 MHz, $CDCl_3$):



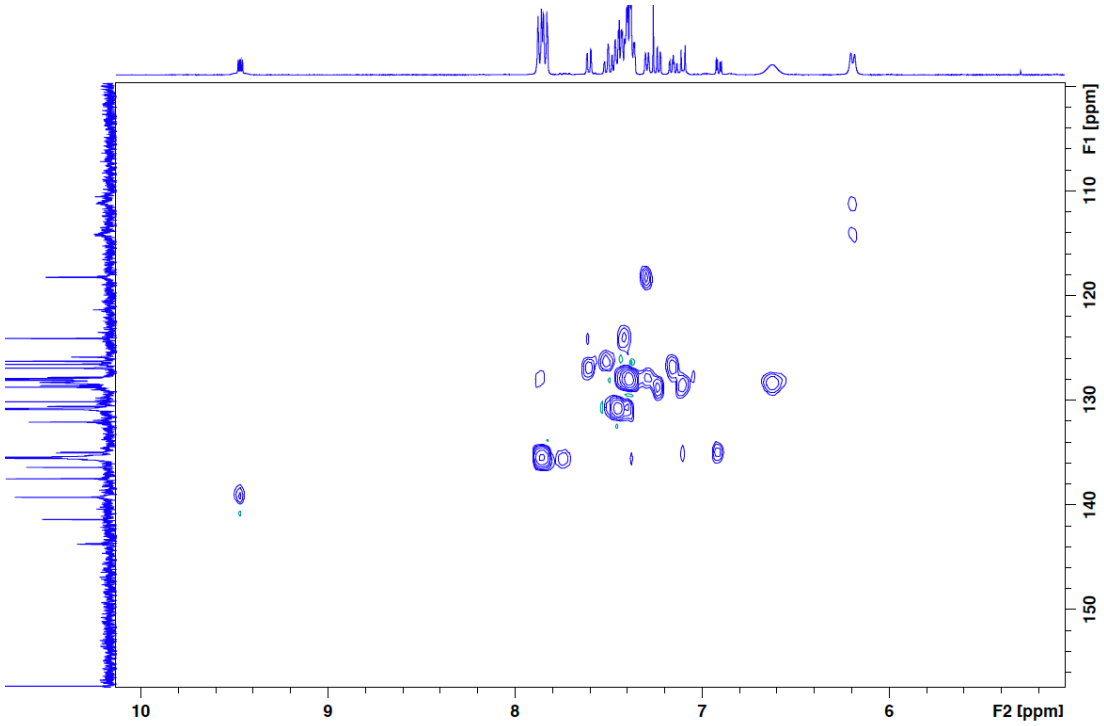
^{31}P-NMR (162 MHz, $CDCl_3$):



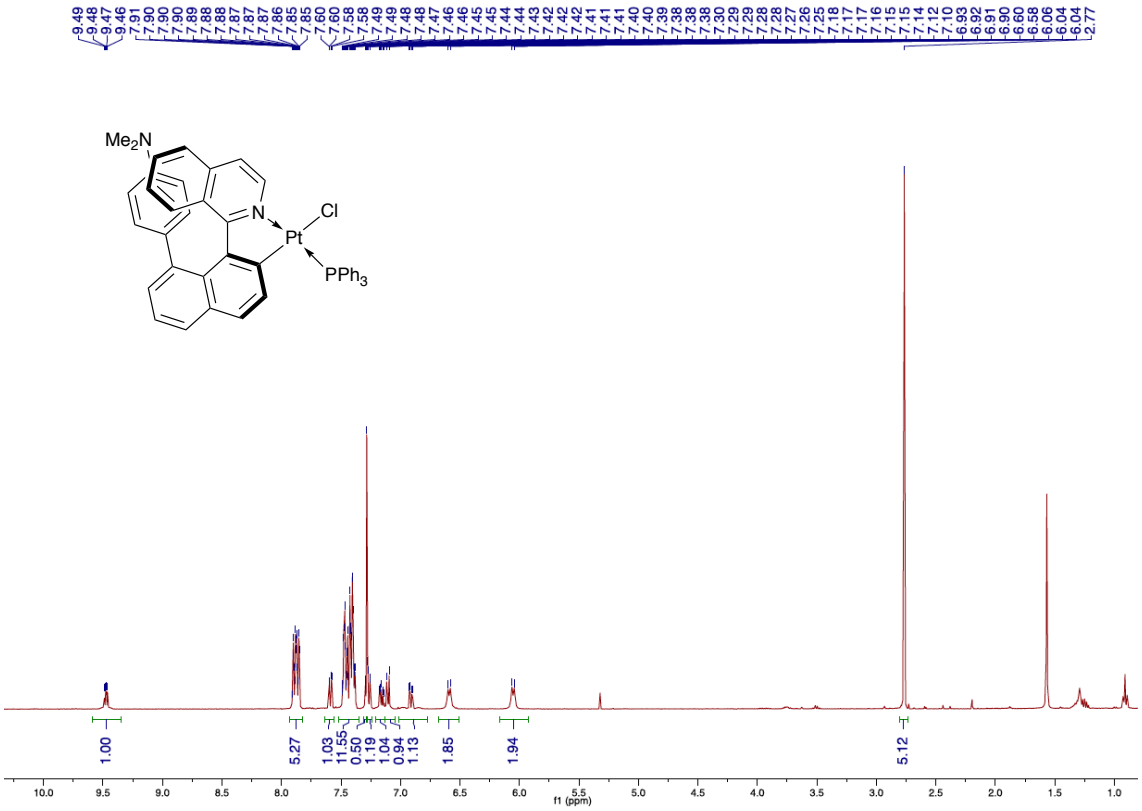
COSY



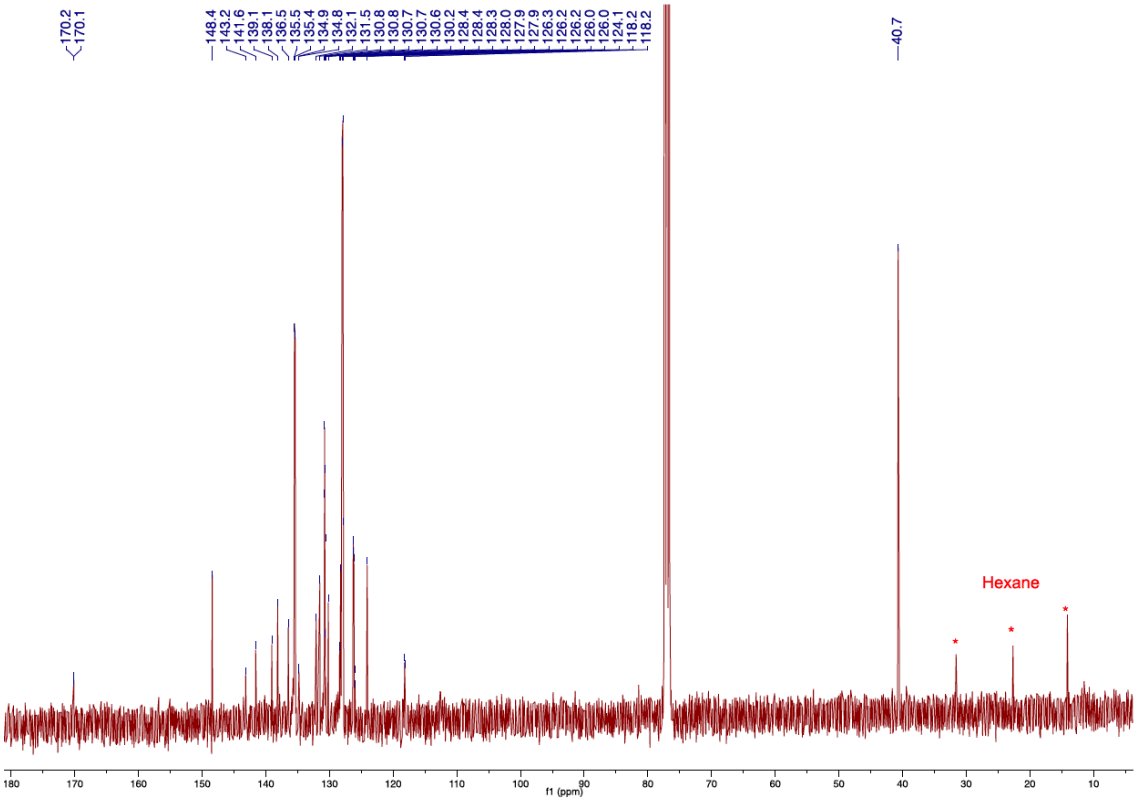
HSQC:



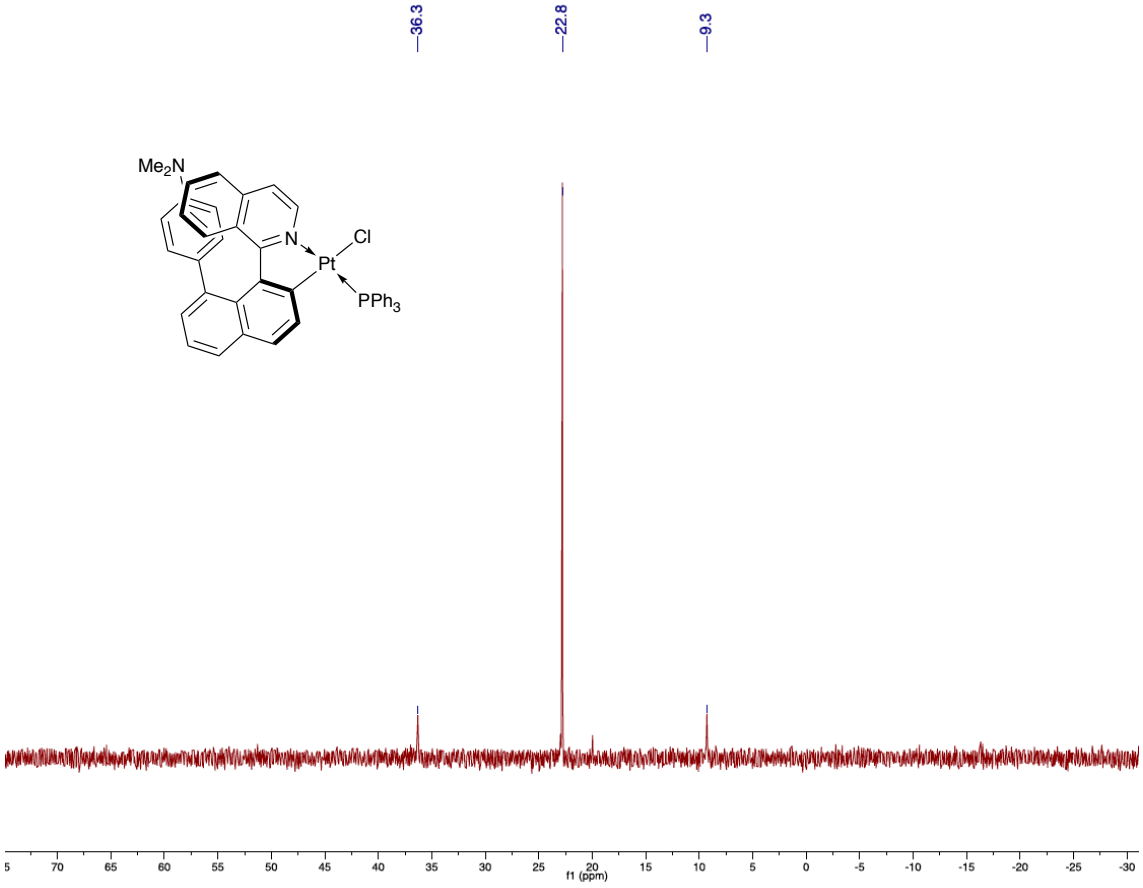
^{1}H-NMR (400 MHz, $CDCl_3$):



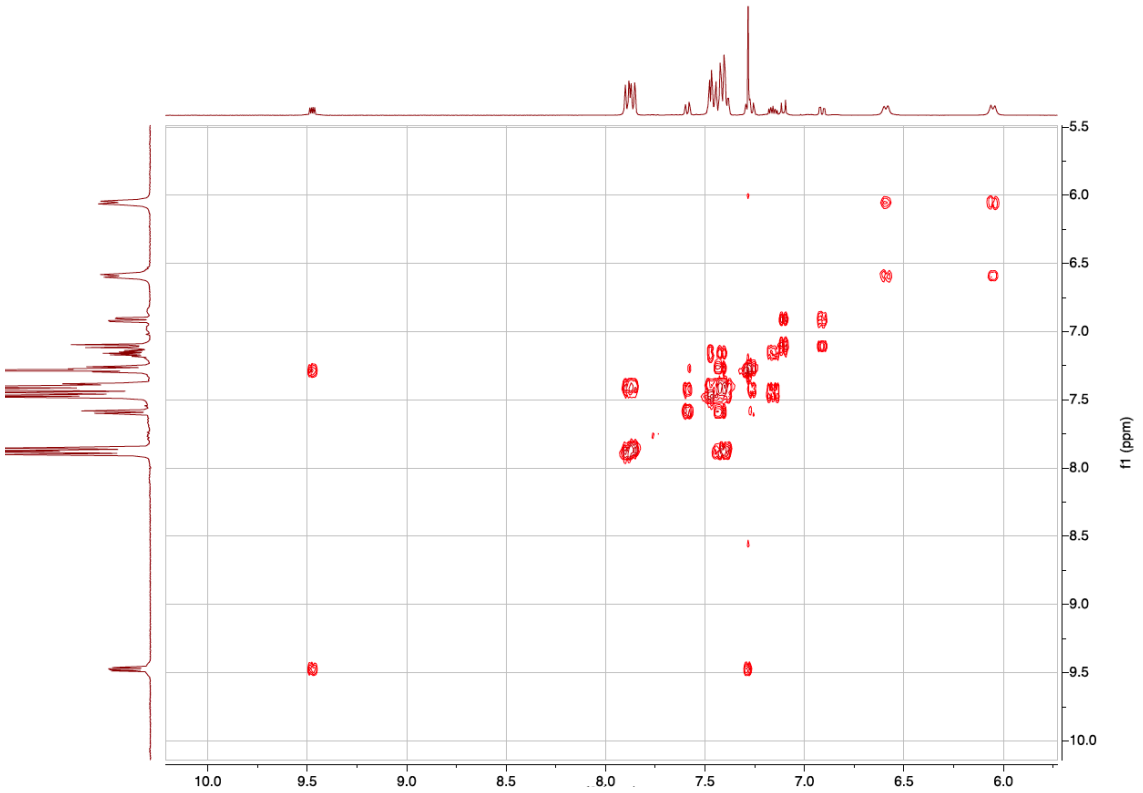
^{13}C-NMR (100 MHz, $CDCl_3$):



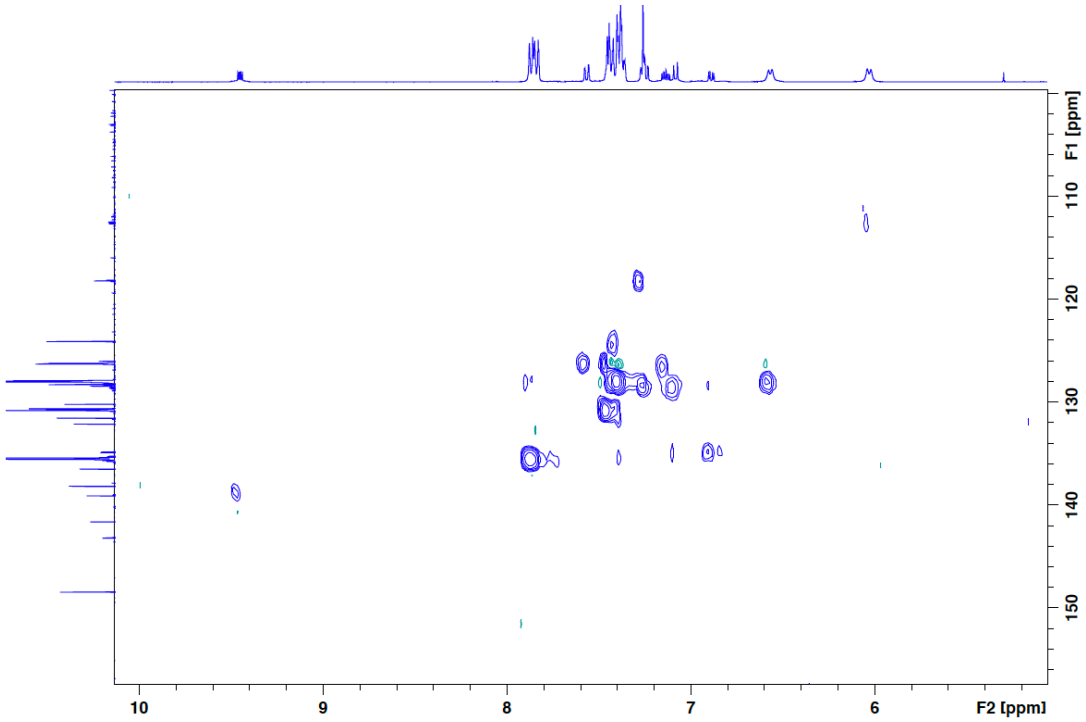
^{31}P-NMR (162 MHz, $CDCl_3$):



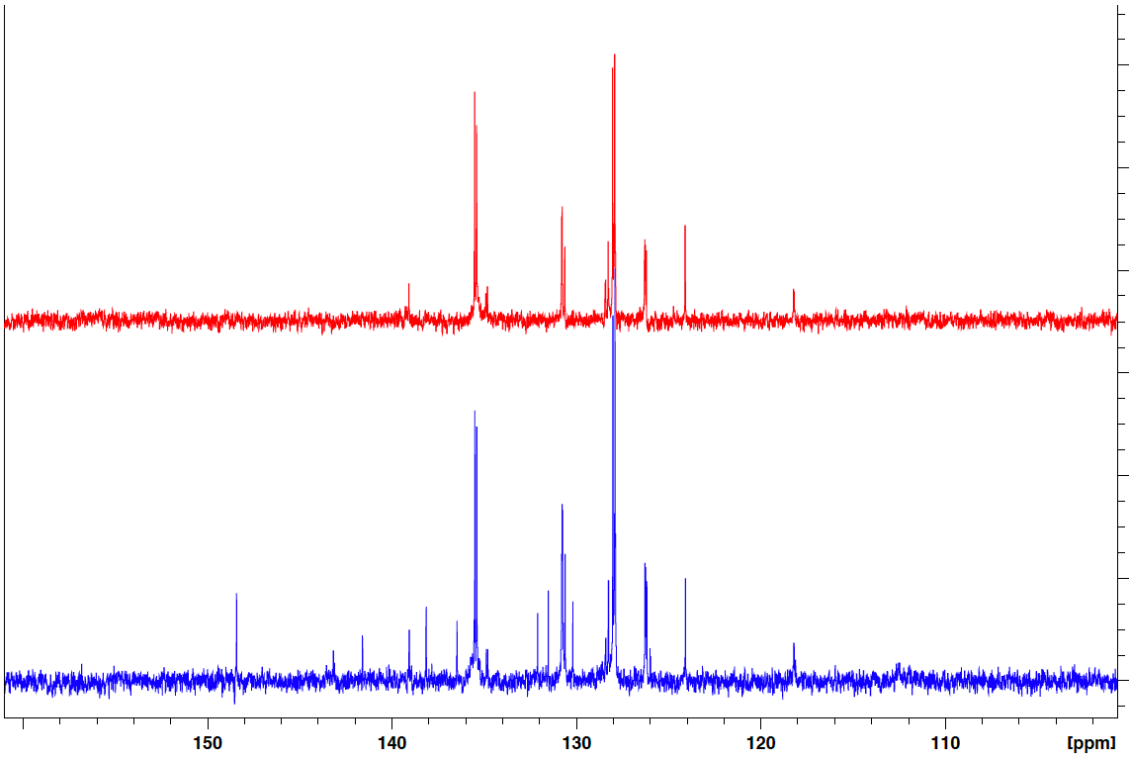
COSY



HSQC:



DEPT-135:



6. Theoretical approaches

The total, transition energies, as well as the geometries and vibrations of all systems have been computed at the (Time-Dependent) Density Functional Theory (TD-DFT) level whereas the environmental effects have been modelled using the polarizable continuum model (PCM).[1] Toluene was considered as solvent as it is the solvent used in the emission experiments. No structure simplification was performed. All calculations have been performed using the Gaussian16.A03 program,[2] but for the SOC calculations that have been achieved with ORCA.[3] We used tightened self-consistent field (10^{-10} a.u.) and geometry optimization (10^{-5} a.u.) convergence thresholds, and a large DFT integration grid (so-called *ultrafine* grid, a pruned 99,590 grid). These (TD-)DFT calculations relied on the M06-2X hybrid functional.[3] The basis used is LanL2DZ for all atoms, augmented by polarization functions on all "heavy" atoms, that is, a *d* function of contraction length 1 with α=0.587, 0.736, 0.961, and 0.648 for C, N, O, and Cl, respectively, and a similar additional *f* orbital with α =0.993 for Pt. The ground states were optimized with DFT, the lowest triplet with U-DFT and the lowest excited singlet with TD-DFT. The nature of the ground-state stationary points was confirmed by analytical Hessian calculations that returned 0 (minima) imaginary vibrational modes. Eventually the spin-orbit coupling elements were computed using the same M06-2X hybrid functional, the ZORA Hamiltonian, the *def2*-TVP basis set and the CPCM(SMD) solvent model for the calculations. The reported SOC values reported in the text have been computed as:

$$\frac{1}{3}\sqrt{S_x^2 + S_y^2 + S_z^2}$$

For the sake of consistency, the S-T gaps given in the main text when studying the ISC process have been computed with ORCA and the same methodology.

Optimal geometries (Cartesian coordinates in Å).

7/S_0

C	2.2472590	-0.5439630	0.3867310
C	3.4415750	-0.9216300	1.0830870
C	3.8581880	-2.2788710	0.9984180
C	3.0085980	-3.2076410	0.3362770
C	1.7738970	-2.7922960	-0.0993790
C	4.1757650	-0.0187240	1.9048090
C	5.0695180	-2.6776960	1.6330240
H	3.2949810	-4.2531660	0.2460400
H	1.0253440	-3.4706770	-0.5010600
C	5.7852280	-1.7752500	2.3900830
C	5.3149670	-0.4419640	2.5544430
H	5.3989790	-3.7116530	1.5370490
H	6.7007910	-2.0874860	2.8900870
H	5.8613580	0.2465480	3.1963430
C	1.7590930	0.8347060	0.2054310
C	0.3577490	0.9469540	0.1999920

C	2.6122750	1.9765150	-0.0067230
C	-0.1856030	2.2643410	0.3090950
C	2.0374040	3.2662190	0.2014720
C	3.9655280	1.9144310	-0.5022070
C	0.6300380	3.3710120	0.3947110
H	-1.2618300	2.4167590	0.3615770
C	2.8537230	4.4314620	0.1600690
C	4.7246090	3.0737410	-0.5336920
H	0.1967600	4.3600270	0.5469910
C	4.1911850	4.3327150	-0.1553170
H	2.3957820	5.4000600	0.3597910
H	5.7388190	3.0241360	-0.9292240
H	4.8215050	5.2192650	-0.1908100
N	1.4030330	-1.4799680	-0.0613830
Pt	-0.5805100	-0.7714990	-0.1487390
Cl	-1.4273760	-2.9879750	-0.8278360
P	-2.7444090	0.0487730	0.0200310
C	-3.2476030	1.1162250	-1.4112050
C	-4.6021190	1.4028320	-1.6521110
C	-2.2630730	1.6254690	-2.2703030
C	-4.9642250	2.2131580	-2.7321640
H	-5.3756610	0.9744100	-1.0138830
C	-2.6298980	2.4361290	-3.3510260
H	-1.2149560	1.3765990	-2.1029520
C	-3.9776330	2.7345290	-3.5799350
H	-6.0150070	2.4299300	-2.9162150
H	-1.8617240	2.8254170	-4.0166400
H	-4.2614370	3.3612200	-4.4238670
C	-4.1208120	-1.1902770	0.1259880
C	-4.7594280	-1.4569100	1.3425480
C	-4.5102880	-1.8715750	-1.0381640
C	-5.7925630	-2.4031590	1.3944390
H	-4.4624320	-0.9333330	2.2504620
C	-5.5463430	-2.8055530	-0.9834550
H	-3.9971810	-1.6805360	-1.9800260
C	-6.1888800	-3.0740470	0.2339160
H	-6.2853840	-2.6099860	2.3428550
H	-5.8439690	-3.3333010	-1.8877280
H	-6.9928530	-3.8072440	0.2754880
C	-2.9795550	1.0538810	1.5644840
C	-3.9465920	2.0642470	1.6577430
C	-2.1826990	0.7412900	2.6757880
C	-4.1128900	2.7618030	2.8601620
H	-4.5604990	2.3244500	0.7965830
C	-2.3588220	1.4329980	3.8792180
H	-1.4193200	-0.0332650	2.5904800
C	-3.3225620	2.4448220	3.9720320
H	-4.8586720	3.5520640	2.9265420

H	-1.7375910	1.1874690	4.7386380
H	-3.4537900	2.9888380	4.9060210
H	3.8187650	0.9996040	2.0373770
C	4.5342100	0.6834900	-1.1212580
C	3.7771580	-0.0620470	-2.0420850
C	5.8362440	0.2575780	-0.8173280
C	4.2945410	-1.2292550	-2.6118100
H	2.7729870	0.2700450	-2.3067650
C	6.3576050	-0.9084810	-1.3880660
H	6.4280850	0.8202650	-0.0952880
C	5.5857160	-1.6618230	-2.2812890
H	3.6880250	-1.7996820	-3.3135300
H	7.3616590	-1.2361260	-1.1225340
H	5.9856140	-2.5763390	-2.7163930

7/S_1

C	2.3307170	-0.5998160	0.6804130
C	3.6714320	-0.9583310	1.0884340
C	4.0672410	-2.3221160	0.9477400
C	3.0846280	-3.2722610	0.5225640
C	1.7777920	-2.8757590	0.3397240
C	4.5850570	-0.0447180	1.6653700
C	5.3884530	-2.7061600	1.2807150
H	3.3490940	-4.3205040	0.4023170
H	0.9870880	-3.5820440	0.0979540
C	6.2858840	-1.7790320	1.7941730
C	5.8699590	-0.4477440	2.0111190
H	5.6825500	-3.7467430	1.1457050
H	7.2987900	-2.0820060	2.0541820
H	6.5581210	0.2703360	2.4541690
C	1.7845170	0.7105710	0.5532750
C	0.3360000	0.7874830	0.7175040
C	2.4996920	1.9314080	0.2510070
C	-0.1910430	2.0113590	1.1993470
C	1.9498510	3.1393870	0.7927020
C	3.6892910	1.9936160	-0.5299300
C	0.6196040	3.1273250	1.3322770
H	-1.2440230	2.0863540	1.4667640
C	2.7095530	4.3251610	0.7412470
C	4.4088760	3.1963970	-0.5723830
H	0.2181440	4.0524040	1.7455590
C	3.9430260	4.3436110	0.0897620
H	2.3141350	5.2312160	1.1995220
H	5.3125810	3.2519460	-1.1773380
H	4.5207770	5.2651080	0.0443160
N	1.3884120	-1.5819220	0.4355660
Pt	-0.5378280	-0.8647160	0.2209360
Cl	-1.4637140	-3.1180960	-0.1452870

P	-2.6748280	0.0691620	-0.0692970
C	-2.7818780	1.4657430	-1.2898240
C	-4.0451420	1.9022730	-1.7272090
C	-1.6235500	2.0605320	-1.8076550
C	-4.1455000	2.9447660	-2.6523390
H	-4.9492260	1.4143760	-1.3605300
C	-1.7276730	3.1022710	-2.7383490
H	-0.6422250	1.7047890	-1.4967040
C	-2.9853610	3.5492830	-3.1561060
H	-5.1265110	3.2778910	-2.9864700
H	-0.8234490	3.5566430	-3.1393380
H	-3.0639390	4.3573700	-3.8816180
C	-4.0053690	-1.0647690	-0.6879710
C	-5.1311090	-1.3770000	0.0801500
C	-3.8627470	-1.5939040	-1.9800680
C	-6.1211760	-2.2182670	-0.4488720
H	-5.2465570	-0.9731690	1.0851390
C	-4.8539690	-2.4235100	-2.5055980
H	-2.9752260	-1.3630900	-2.5703340
C	-5.9860600	-2.7382450	-1.7387520
H	-6.9956970	-2.4630770	0.1514970
H	-4.7398450	-2.8342990	-3.5071100
H	-6.7560630	-3.3909800	-2.1468820
C	-3.3418470	0.7011250	1.5421610
C	-4.0587950	1.8993470	1.6578040
C	-3.1143820	-0.0952240	2.6765710
C	-4.5473800	2.3002420	2.9081520
H	-4.2218230	2.5324530	0.7866170
C	-3.6140250	0.3032040	3.9203270
H	-2.5456820	-1.0221900	2.5833530
C	-4.3295770	1.5024500	4.0374860
H	-5.0954780	3.2365600	2.9974420
H	-3.4369860	-0.3176040	4.7966300
H	-4.7106240	1.8169300	5.0076880
H	4.2778910	0.9812270	1.8550800
C	4.1413380	0.8567390	-1.3697340
C	3.2146800	0.1148820	-2.1252260
C	5.5019410	0.5153370	-1.4387400
C	3.6367430	-0.9611050	-2.9096980
H	2.1583390	0.3852370	-2.1004100
C	5.9259420	-0.5631280	-2.2215330
H	6.2258120	1.0688670	-0.8404920
C	4.9940480	-1.3084730	-2.9552100
H	2.9057710	-1.5292980	-3.4824290
H	6.9812000	-0.8296940	-2.2471550
H	5.3222210	-2.1531850	-3.5587000

7/T_1

C	2.3301240	-0.5679370	0.7671250
C	3.6963100	-0.9053900	1.1233060
C	4.0977100	-2.2643280	1.0083660
C	3.1123530	-3.2366750	0.6545340
C	1.7913390	-2.8562750	0.5104600
C	4.6182230	0.0369840	1.6382240
C	5.4364410	-2.6297970	1.3053910
H	3.3831670	-4.2854910	0.5566830
H	0.9973560	-3.5735700	0.3155550
C	6.3357510	-1.6814620	1.7604760
C	5.9137050	-0.3441230	1.9519550
H	5.7356090	-3.6713310	1.1920550
H	7.3597740	-1.9658150	1.9966640
H	6.6099990	0.3908640	2.3518820
C	1.7908820	0.7165460	0.5591000
C	0.3168670	0.8100670	0.7195000
C	2.5203820	1.9381000	0.2105900
C	-0.1473600	2.0100080	1.2520990
C	2.0137770	3.1398480	0.7900160
C	3.6451890	1.9805510	-0.6399550
C	0.7070830	3.1196590	1.4091300
H	-1.1938980	2.1192610	1.5348050
C	2.7621270	4.3235810	0.6726470
C	4.3628700	3.1880720	-0.7548950
H	0.3331990	4.0387710	1.8576690
C	3.9446360	4.3365680	-0.0769660
H	2.4023430	5.2341440	1.1508150
H	5.2323270	3.2274260	-1.4094690
H	4.5169990	5.2580470	-0.1708730
N	1.3975480	-1.5672990	0.5835360
Pt	-0.5524280	-0.8764810	0.2741200
Cl	-1.4151880	-3.1589390	-0.1354850
P	-2.6603360	0.0578050	-0.0712680
C	-2.7454890	1.3983370	-1.3548480
C	-3.9997360	1.8026810	-1.8452360
C	-1.5789710	1.9901120	-1.8576640
C	-4.0840510	2.8087840	-2.8117310
H	-4.9090730	1.3193070	-1.4858350
C	-1.6670720	2.9953380	-2.8291950
H	-0.6052290	1.6625680	-1.4974790
C	-2.9165050	3.4092630	-3.3025480
H	-5.0583740	3.1169020	-3.1869670
H	-0.7564860	3.4480800	-3.2175400
H	-2.9823810	4.1890650	-4.0596380
C	-4.0121840	-1.0807440	-0.6344740
C	-5.1878450	-1.2558050	0.1027640
C	-3.8448040	-1.7391200	-1.8627350
C	-6.2025690	-2.0879070	-0.3932630

H	-5.3235480	-0.7510260	1.0584450
C	-4.8608640	-2.5578880	-2.3573070
H	-2.9177320	-1.6189360	-2.4233510
C	-6.0427070	-2.7341590	-1.6218530
H	-7.1155140	-2.2254110	0.1836790
H	-4.7274470	-3.0689970	-3.3090380
H	-6.8318820	-3.3788610	-2.0055660
C	-3.3260010	0.7813370	1.5016060
C	-4.0223640	1.9958740	1.5495100
C	-3.1225650	0.0403180	2.6770560
C	-4.5144190	2.4686740	2.7733690
H	-4.1666820	2.5854980	0.6450100
C	-3.6252410	0.5099980	3.8943010
H	-2.5686390	-0.8991280	2.6358870
C	-4.3202930	1.7259880	3.9438340
H	-5.0465730	3.4176700	2.8097870
H	-3.4666530	-0.0682010	4.8027380
H	-4.7038970	2.0959610	4.8932680
H	4.3055330	1.0651360	1.8050840
C	4.0663400	0.8064720	-1.4481870
C	3.1149610	0.0379450	-2.1424820
C	5.4211790	0.4489840	-1.5358020
C	3.5064330	-1.0814290	-2.8813740
H	2.0616320	0.3193710	-2.1034890
C	5.8158130	-0.6707370	-2.2761570
H	6.1656160	1.0270920	-0.9879720
C	4.8592390	-1.4433450	-2.9461700
H	2.7555050	-1.6694940	-3.4063740
H	6.8684090	-0.9458970	-2.3189720
H	5.1641930	-2.3192960	-3.5164040

8/S_0

C	-1.9994680	-0.1564470	-0.6175360
C	-3.1822360	-0.3151300	-1.4121390
C	-3.7174000	-1.6254190	-1.5534810
C	-2.9921260	-2.7166180	-1.0008700
C	-1.7522850	-2.4870670	-0.4561490
C	-3.7889840	0.7629320	-2.1184690
C	-4.9176800	-1.8131740	-2.2979710
H	-3.3735540	-3.7322400	-1.0792310
H	-1.0897000	-3.2845480	-0.1295160
C	-5.5075580	-0.7472280	-2.9425080
C	-4.9188370	0.5472100	-2.8774620
H	-5.3360600	-2.8161440	-2.3774810
H	-6.4128340	-0.8966270	-3.5290230
H	-5.3662870	1.3708250	-3.4307070
C	-1.3998360	1.1284460	-0.2125500
C	0.0036580	1.1004440	-0.1364930

C	-2.1535890	2.3084740	0.1332460
C	0.6711990	2.3598410	-0.0316150
C	-1.4515440	3.5514540	0.1369050
C	-3.5291100	2.3111880	0.5683660
C	-0.0325020	3.5427210	0.0137780
H	1.7579330	2.4111260	-0.0199220
C	-2.1566240	4.7744360	0.3174990
C	-4.1770830	3.5244720	0.7419510
H	0.4979490	4.4953760	0.0242450
C	-3.5114880	4.7649240	0.5681560
H	-1.6010990	5.7111990	0.2768050
H	-5.2093780	3.5196310	1.0912600
H	-4.0575290	5.6958200	0.7094750
N	-1.2659250	-1.2244810	-0.2829260
Pt	0.7650070	-0.7330780	-0.0100460
Cl	1.3792070	-3.0972220	0.3466370
P	2.9980150	-0.1022200	0.0387950
C	3.5007950	0.7091230	1.6300730
C	4.8579160	0.8456440	1.9685630
C	2.5122190	1.1675430	2.5125880
C	5.2205540	1.4592230	3.1711960
H	5.6306100	0.4511090	1.3078690
C	2.8793950	1.7805420	3.7164570
H	1.4592130	1.0314430	2.2656300
C	4.2312540	1.9315900	4.0441930
H	6.2731090	1.5601020	3.4299660
H	2.1074290	2.1305450	4.3992620
H	4.5151340	2.4043560	4.9830480
C	4.2793090	-1.4274060	-0.1707160
C	4.9960900	-1.5614200	-1.3654330
C	4.5267480	-2.3006750	0.9003330
C	5.9664660	-2.5661780	-1.4869850
H	4.8099050	-0.8888000	-2.2016990
C	5.5014830	-3.2924170	0.7786450
H	3.9533410	-2.2094910	1.8221860
C	6.2228040	-3.4277980	-0.4166000
H	6.5207020	-2.6687310	-2.4183740
H	5.6898150	-3.9677380	1.6112750
H	6.9788150	-4.2057180	-0.5115270
C	3.4061660	1.0791760	-1.3359060
C	4.4404240	2.0194730	-1.2321040
C	2.6706720	0.9747830	-2.5259500
C	4.7348020	2.8553900	-2.3159980
H	5.0079180	2.1189410	-0.3078370
C	2.9747860	1.8040560	-3.6110670
H	1.8552070	0.2536120	-2.5949780
C	4.0057560	2.7460520	-3.5067270
H	5.5326350	3.5908960	-2.2286810

H	2.4009520	1.7193790	-4.5321490
H	4.2368540	3.3971010	-4.3482880
H	-3.3418400	1.7531250	-2.0753280
C	-4.2374190	1.0622880	0.9604740
C	-3.6039270	0.1024300	1.7746530
C	-5.5424170	0.8013310	0.5324230
C	-4.2334240	-1.0949390	2.0990620
H	-2.5967910	0.2915320	2.1467580
C	-6.1935890	-0.3989580	0.8483110
H	-6.0500780	1.5236310	-0.1067290
C	-5.5286810	-1.3617790	1.6201420
H	-3.7372410	-1.8436300	2.7139780
H	-7.1965780	-0.5745620	0.4679620
O	-6.0517140	-2.5737420	1.9536910
C	-7.3459690	-2.8737050	1.4648920
H	-7.3687400	-2.8581690	0.3655870
H	-7.5807300	-3.8806570	1.8185320
H	-8.0934860	-2.1682160	1.8543640

8/S_1

C	-2.0659100	-0.1009560	-0.9391340
C	-3.3915270	-0.2496090	-1.4965660
C	-3.9233810	-1.5692520	-1.6052730
C	-3.0669240	-2.6713470	-1.2878120
C	-1.7439150	-2.4443230	-0.9756510
C	-4.1628280	0.8341190	-1.9753180
C	-5.2452280	-1.7531250	-2.0766070
H	-3.4344630	-3.6926420	-1.3582130
H	-1.0382970	-3.2572650	-0.8221000
C	-6.0061350	-0.6664580	-2.4909230
C	-5.4491480	0.6296450	-2.4644020
H	-5.6458570	-2.7652880	-2.1336050
H	-7.0186690	-0.8160210	-2.8625560
H	-6.0276570	1.4768690	-2.8292770
C	-1.4312940	1.1034770	-0.5103080
C	0.0276550	1.0723680	-0.5548640
C	-2.0751170	2.2977470	-0.0064610
C	0.6908360	2.3162310	-0.7006020
C	-1.3809970	3.5351670	-0.2160610
C	-3.3315910	2.3112580	0.6688430
C	-0.0100040	3.5099370	-0.6355390
H	1.7662810	2.3470370	-0.8675260
C	-2.0463990	4.7510090	0.0340680
C	-3.9587410	3.5438660	0.9103670
H	0.5022480	4.4580540	-0.7979360
C	-3.3382550	4.7529490	0.5641350
H	-1.5350250	5.6902120	-0.1752570
H	-4.9156070	3.5567510	1.4303260

H	-3.8431790	5.6964950	0.7635460
N	-1.2324610	-1.1987850	-0.8259000
Pt	0.7340400	-0.7262870	-0.4133960
Cl	1.4375800	-3.0896190	-0.5125400
P	2.9293670	-0.0888150	0.1302450
C	3.0987370	0.9572600	1.6569930
C	4.3702060	1.1514130	2.2254780
C	1.9708180	1.5197680	2.2696040
C	4.5118860	1.9267870	3.3794520
H	5.2464790	0.6795890	1.7789440
C	2.1157810	2.2928020	3.4287080
H	0.9802570	1.3445570	1.8520220
C	3.3837570	2.5024650	3.9804520
H	5.4991460	2.0730940	3.8140920
H	1.2345750	2.7231240	3.9011550
H	3.4938690	3.1011170	4.8832590
C	4.1378320	-1.4505840	0.4845830
C	5.2707020	-1.6612410	-0.3073800
C	3.8993820	-2.2609070	1.6056400
C	6.1711030	-2.6841370	0.0258130
H	5.4607240	-1.0384690	-1.1806240
C	4.8021600	-3.2712720	1.9386690
H	3.0061370	-2.1060820	2.2116060
C	5.9406180	-3.4856300	1.1469760
H	7.0507730	-2.8491780	-0.5939730
H	4.6132600	-3.8996830	2.8071740
H	6.6410550	-4.2787790	1.4036320
C	3.7210130	0.8479170	-1.2621170
C	4.5675290	1.9465520	-1.0626010
C	3.4576620	0.3903580	-2.5634300
C	5.1500650	2.5860960	-2.1645310
H	4.7605700	2.3206160	-0.0580190
C	4.0505470	1.0245850	-3.6597960
H	2.7870130	-0.4573800	-2.7143600
C	4.8963730	2.1239590	-3.4613510
H	5.7997650	3.4453310	-2.0073180
H	3.8452710	0.6653650	-4.6665230
H	5.3511310	2.6226180	-4.3157120
H	-3.7435430	1.8382940	-1.9701360
C	-3.9569860	1.0697170	1.1694270
C	-3.1801360	0.0607960	1.7778030
C	-5.3274680	0.8382920	0.9982210
C	-3.7451200	-1.1523960	2.1463160
H	-2.1174740	0.2302800	1.9537610
C	-5.9120610	-0.3830200	1.3506570
H	-5.9435690	1.5964280	0.5151540
C	-5.1122370	-1.3928990	1.9077170
H	-3.1464970	-1.9395780	2.6005450

H	-6.9704050	-0.5406710	1.1612090
O	-5.5668190	-2.6250040	2.2503120
C	-6.9251770	-2.9159870	1.9708750
H	-7.1364740	-2.8167300	0.8967230
H	-7.0846910	-3.9517890	2.2797400
H	-7.5983690	-2.2589760	2.5390270

8/T_1

C	-2.0623660	-0.0162290	-1.0468660
C	-3.4228270	-0.1304470	-1.5376440
C	-3.9648450	-1.4339820	-1.7001200
C	-3.1072880	-2.5566040	-1.4858730
C	-1.7668070	-2.3547000	-1.2149680
C	-4.2035890	0.9876140	-1.9127820
C	-5.3087940	-1.5861540	-2.1294830
H	-3.4861920	-3.5698810	-1.5979060
H	-1.0612080	-3.1775470	-1.1256130
C	-6.0721240	-0.4753260	-2.4456010
C	-5.5049790	0.8186120	-2.3607970
H	-5.7181520	-2.5909380	-2.2318680
H	-7.0991870	-0.5952880	-2.7866140
H	-6.0929260	1.6874670	-2.6513210
C	-1.4299090	1.1343500	-0.5346000
C	0.0551050	1.1107130	-0.5902410
C	-2.0772100	2.3077700	0.0571780
C	0.6618550	2.3497120	-0.7807930
C	-1.4217040	3.5547260	-0.1749020
C	-3.2599820	2.2620090	0.8272000
C	-0.0764280	3.5477680	-0.7037940
H	1.7330330	2.4171730	-0.9668830
C	-2.0703660	4.7466090	0.1884920
C	-3.8772830	3.4757270	1.1938130
H	0.4122680	4.5033410	-0.8877720
C	-3.3060870	4.7024820	0.8476810
H	-1.5941680	5.7028100	-0.0264130
H	-4.7917350	3.4461680	1.7847610
H	-3.8012510	5.6292190	1.1334010
N	-1.2438400	-1.1248320	-1.0220100
Pt	0.7380880	-0.7148280	-0.4985900
Cl	1.3461430	-3.1141780	-0.5153160
P	2.8982720	-0.1003130	0.1252350
C	3.0181100	0.8626190	1.7099360
C	4.2645710	0.9953080	2.3470180
C	1.8770930	1.4336490	2.2901340
C	4.3696080	1.7147860	3.5407470
H	5.1495040	0.5203110	1.9216930
C	1.9856560	2.1511760	3.4881660
H	0.9060940	1.3109000	1.8132410

C	3.2294340	2.2972210	4.1111840
H	5.3376660	1.8125230	4.0289580
H	1.0944390	2.5886180	3.9346730
H	3.3107600	2.8524910	5.0442950
C	4.1141360	-1.4681800	0.4278080
C	5.2634480	-1.6256460	-0.3532330
C	3.8634870	-2.3412390	1.4981700
C	6.1682740	-2.6566840	-0.0590800
H	5.4633340	-0.9541920	-1.1873960
C	4.7708440	-3.3591160	1.7934250
H	2.9561160	-2.2294710	2.0918900
C	5.9261150	-3.5191000	1.0134310
H	7.0608170	-2.7795400	-0.6702450
H	4.5722350	-4.0358320	2.6225560
H	6.6302770	-4.3180600	1.2403090
C	3.7158570	0.9241370	-1.1879780
C	4.5753970	1.9908680	-0.8937510
C	3.4636550	0.5732420	-2.5239150
C	5.1813610	2.7053580	-1.9351980
H	4.7598980	2.2823980	0.1393310
C	4.0790600	1.2820840	-3.5605610
H	2.7811040	-0.2479820	-2.7482550
C	4.9375770	2.3499180	-3.2671120
H	5.8409230	3.5399590	-1.7037960
H	3.8808660	1.0064390	-4.5947140
H	5.4096990	2.9072900	-4.0744840
H	-3.7756510	1.9866550	-1.8618460
C	-3.8498190	0.9749960	1.2685040
C	-3.0367220	-0.0599810	1.7740560
C	-5.2207100	0.7322010	1.1349870
C	-3.5688070	-1.3069500	2.0776440
H	-1.9692790	0.1125390	1.9183150
C	-5.7760790	-0.5190610	1.4339360
H	-5.8669830	1.5124990	0.7330120
C	-4.9424670	-1.5508830	1.8878640
H	-2.9398520	-2.1126490	2.4518630
H	-6.8408140	-0.6774580	1.2844290
O	-5.3676490	-2.8108240	2.1709690
C	-6.7386130	-3.0938370	1.9565640
H	-7.0160940	-2.9338170	0.9047460
H	-6.8767200	-4.1470150	2.2128610
H	-7.3791690	-2.4756210	2.6011320

9/S_0

C	-1.9130410	0.0744890	-0.7269040
C	-3.1106340	0.0435990	-1.5167120
C	-3.6924880	-1.2241490	-1.7948860
C	-3.0000470	-2.3936360	-1.3757410

C	-1.7489720	-2.2678160	-0.8240070
C	-3.6867330	1.2113140	-2.0941240
C	-4.9032630	-1.2897240	-2.5425090
H	-3.4147540	-3.3814140	-1.5663900
H	-1.1120760	-3.1184150	-0.5947540
C	-5.4631370	-0.1407030	-3.0580850
C	-4.8304690	1.1180750	-2.8575060
H	-5.3544330	-2.2638290	-2.7298980
H	-6.3778890	-0.1952220	-3.6463780
H	-5.2544620	2.0122990	-3.3105530
C	-1.2582670	1.2873160	-0.2021330
C	0.1430670	1.1940290	-0.1395430
C	-1.9573660	2.4637540	0.2544800
C	0.8639360	2.4127740	0.0555590
C	-1.2050560	3.6728790	0.3490570
C	-3.3249850	2.4811960	0.7137070
C	0.2110300	3.6165940	0.2031720
H	1.9520590	2.4171830	0.0563090
C	-1.8589300	4.9032610	0.6392730
C	-3.9228380	3.7007090	0.9934290
H	0.7812060	4.5429130	0.2804960
C	-3.2105390	4.9243910	0.9086660
H	-1.2676040	5.8183280	0.6670740
H	-4.9501080	3.7067590	1.3574350
H	-3.7173300	5.8611980	1.1332720
N	-1.2156390	-1.0491950	-0.5211630
Pt	0.8238940	-0.6752520	-0.1702710
Cl	1.3349850	-3.0886680	-0.0608640
P	3.0767910	-0.1563720	0.0487200
C	3.5182400	0.5235590	1.7184300
C	4.8582050	0.5718230	2.1396820
C	2.5017720	0.9696030	2.5752650
C	5.1779580	1.0875580	3.3990450
H	5.6495070	0.1837400	1.4973670
C	2.8259680	1.4846470	3.8361040
H	1.4596500	0.9009530	2.2634570
C	4.1619500	1.5494820	4.2466240
H	6.2173240	1.1205870	3.7209670
H	2.0320490	1.8265440	4.4975320
H	4.4117420	1.9465640	5.2292180
C	4.3048510	-1.5301890	-0.1680760
C	5.0930470	-1.6229270	-1.3205710
C	4.4334430	-2.4866860	0.8516960
C	6.0177860	-2.6689320	-1.4505020
H	4.9978340	-0.8863140	-2.1173680
C	5.3621320	-3.5205460	0.7223580
H	3.8036180	-2.4271100	1.7388210
C	6.1562590	-3.6138630	-0.4300580

H	6.6283800	-2.7387400	-2.3490890
H	5.4582470	-4.2606750	1.5147130
H	6.8766200	-4.4241790	-0.5310240
C	3.6248960	1.0883870	-1.2164090
C	4.6964120	1.9635480	-0.9913360
C	2.9564510	1.1010020	-2.4496580
C	5.0959890	2.8504810	-1.9981230
H	5.2114740	1.9726550	-0.0318070
C	3.3653550	1.9811410	-3.4575930
H	2.1114930	0.4302630	-2.6116950
C	4.4344410	2.8572750	-3.2324540
H	5.9227660	3.5350970	-1.8168550
H	2.8434570	1.9875190	-4.4127870
H	4.7473120	3.5478140	-4.0139370
H	-3.2060510	2.1756960	-1.9504730
C	-4.0677220	1.2286630	1.0098040
C	-3.4555660	0.1749340	1.7074280
C	-5.3892860	1.0366910	0.5849870
C	-4.1048570	-1.0397330	1.9204760
H	-2.4356450	0.2942830	2.0746820
C	-6.0563930	-0.1717160	0.7882140
H	-5.8925650	1.8277030	0.0281940
C	-5.4239720	-1.2497970	1.4517410
H	-3.5709250	-1.8261170	2.4467510
H	-7.0660400	-0.2775810	0.4009450
C	-7.2500550	-2.7322740	0.8289950
H	-7.0431380	-2.6483830	-0.2523370
H	-7.6100030	-3.7434190	1.0390670
H	-8.0622690	-2.0384010	1.0781610
C	-5.2539990	-3.6147990	2.0011580
H	-4.4405310	-3.7953810	1.2774750
H	-4.8065800	-3.4795830	2.9933230
H	-5.8866870	-4.5057140	2.0477910
N	-6.0748520	-2.4664000	1.6444240

9/S_1

C	-2.0059190	0.1273200	-0.8685170
C	-3.3127010	0.0660140	-1.4783070
C	-3.8946010	-1.2212560	-1.6981720
C	-3.0922240	-2.3812440	-1.4357990
C	-1.7774830	-2.2223620	-1.0576230
C	-4.0354840	1.2091460	-1.8983360
C	-5.2084270	-1.3145070	-2.2103450
H	-3.4875790	-3.3783840	-1.6183810
H	-1.1022040	-3.0677310	-0.9481550
C	-5.9242380	-0.1701950	-2.5587620
C	-5.3190430	1.0943130	-2.4276890
H	-5.6414010	-2.3045570	-2.3603790

H	-6.9321770	-0.2548230	-2.9625000
H	-5.8529530	1.9893720	-2.7435620
C	-1.3222680	1.2922720	-0.3715250
C	0.1231300	1.2026060	-0.3731230
C	-1.9285480	2.4736230	0.1881530
C	0.8442680	2.4193690	-0.3177470
C	-1.1785640	3.6954900	0.1508030
C	-3.2260930	2.4925840	0.7993970
C	0.2075350	3.6464590	-0.1684910
H	1.9279120	2.4167170	-0.4181960
C	-1.8277950	4.9115920	0.4579330
C	-3.8480040	3.7257990	1.0684410
H	0.7756980	4.5751390	-0.2142170
C	-3.1610620	4.9312310	0.8729740
H	-1.2667520	5.8427090	0.3764880
H	-4.8386270	3.7345800	1.5214210
H	-3.6449810	5.8765380	1.1109340
N	-1.2295170	-1.0129790	-0.7863690
Pt	0.7628530	-0.6519950	-0.3784280
Cl	1.3002900	-3.0798630	-0.3562240
P	3.0103950	-0.1468700	0.0625710
C	3.3224310	0.6590410	1.7100950
C	4.6232650	0.7076690	2.2411510
C	2.2536260	1.1943420	2.4424940
C	4.8536280	1.3104860	3.4812150
H	5.4533380	0.2550940	1.6974760
C	2.4874420	1.7958840	3.6854600
H	1.2404380	1.1307140	2.0467210
C	3.7853880	1.8596650	4.2034170
H	5.8635610	1.3433220	3.8863960
H	1.6520870	2.2069910	4.2495810
H	3.9646340	2.3242390	5.1718080
C	4.2343760	-1.5435920	0.0993400
C	5.2371950	-1.6686630	-0.8677970
C	4.1526520	-2.4710850	1.1502920
C	6.1631360	-2.7190310	-0.7817100
H	5.3079300	-0.9554880	-1.6879020
C	5.0819820	-3.5083190	1.2387450
H	3.3592000	-2.3841600	1.8922190
C	6.0900320	-3.6348810	0.2709540
H	6.9401550	-2.8142350	-1.5383760
H	5.0139310	-4.2254890	2.0548450
H	6.8109920	-4.4482160	0.3379510
C	3.7267640	0.9840360	-1.2272930
C	4.7255820	1.9248170	-0.9415280
C	3.2556370	0.8404390	-2.5415650
C	5.2505860	2.7199660	-1.9678720
H	5.0845220	2.0570580	0.0782080

C	3.7898610	1.6288740	-3.5665120
H	2.4646380	0.1203210	-2.7560430
C	4.7870860	2.5700120	-3.2807280
H	6.0196310	3.4560750	-1.7399080
H	3.4203540	1.5135450	-4.5838770
H	5.1967260	3.1893210	-4.0771160
H	-3.5762820	2.1923380	-1.8193110
C	-3.8702000	1.2534980	1.2130390
C	-3.1034900	0.1774100	1.7306370
C	-5.2531370	1.0367930	1.0050860
C	-3.6407730	-1.0817600	1.8911830
H	-2.0576020	0.3460000	1.9848710
C	-5.8042970	-0.2252240	1.1197430
H	-5.8736880	1.8519670	0.6348370
C	-4.9894670	-1.3392750	1.4951600
H	-3.0130180	-1.8807510	2.2738490
H	-6.8499930	-0.3699050	0.8659080
C	-6.8531210	-2.8497080	1.0567900
H	-7.0265340	-2.4533070	0.0467520
H	-7.0373040	-3.9257370	1.0424940
H	-7.5712650	-2.3854920	1.7468290
C	-4.6315170	-3.7262330	1.8640340
H	-3.7123790	-3.7433180	1.2649820
H	-4.3623550	-3.6711330	2.9280160
H	-5.1725720	-4.6592630	1.6939090
N	-5.4793920	-2.6047650	1.4740130

9/T_1

C	-1.9749220	0.2187050	-1.0815770
C	-3.3358250	0.1888360	-1.5843830
C	-3.9147930	-1.0778400	-1.8686490
C	-3.0931480	-2.2416370	-1.7558710
C	-1.7522030	-2.1060400	-1.4564540
C	-4.0827210	1.3581970	-1.8605150
C	-5.2588350	-1.1505730	-2.3172550
H	-3.4999770	-3.2271390	-1.9722760
H	-1.0702060	-2.9531700	-1.4399340
C	-5.9873070	0.0058780	-2.5368700
C	-5.3839330	1.2691540	-2.3311820
H	-5.6955070	-2.1296120	-2.5146070
H	-7.0144780	-0.0527890	-2.8933380
H	-5.9439770	2.1778810	-2.5446530
C	-1.3005090	1.3076110	-0.4854270
C	0.1820400	1.2256690	-0.5366150
C	-1.8953790	2.4684340	0.1789920
C	0.8462350	2.4444790	-0.6476200
C	-1.1854270	3.6987650	0.0229660
C	-3.0836630	2.4283850	0.9422300

C	0.1610450	3.6672640	-0.5006200
H	1.9211350	2.4729750	-0.8240940
C	-1.7880950	4.8933990	0.4482710
C	-3.6572230	3.6462680	1.3674540
H	0.6907490	4.6103740	-0.6263250
C	-3.0331390	4.8642020	1.0938650
H	-1.2714850	5.8397530	0.2906890
H	-4.5785890	3.6216250	1.9478900
H	-3.4924730	5.7940660	1.4257160
N	-1.1954100	-0.9142630	-1.1453640
Pt	0.7938820	-0.6255660	-0.5751160
Cl	1.3444040	-3.0264960	-0.8500400
P	2.9640500	-0.1477840	0.1265750
C	3.1029090	0.7323910	1.7575990
C	4.3477630	0.7840340	2.4095970
C	1.9795550	1.3162260	2.3589270
C	4.4700190	1.4375780	3.6389870
H	5.2174010	0.2966610	1.9670010
C	2.1049030	1.9669190	3.5930070
H	1.0088500	1.2560990	1.8698380
C	3.3479180	2.0338160	4.2307920
H	5.4369790	1.4732930	4.1377550
H	1.2269470	2.4150240	4.0549750
H	3.4422700	2.5381250	5.1912180
C	4.1009290	-1.5896260	0.3910050
C	5.2619830	-1.7675870	-0.3675620
C	3.7776660	-2.4994050	1.4099100
C	6.1061530	-2.8563870	-0.1024090
H	5.5175150	-1.0676050	-1.1621460
C	4.6242500	-3.5761180	1.6762510
H	2.8616530	-2.3694450	1.9869220
C	5.7913650	-3.7568150	0.9186560
H	7.0081110	-2.9948070	-0.6961660
H	4.3696700	-4.2812370	2.4654860
H	6.4482230	-4.6008780	1.1230850
C	3.8567980	0.8919140	-1.1243300
C	4.7506090	1.9110990	-0.7698600
C	3.6228360	0.6020850	-2.4783750
C	5.4100540	2.6384280	-1.7691960
H	4.9213970	2.1564550	0.2775070
C	4.2917010	1.3230840	-3.4726210
H	2.9136560	-0.1816600	-2.7501520
C	5.1851500	2.3429110	-3.1189170
H	6.0966370	3.4361150	-1.4909910
H	4.1079180	1.0944630	-4.5208020
H	5.6993670	2.9097970	-3.8933180
H	-3.6282300	2.3358760	-1.7153880
C	-3.7179140	1.1435790	1.3050340

C	-2.9470410	0.0431670	1.7193030
C	-5.0988110	0.9468930	1.1533660
C	-3.5093010	-1.2153660	1.9048890
H	-1.8749270	0.1674160	1.8803350
C	-5.6814200	-0.3070980	1.3286240
H	-5.7253540	1.7748480	0.8202460
C	-4.8949300	-1.4286280	1.6899220
H	-2.8621090	-2.0344540	2.2059540
H	-6.7478710	-0.4147020	1.1514900
C	-6.7964470	-2.9020800	1.3118250
H	-6.8717810	-2.6534560	0.2393590
H	-7.0700220	-3.9520140	1.4471040
H	-7.5325010	-2.2978360	1.8572570
C	-4.5625340	-3.8332180	1.8980110
H	-3.8901000	-3.8878800	1.0256100
H	-3.9460560	-3.7996840	2.8050180
H	-5.1573750	-4.7496820	1.9402270
N	-5.4577360	-2.6867690	1.8375820

7. References

[1] Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev*. **2005**, *105*, 2999–3094.

[2] 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, 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 16 Revision A.03, **2016**, Gaussian Inc. Wallingford CT.

[3] Neese, F. *WIREs Comput. Mol. Sci.* **2018**, *8*, e1327

[4] Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc*., **2008**, *120*, 215–241.