Hybrids of Cationic [4]Helicene and N-Heterocyclic Carbene as Ligands for Complexes Exhibiting (Chir)optical Properties in the Far Red Spectral Window

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Supporting Information

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† Electronic Supplementary Information (ESI) available: experimental conditions, full characterizations of new compounds; UV-Vis, ECD, fluorescence and CPL spectra; computational details. See DOI: 10.1039/x0xx00000x. In addition, the dataset for this article can be found at the following DOI: 10.26037/yareta:526n2fl7gbe4jibfdcpbmtnpem. It will be preserved for 10 years.

Contents

General remarks and analysis conditions

Reagents

All commercial chemicals were used as received unless otherwise noted. Cationic diaza [4]helicene **1a**(BF_4) was prepared according literature procedures,[1] and was resolved into single enantiomers *via* Pummerer-like chemistry.[2] **1a**(BF_4) (racemic or enantiopure) was converted into amino **1b**(BF_4) in a two-step sequence (nitration then reduction) following reported procedures.[3] Au(C^N^C)Cl was obtained following already described procedure.[4] Reactions were monitored by thin-layer chromatography (TLC) carried out on silica gel plates (60F254) using UV light as visualizing agent, $KMnO_4$/K_2CO_3/NaOH in water for staining. Column chromatography were performed with Silica Gel (spherical, particle size 40 µm, neutral).

Analytical methods and apparatus

Melting points were measured on a standard melting point apparatus in open capillary tubes and are uncorrected. **NMR spectra** ^{1}H (400 MHz), ^{1}H (600 MHz), ^{13}C (101 MHz), ^{13}C (151 MHz), ^{19}F (376 MHz), ^{31}P (162 MHz) and ^{77}Se (76 MHz) were recorded on Brucker spectrometer with complete proton decoupling for nucleus other than ^{1}H. Variable temperature (VT) ^{1}H (500 MHz) were recorded on Brucker spectrometer. NMR Chemical shifts are reported in parts per million with the solvent resonance as the internal standard ($CDCl_3$, ^{1}H: δ 7.26 ppm, ^{13}C: δ 77.16 ppm; CD_2Cl_2, ^{1}H: δ 5.32 ppm, ^{13}C: δ 53.84 ppm; Acetone-d6, ^{1}H: 2.05 ppm); ^{19}F chemical shifts are reported with $CFCl_3$ (δ = 0.0 ppm) as the internal standard; ^{31}P chemical shifts are reported with H_3PO_4 (δ = 0.0 ppm) as the internal standard; ^{77}Se chemical shifts are reported with external KSeCN in D_2O at a specific concentration with a chemical shift of –316.5 ppm (4.0 mol/L) and –329.0 ppm (0.25 mol/L). Coupling constants (J) are reported in Hertz (Hz). Multiplicities are reported using following abbrevations: s = singlet, br. s = broad singlet, d = doublet, dd = double doublet, ddd = double double doublet, dt = double triplet, t = triplet, q = quartet, quint = quintet, sept = septet, m = multiplet. **High-resolution mass spectroscopy (HMRS)** were recorded on a Q-TOF. ***In situ* IR** monitoring was performed on a ReactIR 45m from Mettler Toledo.

(Chir)Optical properties

Optical rotation were measured on a Perkin Elmer 241 polarimeter at 20 °C using a Hg lamp (365 nm). **UV-Vis-NIR absorption spectra** were recorded on a JASCO V-650 spectrophotometer at 20°C. Measurement were performed in acetonitrile analytical grade at precise concentrations *ca*. 1 10^{-5} M. **Electronic Circular dichroism (ECD) spectra** were recorded on a JASCO J-815 spectrophotometer at 20°C. Measurement were performed in analytical grade acetonitrile at precise concentrations *ca*. 1 10^{-5} M. **Steady-state fluorescence spectra** were measured using a FluoroMax+ spectrofluorometer from Horiba scientific. All fluorescence spectra were corrected for the wavelength-dependent sensitivity of the detection. Fluorescence quantum yields Φ were measured in diluted solution with an optical density lower than 0.1 using the following equation:

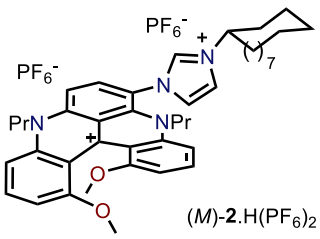
$$\frac{\Phi_x}{\Phi_r} = \left(\frac{\mathrm{A}_r(\lambda)}{\mathrm{A}_x(\lambda)}\right)\left(\frac{n_x^2}{n_r^2}\right)\left(\frac{\mathrm{D}_x}{D_r}\right)$$

where A is the absorbance at the excitation wavelength (λ), n the refractive index and D the integrated intensity. “r” and “x” stand for reference and sample. The fluorescence quantum yields were measured relative to cresyl violet in methanol (Φ = 0.54). Excitations of reference and sample compounds were performed at the same wavelength.

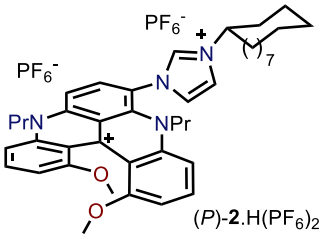
Circularly polarized luminescence (CPL) spectra were recorded with a home-made instrument,[5] on 10^{-5} M acetonitrile solutions under 517 nm irradiation from a LED source. A 90° geometry between excitation and detection was employed.

Synthesis and characterization of new compounds

Compound **2**.H$(PF_6)_2$:



(*M*)-**2**.H$(PF_6)_2$

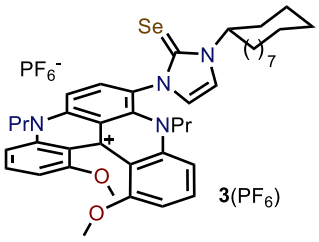


(*P*)-**2**.H$(PF_6)_2$

In a microwave tube (10 mL) were placed (*rac*)-**1b**(BF_4) (100 mg, 0.19 mmol, 1.0 equiv.), cyclododecylamine (36 mg, 0.19 mmol, 1.0 equiv.), $MgSO_4$ (47 mg, 0.39 mmol, 2 equiv.) and acetic acid (300 µL) then the mixture was heated at 60 °C for 5 min. To the green homogeneous mixture, glyoxal (24 µL, 0.21 mmol, 1.1 equiv., 40 % weight in aqueous solution), $ZnCl_2$ (235 µL, 0.235 mmol, 1.2 equiv., 1M in Et_2O) and formaldehyde (16 µL, 0.21 mmol, 1.1 equiv., 37 % weight in aqueous solution) were successively added. The tube was sealed with a septum and the resulting mixture was stirred at 60 °C for 1 hour then cooled down to room temperature. An aliquot of the crude reaction mixture was taken and a ^{1}H NMR was recorded to determine the selectivity of the reaction, which was calculated by integration of characteristic signals of the different compounds (cf NMR ^{1}H - Selectivity). The solvent was removed under reduced pressure and the crude mixture (diluted in a 1/1: milli-Q water / acetone solution) was loaded on an anion exchange resin Dowex®6 (minimum 1.9 cm of resin for 0.19 mmol of acetate salt) and eluted with milli-Q water / acetone (1/1). The solvents were evaporated under reduced pressure, then KPF_6 (107 mg, 0.58 mmol, 3 equiv.), CH_2Cl_2 (25 mL) and water (5 mL) were added and the mixture was stirred at room temperature for 1 hour. The organic layer was separated, and the aqueous layer was extracted with 3 x 25 mL of CH_2Cl_2. The organic layers were combined, dried over magnesium sulfate, filtered and the solvent was evaporated under reduced pressure. The mixture was purified by flash chromatography on silica gel (eluent: CH_2Cl_2/MeOH: 98/2, R*f* = 0.24) to afford the desired imidazolium salt **2**.H$(PF_6)_2$ as a dark green solid (138 mg, 76%). **m.p.** = 166 °C. ^{1}H **NMR (600 MHz, $CDCl_3$) δ** 9.24 (br. s, 1H), 8.21 (d, *J* = 9.3 Hz, 1H), 8.05 (dd, *J* = 8.9, 8.1 Hz, 1H), 7.90(dd, *J* = 8.3, 8.5 Hz, 1H), 7.77 (t, *J* = 1.9 Hz, 1H), 7.74 – 7.71 (m, 1H), 7.70 (d, *J* = 9.3 Hz, 1H), 7.51 (d, *J* = 8.9 Hz, 1H), 7.39 (d, *J* = 8.6 Hz, 1H), 7.00 (d, *J* = 8.1 Hz, 1H), 6.92 (d, *J* = 7.7 Hz, 1H), 4.71-4.78 (m, 2H), 4.54-4.62 (m, 1H), 4.30-4.37 (m, 1H), 3.80 (s, 3H), 3.76 (s, 3H), 3.23 (dt, 13.8 Hz, 7.6 Hz, 1H), 2.15-2.31 (m, 4H), 1.90-1.99 (m, 2H), 1.35-1.64 (m, 20H), 1.27 (t, *J* = 7.4Hz, 3H), 0.44 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (151 MHz, CD_2Cl_2) δ** 160.3, 159.5, 143.7, 143.4, 142.4, 139.4, 139.3, 138.0, 136.4, 135.8, 124.7, 123.5, 123.5, 121.6, 117.4, 116.3, 114.9, 110.6, 108.0, 107.9, 105.0, 104.9, 61.0, 53.2, 56.5, 56.4, 54.0, 30.8, 30.7, 24.1, 23.9, 23.9, 23.9, 23.9, 23.8, 23.8, 22.5, 22.0, 21.8, 21.0, 11.4, 10.5. **^{19}F NMR (376 MHz, CD_2Cl_2) δ** -72.4 (d, *J* = 712 Hz). **^{31}P NMR (162 MHz, CD_2Cl_2) δ** -144.4 (sept, J = 712 Hz). **HRMS (ESI)** calcd. for $C_{42}H_{54}N_4O_2^{++}$ (M-2PF_6): m/z 323.2118, found: 323.2122 (1 ppm). Following the same procedure, the two enantiomers of **1b**(BF_4) were employed to afford (*M*)-**2**.H$(PF_6)_2$ in 74% yield and (*P*)-**2**.H$(PF_6)_2$ in 67% yield.

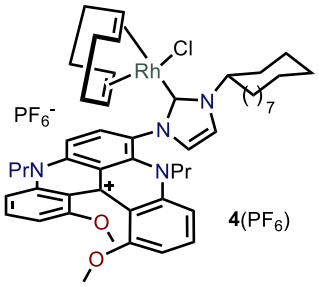
Figure S1. Picture of *rac*-**2**.H$(PF_6)_2$ at 77 K in MeTHF irradiated at 254nm.

Compound **3**(PF_6):



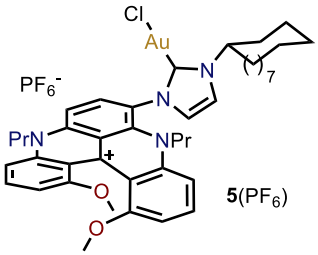
In a round-bottomed flask, **2**.H(PF_6)$_2$ (50 mg, 0.05 mmol, 1 equiv.), tBuOK (11 mg, 0.1 mmol, 2 equiv.) and metallic Se (6 mg, 0.07 mmol, 1.5 equiv.) were dissolved in THF (2 mL). The resulting dark green solution was stirred at room temperature overnight. Then, the mixture was filtered over celite and the solvents were removed. The dark solid was dissolved in dichloromethane (10 mL) and KPF_6 (18 mg, 0.1 mmol, 2 equiv.) and water (2 mL) were added. The heterogenous solution was stirred for 1 hour at room temperature. Then, the organic layer was separated, dried over $MgSO_4$ and evaporated under reduced pressure. The crude product was purified by flash chromatography on silica gel (eluent: Dichloromethane/Acetone: 98/2 then 95/5) to afford the selenocomplex **3**(PF_6) as a dark green solid (29 mg, 75%). Mixture of 2 atropoisomers with [a]major/[b]minor = 0.6/0.4 : **^{1}H NMR (400 MHz, CD_2Cl_2) δ** 8.34 [a] (d, *J* = 9.2Hz, 0.6H), 7.97-8.03[a,b] (m, 1.4H), 7.81–7.85[a,b] (m, 1H), 7.58–7.61[a,b] (m, 1H), 7.44–7.50[a,b] (m, 1.4H), 7.23–7.29[a,b] (m, 2H), 6.93–6.98 (m, 1.6H), 6.83–6.87[a,b] (m, 1H), 5.29–5.36[a] (m, 0.6H), 5.20–5.26[b] (m, 0.4H), 4.65–4.77[a,b] (m, 1H), 4.47–4.57[a,b] (m, 1H), 4.20–4.27[a,b] (m, 0.4H), 3.71–3.80[a,b] (m, 6.6H), 3.31–3.38[a,b] (m, 1H), 1.95–2.34[a,b] (m, 4H), 1.86–1.24[a,b] (m, 25H), 0.48–0.55[a,b] (m, 3H). **^{13}C NMR (101 MHz, CD_2Cl_2) δ** 160.2 160.2, 159.8, 159.6, 159.2, 159.1, 143.8, 143.7, 143.2, 143.2, 142.2, 142.2, 140.6, 138.6, 138.4, 138.4, 138.3, 137.2, 137.2, 137.1, 137.0, 122.2, 121.8, 120.9, 120.8, 120.7, 119.9, 119.2, 119.0, 116.9, 116.9, 114.5, 114.4, 110.7, 110.0, 107.9, 107.8, 106.7, 106.6, 104.6, 104.3, 104.2, 103.9, 56.7, 56.7, 56.5, 56.4, 56.3, 56.2, 31.6, 31.2, 30.7, 30.6, 30.2, 25.0, 24.9, 24.8, 24.6, 24.2, 24.2, 24.0, 23.9, 23.9, 23.8, 23.5, 22.4, 22.7, 22.6, 22.5, 22.3, 22.2, 21.0, 20.9, 11.5, 11.4, 11.3, 11.2. **^{19}F NMR (376 MHz, CD_2Cl_2) δ** -73.4 (d, *J* = 710 Hz). **^{31}P NMR (162 MHz, CD_2Cl_2) δ** -144.5 (sept, *J* = 711 Hz). **^{77}Se NMR (76 Hz, Acetone-d6) δ** 64.9 (s), 49.2 (s). **HRMS (ESI)** calcd. for $C_{42}H_{53}N_4O_2Se^+$ (M-PF_6): m/z 725.3328, found: 725.3334 (1 ppm). Single-crystals of **3** were obtained by slow evaporation of a saturated solution in dichloromethane/pentane. No apparent luminescence at 77k in MeTHF, 254 nm.

Complex **4**(PF_6):



In a flame-dried Schlenk tube were placed [Rh(cod)Cl]$_2$ (7 mg, 0.014 mmol, 0,5 equiv.), tBuOK (6 mg, 0.05 mmol, 2.0 equiv.) and THF (2 mL) under argon atmosphere. The mixture was stirred at room temperature for 10 min and **2**.H(PF_6)$_2$ (25mg, 0.027 mmol, 1 equiv.) was added and the resulting mixture was stirred for 2 h at room temperature. The solvent was removed under reduced pressure and the mixture was dissolved in dichloromethane (20 mL). Water (2 mL) and KPF_6 (15 mg, 0.08 mmol, 3 equiv.) was added. The resulting mixture was stirred at room temperature for 1 hour. The organic layer was separated, dried with $MgSO_4$ and evaporated under reduced pressure. The crude product was purified by flash chromatography on silica gel (eluent: Dichloromethane/Acetone: 98/2) to afford the rhodium complex **4**(PF_6) as a dark green solid (19 mg, 69%). Mixture of 2 atropoisomers with [a]major/[b]minor = 0.6/0.4 : **^{1}H NMR (600 MHz, CD_2Cl_2) δ** 10.13[a] (d, *J* = 9.2 Hz, 0.6H), 7.98–8.06[a,b] (m, 1H), 7.92[b] (d, *J* = 9.0 Hz, 0.4H), 7.79–7.87[a,b] (m, 2H), 7.62[b] (d, *J* = 9.0 Hz, 0.4H), 7.47–7.54[a,b] (m, 1H), 7.46[b] (d, *J* = 1.9 Hz, 0.4H), 7.28–7.31[a,b] (m, 1H), 7.22–7.27[a] (m, 0.6H), 7.14 (d, *J* = 1.9 Hz, 0.6H), 6.93–7.0[a,b] (m, 1H), 6.83–6.88[a,b] (m, 1H), 5.85–5.91[a] (m, 0.6H), 5.70–5.74[b] (m, 0.4H), 5.20–5.23[a] (m, 0.6H), 5.03–5.08[a] (m, 0.6H), 4.72–4.86[a,b] (m, 1.4H), 4.54–4.63[a,b] (m, 1.4H), 4.15–4.20[a] (m, 0.6H), 3.75–3.81[a,b] (m, 6H), 3,62–3.64 (m, 0.4H), 3.31–3.41[a,b] (m, 1H), 2.98–3.08[a] (m, 1.2H), 2.57–2.64[a] (m, 0.6H), 1.25–2.31 (m, 37H), 0.40–0.47[a,b] (m, 3H). **^{13}C NMR (101 MHz, CD_2Cl_2) δ** 185.2, 184.7, 184.1, 183.6, 160.2, 160.2, 159.8, 159.0, 144.9, 143.8, 143.6, 142.6, 142.5, 142.4, 138.8, 138.4, 138.3, 138.2, 137.8, 137.6, 137.4, 137.1, 136.6, 134.8, 123.3, 123.0, 122.8, 122.5, 122.3, 121.7, 121.0, 120.8, 117.3, 116.6, 114.8, 114.2, 113.6, 109.5, 108.0, 107.9, 106.6, 106.5, 104.6, 104.4, 104.4, 103.6, 100.5, 100.5, 98.6, 98.5, 98.5, 70.9, 70.7, 70.0, 69.8, 68.3, 68.2, 66.5, 66.3, 59.9, 59.1, 56.5, 56.4, 56.3, 56.2, 55.4, 51.0, 34.6, 34.2, 32.6, 32.1, 31.9, 31.0, 30.9, 30.7, 30.2, 29.1, 28.0, 27.7, 25.6, 25.3, 25.2, 24.9, 24.7, 24.6, 24.3, 23.8, 23.7, 23.5, 23.4, 23.4, 22.8, 22.6, 22.5, 22.5, 21.1, 20.8, 11.5, 11.4, 10.6. **^{19}F NMR (376 MHz, CD_2Cl_2) δ** -73.4 (d, *J* = 710 Hz). **^{31}P NMR (162 MHz, CD_2Cl_2) δ** -144.5 (sept, *J* = 711 Hz). **HRMS (ESI)** calcd. for $C_{50}H_{65}N_4O_2ClRh^+$ (M-PF_6): m/z 891.3851, found: 891.3882 (3.5 ppm). Single-crystals of **4**(PF_6) were obtained by slow diffusion of pentane into a saturated solution in dichloromethane.

Complex **5**(PF_6):



5(PF_6)

In the glovebox, **2**.H(PF_6)$_2$ (100 mg, 0.1 mmol, 1 equiv.) and tBuOK (24 mg, 0.2 mmol, 2 equiv.) were dissolved in THF (5 mL). The resulting mixture was stirred at room temperature for 10 minutes. Then, AuCl.SMe_2 (32 mg, 0.1 mmol, 1 equiv.) was added and the resulting mixture was stirred at room temperature for 3 hours. Outside the glovebox, the solvent was removed and the mixture was dissolved in dichloromethane (50 mL). Water (5 mL) and KPF_6 (58 mg, 0.3 mmol, 3 equiv.) was added. The resulting mixture was stirred at room temperature for 1 hour. The organic layer was separated, dried with $MgSO_4$ and evaporated under reduced pressure. Then, the dark green solid was purified by flash chromatography on silica gel (eluent: Dichloromethane/Acetone: 98/2) to afford the gold complex **5**(PF_6) as a dark green solid (55 mg, 51%). Mixture of 2 atropoisomers with [a]major/[b]minor = 0.6/0.4: **^{1}H NMR (400 MHz, CD_2Cl_2) δ** 8.42[a] (d, *J* = 9.2 Hz, 0.6H), 7.99-8.07[a,b] (m, 1.4H), 7.84-7.91[a,b] (m, 1H), 7.62-7.67 [a,b] (m, 1.4H), 7.41-7.51[a,b] (m, 2H), 7.32[a] (d, *J* = 8.7 Hz, 0.6H), 7.24[b] (d, *J* = 8.7 Hz, 0.4H), 7.20[a] (m, 0.6H) 6.95-6.99 [a,b] (m, 1H), 6.89[a,b] (d, *J* = 8.2 Hz, 1H), 5.12-5.19[a] (m, 0.6H), 4.99-5.05f [b] (m, 0.4H), 4.68-4.78[a,b] (m, 1H), 4.49-4.60[a,b] (m, 1H), 4.15-4.29[a,b] (m, 1H), 3.73–3.82[a,b] (m, 6H), 3.42[a] (dt, *J* = 14.3, 7.3Hz, 0.6H), 3.18[b] (dt, *J* = 14.5, 7.5Hz, 0.4H), 2.06-2.38f [a,b] (m, 4H), 1.90-1.25 [a,b] (m, 25H), 0.44-0.52 [a,b] (m, 3H). **^{13}C NMR (101 MHz, CD_2Cl_2) δ** 173.2, 172.3, 160.2, 159.5, 144.4, 144.0, 143.4, 143.3, 142.3, 139.0, 138.7, 138.6, 137.9, 137.7, 137.6, 136.7, 136.3, 136.2, 123.9, 123.4, 122.1, 121.4, 121.0, 120.6, 120.4, 117.1, 116.9, 114.7, 110.1, 110.0, 108.0, 107.9, 107.3, 107.3, 104.7, 104.6, 104.5, 104.4, 59.2, 56.5, 56.5, 56.3, 56.3, 53.1, 32.2, 32.0, 31.7, 31.6, 24.8, 24.7, 24.6, 24.3, 24.2, 24.2, 24.0, 23.9, 23.8, 23.6, 23.5, 23.1, 22.6, 22.4, 22.4, 22.2, 22.2, 21.0, 11.4, 11.2, 11.0. **^{19}F NMR (376 MHz, CD_2Cl_2) δ** -73.3 (d, *J* = 711 Hz). **^{31}P NMR (162 MHz, CD_2Cl_2) δ** -144.5 (sept, *J* = 711 Hz). **HRMS (ESI)** calcd. for $C_{42}H_{53}N_4O_2ClAu^+$ (M-PF_6): m/z 877.3517, found: 877.3520 (0 ppm).

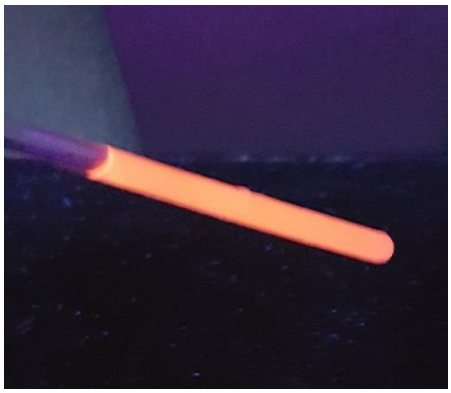
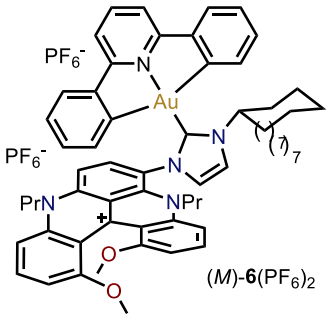
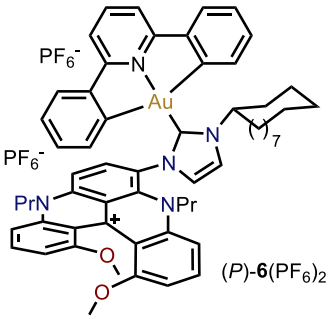


Figure S2. Picture of **5**(PF_6) at 77 K in MeTHF irradiated at 254nm.

Complex **6**(PF_6)$_2$:



(*M*)-**6**(PF_6)$_2$



(*P*)-**6**(PF_6)$_2$

In the glovebox, **2**.H(PF_6)$_2$ (20 mg, 0.02 mmol, 1 equiv.) and tBuOK (5.0 mg, 0.04 mmol, 2 equiv.) were dissolved in MeOH (4 mL). The resulting mixture was stirred at room temperature for 10 minutes. Then, Au(C^N^C)Cl (10 mg, 0.02 mmol, 1 equiv.) was added and the resulting mixture was stirred at room temperature for 3 hours. Outside the glovebox, the solvent was removed and the mixture was dissolved in dichloromethane (10 mL). Water (2 mL) and KPF_6 (11 mg) was added. The resulting mixture was stirred at room temperature for 1 hour. The organic layer was separated, dried over $MgSO_4$ and evaporated under reduced pressure. The crude product was successively washed with Et_2O (3x10 mL), then pentane (10 mL). The dark solid was purified by flash chromatography on silica gel (eluent: Dichloromethane/Acetone: 9/1) to afford the gold complex **6**(PF_6)$_2$ as a dark green solid (22 mg, 81%, dr > 20:1). **^{1}H NMR (400 MHz, CD_2Cl_2) δ** 8.28-8.31 (m, 2H), 7.88-7.98 (m, 3H), 7.72–7.75 (m, 1H), 7.55-7.63 (m, 3H), 7.51 (d, *J* = 8.1 Hz, 1H), 7.38 (d, *J* = 9.0 Hz, 1H), 7.34 (d, *J* = 6.9 Hz, 1H), 6.95–7.22 (m, 5H), 6.87 (d, *J* = 8.1 Hz, 1H), 6.54 (d, *J* = 8.1 Hz, 1H), 6.39 (d, *J* = 7.2 Hz, 1H), 5.88 (d, *J* = 8.7 Hz, 1H), 4.73-4.78 (m, 1H), 4.53-4.61 (m, 1H), 4.16-4.35 (m, 2H), 3.57-3.83 (m, 1H), 3.64 (s, 3H), 3.57 (s, 3H), 2.31-2.43 (m, 1H), 1.96-2.20 (m, 4H), 1.70-1.82 (m, 1H), 0.83–1.61 (m, 23H), 0.36 (t, *J*

= 7.3 Hz, 3H). **^{13}C NMR (101 MHz, CD_2Cl_2) δ** 164.4, 164.3, 164.2, 162.3, 159.9, 159.5, 155.9, 150.7, 148.2, 144.6, 142.8, 142.1, 142.0, 139.1, 138.3, 138.1, 137.5, 136.7, 136.4, 135.7, 133.5, 132.1, 129.7, 128.1, 127.6, 126.2, 125.0, 123.3, 120.9, 120.6, 118.7, 118.1, 115.0, 114.3, 108.5, 108.4, 108.0, 104.7, 104.0, 60.6, 56.4, 56.3, 55.2, 31.6, 31.4, 30.2, 24.9, 24.8, 24.2, 23.6, 23.3, 22.7, 22.6, 22.5, 22.2, 21.5, 21.0, 11.3, 11.0. **^{19}F NMR (376 MHz, CD_2Cl_2) δ** -72.9 (d, *J* = 711 Hz). **^{31}P NMR (162 MHz, CD_2Cl_2) δ** -144.3 (sept, *J* = 711 Hz). **HRMS (ESI)** calcd. for $C_{59}H_{64}N_5O_2Au^{++}$ (M-2PF_6): m/z 535.7357, found: 535.7364 (1 ppm).

The reaction was performed with the separated enantiomers of **2**.H(PF_6)$_2$. (*M*)-**2**.H(PF_6)$_2$ afforded (*M*)-**6**(PF_6)$_2$ in 64% yield, (*P*)-**2**.H(PF_6)$_2$ afforded (*P*)-**6**(PF_6)$_2$ in 69% yield**.**

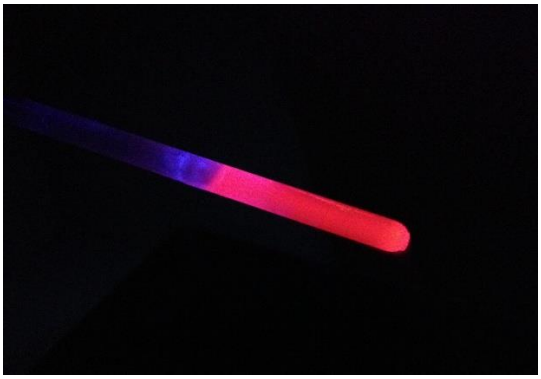
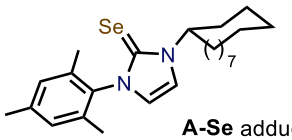


Figure S3. Picture of *rac*-**6**(PF_6)$_2$ at 77 K in MeTHF irradiated at 254nm.

Compound A-Se:



A-Se adduct

In a round-bottomed flask, **A**.H(BF_4) (100 mg, 0.23 mmol, 1 equiv.), tBuOK (51 mg, 0.45 mmol, 2 equiv.) and metallic Se (27 mg, 0.34 mmol, 1.5 equiv.) were dissolved in THF (2 mL). The resulting solution was stirred at room temperature overnight and the solvent was removed under vacuum. Dichloromethane was added and after filtration over Celite and evaporation, the residue was washed with n-pentane and dried to afford the selenium adduct **A-Se** as a white powder (76 mg, 78%). **^{1}H NMR (400 MHz, $CDCl_3$) δ** 7.01 (d, *J* = 2.3 Hz, 1H), 6.97 (s, 2H), 6.78 (d, *J* = 2.3 Hz, 1H), 5.29-5.23 (m, 1H), 2.32 (s, 3H), 1.97–2.05 (m, 2H), 2.01 (s, 6H), 1.55 – 1.78 (m, 4H), 1.49 – 1.29 (m, 16H). **^{13}C NMR (101 MHz, $CDCl_3$) δ** 156.8, 139.2, 135.7, 134.5, 129.3, 119.4, 116.8, 56.0, 30.1, 23.8, 23.7, 23.6, 21.8, 21.3, 18.2. **^{77}Se NMR (115 MHz, $CDCl_3$) δ** 10.2 (s). **HRMS (ESI)** calcd. for $C_{24}H_{37}N_2Se$ (M+H): m/z 432.2122, found: 432.2129 (0 ppm).

Optical and chiroptical properties

Absorption, fluorescence, ECD and CPL spectra

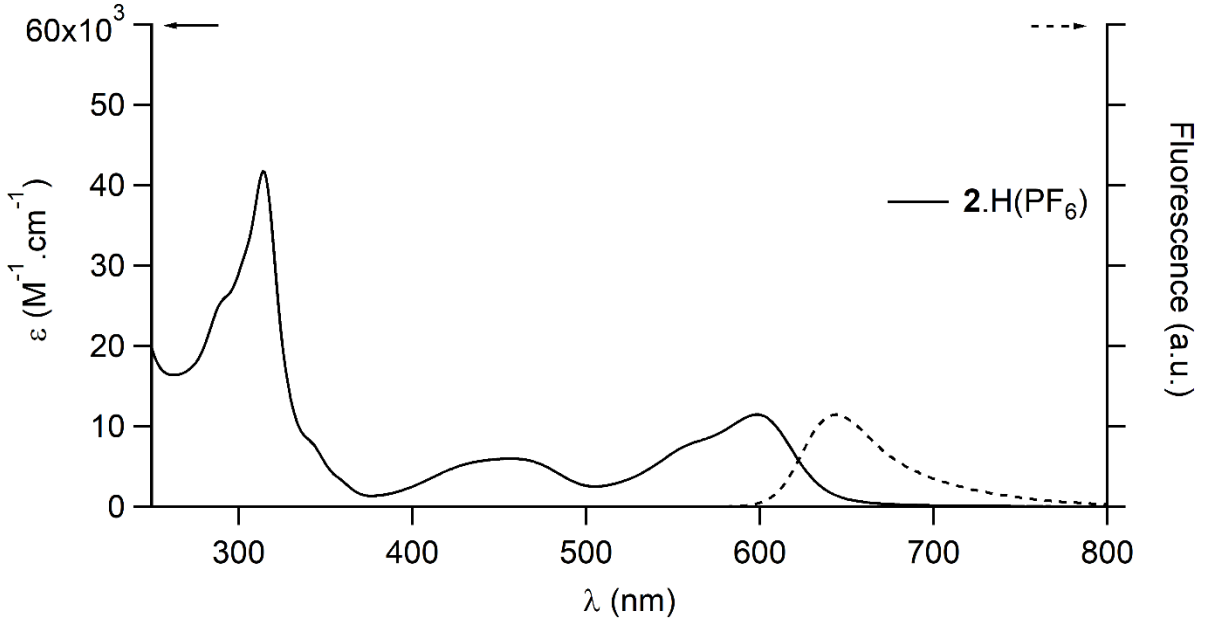


Figure S4. Absorption (plain line) and fluorescence (dashed line) spectra of **2**.H$(PF_6)_2$ in acetonitrile solution (C = 0.82 10^{-5} M).

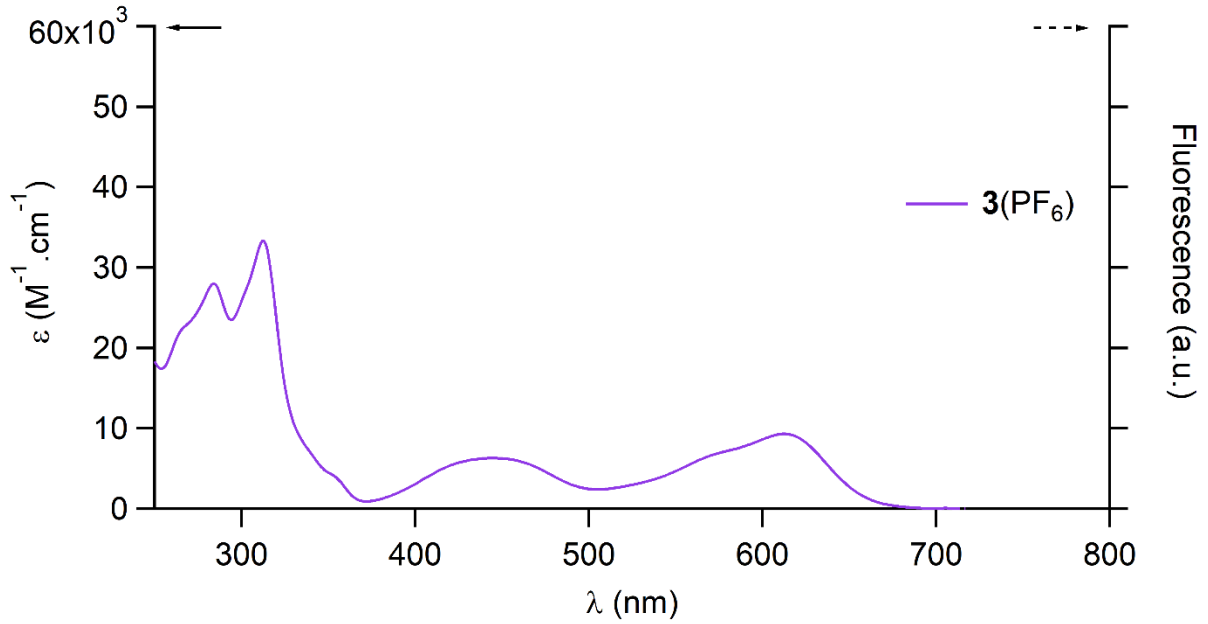


Figure S5. Absorption (plain line) spectrum of **3**(PF_6) in acetonitrile solution (C = 1.07 10^{-5} M).

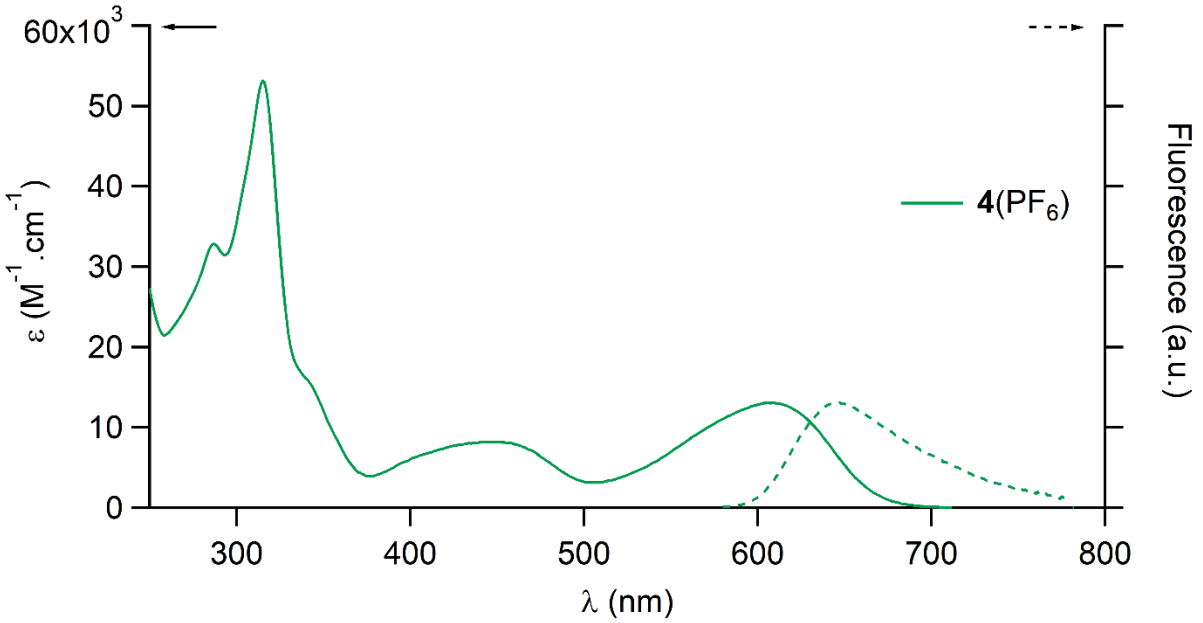


Figure S6. Absorption (plain line) and fluorescence (dashed line) spectra of **4**(PF_6) in acetonitrile solution (C = 0.98 10^{-5} M).

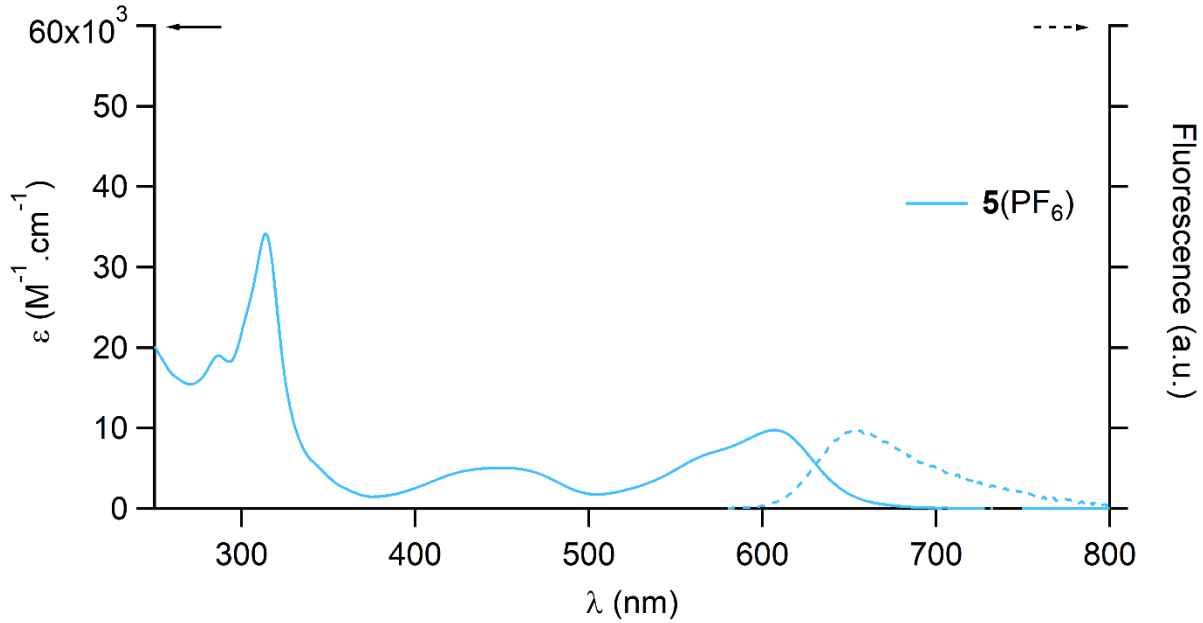


Figure S7. Absorption (plain line) and fluorescence (dashed line) spectra of **5**(PF_6) in acetonitrile solution (C = 1.21 10^{-5} M).

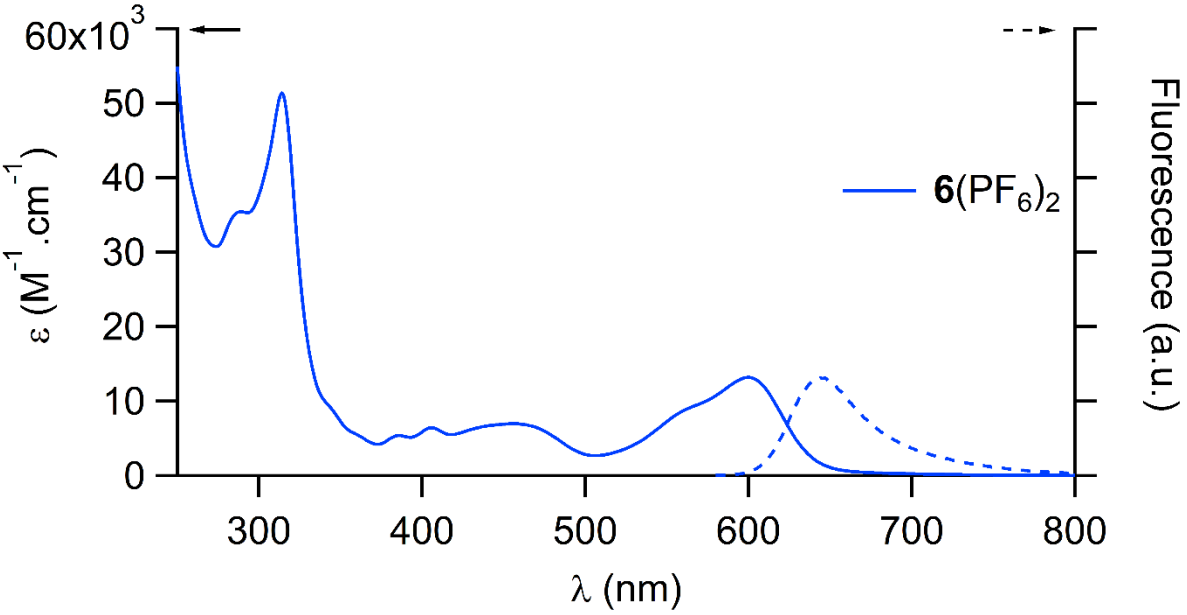


Figure S8. Absorption (plain line) and fluorescence (dashed line) spectra of **6**$(PF_6)_2$ in acetonitrile solution (C = 1.04 10^{-5} M).

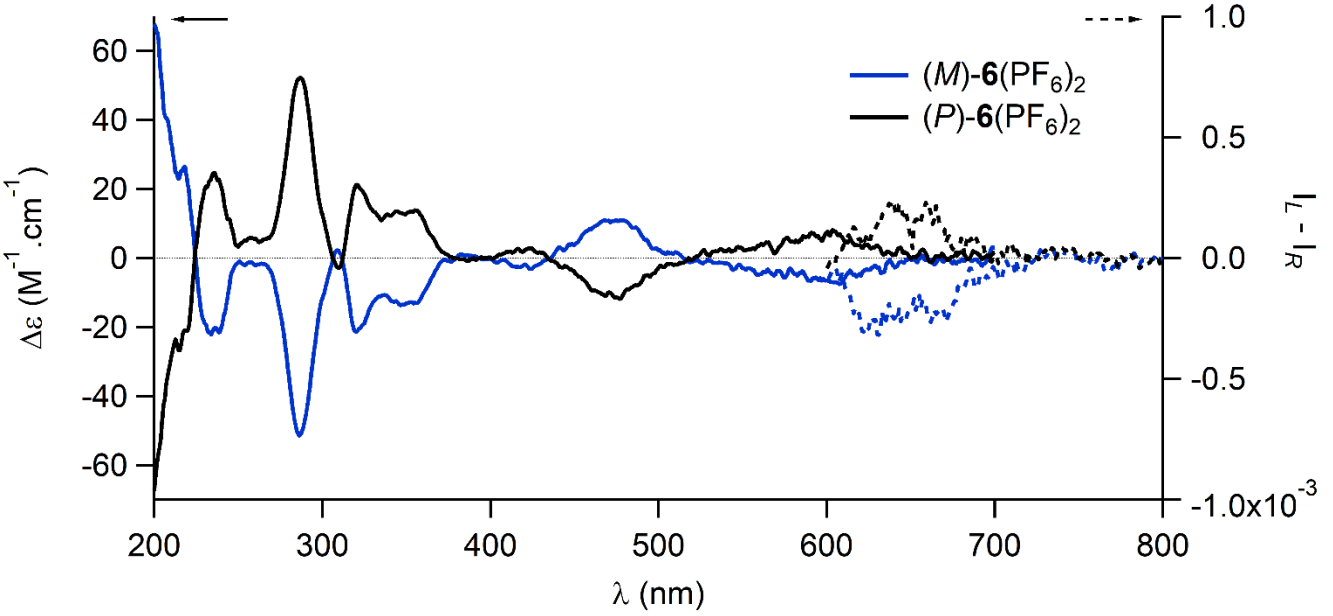


Figure S9. ECD (plain line) and CPL (dashed line) spectra in acetonitrile solutions of (*M*)-**6**$(PF_6)_2$ (blue lines, $[\alpha]_{365}^{20}$ –4000, C = 0.99 10^{-5} M) and (*P*)-**6**$(PF_6)_2$ (blak lines, $[\alpha]_{365}^{20}$ +4000, C = 0.98 10^{-5} M).

Computational details

General considerations

All geometries were fully optimized in gas phase at the B3PLYP level[7] of theory without any constraints at 298 K and 1 atm. The Berny algorithm was used for geometry optimizations.[8] 6-311G(d,p) Pople basis set was used for all atoms.[9] Frequency calculations were performed at the same level for all intermediates and transition states to confirm minima (no imaginary frequencies) and first order saddle points (one imaginary frequency representing the desired reaction coordinate), respectively. Furthermore, transition states were further confirmed by either intrinsic reaction coordinates (IRC).[10] DFT and TD-DFT calculations were performed using the Gaussian 09, Revision D.01 program.[11]

Nomenclature

In the geometrical analyses (see below), the atropisomeric situation around the C(sp^2)–N(sp^2) bond linking the helicene and the imidazole moieties will be described using standard IUPAC descriptors.

The orientation of the propyl side chain adopting a *gauche* conformation will also be described using the IUPAC descriptors for atropisomers.[12] The particular case of N(sp^2)–C(sp^3) bonds is reminded here. The Newman projection of this bond from the N(sp^2) to the C(sp^3) allows to determine the dihedral angle θ between the substituents. Four main types of dihedral angles can be defined. For $0°<\theta<\pm30°$, the substituents are designated as synperiplanar (*sp*) and for $\pm150°< \theta <180°$ they are named antiperiplanar (*ap*). For $30°<\theta<90°$ (+*sc*) or $-30°<\theta<-90°$ (–*sc*) the synclinal (*sc*) terminology is used and for $90°<\theta<150°$ (+*ac*) or $-90°<\theta<-150°$ (–*ac*) the anticlinal (*ac*) terminology is used (Figure S10).

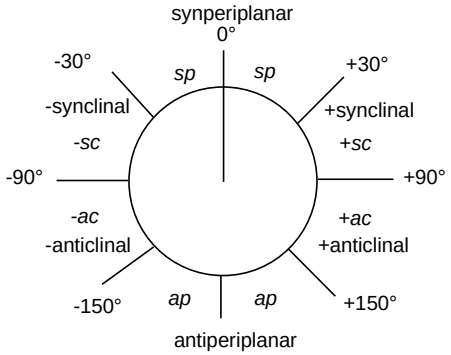


Figure S10. General IUPAC nomenclature of atropisomers.

The CIP priority rules are used to characterize the substituents. In the particular case of two identical groups, here A, linked to the C(sp^3) atom, the third group C is taken as reference irrespective of the CIP priority rules (Figure S11, with X > Y).

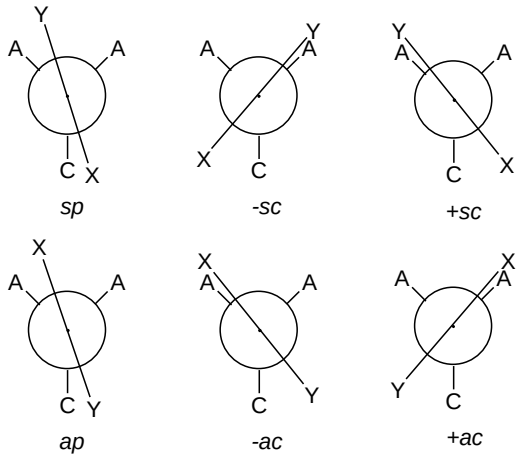


Figure S11. Nomenclature rules for atropisomerism around C(sp^3)–N(sp^2) bonds when two identical substituents are linked to the C(sp^3) atom.

For the Helicene-NHC hybrids, the X and Y priority of the substituents linked to the N(sp^2) atom is attributed according to the CIP priority rules. For the propyl chain, the two H atoms linked to the C(sp^3) are designed as A and the adjacent CH_2 groups take the priority (C). According to solid-state structures and computational analyses, the propyl chain can adopt either a *–sc* or *–ac* conformation (negative value of the torsion angle) or a *+sc* or *+ac* conformation (positive value of the torsion angle) depending on the face of the helicene it is pointing toward. The orientation of the propyl chain will thus be designed as (–) or (+) (see Figure S12).

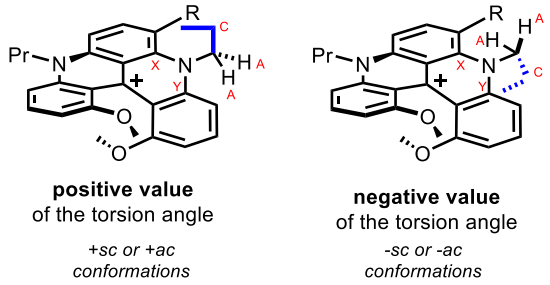


Figure S12. Orientation of the propyl chain: (+) and (–) torsion angles.

Results

*Geometrical analysis of analogues of selenium adduct **3**(PF_6)*

The crystal structure of **3**(PF_6) was used as starting point. With the aim to limit unwanted irrelevant conformational local minima, the structure was simplified: the propyl side chain away from the imidazolidinene has been truncated to a methyl residue, and the cyclododecyl moiety has been exchanged for a conformationally rigid cyclohexyl residue. Those modifications appear in grey color in Figure S13. The (*P*)-helicity has been arbitrary assign to all stereoisomers. The conformation of the biaryl can be either *aS* or *aR* and the torsion angle of the propyl chain can be either (+) or (–). Those modifications are highlighted in blue color in Figure S13. The dihedral angle a-b-c-d will be used to describe further the atropoisomery at the helicene-imidazole junction. The four possible stereoisomers are depicted in Figure SX.

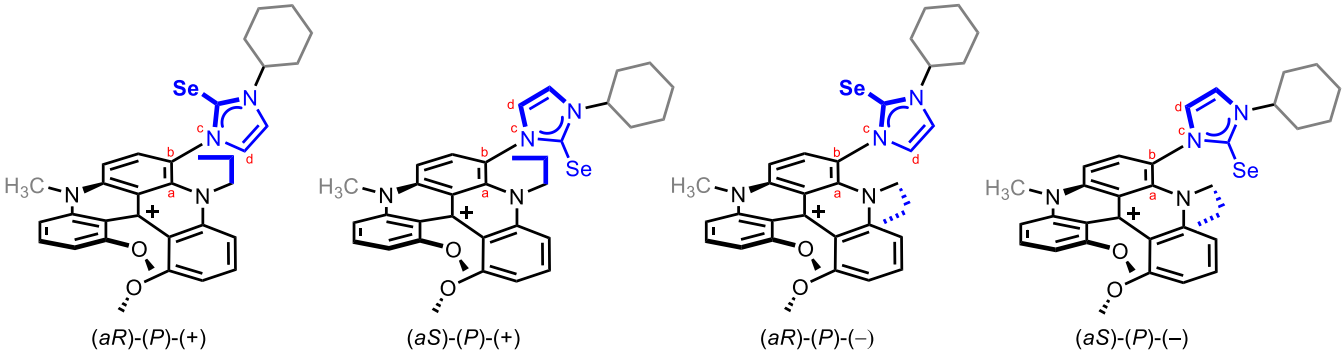


Figure S13. Four possible stereoisomers of simplified selenium adduct **3**. Simplifications are highlighted in grey color, the varying stereo elements are indicated in blue color, the a-b-c-d dihedral angle describes the atropoisomers.

The optimized geometries of the four possible stereoisomers are depicted in Figure S14 along with their ΔG(298 K) energies relative to that of the most stable isomer arbitrary set at 0.0 kcal mol^{-1}. The aS-P-(+) stereoisomer was found to be the most stable of the series. This is somewhat surprising as the aR-P-(+) stereoisomer was found in the crystal packing of **3**(PF_6). Computationally, this stereoisomer was found to less stable by only 0.2 kcal mol^{-1}. This would correspond to a 0.58:0.42 ratio at 298 K, which is close to the experimental ratio of 0.6:0.4 determined experimentally for **3**(PF_6) by ^{77}Se NMR spectroscopy (See Figure SX). Interestingly for the aR-P-(+), the computed structure is very similar to that observed in the crystal structure of **3**(PF_6), indicating that the simplifications used for the calculation (appearing in grey color in Figure SX) do not alter the global geometry of the helicene-imidazol moiety. The a-b-c-d dihedral angle values is of +65.5° while it reaches +63.6° in the X-ray structure of **3**(PF_6). The interaction between the propyl side chain and the Se atom prevent the biayrl to adopt a preferential 90° conformation.

The two structures exhibiting a (–) orientation of the propyl side chain were found to be less stable. In the case of aR-P-(–), the structure is clearly destabilized and was located at +14.1 kcal mol^{-1}. In this case, the dihedral angle between the helicene and the imidazole units is +100.8°. Concerning its epimer aS-P-(–), the propyl chain does not adopt a gauche conformation but a distorted antiperiplanar instead. This stabilises somehow this isomer that lies at +1.0 kcal mol^{-1} (a-b-c-d = –118.1°). However, this conformation of the propyl side chain is not observed experimentally by ^{1}H NMR spectroscopy.

Finally, the isomerization from aS-P-(+) to aR-S-(+) was also computed. In the transition state, the aniline and imidazole moieties are almost coplanar, with a dihedral angle of –6.3°. This TS was located at +17.2 kcal mol^{-1}. Considering a first order kinetic, this values would correspond to a kinetic constant of 1.50 s^{-1} and a half-life T½ of 0.46 s. This is consistent with a facile isomerization and yet the possibility to distinguish the two species by NMR spectroscopy.

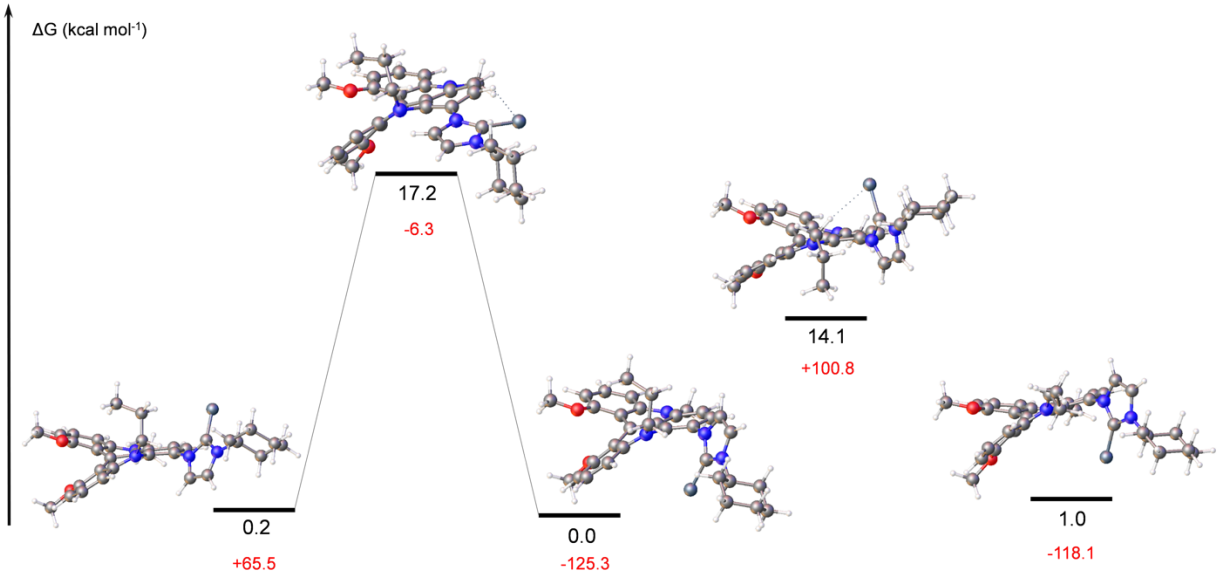


Figure S14. Computed optimized geometries of the four possible stereoisomers of simplified selenium adduct **3**. The Gibb's free energy (298 K) are given in kcal mol^{-1}. The values of the dihedral angle a-b-c-d are also given. The reaction coordinates of the isomerization aR-P-(+) → aS-P-(+) were also computed and the structure of the TS is depicted.

*Geometrical analysis of analogues of rhodium (I) complex **4**(PF_6)*

The optimized geometries of the two possible stereoisomers with the appropriate *gauche* conformation of the propyl side chain are depicted in Figure S15 along with their ΔG(298 K) energies relative to that of the most stable stereoisomer arbitrary set at 0.0 kcal mol^{-1}. Similarly to the case of the Se adduct, the (*aS*)-(*P*) stereoisomer was found to be the most stable by 1.6 kcal mol^{-1}.

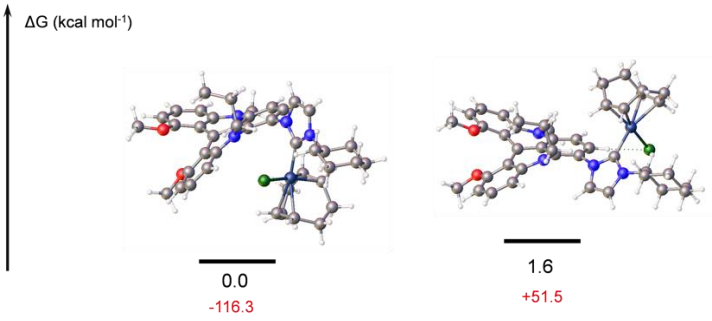


Figure S15. Computed optimized geometries of two possible stereoisomers with the appropriate *gauche* conformation of the propyl side chain of simplified rhodium (I) complex **4**. The Gibb's free energy (298 K) are given in kcal mol^{-1}. The values of the dihedral angle a-b-c-d are also given.

*Geometrical analysis of analogues of gold (I) complex **5**(PF_6)*

The optimized geometries of the two possible stereoisomers with the appropriate *gauche* conformation of the propyl side chain are depicted in Figure S16 along with their ΔG(298 K) energies relative to that of the most stable stereoisomer arbitrary set at 0.0 kcal mol^{-1}. Similarly to the case of the Se adduct, the (*aS*)-(*P*) stereoisomer was found to be the most stable by 1.1 kcal mol^{-1}.

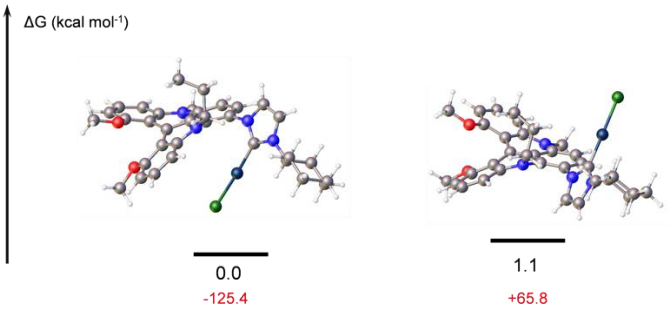


Figure S16. Computed optimized geometries of two possible stereoisomers with the appropriate *gauche* conformation of the propyl side chain of simplified gold (I) complex **5**. The Gibb's free energy (298 K) are given in kcal mol^{-1}. The values of the dihedral angle a-b-c-d are also given.

*Geometrical analysis of analogues of gold(III) complex **6**(PF_6)$_2$*

The optimized geometries of the two possible stereoisomers with the appropriate *gauche* conformation of the propyl side chain are depicted in Figure S17 along with their ΔG(298 K) energies relative to that of the most stable stereoisomer arbitrary set at 0.0 kcal mol^{-1}. The (*aS*)-(*P*) stereoisomer was found to be more stable by only 0.1 kcal mol^{-1}. As such, the two stereoisomer should be obtained in a 54:46 ratio. As a reminder, only one stereoisomer could be observed by NMR spectroscopy. This could be rationalized by either (i) isochronous spectra of the two stereoisomers in NMR spectroscopy or (ii) a facile isomerization, faster than the NMR time scale. The (*aS*)-(*P*) → (*aR*)-(*P*) isomerization process was also investigated computationally. In the transition state, the dihedral angle of the aniline and imidazole moieties reaches –26.0°, consequence of the high steric hindrance of the bulky cyclometalated Au (III) moiety. This TS was located at +13.5 kcal mol^{-1}. Considering a first order kinetic, this values corresponds to a kinetic constant of 777 s^{-1} and a half-life T½ of 9 10^{-4} s. Clearly, the isomerization is faster than the NMR time scale and the two stereoisomers are not distinguishable with this technics.

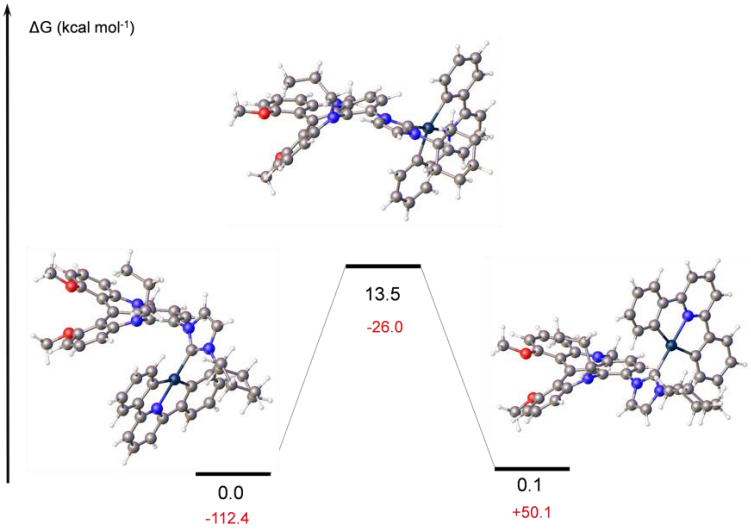


Figure S17. Computed optimized geometries of two possible stereoisomers with the appropriate *gauche* conformation of the propyl side chain of simplified gold (III) complex **5**. The Gibb's free energy (298 K) are given in kcal mol^{-1}. The values of the dihedral angle a-b-c-d are also given. The reaction coordinates of the isomerization aR-P-(+) → aS-P-(+) were also computed and the structure of the TS is depicted.

Experimental and computed diastereomeric ratios

The diastereomeric ratios determined experimentally through ^{1}H (and ^{77}Se) NMR spectroscopy are summarized in Table S1 and compared with the computed ratios gained on simplified analogues.

Compound	Exp ratio (NMR)	Computed ratio	Computed ΔE (kcal mom^{-1})
3	0.6:0.4 at 298 K	0.58:0.52	0.2
4	0.6:0.4 at 298 K	0.93:0.07	1.6
5	0.6:0.4 at 298 K	0.86:0.14	1.1
6	0.52:0.48 at 233 K	0.54:0.46	0.1

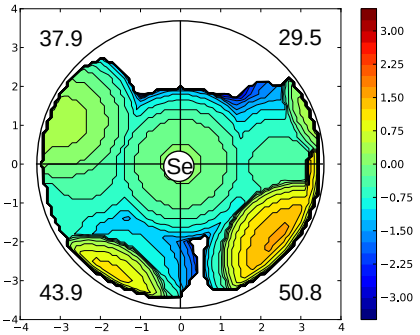
Table S1. Comparison of experimental and computed diastereomeric ratios.

Steric and electronic parameters of 2(PF$_6$).

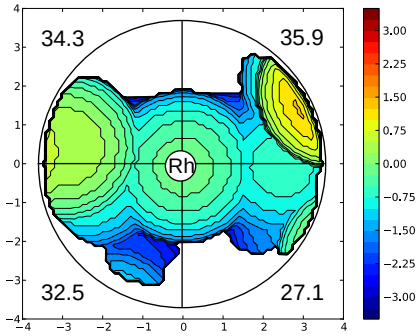
Topographical steric maps of **3**(PF$_6$) and **4**(PF$_6$)

The topographical steric maps of **3**(PF$_6$) (left) and **4**(PF$_6$) (right) were established using the SamBVca web application.[13] Values given in the four corners of the maps are the %Vbur of the ligands in the corresponding quadrant:

The structural parameters of the selenium adduct (*R*)(*P*)-**3**(PF$_6$) evidenced the steric hindrance notably caused by the *ortho* N-propyl group of the [4]helicene fragment in the southwest quadrant. Regarding (NHC)RhCl(COD) (*R*)(*P*)-**4**(PF$_6$), a degree of rotational freedom around the N-helicene bond keeps the *ortho* N-propyl group (southwest quadrant) away from the metal center and allows for an efficient decrease of the steric congestion in proximity of the rhodium coordination sphere.



3(PF$_6$) %Vbur = 40.5



4(PF$_6$) %Vbur = 32.4

Figure S18. Steric maps of selenium adduct **3**(PF$_6$) (left) and complex **4**(PF$_6$) (right).

Electronic parameters (Tolman Electronic Parameter)

Procedure: A solution of **4**(PF_6) (5 mg) in dichloromethane (3 mL) was placed in a ReactIR schlenk tube. The mixture was degassed by bubbling with N_2. *In situ* IR spectra were collected every minute during two hours (Figure S19, top). Five minutes after the beginning of the measurement, the solution was saturated with CO by bubbling for 30 minutes. The mixture was next degassed by bubbling with N_2. After two hours of measurement, two bands at 2088 and 2006 cm^{-1} were identified for the CO ligands (resolution 4 cm^{-1}, Figure S19, bottom). Next, the residue was precipitated with pentane. ^1H NMR spectroscopy (CD_3CN) confirmed the disappearance of the cod ligand signals and mass spectroscopy established the formation of the expected complex.

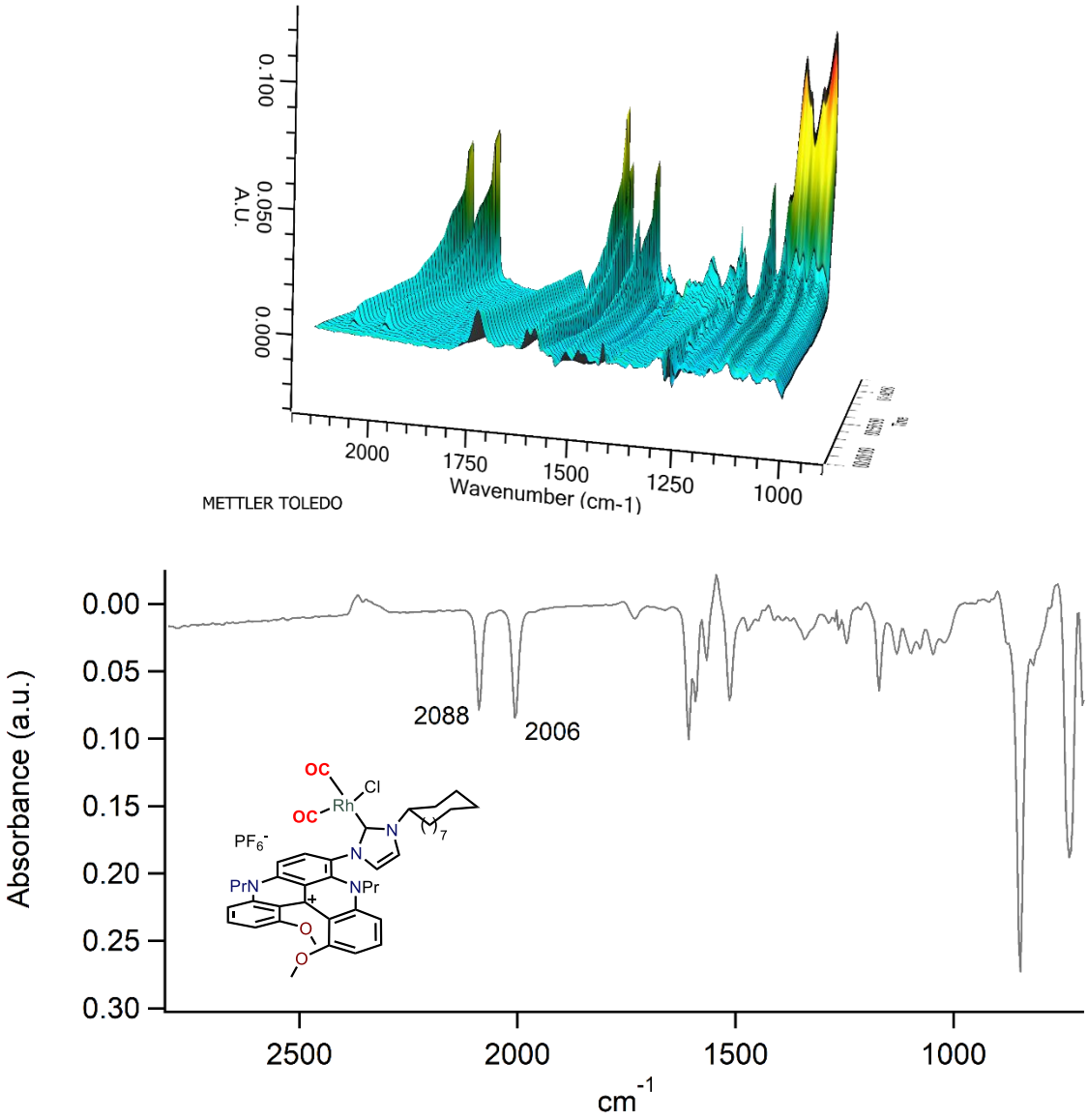


Figure S19. Top: *In situ* IR monitoring. Bottom: *in situ* IR spectrum of [(**2**)Rh(CO)$_2$Cl](PF_6) after 1h50 measurement (CH_2Cl_2 solution, C ~ 5 10^{-3} M).

A TEP of 2055.1 ± 4 cm^{-1} was calculated according to equations (1) and (2):[14]

$$TEP = 0.847\nu_{av}(CO)[Ir] + 336\ cm^{-1} \quad (1)$$

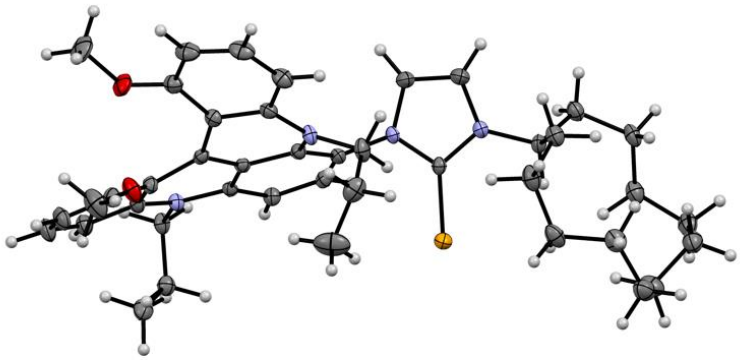
$$\nu_{av}(CO)[Ir] = 0.8695\nu_{av}(CO)[Rh] + 250.7\ cm^{-1} \quad (2)$$

X-ray structure determination

Intensity data were collected at low temperature on an APEXII, Bruker-AXS diffractometer, Mo-Kα radiation (λ = 0.71073 Å). The structure was solved by dual-space algorithm using the SHELXT program,[15] and then refined with full-matrix least-square methods based on F2 (SHELXL-2014).[16] All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions.

Compound **3**(PF_6) (CCDC 2061398)

Table S2. Crystal data and structure refinement for compound **3**(PF_6).

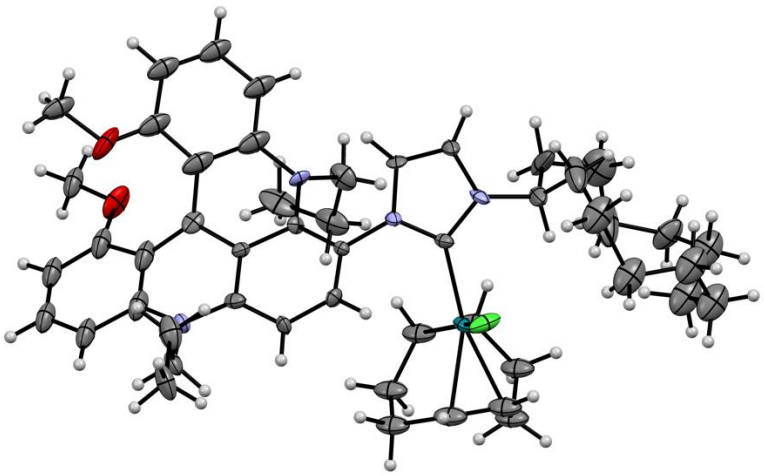


Empirical formula	$C_{44}H_{57}Cl_4F_6N_4O_2PSe$
Formula weight	1039.66
Temperature/K	150 (2)
Crystal system	triclinic
Space group	P-1
a/Å	9.8906(6)
b/Å	12.5154(9)
c/Å	19.2461(13)
α/°	88.465(2)
β/°	86.617(2)
γ/°	87.886(2)
Volume/Å^3	2375.9(3)
Z	2
ρ_{calc}g/cm^3	1.453
μ/mm^{-1}	1.113
F(000)	1072
Crystal size/mm^3	0.600 × 0.310 × 0.150
Radiation	Mo-Kα (λ = 0.71073)
2Θ range for data collection/°	1.060 to 27.561
Index ranges	$-8 \le h \le 12$, $-16 \le k \le 16$, $-24 \le l \le 25$
Reflections collected	58793
Independent reflections	10952 [R_{int} = 0.0651]
Data/restraints/parameters	10952/0/563
Goodness-of-fit on F^2	1.064
Final R indexes [I>=2σ (I)]	R_1 = 0.0521, wR_2 = 0.1298
Final R indexes [all data]	R_1 = 0.0920, wR_2 = 0.1585
Largest diff. peak/hole / e Å^{-3}	1.130/-1.240

Compound **4**(PF_6) (CCDC 2061397)

Table S3. Crystal data and structure refinement for compound **4**(PF_6).

Empirical formula	$C_{51}H_{67}Cl_3F_6N_4O_4PRh$
Formula weight	1122.31
Temperature/K	150(2)
Crystal system	Monoclinic
Space group	P $2_1/n$
a/Å	9.8537(11)
b/Å	22.588(3)
c/Å	22.749(3)
α/°	90
β/°	97.220(4)
γ/°	90
Volume/Å^3	5023.2(10)
Z	4
ρ_{calc}g/cm^3	1.484
μ/mm^{-1}	0.598
F(000)	2328
Crystal size/mm^3	0.600 × 0.080 × 0.070
Radiation	Mo-Kα (λ = 0.71073)
2Θ range for data collection/°	2.980 to 27.485
Index ranges	$-11 \leq h \leq 12$, $-29 \leq k \leq 29$, $-29 \leq l \leq 29$
Reflections collected	55032
Independent reflections	11457 [R_{int} = 0.0839]
Data/restraints/parameters	11457/4/515
Goodness-of-fit on F^2	1.306
Final R indexes [I>=2σ (I)]	R_1 = 0.1684, wR_2 = 0.3600
Final R indexes [all data]	R_1 = 0.1891, wR_2 = 0.3689
Largest diff. peak/hole / e Å^{-3}	1.899/-5.368



^{1}H, ^{13}C, ^{19}F, ^{31}P NMR spectra of new compounds

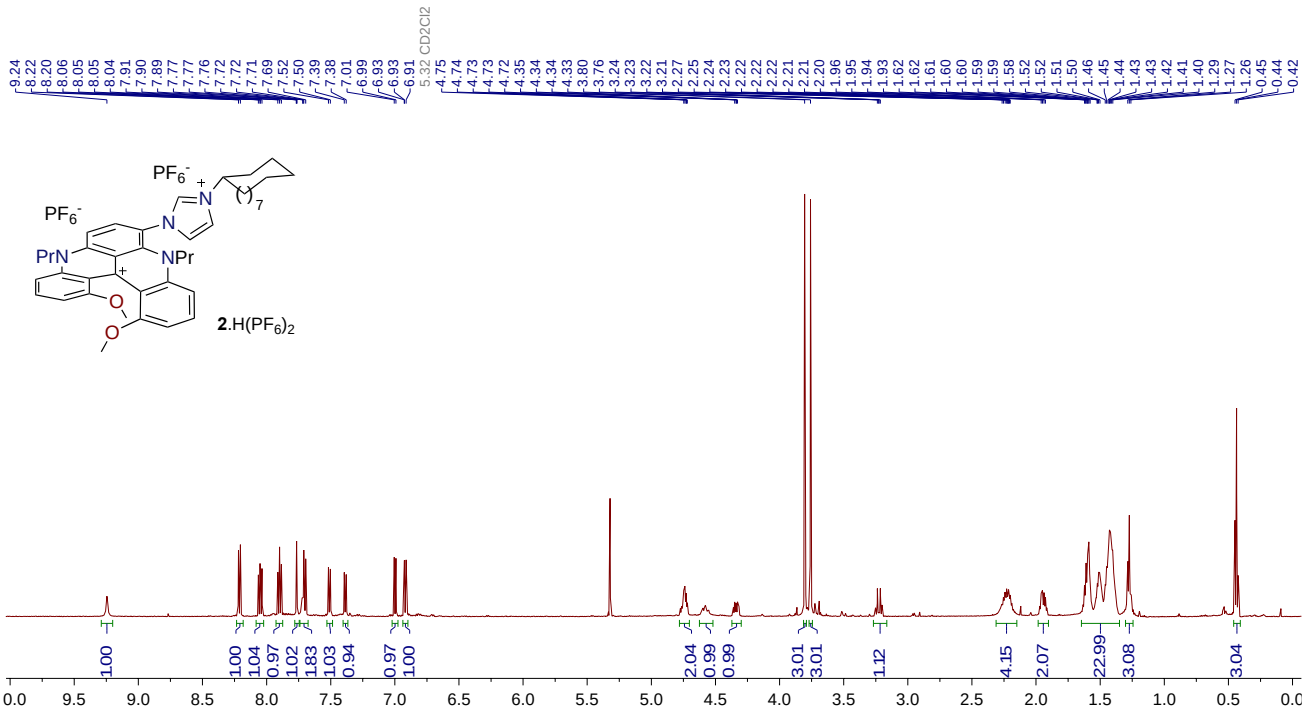


Figure S20. ^{1}H NMR (600 MHz, CD_2Cl_2) spectrum of **2**.H$(PF_6)_2$

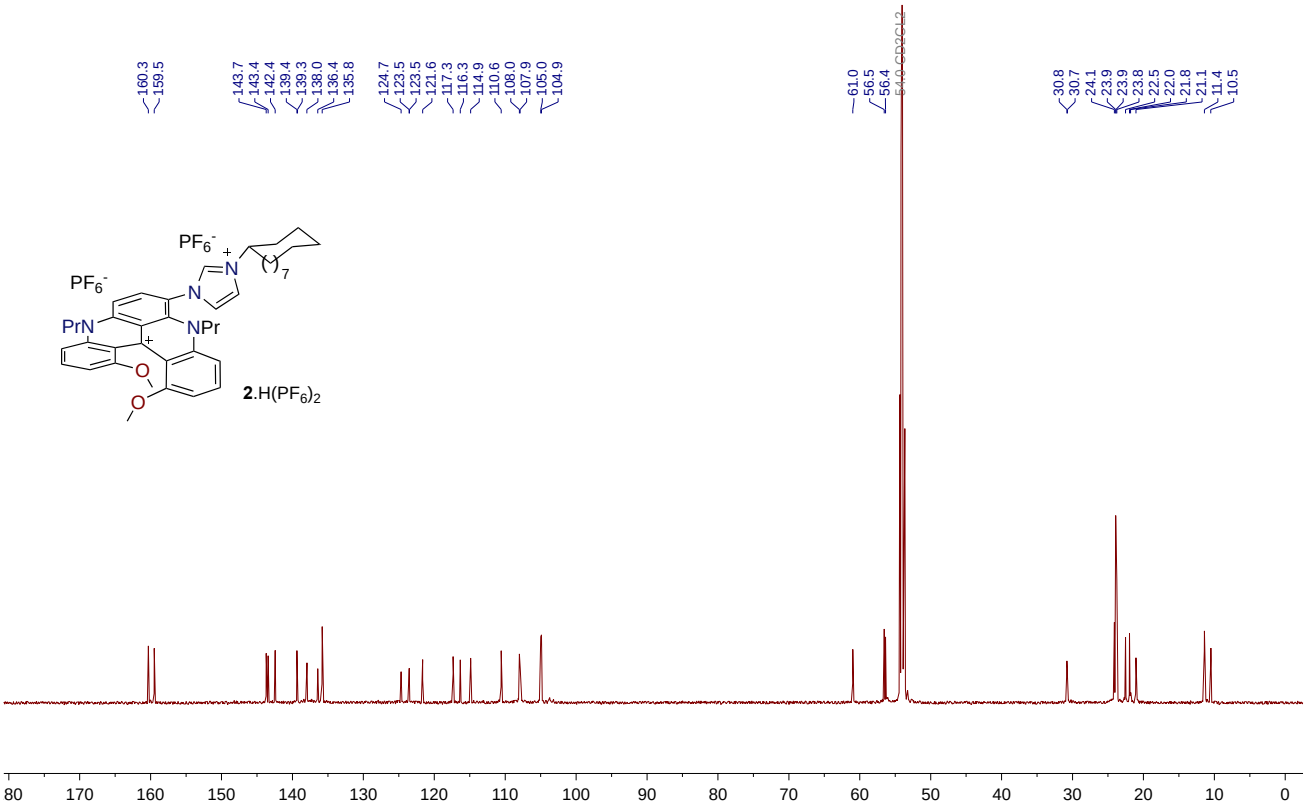


Figure S21. ^{13}C NMR (151 MHz, CD_2Cl_2) spectrum of **2**.H$(PF_6)_2$

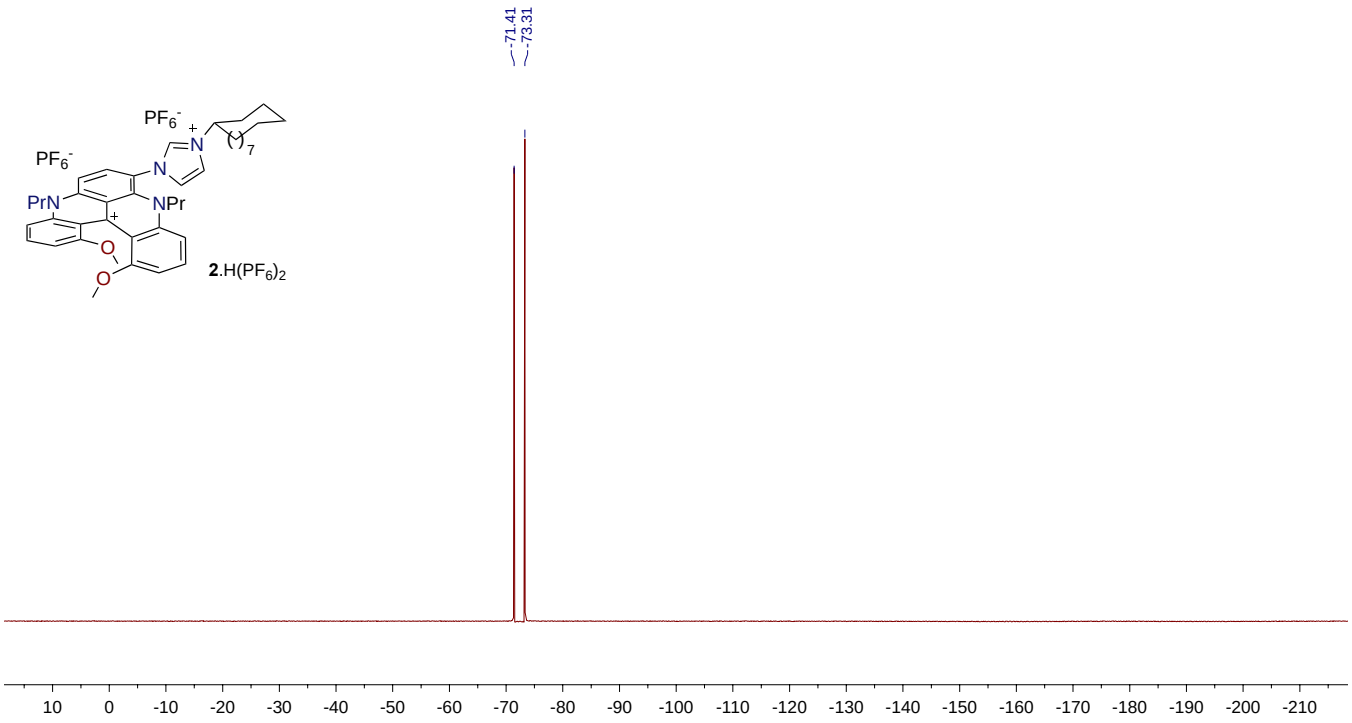


Figure S22. ^{19}F NMR (376 MHz, CD_2Cl_2) spectrum of **2**.H$(PF_6)_2$

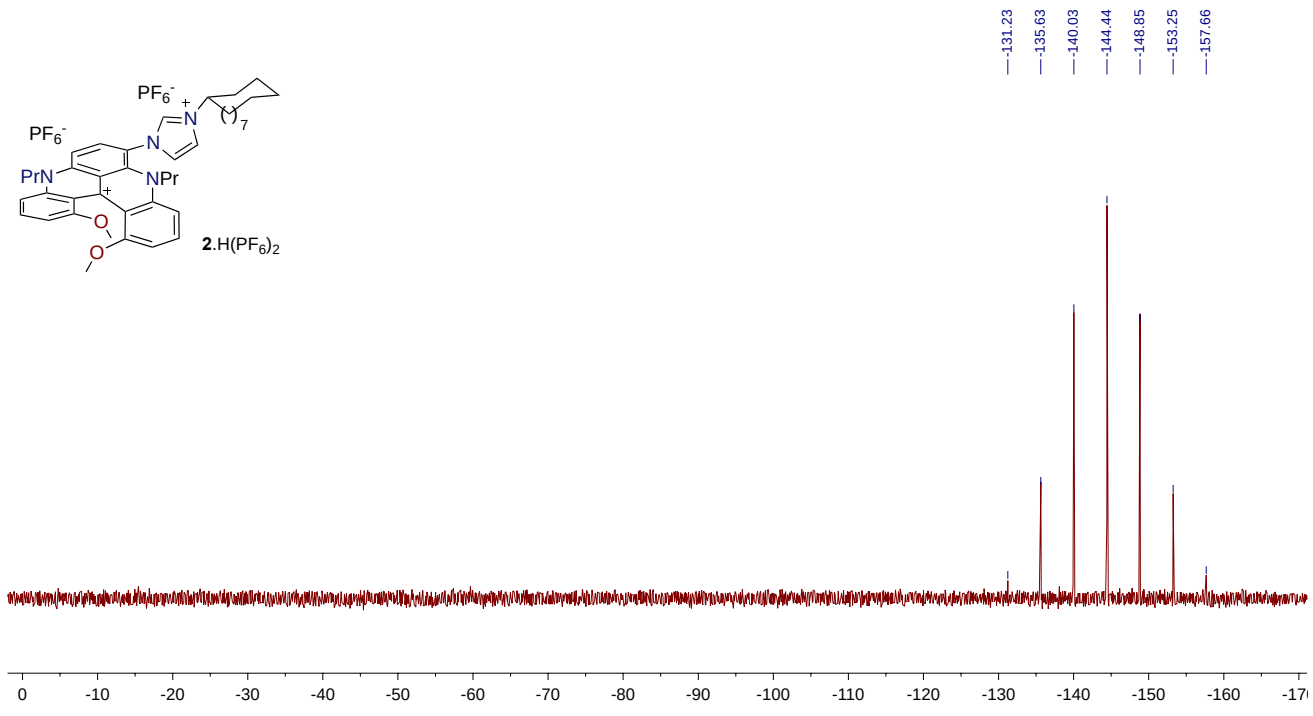


Figure S23. ^{31}P NMR (162 MHz, CD_2Cl_2) spectrum of **2**.H$(PF_6)_2$

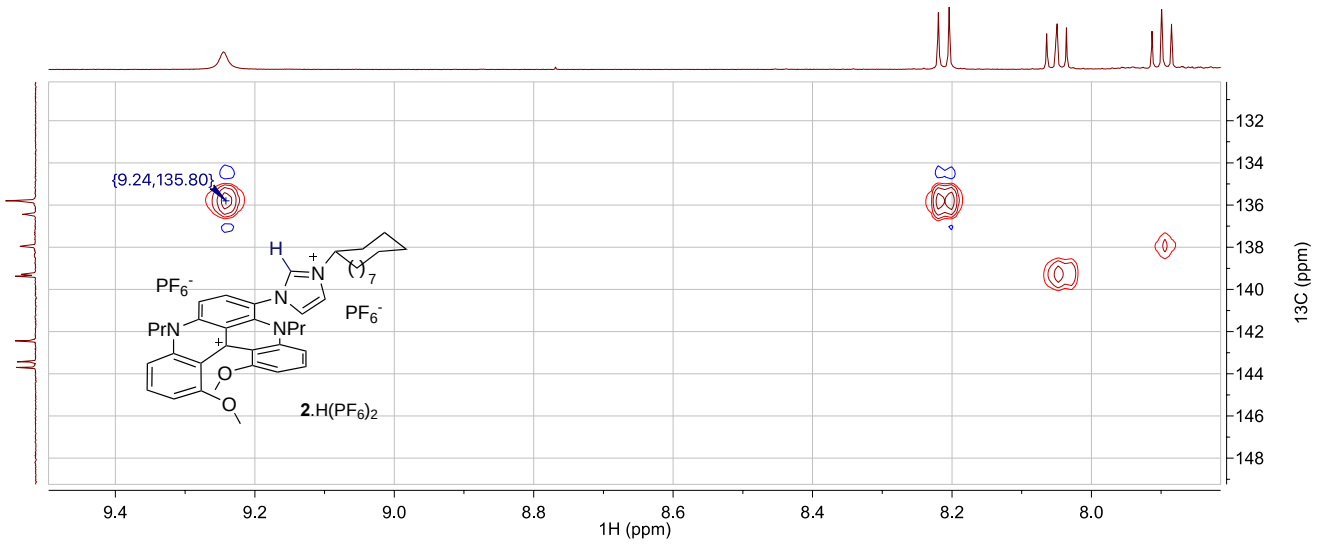


Figure S24. 2D HSQC spectrum zoom of **2**.H(PF$_6$)$_2$

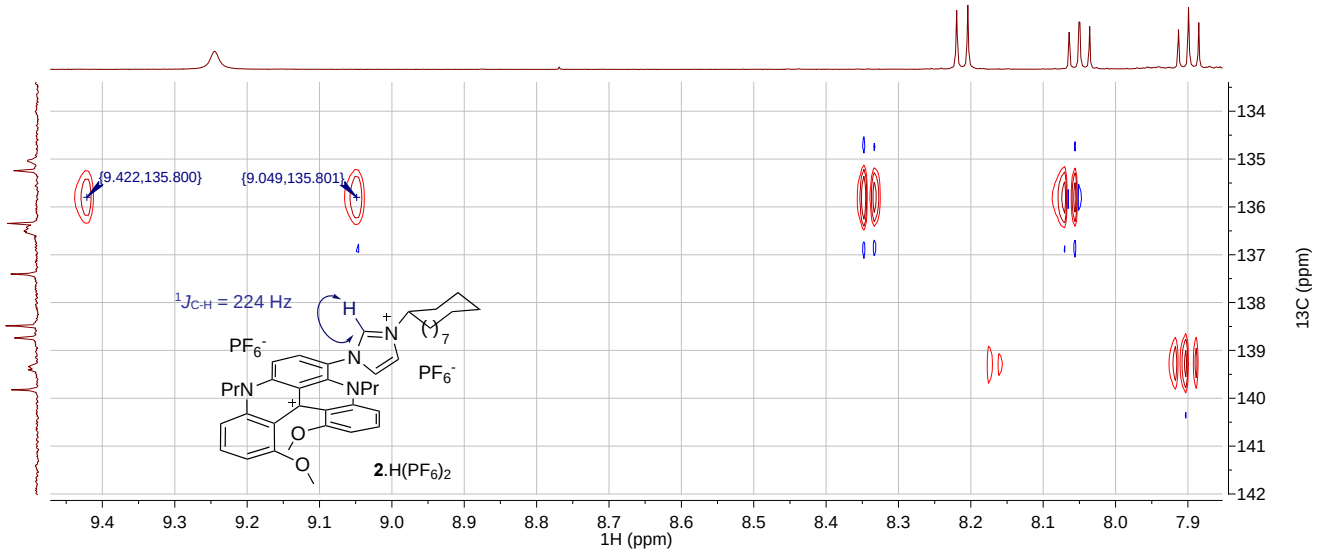


Figure S25. 600.47 MHz 2D HSQC $^1J_{CH}$ spectrum zoom of **2**.H(PF$_6$)$_2$

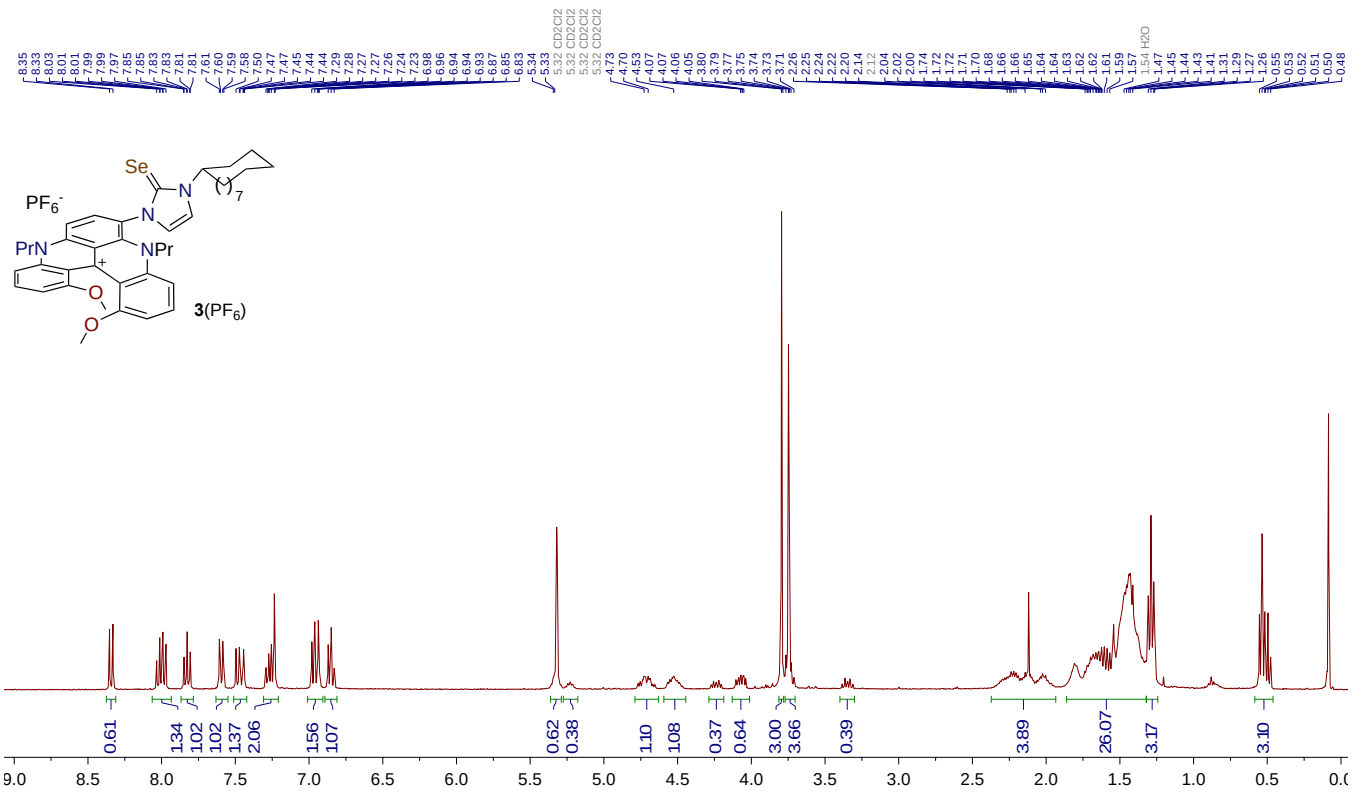


Figure S26. ^{1}H NMR (400 MHz, CD_2Cl_2) spectrum of **3**(PF_6)

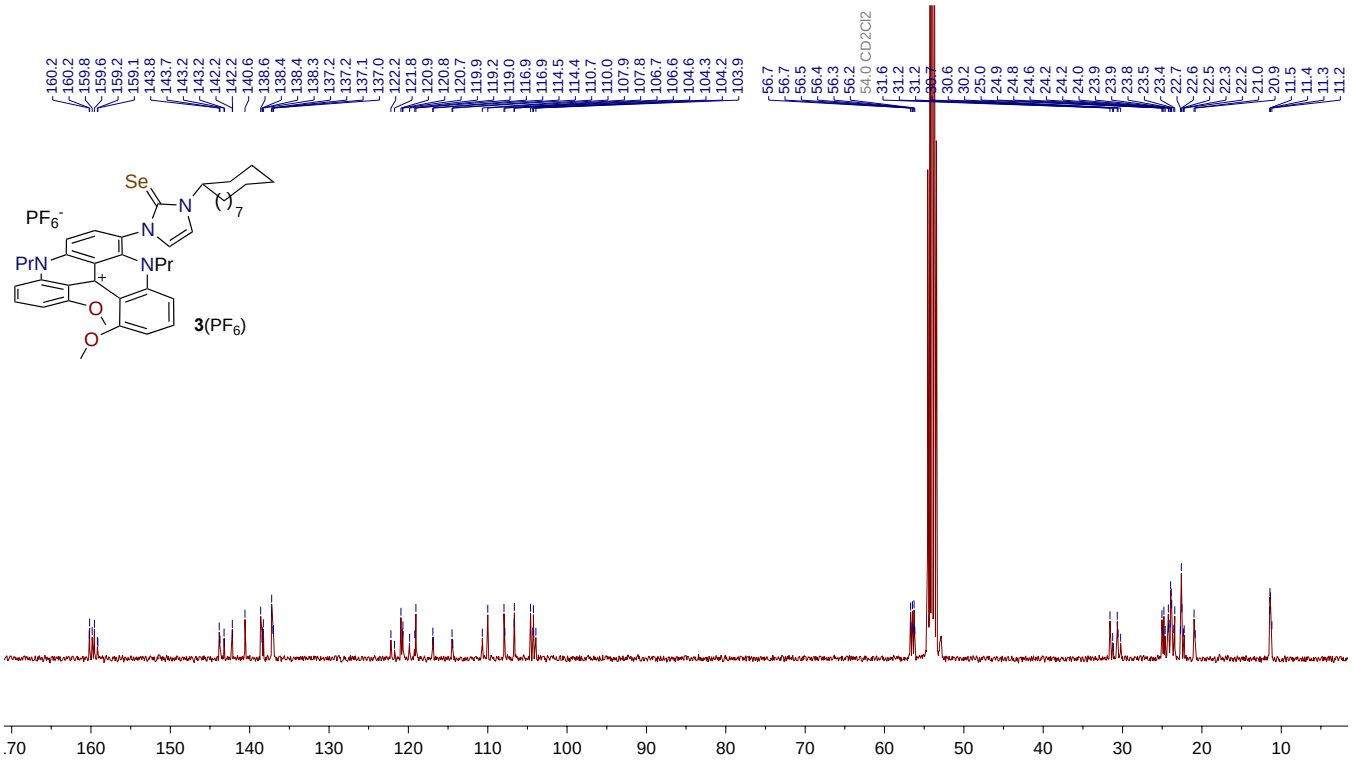


Figure S27. ^{13}C NMR (101 MHz, CD_2Cl_2) spectrum of **3**(PF_6)

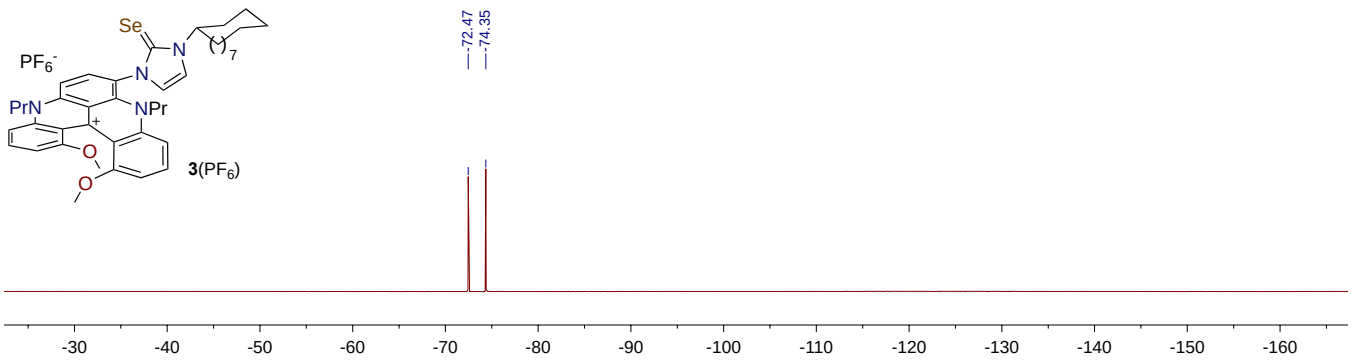


Figure S28. ^{19}F NMR (376 MHz, CD_2Cl_2) spectrum of **3**(PF_6)

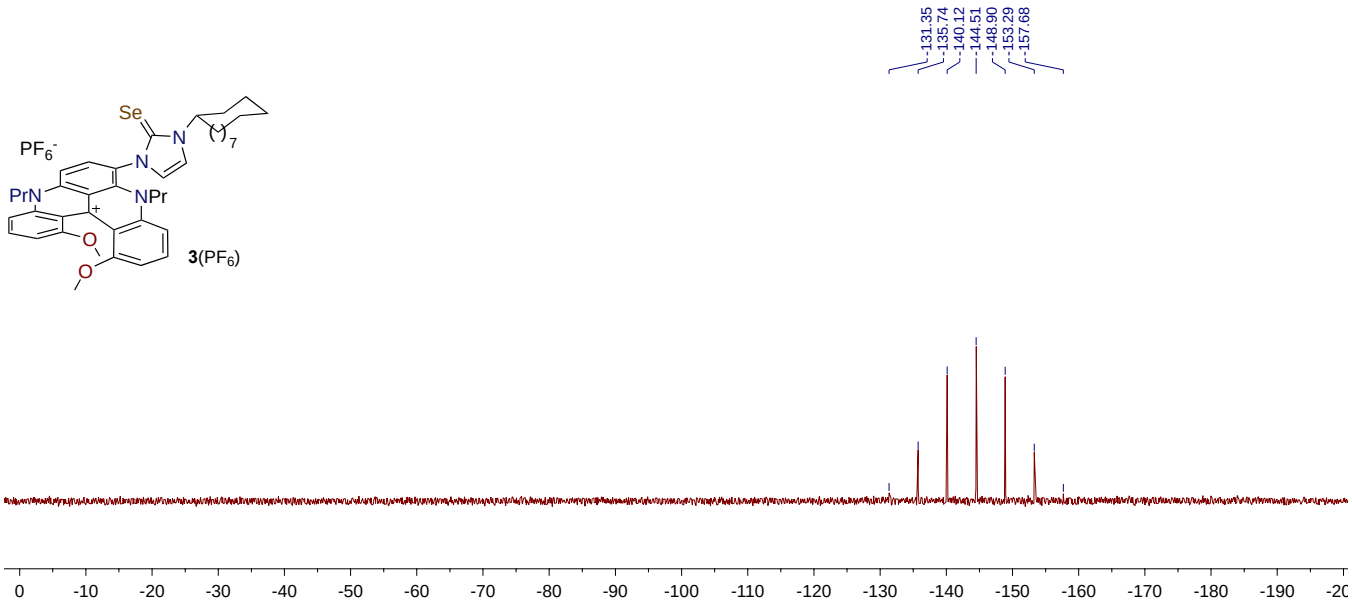


Figure S29. ^{31}P NMR (162 MHz, CD_2Cl_2) spectrum of **3**(PF_6)

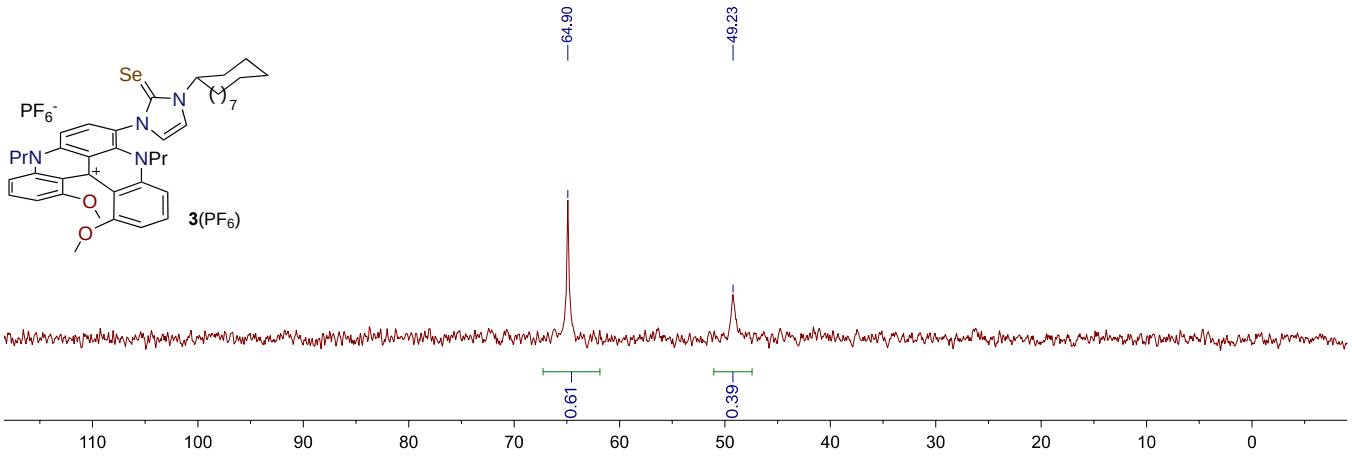


Figure S30. ^{77}Se NMR (76 MHz, CD_2Cl_2) spectrum of **3**(PF_6)

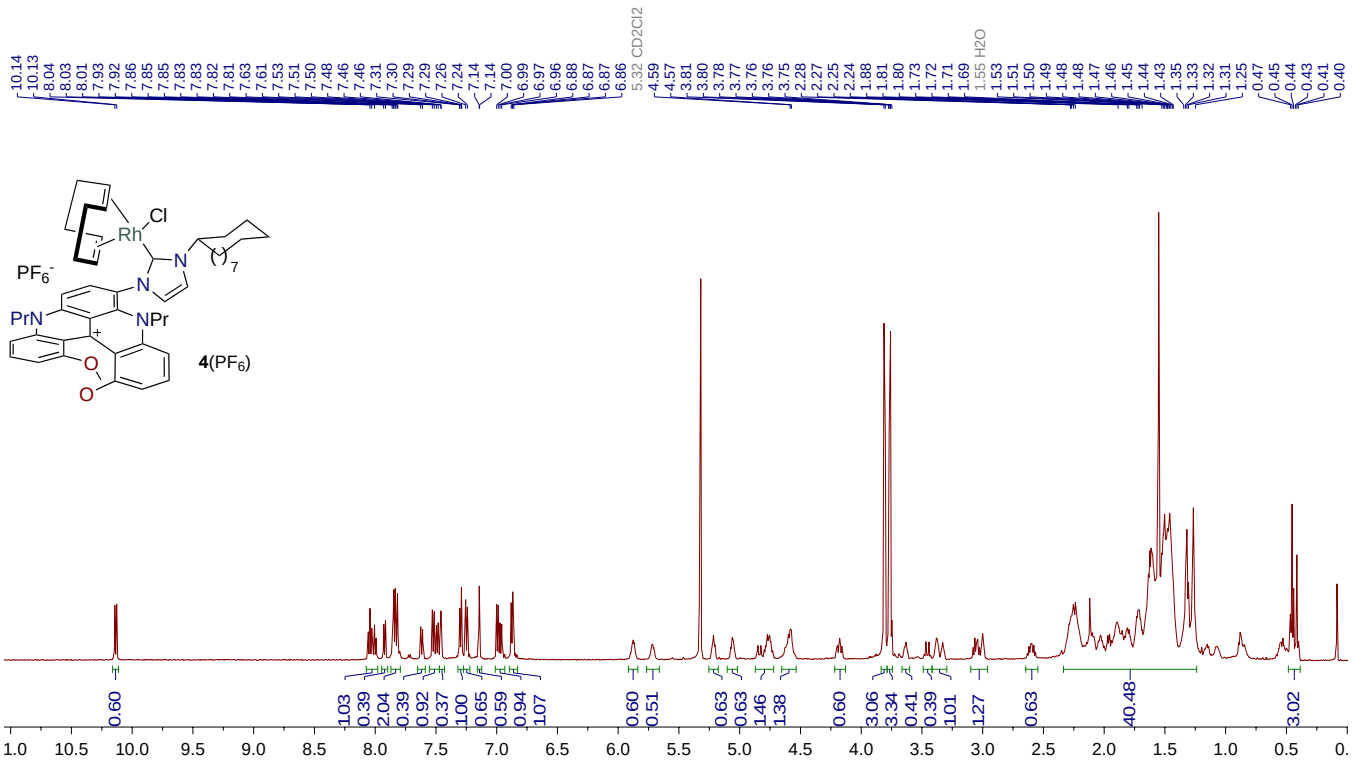


Figure S31. ^{1}H NMR (600 MHz, CD_2Cl_2) spectrum of **4**(PF_6)

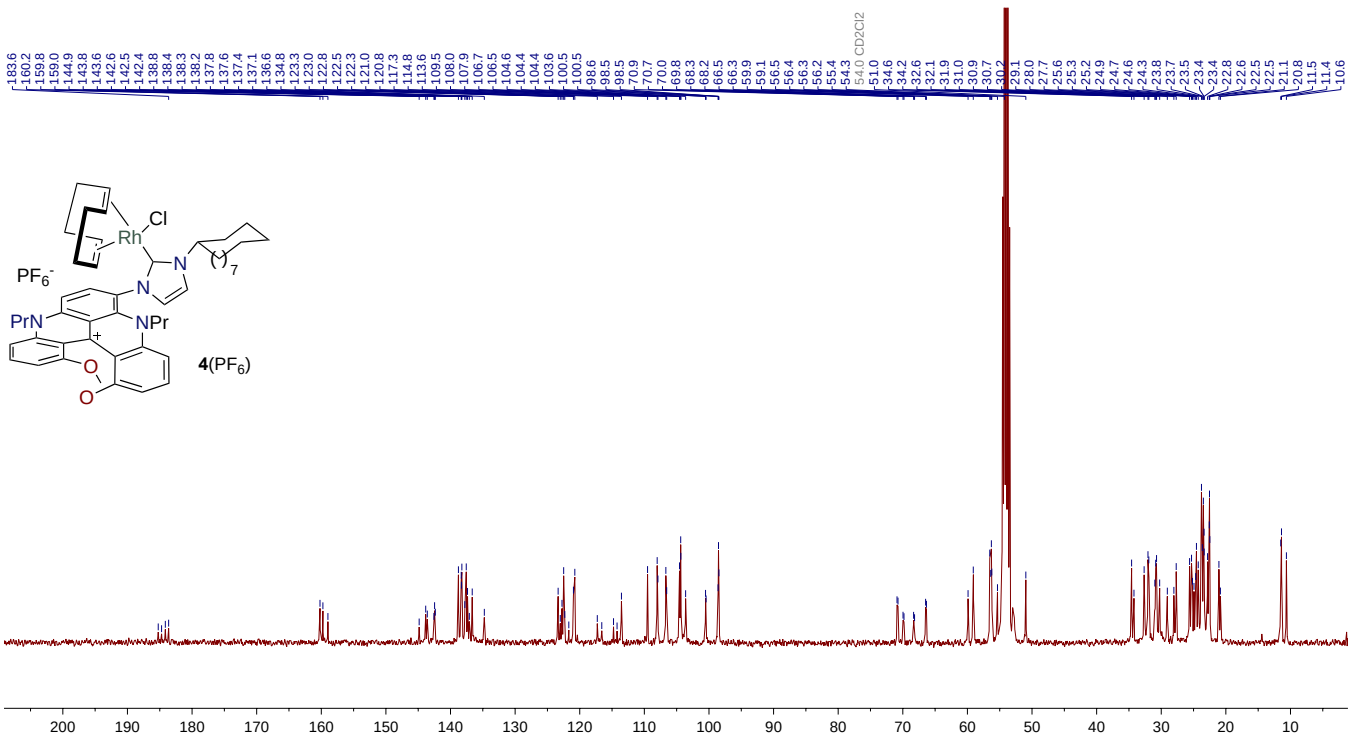


Figure S32. ^{13}C NMR (101 MHz, CD_2Cl_2) spectrum of **4**(PF_6)

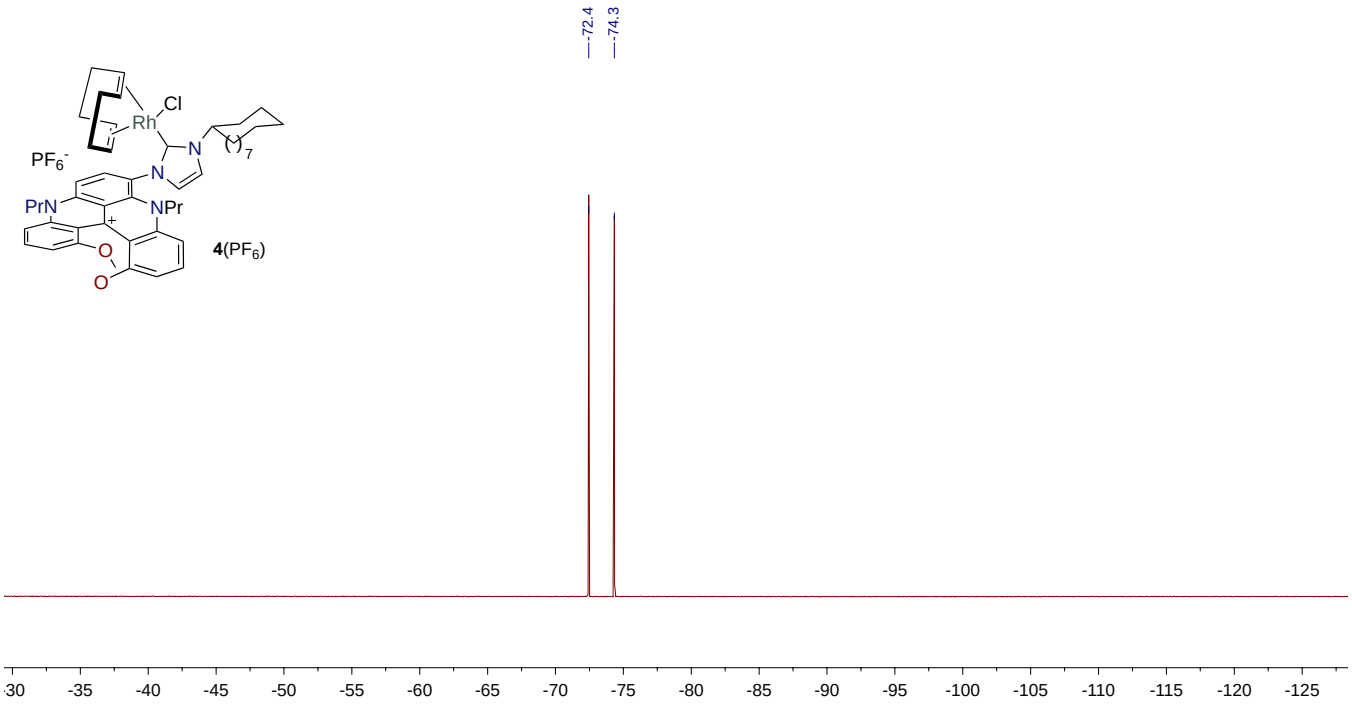


Figure S33. ^{19}F NMR (376 MHz, CD_2Cl_2) spectrum of **4**(PF_6)

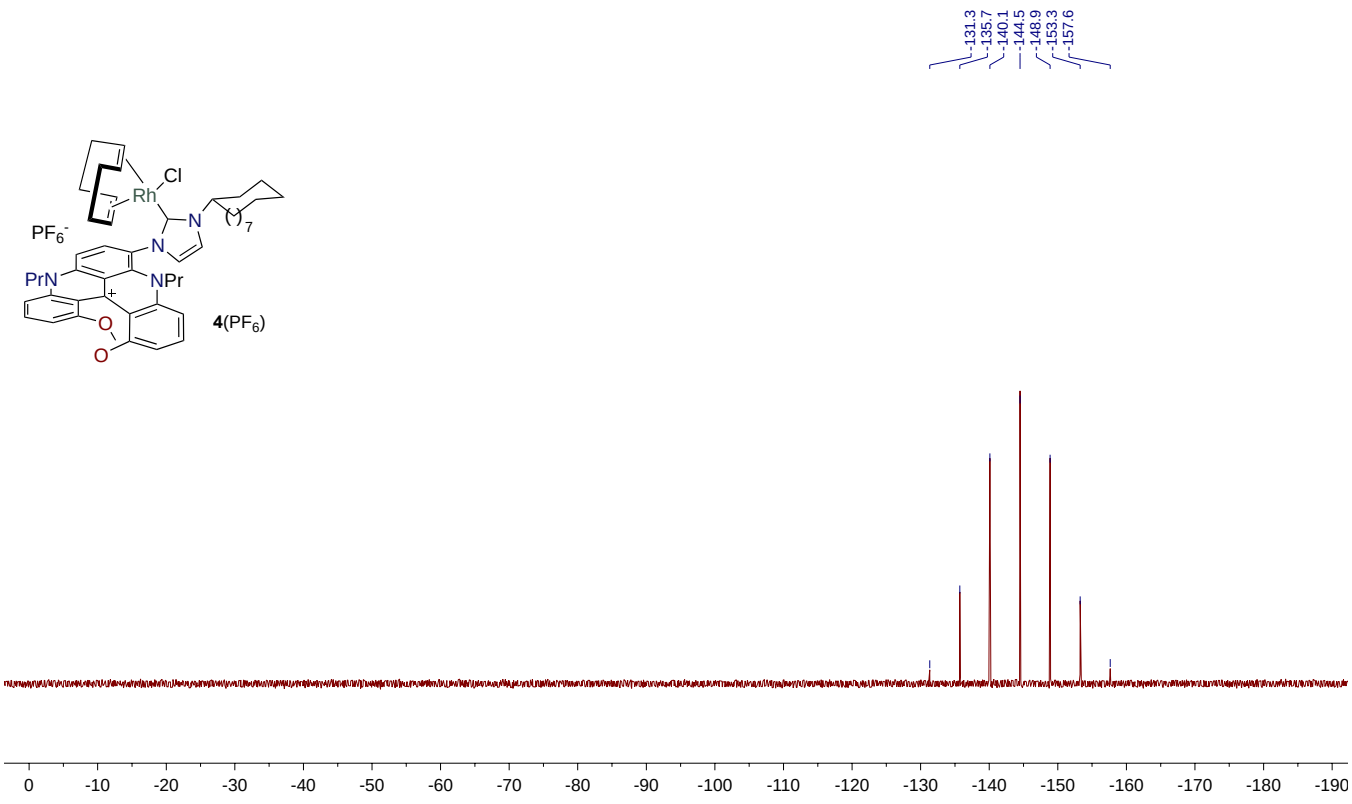


Figure S34. ^{31}P NMR (162 MHz, CD_2Cl_2) spectrum of **4**(PF_6)

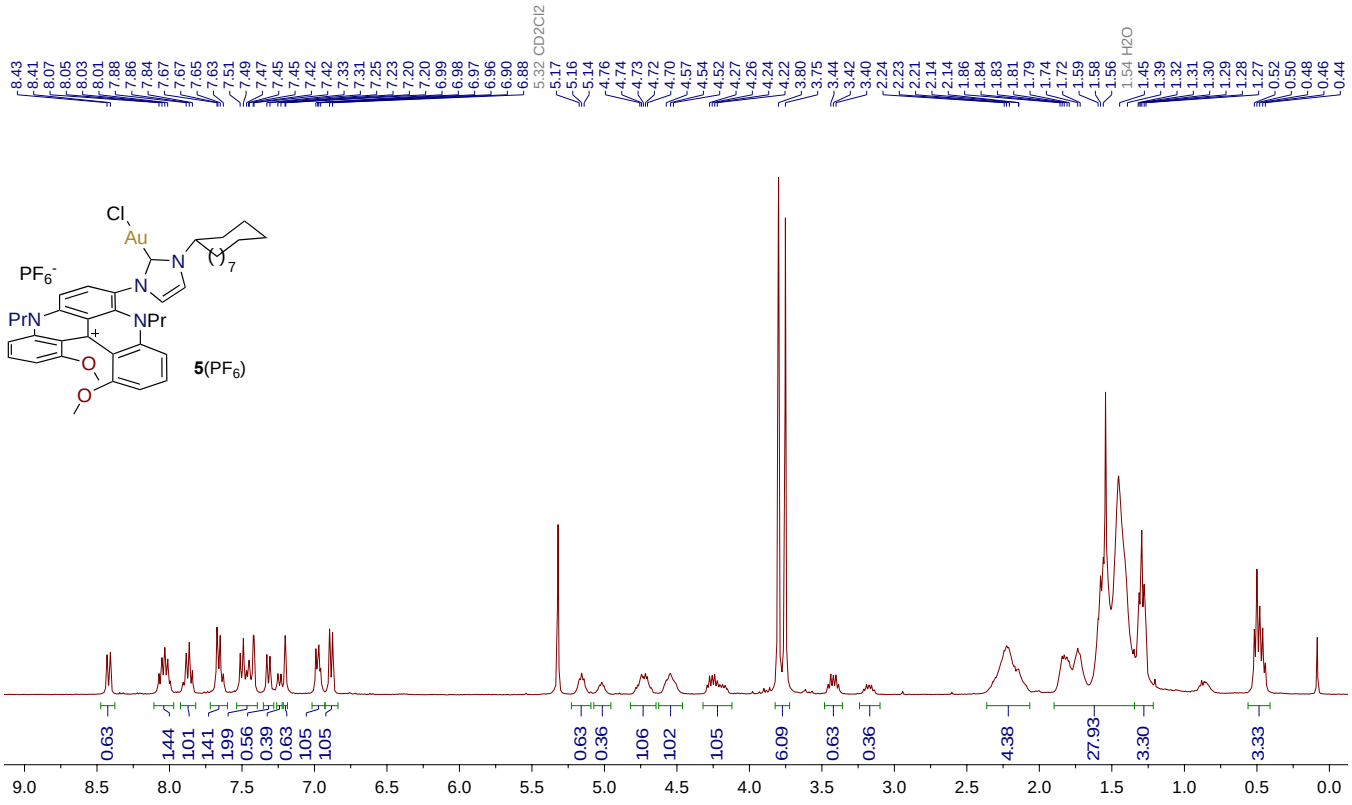


Figure S35. ^{1}H NMR (400 MHz, CD_2Cl_2) spectrum of **5**(PF_6)

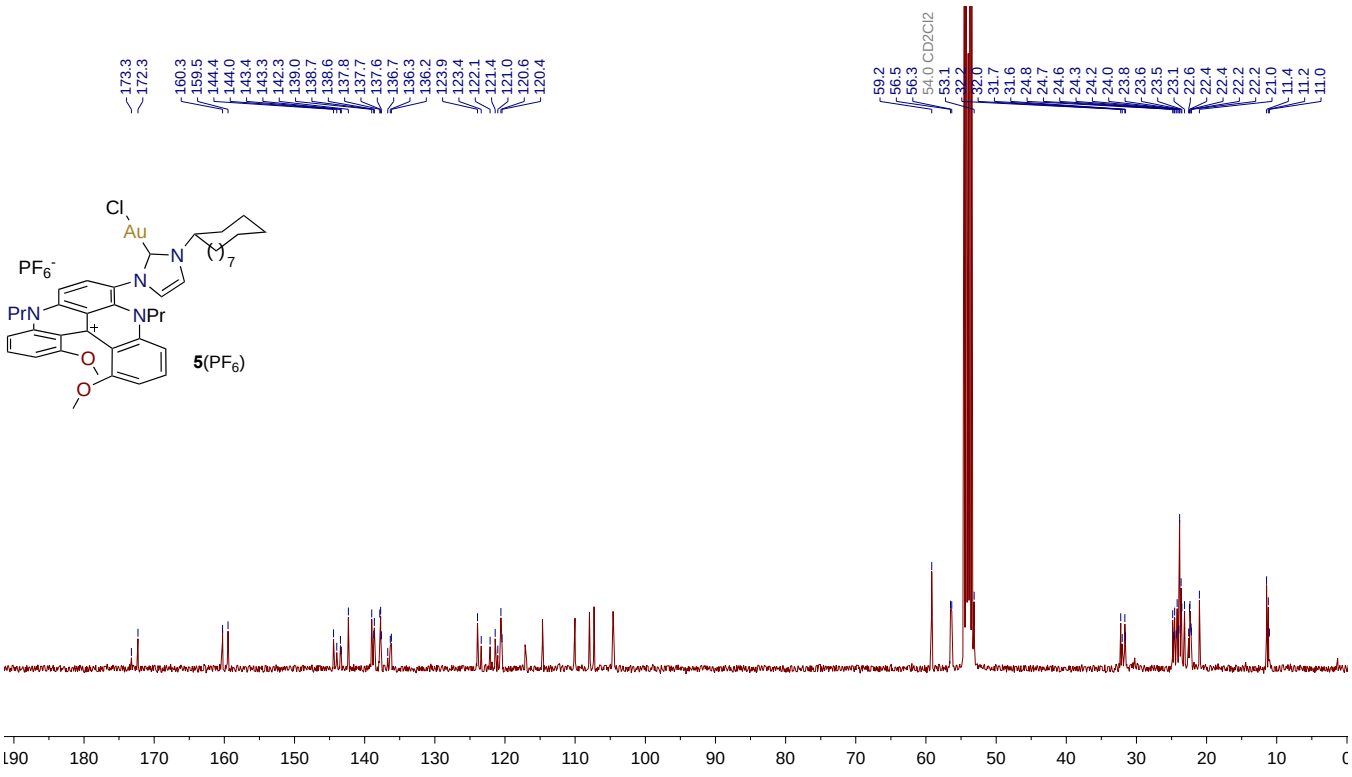


Figure S36. ^{13}C NMR (101 MHz, CD_2Cl_2) spectrum of **5**(PF_6)

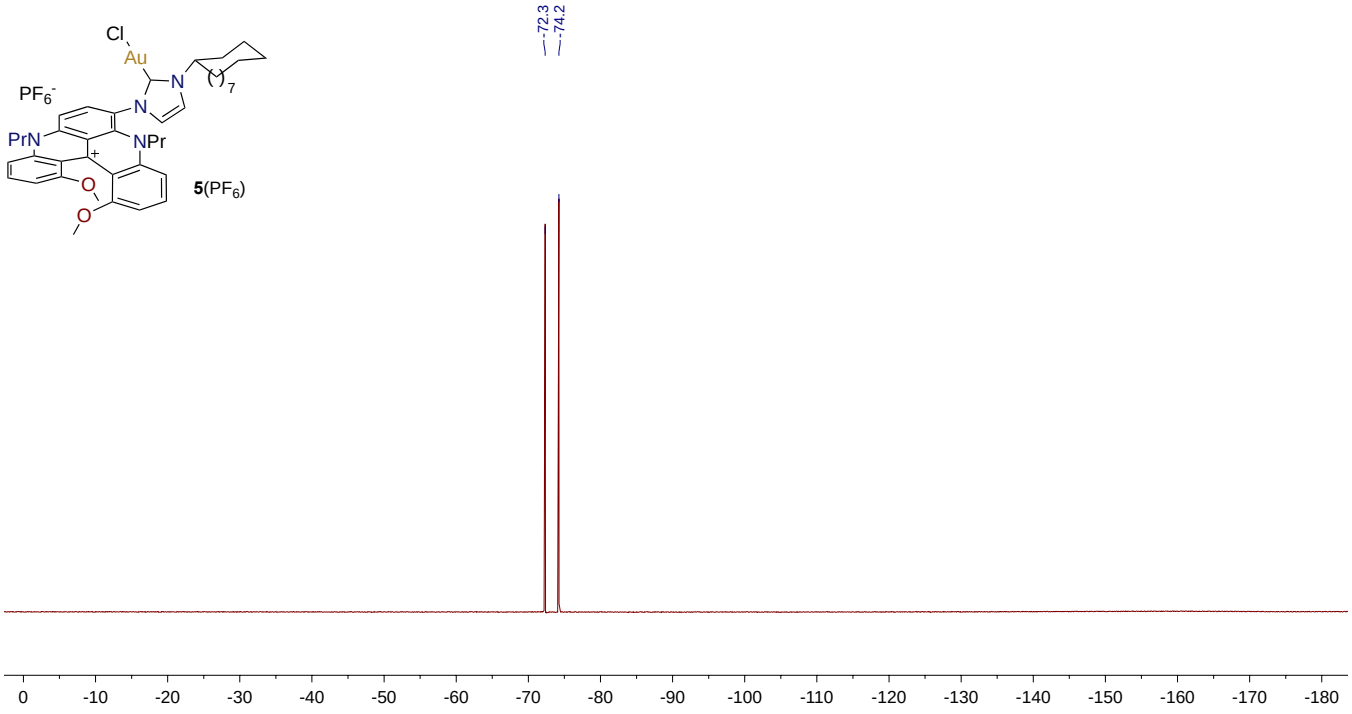


Figure S37. ^{19}F NMR (376 MHz, CD_2Cl_2) spectrum of **5**(PF_6)

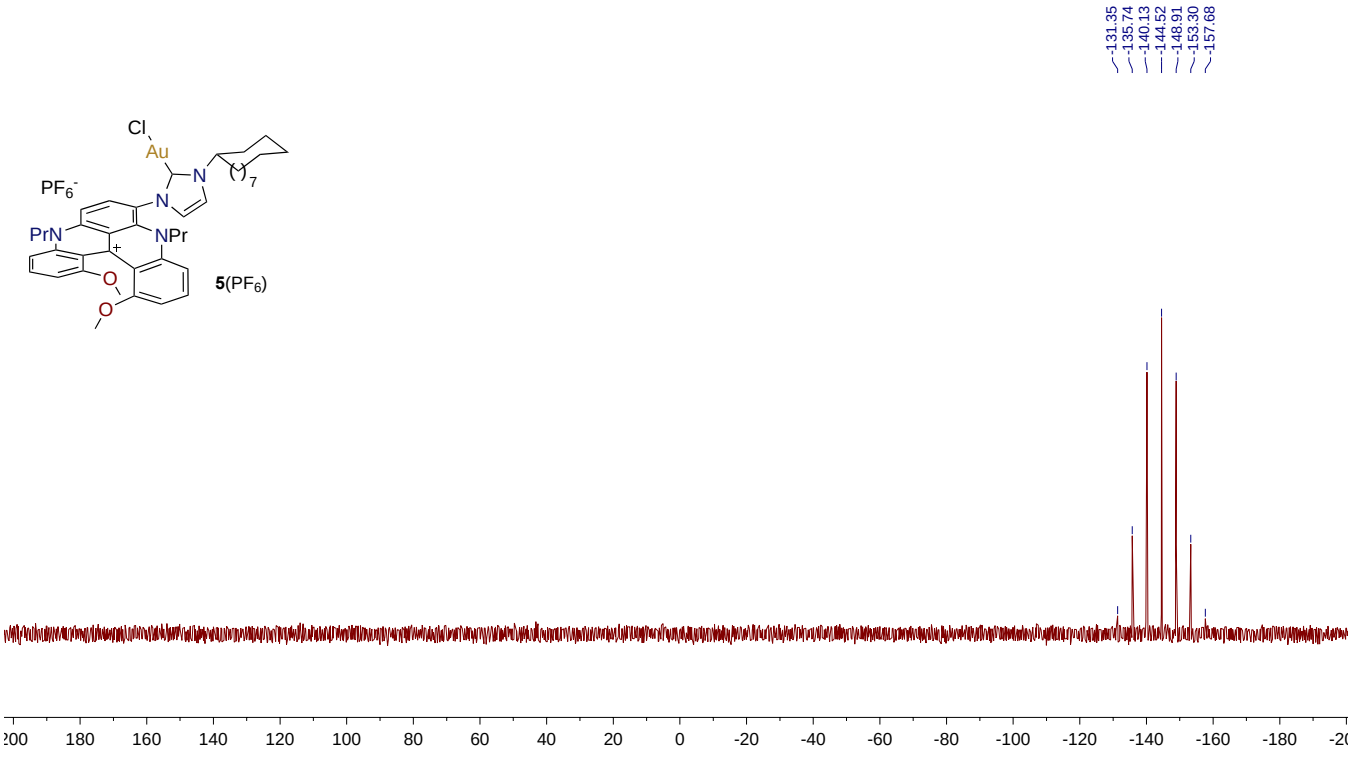


Figure S38. ^{31}P NMR (162 MHz, CD_2Cl_2) spectrum of **5**(PF_6)

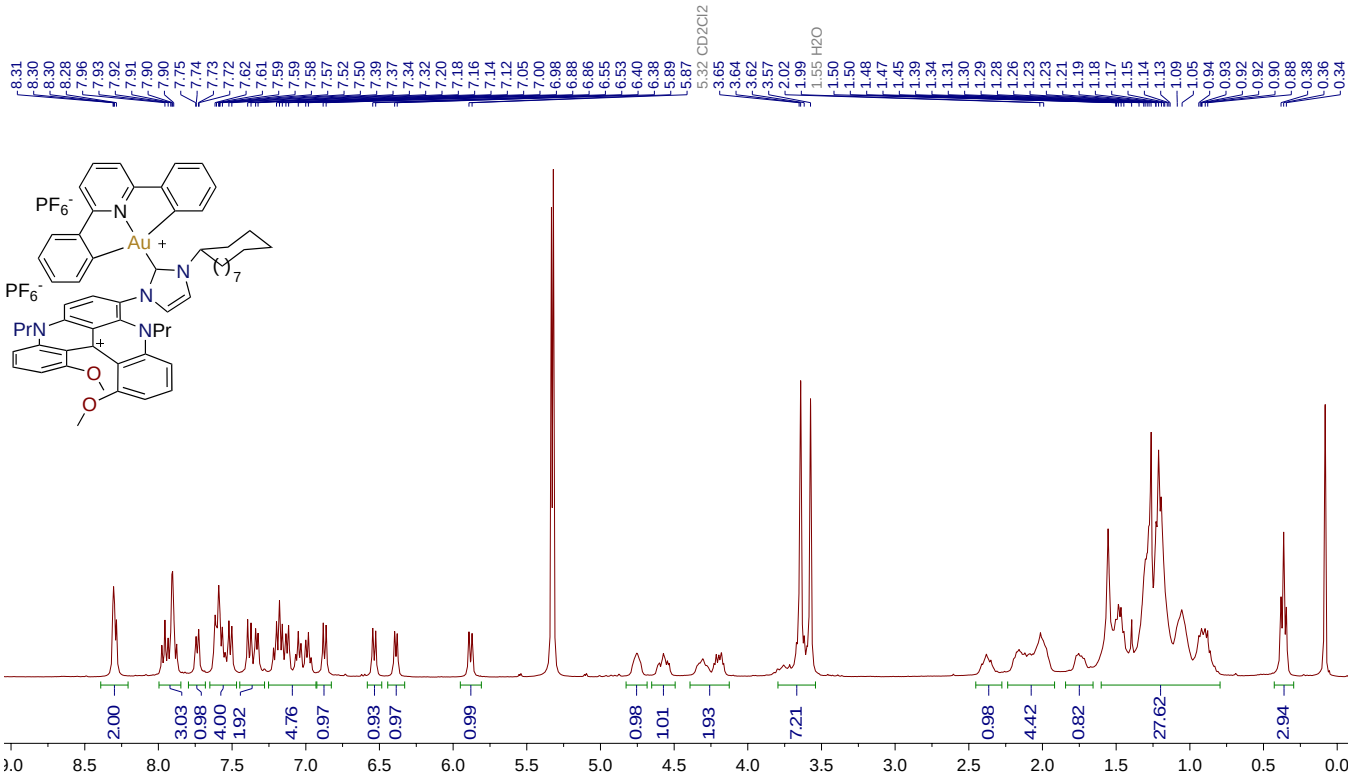


Figure S39. ^{1}H NMR (400 MHz, CD_2Cl_2) spectrum of **6**$(PF_6)_2$

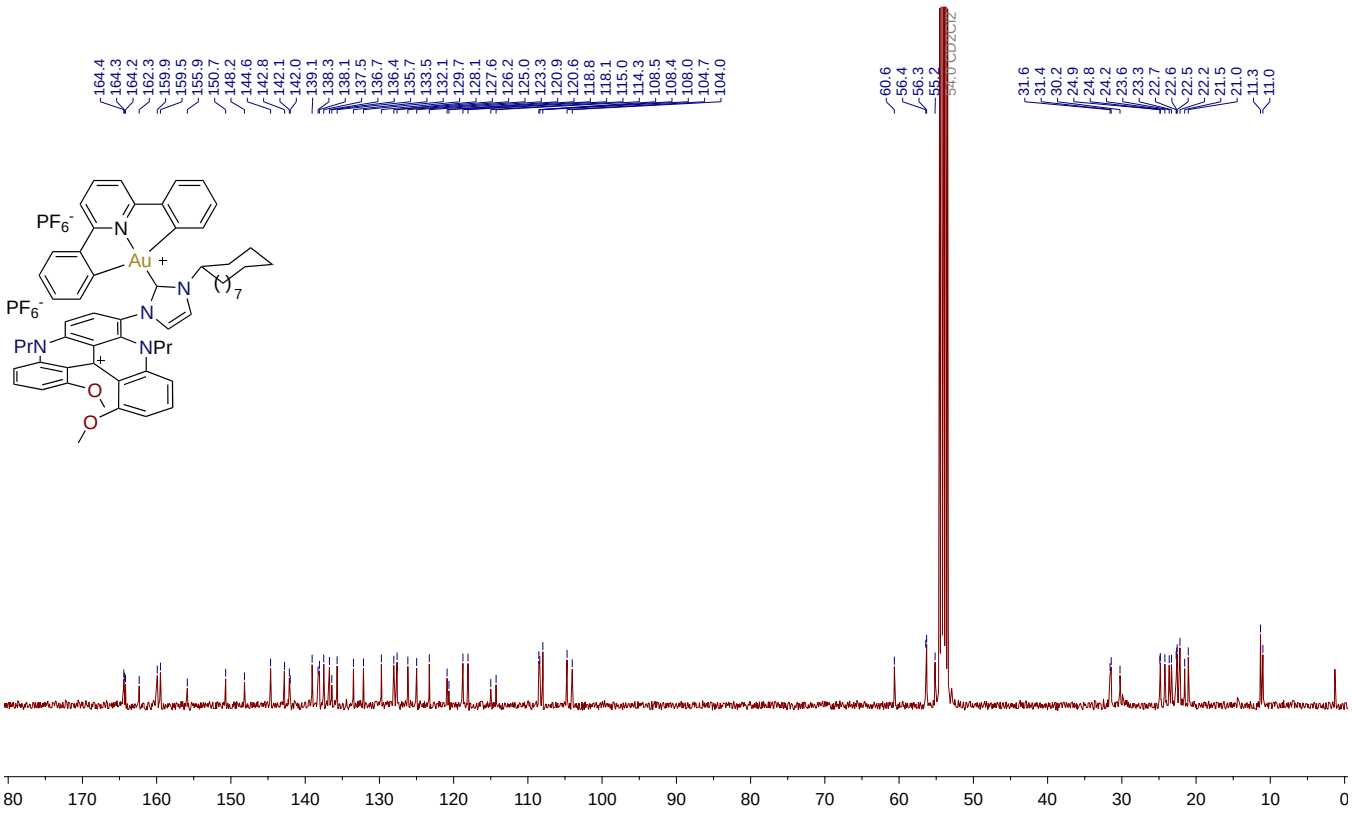


Figure S40. ^{13}C NMR (101 MHz, CD_2Cl_2) spectrum of **6**$(PF_6)_2$

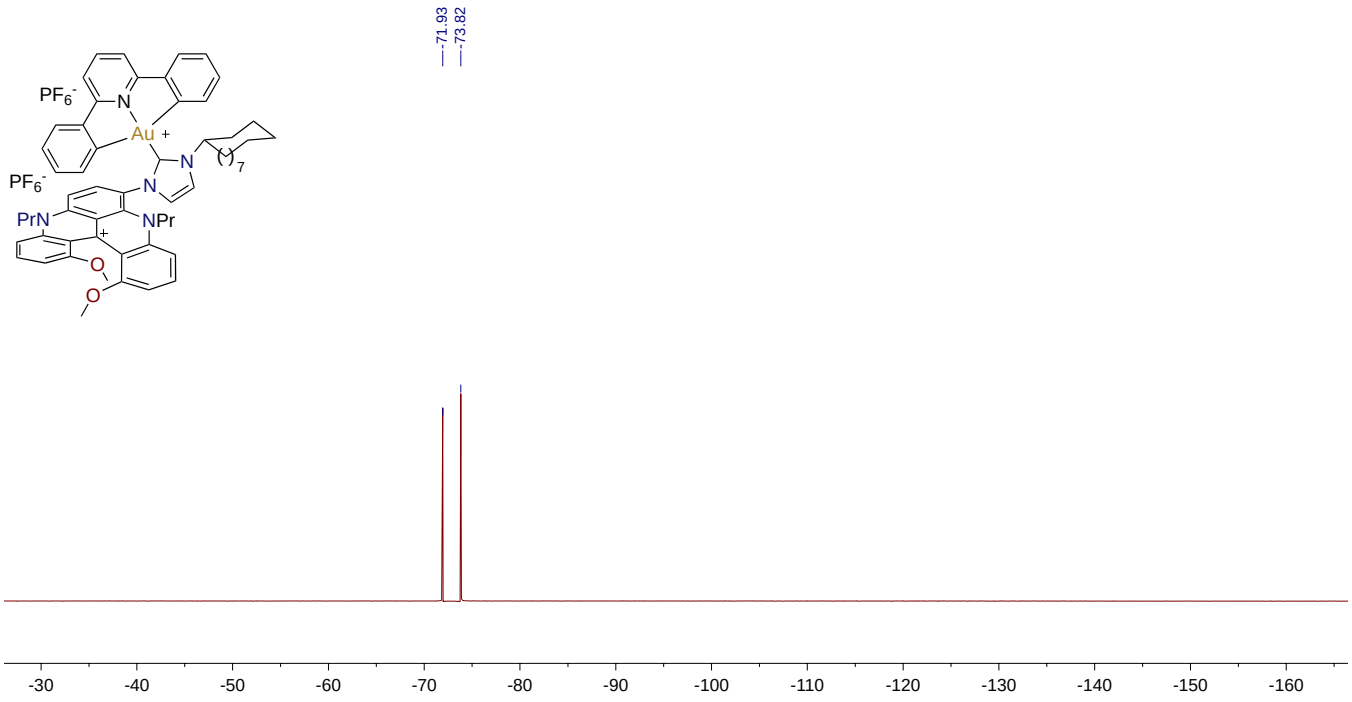


Figure S41. ^{19}F NMR (376 MHz, CD_2Cl_2) spectrum of **6**$(PF_6)_2$

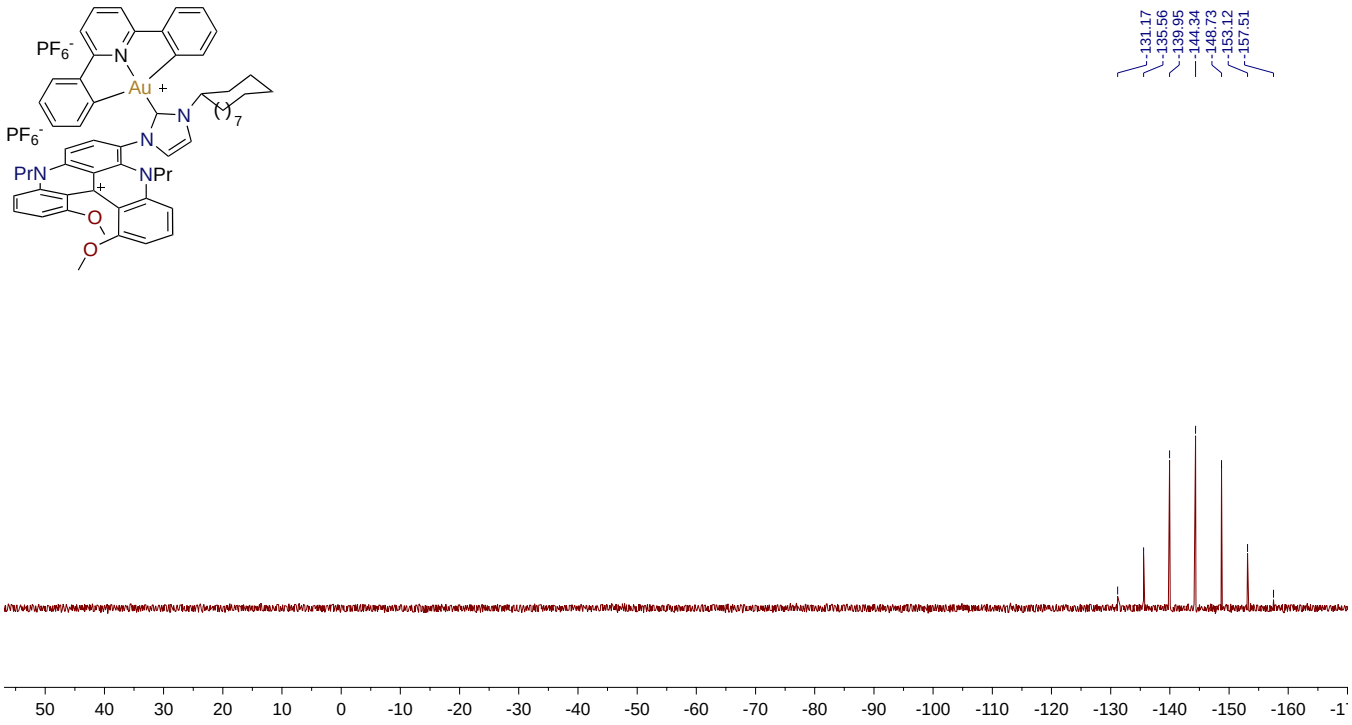


Figure S42. ^{31}P NMR (162 MHz, CD_2Cl_2) spectrum of **6**$(PF_6)_2$

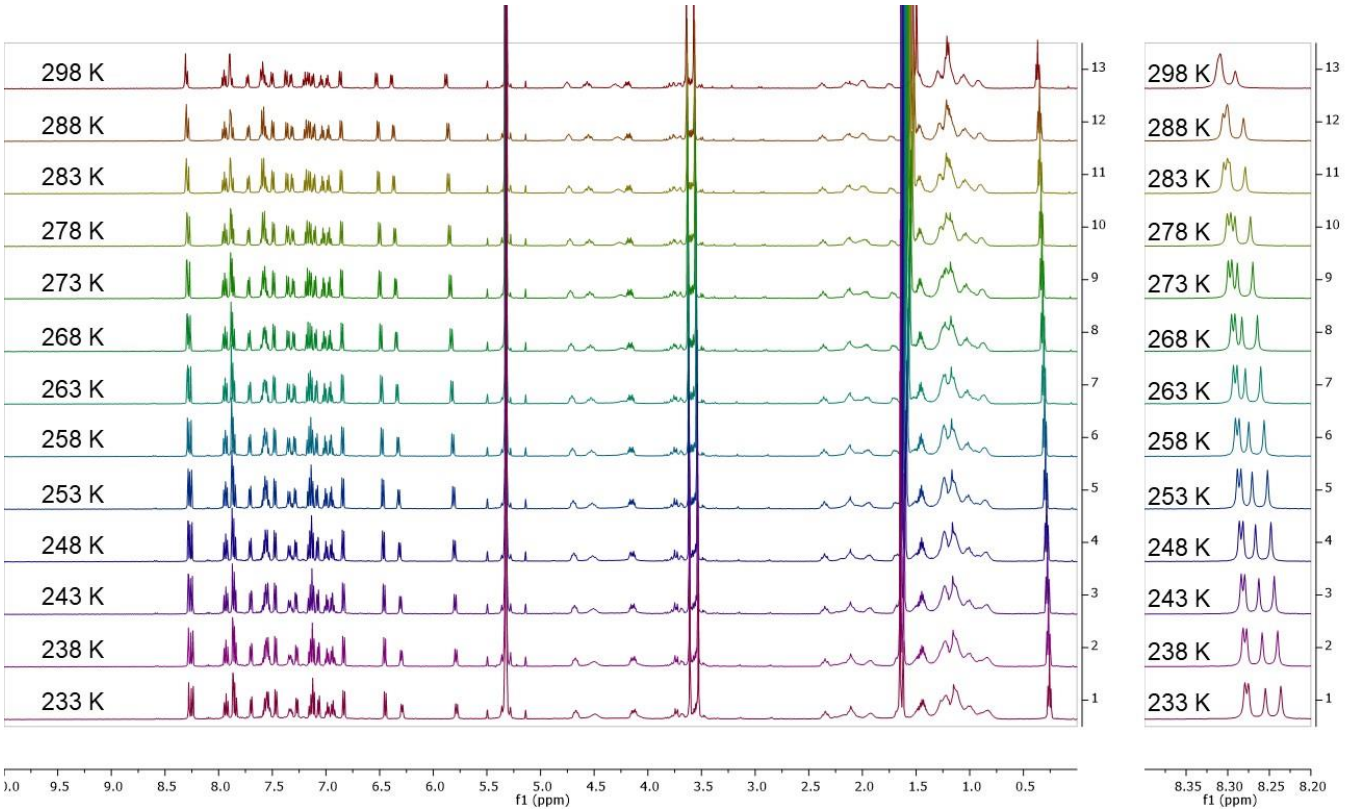


Figure S43. ^{1}H NMR (500 MHz, CD_2Cl_2) spectra of **6**$(PF_6)_2$ at variable temperatures.

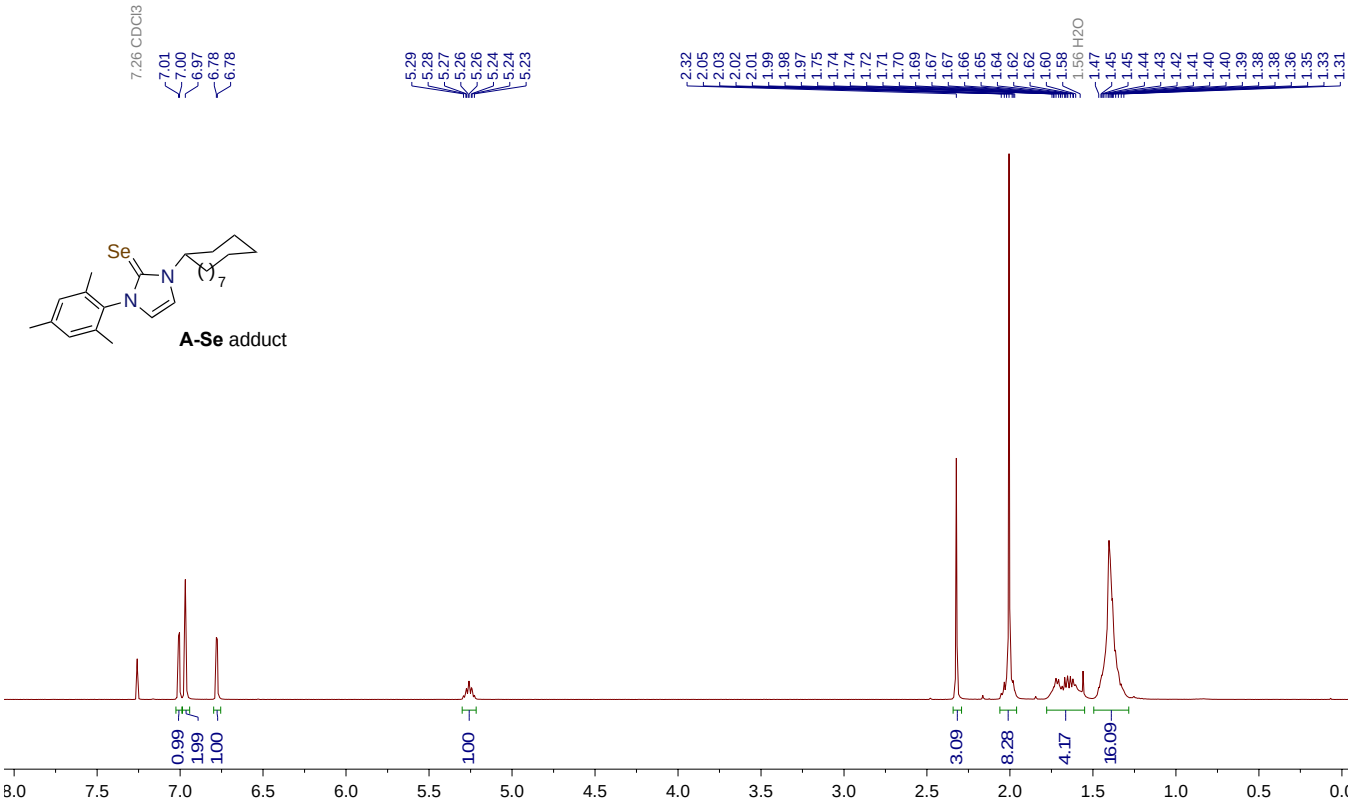


Figure S44. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **A-Se** adduct.

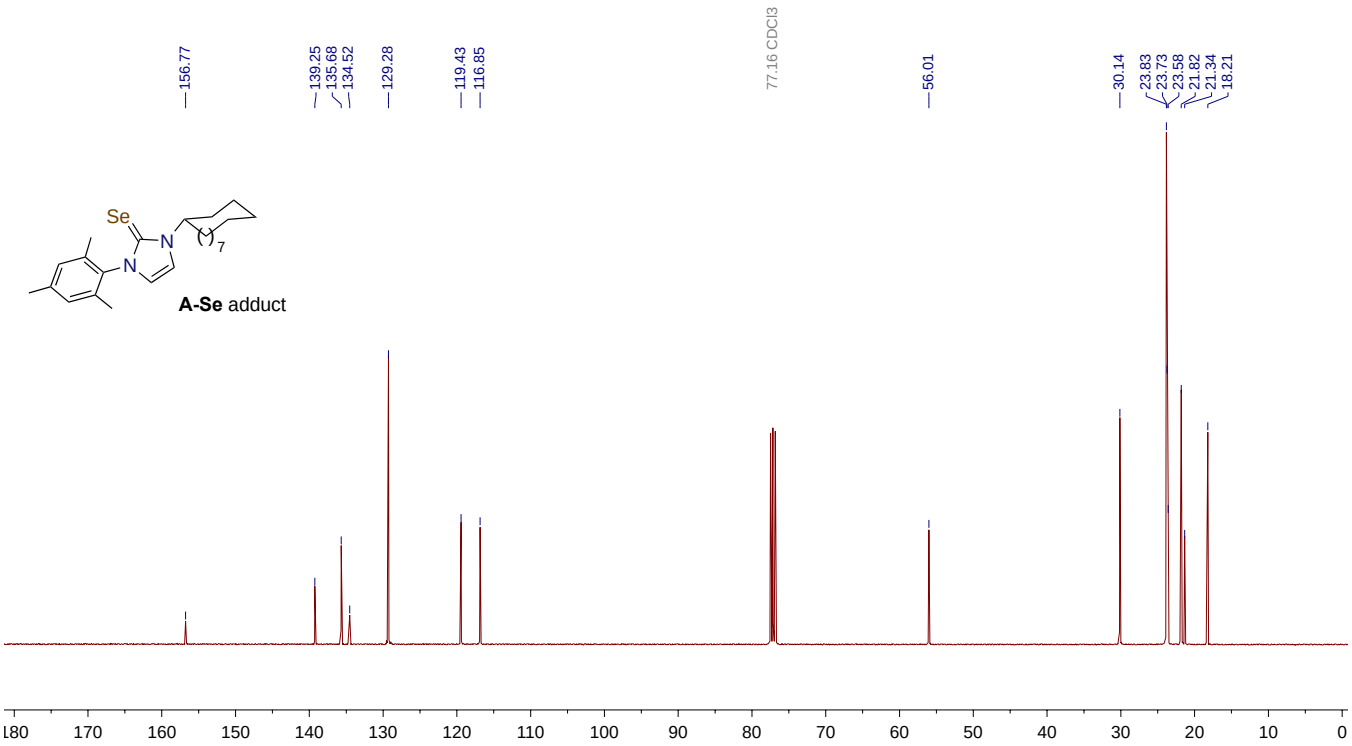


Figure S45. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **A-Se** adduct

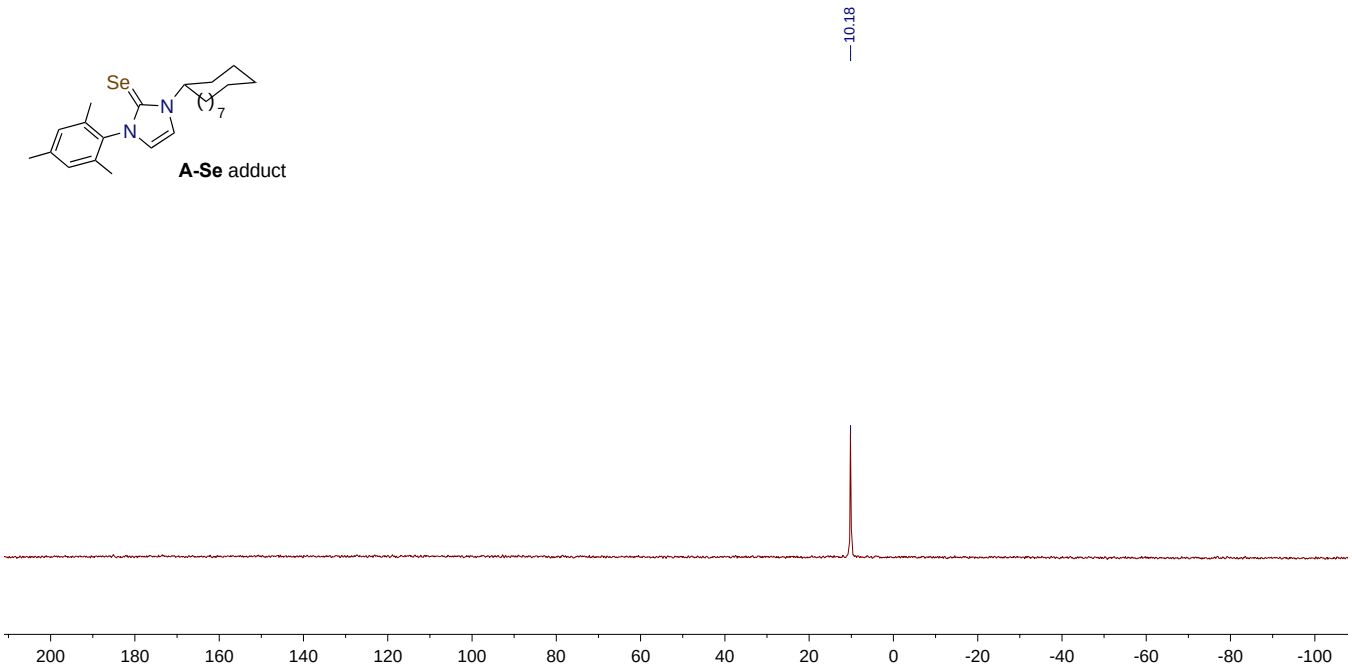


Figure S46. ^{77}Se NMR (115 MHz, $CDCl_3$) spectrum of **A-Se** adduct.

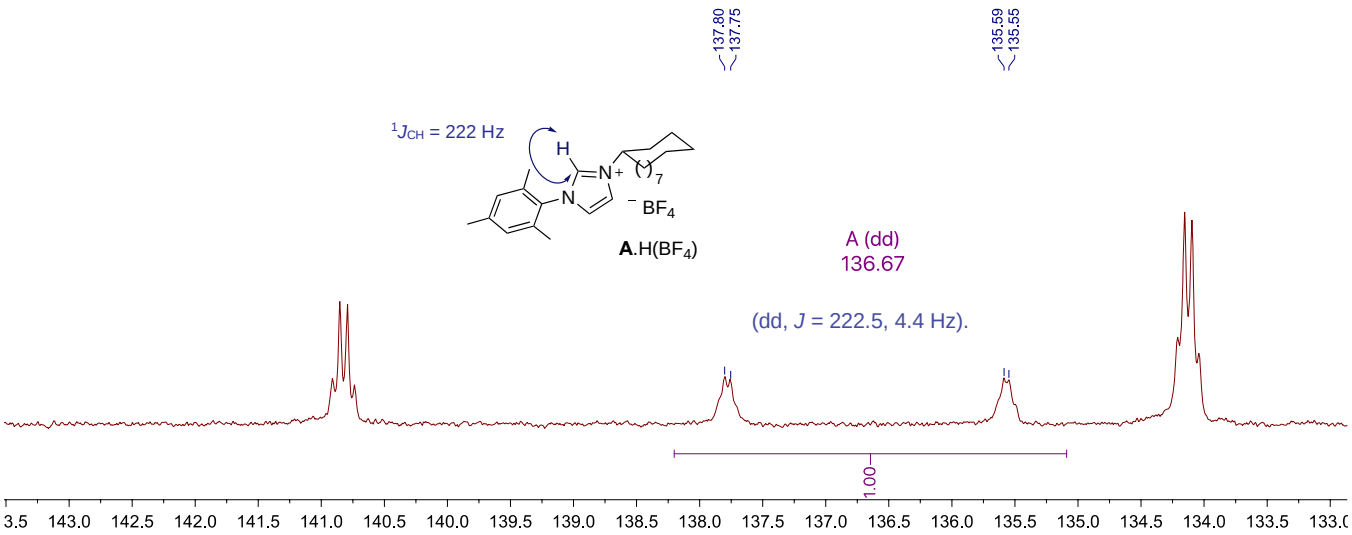
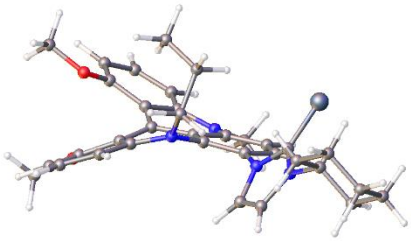


Figure S47. ^{13}C-1H NMR spectrum zoom of **A**.H(BF_4) and $^1J_{CH}$ coupling constant measurement.

Energies and Cartesian coordinates

(*aR*)-(*P*)-**3**-(+)



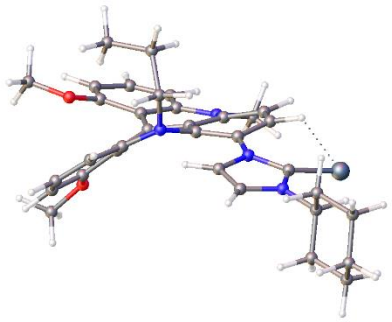
Geometry optimization, B3LYP/6-311G, gas phase**

SCF Done: E(RB3LYP) = -1696.93514806
Zero-point correction= 0.651844 (Hartree/Particle)
Thermal correction to Energy= 0.688608
Thermal correction to Enthalpy= 0.689553
Thermal correction to Gibbs Free Energy= 0.582138
Sum of electronic and zero-point Energies= -1696.283304
Sum of electronic and thermal Energies= -1696.246540
Sum of electronic and thermal Enthalpies= -1696.245595
Sum of electronic and thermal Free Energies= -1696.353010

Cartesian coordinates:

N	0.028279	-3.988408	0.730582	H	3.609943	0.132258	5.330683
C	-0.004897	-2.750759	0.121760	H	-0.734398	-4.323682	5.932255
C	0.293831	-1.597736	0.908905	H	-0.903519	-6.326286	4.520996
C	0.608058	-1.743619	2.278340	H	-0.604025	-6.203547	2.105523
C	0.163356	-2.949120	2.917776	H	-0.934178	-5.542791	-0.366183
C	-0.076993	-4.098667	2.108150	H	0.592690	-5.984247	0.436632
C	0.289420	-0.292496	0.311743	H	-0.157039	2.498572	0.031505
C	0.087578	-0.192345	-1.071703	H	-0.103976	2.711719	1.769196
C	-0.199300	-1.340393	-1.814462	H	-2.404858	2.666545	0.865634
C	-0.262704	-2.597992	-1.244457	H	-2.192469	1.036798	0.294130
C	1.347216	-0.665763	2.879703	H	-1.854985	0.254785	2.710742
C	1.200922	0.635570	2.319548	H	-3.409625	1.049250	2.478904
N	0.453338	0.800371	1.156283	H	-2.083927	1.919819	3.253066
C	2.282582	-0.842863	3.949626	H	4.518128	-1.996604	4.970506
C	2.904748	0.254373	4.522047	H	3.590312	-3.465497	5.368521
C	2.647823	1.535053	4.020290	H	3.270752	-1.951505	6.253239
C	1.824531	1.737137	2.932288	H	-1.536849	-2.205763	6.501889
C	-0.424143	-5.324777	2.704846	H	-0.429964	-0.820447	6.681952
C	-0.614243	-5.384670	4.069523	H	0.170027	-2.473978	6.972437
C	-0.505121	-4.249538	4.879601	C	-0.021212	3.544087	-5.481714
C	-0.146843	-3.036586	4.315164	H	-1.724498	3.293560	-4.188419
N	0.246763	1.032520	-1.777908	C	-0.689296	4.505525	-6.476624
C	-0.705391	1.621954	-2.594182	H	1.043582	3.794847	-5.393217
N	-0.074312	2.705558	-3.141976	H	-0.080474	2.513398	-5.842522
C	1.237736	2.777366	-2.693744	C	-0.701244	5.947023	-5.950470
C	1.448363	1.743115	-1.854127	H	-0.171918	4.453619	-7.438543
Se	-2.435815	1.051494	-2.862860	H	-1.718887	4.175320	-6.659038
C	-0.692538	3.642063	-4.103562	C	-1.360145	6.032695	-4.566784
C	-0.390070	2.021775	0.980235	H	0.329078	6.319824	-5.886130
C	-1.890821	1.725499	1.087485	H	-1.223509	6.599861	-6.655348
C	-2.329322	1.207446	2.459345	C	-0.695145	5.078614	-3.562078
O	2.545078	-2.117545	4.298552	H	-1.314840	7.056037	-4.183926
C	3.544524	-2.382033	5.285584	H	-2.423580	5.779574	-4.652930
O	-0.132495	-1.874507	4.992867	H	0.335287	5.408979	-3.378956
C	-0.507687	-1.860013	6.372483	H	-1.218143	5.105547	-2.601430
C	0.069277	-5.198216	-0.101466	C	10.048142	7.815646	-0.961704
H	0.629101	-4.985009	-1.008816	C	10.640290	6.968769	-1.892683
H	2.326496	1.436454	-1.314343	C	10.004878	6.774422	-3.107886
H	1.911265	3.551363	-3.016469	C	8.797376	7.409402	-3.413380
H	-0.366862	-1.227071	-2.876794	C	8.257663	8.281814	-2.463396
H	-0.519967	-3.442242	-1.865558	O	7.099554	8.929707	-2.747480
H	1.723991	2.727890	2.514930	H	8.400711	9.154515	-0.518149
H	3.150249	2.384559	4.467869				

TS-**3**



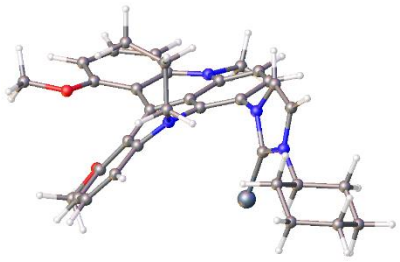
Geometry optimization, B3LYP/6-311G, gas phase**

SCF Done: E(RB3LYP) = -1696.90882931
Zero-point correction= 0.651142 (Hartree/Particle)
Thermal correction to Energy= 0.687018
Thermal correction to Enthalpy= 0.687962
Thermal correction to Gibbs Free Energy= 0.582884
Sum of electronic and zero-point Energies= -1696.257687
Sum of electronic and thermal Energies= -1696.221812
Sum of electronic and thermal Enthalpies= -1696.220868
Sum of electronic and thermal Free Energies= -1696.325945

Cartesian coordinates:

N	6.607083	8.878621	10.667452	H	5.097770	11.900722	7.619741
C	6.347366	10.162202	10.228772	H	5.167322	9.654238	8.487118
C	6.797371	11.263721	11.004479	H	7.984756	15.564177	12.890513
C	7.449998	11.034694	12.239268	H	9.884803	15.237414	14.413304
C	7.290603	9.740713	12.828398	H	10.875867	13.018991	14.755136
C	6.924380	8.643775	11.991053	H	7.447214	7.993594	15.789117
C	6.631457	12.600025	10.531642	H	7.063851	6.116577	14.246722
C	6.233657	12.819433	9.195561	H	6.624600	6.498749	11.883169
C	5.609084	11.726042	8.555428	H	5.465574	7.307820	9.778685
C	5.659272	10.431455	9.039380	H	7.214702	7.002351	9.948485
C	8.216521	12.142681	12.777359	H	5.197547	14.815962	10.797683
C	7.775853	13.450711	12.459301	H	5.954566	15.387246	12.263176
N	6.791462	13.625492	11.474466	H	3.635610	14.482879	12.526232
C	9.395776	12.001382	13.561141	H	4.192320	12.890437	12.059607
C	9.982125	13.111058	14.152963	H	5.634174	12.782944	14.146941
C	9.418387	14.379957	13.942570	H	3.951859	13.115720	14.549333
C	8.341582	14.564328	13.103335	H	5.137059	14.426353	14.564590
C	6.882809	7.329689	12.506078	H	11.949676	11.139041	13.856111
C	7.117407	7.127185	13.850607	H	11.370819	9.493191	14.218447
C	7.350299	8.191507	14.727256	H	11.071970	10.805504	15.385323
C	7.412137	9.480570	14.240961	H	6.650663	9.910974	16.819733
N	6.432125	14.041196	8.485111	H	7.613222	11.410672	16.853078
C	6.360329	14.210429	7.084573	H	8.436302	9.835122	16.748090
N	6.738283	15.505059	6.864104	C	8.302706	16.319981	5.124324
C	7.126289	16.110189	8.048326	H	6.357960	15.443779	4.850472
C	6.952629	15.224971	9.047197	C	8.400329	16.958202	3.727745
Se	6.010848	13.013687	5.707605	H	8.824030	16.960200	5.850889
C	6.838497	16.152530	5.534177	H	8.799835	15.348066	5.131740
C	5.604153	14.493068	11.751348	C	7.626579	18.278681	3.647528
C	4.500728	13.807529	12.570479	H	9.449094	17.114818	3.465693
C	4.833500	13.517657	14.034711	H	8.001947	16.256395	2.980080
O	9.912393	10.754888	13.643043	C	6.162328	18.101664	4.088068
C	11.149264	10.553709	14.322459	H	8.109541	19.021749	4.295753
O	7.502382	10.569038	15.029617	H	7.658169	18.682309	2.632470
C	7.554877	10.407636	16.446219	C	6.067458	17.477553	5.491670
C	6.467627	7.757770	9.727479	H	5.635867	19.057576	4.082240
H	6.645353	8.122213	8.719611	H	5.645092	17.452577	3.373797
H	7.211274	15.310317	10.082643	H	6.477751	18.182966	6.230879
H	7.496134	17.119549	8.090216	H	5.015693	17.306342	5.766975

(*aS*)-(*P*)-**3**-(+)



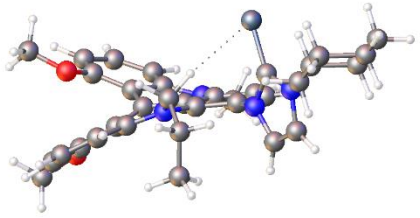
Geometry optimization, B3LYP/6-311G, gas phase**

SCF Done: E(RB3LYP) = -1696.93518224
Zero-point correction= 0.651766 (Hartree/Particle)
Thermal correction to Energy= 0.688548
Thermal correction to Enthalpy= 0.689492
Thermal correction to Gibbs Free Energy= 0.581844
Sum of electronic and zero-point Energies= -1696.283416
Sum of electronic and thermal Energies= -1696.246634
Sum of electronic and thermal Enthalpies= -1696.245690
Sum of electronic and thermal Free Energies= -1696.353338

Cartesian coordinates:

N	-1.043206	-3.886289	0.861533	H	-2.547957	-0.880542	-2.211464
C	-1.181624	-2.612916	0.345895	H	-2.556072	-3.121512	-1.247562
C	-0.450165	-1.547521	0.953622	H	2.103410	2.449424	1.791836
C	0.378742	-1.817680	2.068248	H	4.140390	1.823325	2.974726
C	0.087819	-3.009097	2.816733	H	4.593684	-0.509018	3.592186
C	-0.591775	-4.074509	2.158239	H	0.330783	-4.471436	5.912054
C	-0.533155	-0.214519	0.431269	H	-0.625267	-6.355133	4.660888
C	-1.286254	-0.003988	-0.740865	H	-1.312861	-6.113724	2.334378
C	-1.988968	-1.067979	-1.302533	H	-2.530098	-5.278052	0.228160
C	-1.970095	-2.347677	-0.775798	H	-0.864334	-5.899836	0.314207
C	1.429711	-0.876747	2.319390	H	-0.413260	2.633451	0.243859
C	1.243893	0.463738	1.871509	H	0.175551	2.719312	1.890152
N	0.103300	0.783761	1.145589	H	-2.244564	3.207187	1.697475
C	2.690568	-1.229563	2.904201	H	-2.555392	1.571802	1.164898
C	3.638459	-0.254156	3.157470	H	-1.651130	0.686168	3.373606
C	3.378629	1.073490	2.796512	H	-3.011474	1.782753	3.605451
C	2.214870	1.439962	2.155810	H	-1.366250	2.349019	3.896538
C	-0.808092	-5.295253	2.823562	H	4.965007	-2.705148	2.886527
C	-0.436929	-5.420337	4.146167	H	4.100074	-4.070004	3.639210
C	0.120409	-4.354217	4.859348	H	4.388140	-2.581339	4.576843
C	0.360812	-3.150597	4.216618	H	0.089098	-2.327367	6.793495
N	-1.300217	1.227797	-1.456043	H	1.326349	-1.072053	6.527479
C	-0.213076	1.754084	-2.139886	H	1.796099	-2.791655	6.518053
N	-0.720091	2.818943	-2.835906	C	0.059337	5.149746	-3.218906
C	-2.086771	2.930055	-2.621734	H	1.088843	3.305080	-3.643342
C	-2.456879	1.945108	-1.777881	C	0.907614	6.044628	-4.136083
Se	1.516575	1.131309	-2.107798	H	-0.971314	5.526375	-3.198310
C	0.072224	3.698172	-3.719738	H	0.435431	5.185472	-2.192043
C	-0.464822	2.155202	1.219016	C	0.456707	5.945116	-5.599618
C	-1.889625	2.175380	1.787347	H	0.853779	7.080168	-3.788620
C	-1.981901	1.720581	3.246594	H	1.959409	5.744057	-4.057745
O	2.896228	-2.544340	3.113025	C	0.456367	4.489707	-6.086834
C	4.171245	-2.986119	3.583988	H	-0.553700	6.362326	-5.698135
O	0.788336	-2.041522	4.847148	H	1.106565	6.553816	-6.234507
C	1.009639	-2.077167	6.258985	C	-0.393534	3.587259	-5.178679
C	-1.476255	-5.037849	0.060485	H	0.083823	4.429730	-7.113124
H	-1.318499	-4.815733	-0.992233	H	1.485545	4.111569	-6.106964
H	-3.416914	1.697538	-1.361164	H	-1.446908	3.885641	-5.255393
H	-2.677788	3.703017	-3.080179	H	-0.329459	2.544514	-5.502151

(*aR*)-(*P*)-**3**-(–)



Geometry optimization, B3LYP/6-311G, gas phase**

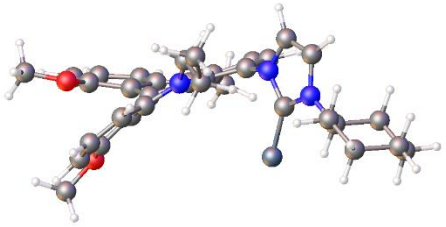
SCF Done: E(RB3LYP) = -1696.92689290

Zero-point correction=	0.652787	(Hartree/Particle)
Thermal correction to Energy=	0.689229	
Thermal correction to Enthalpy=	0.690173	
Thermal correction to Gibbs Free Energy=	0.584139	
Sum of electronic and zero-point Energies=	-1696.274105	
Sum of electronic and thermal Energies=	-1696.237664	
Sum of electronic and thermal Enthalpies=	-1696.236720	
Sum of electronic and thermal Free Energies=	-1696.342754	

Cartesian coordinates:

C	7.365926	17.591575	6.285539	C	6.218899	10.704825	16.323357
C	6.671704	16.230976	6.128740	Se	5.109399	14.396464	8.484131
C	6.483591	15.845226	4.654017	H	7.706902	7.529559	9.032617
C	5.719108	16.944800	3.900665	H	9.900158	13.213714	7.620734
C	6.399634	18.312419	4.048624	H	9.324062	15.273607	5.904881
C	6.595144	18.682256	5.525250	H	7.085254	11.419224	7.214914
N	7.389484	15.172730	6.868973	H	6.728079	9.198213	8.154196
C	6.834310	14.391540	7.843839	H	9.287173	14.998319	13.011557
N	7.857274	13.557199	8.267379	H	10.349114	14.437097	15.118637
C	8.998008	13.783137	7.487991	H	10.547664	12.105591	15.877257
C	8.706126	14.790967	6.641244	H	5.766552	8.289292	15.827813
C	7.646945	12.360313	9.028682	H	5.493413	6.329405	14.374291
C	7.847652	12.218599	10.421136	H	6.063835	6.424097	12.003201
C	7.631757	10.909342	10.989360	H	6.044053	7.148241	9.541138
C	7.239805	9.805587	10.167281	H	7.441970	6.518878	10.446217
C	7.058484	9.997707	8.799067	H	7.029834	14.677061	10.323429
C	7.252108	11.258902	8.272763	H	7.542658	15.096347	11.918609
C	7.812357	10.689697	12.374904	H	9.076796	16.471740	10.958308
C	7.152464	9.546357	12.951249	H	8.789800	15.805317	9.376994
C	6.848174	8.444305	12.104919	H	10.882844	14.805686	11.386483
N	7.094644	8.560624	10.746491	H	11.136716	15.587005	9.830630
N	8.186073	13.242918	11.293753	H	10.489639	13.952456	9.898334
C	8.697003	12.957791	12.553293	H	11.282379	9.909745	15.581568
C	8.616410	11.637597	13.079133	H	10.168167	8.525844	15.719443
C	6.288736	7.268440	12.636035	H	9.826380	10.028857	16.616260
C	5.947132	7.227361	13.971818	H	5.145250	10.501139	16.291909
C	6.113601	8.336291	14.806319	H	6.387994	11.725891	16.657250
C	6.688637	9.494322	14.306674	H	6.710278	10.008446	17.008984
C	9.273732	13.974240	13.344629	H	5.691402	16.274001	6.609348
C	9.886776	13.649833	14.534786	H	7.464041	15.695800	4.184238
C	9.983899	12.326602	14.983200	H	5.948273	14.893383	4.593798
C	9.368435	11.322501	14.260033	H	5.633051	16.672309	2.845169
C	7.056947	7.369722	9.889764	H	4.696164	17.002469	4.291272
C	7.896570	14.670738	10.981338	H	7.375341	18.290219	3.546544
C	9.054530	15.531459	10.398564	H	5.809074	19.082337	3.544351
C	10.465297	14.928815	10.386502	H	7.126013	19.634112	5.614598
O	9.465826	10.013496	14.557975	H	5.616003	18.826181	5.997421
C	10.236337	9.610900	15.692307	H	8.389281	17.534522	5.893714
O	6.790938	10.634424	15.014599	H	7.441501	17.843717	7.347537

(*aS*)-(*P*)-**3**-(–)



Geometry optimization, B3LYP/6-311G, gas phase**

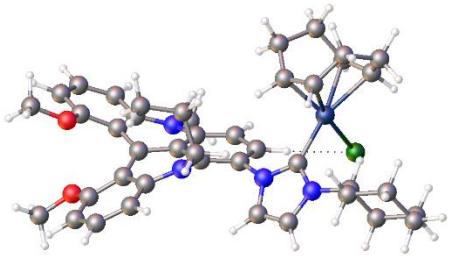
SCF Done: E(RB3LYP) = -1696.93123708

Zero-point correction=	0.652190 (Hartree/Particle)
Thermal correction to Energy=	0.688882
Thermal correction to Enthalpy=	0.689826
Thermal correction to Gibbs Free Energy=	0.582194
Sum of electronic and zero-point Energies=	-1696.279047
Sum of electronic and thermal Energies=	-1696.242355
Sum of electronic and thermal Enthalpies=	-1696.241411
Sum of electronic and thermal Free Energies=	-1696.349043

Cartesian coordinates:

C	9.659801	11.020613	13.981876	O	9.756665	9.682195	14.082620
C	8.739753	11.503686	12.993532	C	10.719607	9.117839	14.975772
C	8.789128	12.883074	12.638162	H	6.893871	8.012047	8.682592
C	9.501251	13.776220	13.464055	H	5.869247	14.983843	8.334763
C	10.283498	13.283072	14.485833	H	7.399694	16.572253	6.702760
C	10.414548	11.909397	14.724248	H	6.472780	12.067005	7.418357
C	7.779874	10.678727	12.329145	H	5.903053	9.824830	8.203165
C	7.389582	11.080284	11.030619	H	9.493579	14.835860	13.275545
C	7.633067	12.424591	10.583902	H	10.855309	13.977255	15.090441
N	8.110746	13.333465	11.514430	H	11.109189	11.560830	15.473954
C	6.784486	10.123492	10.156981	H	6.254506	7.883376	15.756091
C	6.401996	10.509192	8.871915	H	5.611499	6.157181	14.132488
C	6.695997	11.788828	8.441279	H	5.739969	6.570125	11.731244
C	7.320295	12.738288	9.245476	H	5.325958	7.615304	9.428580
C	7.160216	9.492735	12.862518	H	6.824700	6.828961	9.980332
C	6.643148	8.530600	11.948815	H	6.853310	14.847107	10.822673
N	6.643449	8.822240	10.594657	H	7.421675	15.037580	12.461900
C	6.123383	7.309788	12.416651	H	8.976359	15.668585	9.909873
C	6.031728	7.089734	13.774815	H	9.760875	15.586528	11.453776
C	6.409613	8.064388	14.702894	H	7.390425	17.442272	10.791693
C	6.945206	9.264004	14.261582	H	9.077786	17.936339	10.914908
N	7.749089	13.929371	8.586862	H	8.217771	17.382609	12.351797
C	9.023404	14.062921	8.052715	H	11.732148	9.429553	14.705615
N	8.956838	15.179289	7.262340	H	10.626162	8.040557	14.860207
C	7.667063	15.695093	7.264940	H	10.509359	9.396004	16.012722
C	6.910171	14.920330	8.070040	H	5.880041	10.005507	16.647001
C	10.079109	15.701495	6.455299	H	7.234671	11.133556	16.910991
C	9.831806	15.472772	4.956613	H	7.530485	9.376065	16.938059
C	11.014635	15.994774	4.126698	H	10.933702	15.096130	6.767033
C	11.319418	17.466575	4.436586	H	9.481939	17.785858	6.553450
C	11.550755	17.685513	5.938003	H	10.575042	17.285093	7.842727
C	10.366475	17.174991	6.774328	H	11.717598	18.745427	6.149247
Se	10.454849	12.952199	8.358351	H	12.461853	17.158843	6.246414
C	6.394409	7.757820	9.614439	H	10.480461	18.090714	4.102995
C	7.740600	14.777330	11.449213	H	12.195043	17.796299	3.870500
C	8.800518	15.782949	10.975520	H	10.800295	15.864352	3.062349
C	8.343604	17.214450	11.277752	H	11.900405	15.385341	4.342341
O	7.232275	10.291892	15.082113	H	8.914471	15.993113	4.652586
C	6.946416	10.178395	16.478218	H	9.674042	14.405924	4.775156

(*aR*)-(*P*)-**4**



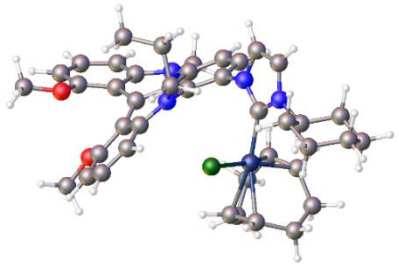
Geometry optimization, B3LYP/6-311G, gas phase**

SCF Done: E(RB3LYP) = -2570.59686179
Zero-point correction= 0.835190 (Hartree/Particle)
Thermal correction to Energy= 0.881827
Thermal correction to Enthalpy= 0.882771
Thermal correction to Gibbs Free Energy= 0.754565
Sum of electronic and zero-point Energies= -2569.761672
Sum of electronic and thermal Energies= -2569.715035
Sum of electronic and thermal Enthalpies= -2569.714091
Sum of electronic and thermal Free Energies= -2569.842297

Cartesian coordinates:

C	6.229828	17.419083	5.931588	H	6.360546	6.412672	14.822734
C	6.472463	15.936531	5.609583	H	6.636864	6.494135	12.397835
C	7.437009	15.752069	4.426775	H	6.313948	7.069887	9.889676
C	6.926566	16.510222	3.190972	H	7.847512	6.737798	10.736938
C	6.677074	17.994737	3.495434	H	6.186432	14.809946	10.044882
C	5.722911	18.167292	4.686838	H	6.782351	15.553366	11.510842
N	6.946444	15.191729	6.797720	H	4.309252	15.170434	11.455340
C	6.344864	14.075304	7.285124	H	4.563990	13.439012	11.371441
N	7.166660	13.677955	8.322107	H	5.572360	13.459334	13.692077
C	8.271439	14.531154	8.435639	H	3.968580	14.192803	13.689101
C	8.123067	15.476457	7.481194	H	5.404237	15.219933	13.748732
C	7.046590	12.460735	9.055633	H	11.543679	11.078843	15.142593
C	7.213737	12.403988	10.450251	H	10.715154	9.557949	15.575430
C	7.284079	11.116799	11.083271	H	10.296617	11.070145	16.426656
C	7.066206	9.925443	10.322225	H	5.552781	10.528252	16.742931
C	6.838746	10.029590	8.944741	H	6.581586	11.981762	16.869175
C	6.864106	11.273304	8.331787	H	7.285523	10.367983	17.165282
C	7.606401	11.024556	12.458556	H	5.517897	15.460261	5.360046
C	7.233212	9.810442	13.129648	H	8.429877	16.134363	4.704083
C	7.055118	8.626476	12.347290	H	7.541099	14.683274	4.216104
N	7.160802	8.705564	10.966976	H	7.646352	16.401251	2.372756
N	7.308663	13.529765	11.273184	H	5.993113	16.045318	2.844905
C	8.064596	13.438208	12.442914	H	7.633753	18.485484	3.723866
C	8.290279	12.157983	13.030634	H	6.270986	18.500967	2.612808
C	6.775065	7.396528	12.976415	H	5.590766	19.228317	4.925333
C	6.597039	7.359082	14.346516	H	4.729410	17.783339	4.415891
C	6.651582	8.519204	15.131401	H	7.167073	17.882048	6.271174
C	6.938538	9.737824	14.533445	H	5.512900	17.509142	6.756735
C	8.615208	14.591586	13.033001	C	3.243404	14.480001	7.346942
C	9.456661	14.463148	14.122972	C	3.503713	13.395759	8.217586
C	9.797316	13.209262	14.648595	C	3.018885	12.778927	5.045857
C	9.239128	12.061660	14.101412	C	3.013962	11.730163	5.947727
C	7.290584	7.479970	10.167591	C	2.122548	14.000584	5.086460
C	6.336228	14.643762	11.108765	C	2.047326	11.594600	7.113961
C	4.981026	14.366480	11.782273	C	1.979651	14.621401	6.496749
C	4.990022	14.304317	13.313180	C	2.615674	12.181302	8.427416
O	9.581344	10.811222	14.477060	H	3.556864	12.623978	4.113387
C	10.595543	10.635659	15.465966	H	3.566710	10.836941	5.666427
O	6.891620	10.917592	15.186202	H	4.152164	13.602191	9.068338
C	6.556498	10.933104	16.574018	H	3.732657	15.422631	7.588538
Rh	4.704882	13.155445	6.476766	H	1.130822	13.759921	4.675674
H	7.857613	7.703154	9.265008	H	2.553755	14.746854	4.410494
H	9.047036	14.375149	9.167039	H	1.130427	14.176703	7.025832
H	8.753996	16.312569	7.227218	H	1.738233	15.684270	6.391537
H	6.762963	11.341255	7.251541	H	1.096084	12.073905	6.865521
H	6.661926	9.155136	8.333489	H	1.817724	10.534651	7.265438
H	8.440283	15.568778	12.603317	H	3.222512	11.414782	8.924456
H	9.905447	15.353061	14.553423	H	1.794572	12.417945	9.122240
H	10.512889	13.146961	15.457659	Cl	6.230016	12.074003	4.939163
H	6.435471	8.457115	16.189496				

(*aS*)-(*P*)-**4**



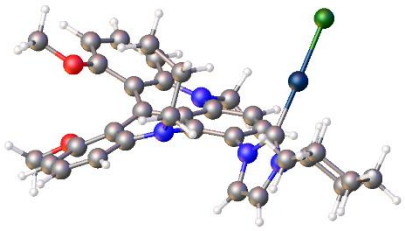
Geometry optimization, B3LYP/6-311G, gas phase**

SCF Done: E(RB3LYP) = -2570.60039343
Zero-point correction= 0.835320 (Hartree/Particle)
Thermal correction to Energy= 0.881861
Thermal correction to Enthalpy= 0.882805
Thermal correction to Gibbs Free Energy= 0.755581
Sum of electronic and zero-point Energies= -2569.765073
Sum of electronic and thermal Energies= -2569.718533
Sum of electronic and thermal Enthalpies= -2569.717589
Sum of electronic and thermal Free Energies= -2569.844812

Cartesian coordinates:

C	9.636595	11.448164	13.798418	H	6.853781	7.811693	8.957479
C	8.614131	11.793097	12.852862	H	4.871021	14.318960	8.212979
C	8.579161	13.128934	12.350137	H	5.853137	16.379540	6.678564
C	9.426070	14.108639	12.898121	H	5.991813	11.743007	7.409546
C	10.336804	13.749000	13.866418	H	5.735166	9.510072	8.358686
C	10.467044	12.425617	14.311647	H	9.454772	15.102018	12.478788
C	7.671946	10.856806	12.324639	H	11.017188	14.500081	14.250106
C	7.198083	11.111362	11.014271	H	11.244664	12.177659	15.019049
C	7.276025	12.439307	10.468710	H	6.474817	8.292864	16.043125
N	7.708066	13.444335	11.313096	H	5.908602	6.382565	14.607917
C	6.647817	10.038188	10.249371	H	5.927110	6.575349	12.176670
C	6.187557	10.287248	8.955387	H	5.352079	7.380436	9.811002
C	6.311595	11.561387	8.428873	H	6.924312	6.748385	10.355512
C	6.858941	12.631765	9.133317	H	7.350190	15.259051	10.279046
C	7.160148	9.683493	12.981614	H	7.604062	15.410808	11.989223
C	6.688701	8.607145	12.177652	H	5.243597	15.810787	11.327281
N	6.628745	8.772495	10.801820	H	5.088118	14.153299	10.791903
C	6.276952	7.402232	12.774889	H	5.562230	13.349711	13.159611
C	6.246756	7.305187	14.151104	H	4.152255	14.405630	13.087582
C	6.581155	8.385699	14.972511	H	5.691993	15.032004	13.679936
C	7.010256	9.574083	14.402271	H	11.795338	9.966768	14.520797
N	6.985957	13.860744	8.410419	H	10.725806	8.619891	14.989494
C	8.159087	14.400475	7.928036	H	10.714033	10.130056	15.936967
N	7.750855	15.469587	7.196435	H	6.000185	10.461386	16.767151
C	6.367969	15.593363	7.201668	H	7.277464	11.701639	16.851078
C	5.880344	14.584666	7.952692	H	7.706376	9.979195	17.016352
C	8.664192	16.405977	6.500592	H	9.661482	16.010528	6.708607
C	8.424163	16.395683	4.984001	H	7.539689	18.194130	6.981058
C	9.393852	17.354734	4.275887	H	8.792330	17.775067	8.158222
C	9.308761	18.774222	4.853395	H	9.416812	19.782550	6.776065
C	9.532355	18.773293	6.371471	H	10.562764	18.468783	6.590274
C	8.565874	17.820146	7.090587	H	8.320575	19.196662	4.630671
Rh	10.111145	13.883300	8.274524	H	10.040757	19.422699	4.363649
Cl	10.201319	15.726579	9.853894	H	9.181085	17.363582	3.203142
C	6.414732	7.610363	9.931785	H	10.418289	16.978063	4.386119
C	7.110220	14.808059	11.235141	H	7.393287	16.704790	4.770648
C	5.601940	14.793527	11.515443	H	8.537634	15.377659	4.598798
C	5.233935	14.369336	12.940262	H	12.550245	14.959629	8.553204
O	7.245146	10.695536	15.107326	H	12.021384	13.225139	10.072336
C	7.040529	10.692497	16.522399	H	8.853899	11.654669	7.416743
O	9.762491	10.133519	14.075791	H	9.624800	13.135827	5.729608
C	10.818519	9.702308	14.935432	H	13.764210	13.515708	6.575247
C	10.369643	12.785603	6.438699	H	12.632689	14.794569	6.199368
C	11.804128	12.814189	5.915020	H	12.227419	11.806910	5.954990
C	12.710808	13.811939	6.672218	H	11.789053	13.086193	4.856596
C	12.349728	13.979843	8.132587	H	12.870115	11.311380	7.916794
C	12.051326	12.965648	9.018607	H	12.447370	10.934054	9.566072
C	12.111883	11.484962	8.683275	H	10.173697	10.622696	9.107103
C	10.747954	10.922560	8.224158	H	10.896194	10.006865	7.633297
C	9.906833	11.920563	7.451865				

(*aR*)-(*P*)-**5**



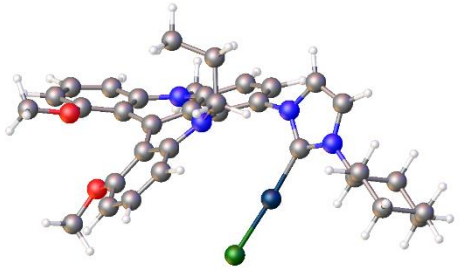
Geometry optimization, B3LYP/6-311G, gas phase**

SCF Done: E(RB3LYP) = -2283.65094456
Zero-point correction= 0.653123 (Hartree/Particle)
Thermal correction to Energy= 0.692030
Thermal correction to Enthalpy= 0.692975
Thermal correction to Gibbs Free Energy= 0.579075
Sum of electronic and zero-point Energies= -2282.997821
Sum of electronic and thermal Energies= -2282.958914
Sum of electronic and thermal Enthalpies= -2282.957970
Sum of electronic and thermal Free Energies= -2283.071869

Cartesian coordinates:

C	6.390084	17.734871	6.530990	Au	4.580200	13.615655	7.257495
C	6.396468	16.301277	5.983199	H	7.765287	7.662249	9.026707
C	7.022117	16.221349	4.583086	H	9.524632	14.119794	8.674631
C	6.300001	17.173060	3.616460	H	9.041336	16.246773	6.994175
C	6.278781	18.612236	4.148344	H	6.882326	11.440341	7.133082
C	5.670044	18.679987	5.555741	H	6.677362	9.228533	8.132992
N	7.063338	15.365704	6.921860	H	8.856462	15.363145	12.594534
C	6.466596	14.283204	7.473700	H	10.214416	14.998542	14.592036
N	7.438700	13.704292	8.248662	H	10.612404	12.740541	15.469386
C	8.630088	14.421540	8.158731	H	6.165580	8.355291	15.915354
C	8.386793	15.462320	7.330567	H	6.006841	6.358085	14.496515
C	7.286814	12.470531	8.953934	H	6.399905	6.473174	12.095038
C	7.453899	12.366896	10.342904	H	6.168260	7.142160	9.617102
C	7.427894	11.059981	10.934260	H	7.657883	6.665406	10.469436
C	7.141547	9.911093	10.137431	H	7.040438	15.172076	10.069318
C	6.929914	10.067195	8.763096	H	7.039459	15.363964	11.809042
C	7.020909	11.324876	8.200066	H	4.767132	15.345473	10.832539
C	7.689866	10.908485	12.316343	H	4.981649	13.714324	10.261212
C	7.203059	9.712097	12.937488	H	5.244303	12.920584	12.679403
C	6.969933	8.566498	12.118124	H	3.701472	13.722520	12.398891
N	7.129393	8.673925	10.745893	H	5.004039	14.584470	13.222209
N	7.602824	13.455232	11.194032	H	11.495581	10.596207	15.154978
C	8.312198	13.278245	12.380588	H	10.528503	9.142950	15.514764
C	8.422862	11.974483	12.943067	H	10.195353	10.663363	16.383824
C	6.576296	7.348207	12.700636	H	5.377748	10.490626	16.447721
C	6.333534	7.293156	14.057164	H	6.503977	11.852857	16.677557
C	6.436300	8.425330	14.872314	H	7.056179	10.187517	16.994661
C	6.841257	9.630566	14.323998	H	5.366934	15.939761	5.929622
C	8.930186	14.370670	13.013490	H	8.083411	16.494127	4.638214
C	9.714854	14.156370	14.127765	H	6.972473	15.191134	4.219143
C	9.936770	12.872382	14.637337	H	6.784600	17.133242	2.637362
C	9.318792	11.783584	14.044560	H	5.271599	16.822888	3.468545
C	7.170376	7.462527	9.914446	H	7.302654	19.006452	4.175360
C	6.773464	14.684886	11.003918	H	5.716666	19.255713	3.466295
C	5.267702	14.399494	11.064143	H	5.711559	19.701756	5.942518
C	4.782032	13.876386	12.418003	H	4.608755	18.408600	5.508803
O	9.550492	10.506214	14.400748	H	7.421522	18.080772	6.673166
C	10.503804	10.226824	15.429559	H	5.905059	17.750936	7.511605
O	6.855231	10.790860	15.003167	Cl	2.423452	12.796864	7.061038
C	6.418516	10.814755	16.365466				

(*aS*)-(*P*)-**5**



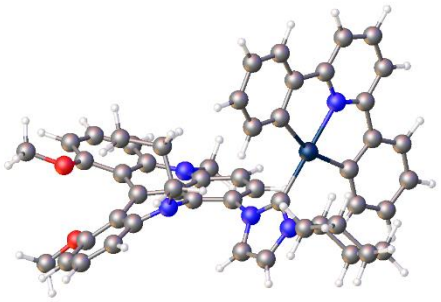
Geometry optimization, B3LYP/6-311G, gas phase**

SCF Done: E(RB3LYP) = -2283.65329035
Zero-point correction= 0.653118 (Hartree/Particle)
Thermal correction to Energy= 0.692000
Thermal correction to Enthalpy= 0.692944
Thermal correction to Gibbs Free Energy= 0.579615
Sum of electronic and zero-point Energies= -2283.000172
Sum of electronic and thermal Energies= -2282.961291
Sum of electronic and thermal Enthalpies= -2282.960346
Sum of electronic and thermal Free Energies= -2283.073675

Cartesian coordinates:

C	5.705279	17.188865	6.429845	Au	5.566847	12.787256	6.334325
C	6.589975	16.085501	5.831291	H	4.840397	10.063852	12.156259
C	7.619956	16.645902	4.841131	H	9.186451	14.731715	9.464313
C	6.917817	17.448726	3.733404	H	8.600300	16.766786	7.708161
C	6.027269	18.555949	4.313608	H	6.859857	13.550719	10.720082
C	5.013206	17.989431	5.316040	H	6.300495	11.585612	12.052810
N	7.236502	15.288276	6.902459	H	8.701743	10.731196	4.589570
C	6.902911	14.013230	7.208587	H	7.908668	8.840334	3.276239
N	7.697506	13.689079	8.280056	H	6.691721	6.982209	4.316266
C	8.492556	14.773225	8.643078	H	8.303840	4.344357	9.764102
C	8.202732	15.769741	7.775623	H	7.063049	4.613281	11.865581
C	7.561108	12.471631	9.021663	H	6.184329	6.782017	12.550905
C	7.795683	11.205195	8.455016	H	6.020430	9.258561	13.220306
C	7.354579	10.048548	9.174438	H	4.799635	8.316640	12.329941
C	6.800997	10.178785	10.482617	H	9.185033	12.864139	6.564425
C	6.683072	11.451804	11.052693	H	9.967058	11.437671	5.914951
C	7.033823	12.563417	10.308818	H	11.401861	12.695583	7.485932
C	7.425038	8.771430	8.564099	H	10.306708	12.354356	8.805618
C	7.384692	7.635670	9.441810	H	10.715989	9.862424	8.493262
C	6.783941	7.789281	10.725837	H	12.204553	10.743411	8.833006
N	6.348410	9.044959	11.123126	H	11.840580	10.234966	7.183282
N	8.442030	10.995619	7.250070	H	4.759376	6.372328	5.527050
C	8.092151	9.884102	6.487381	H	4.892695	5.274115	6.925274
C	7.508778	8.755379	7.135106	H	6.102140	5.188881	5.619000
C	6.641287	6.680566	11.578990	H	10.126756	4.830048	8.420904
C	7.159087	5.460216	11.196501	H	9.938327	5.359264	6.729314
C	7.855651	5.299272	9.995014	H	8.691222	4.326560	7.475523
C	7.995348	6.375321	9.133403	H	5.952345	15.367891	5.309679
C	8.283125	9.875921	5.097033	H	8.323792	17.301797	5.367813
C	7.805607	8.815963	4.354483	H	8.202806	15.825266	4.412001
C	7.120209	7.749334	4.943879	H	7.668649	17.872790	3.061338
C	6.949426	7.719375	6.316503	H	6.306666	16.768682	3.128127
C	5.459395	9.179242	12.284905	H	6.655306	19.303926	4.813953
C	9.560910	11.875530	6.822081	H	5.506430	19.078145	3.506573
C	10.687026	11.955931	7.861010	H	4.422558	18.794868	5.760396
C	11.399059	10.622740	8.105625	H	4.304597	17.337840	4.791267
O	6.217729	6.791375	6.959025	H	6.322937	17.864025	7.035170
C	5.451906	5.854017	6.194701	H	4.966215	16.739639	7.099239
O	8.744694	6.342926	8.018057	Cl	4.090336	11.272309	5.374271
C	9.410039	5.131504	7.652085				

(*aR*)-(*P*)-**6**



Geometry optimization, B3LYP/6-311G, gas phase**

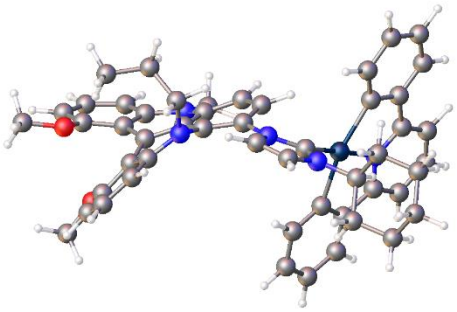
SCF Done: E(RB3LYP) = -2532.44697213
Zero-point correction= 0.881867 (Hartree/Particle)
Thermal correction to Energy= 0.932351
Thermal correction to Enthalpy= 0.933295
Thermal correction to Gibbs Free Energy= 0.796156
Sum of electronic and zero-point Energies= -2531.565106
Sum of electronic and thermal Energies= -2531.514621
Sum of electronic and thermal Enthalpies= -2531.513677
Sum of electronic and thermal Free Energies= -2531.650816

Cartesian coordinates:

C	2.889096	1.358985	-4.423248	C	-3.763945	-3.609087	-1.944496
C	3.009564	1.126217	-3.046168	C	0.626215	1.623755	-2.491372
C	4.290916	1.156972	-2.424643	C	0.569325	2.912415	-1.657136
C	5.451329	1.230908	-3.264017	C	1.596155	3.984673	-2.030006
C	5.308494	1.428650	-4.629027	C	5.045189	-0.964628	2.670266
C	4.030161	1.517316	-5.186921	O	5.763374	3.416371	-1.502724
N	1.878485	0.846441	-2.270894	C	6.444152	4.635981	-1.829371
C	2.045864	0.147864	-1.080710	O	6.632055	1.040187	-2.654654
C	3.287347	0.308566	-0.386282	C	7.831901	0.987274	-3.439280
C	4.344956	1.036038	-0.994092	H	4.592380	-1.943235	2.533942
C	3.481694	-0.280389	0.897077	H	0.992773	-1.743938	-3.068206
C	2.454366	-1.059057	1.448490	H	-1.518526	-2.559396	-3.843113
C	1.298850	-1.281305	0.726463	H	0.549604	-1.942858	1.138323
C	1.071469	-0.703132	-0.525062	H	2.552073	-1.505878	2.425925
C	5.352770	1.552111	-0.120748	H	1.922220	1.353008	-4.904265
C	5.544685	0.919901	1.147467	H	3.933947	1.665933	-6.255966
N	4.692279	-0.107116	1.527608	H	6.173767	1.490559	-5.272316
C	6.585346	1.334608	1.994400	H	7.731872	4.002983	0.237013
C	7.368791	2.410612	1.628053	H	8.156653	2.739625	2.295169
C	7.138334	3.125989	0.448825	H	6.747640	0.864801	2.951770
C	6.129908	2.725804	-0.411397	H	4.709949	-0.534091	3.617473
N	-0.073063	-1.137686	-1.282616	H	6.123354	-1.099234	2.694333
C	-1.376151	-1.220480	-0.874071	H	-0.222339	0.990649	-2.249727
N	-2.051557	-1.793377	-1.890588	H	0.557210	1.855514	-3.551486
C	-1.186876	-2.086573	-2.935819	H	-0.439754	3.316179	-1.785275
C	0.046650	-1.687049	-2.560715	H	0.652374	2.655814	-0.595763
Au	-2.196050	-0.688818	0.914715	H	2.623601	3.659166	-1.853617
C	-1.884653	-2.494375	1.978980	H	1.431617	4.884042	-1.432690
C	-2.356017	-2.377486	3.315407	H	1.511060	4.268811	-3.082595
C	-2.279820	-3.470127	4.186251	H	7.783874	0.175090	-4.168788
C	-1.751355	-4.680978	3.748908	H	8.632353	0.794430	-2.729357
C	-1.300082	-4.807200	2.438797	H	8.011277	1.938130	-3.947811
C	-1.368335	-3.717763	1.562872	H	6.324760	5.373466	-1.031925
C	-2.947115	-1.087722	3.712299	H	5.968123	4.997045	-2.737551
N	-2.992576	-0.168269	2.717007	H	7.505319	4.453642	-2.016635
C	-3.517900	1.075934	2.833960	H	-3.885930	-1.700477	-0.957006
C	-4.035968	1.453684	4.072325	H	-3.319841	-4.030322	-2.854254
C	-4.001032	0.543587	5.125256	H	-3.273320	-4.088191	-1.092788
C	-3.462599	-0.729417	4.957455	H	-5.431915	-4.979150	-2.003461
C	-3.485796	1.861611	1.588773	H	-5.694551	-3.587090	-0.970759
C	-4.050517	3.137807	1.489404	H	-5.671302	-3.583822	-4.035854
C	-4.053156	3.811051	0.271632	H	-7.075045	-3.358969	-3.009618
C	-3.496729	3.209324	-0.852774	H	-6.199906	-1.168707	-3.888911
C	-2.918978	1.938110	-0.758228	H	-6.171333	-1.229669	-2.137079
C	-2.893857	1.250532	0.449454	H	-3.794358	-1.687289	-4.012271
C	-3.511828	-2.094755	-1.904906	H	-4.041481	-0.285225	-2.971278
C	-4.217365	-1.361563	-3.054512	H	-3.448156	-1.430986	5.779465
C	-5.724696	-1.664938	-3.039221	H	-4.403788	0.828881	6.089961
C	-6.000027	-3.173819	-3.072993	H	-4.462658	2.436907	4.211350
C	-5.273484	-3.900287	-1.933898	H	-1.015222	-3.848863	0.545137

H	-0.899957	-5.753676	2.092845	H	-4.500171	4.794988	0.199922
H	-1.701681	-5.524168	4.426947	H	-4.504120	3.608691	2.353706
H	-2.500668	1.487817	-1.651503	H	-2.640375	-3.389466	5.205146
H	-3.517498	3.724727	-1.806744				

TS-**6**



Geometry optimization, B3LYP/6-311G, gas phase**

SCF Done: E(RB3LYP) = -2532.42649571

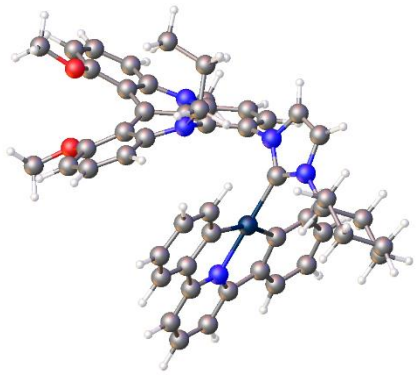
Zero-point correction=	0.881091 (Hartree/Particle)
Thermal correction to Energy=	0.930780
Thermal correction to Enthalpy=	0.931724
Thermal correction to Gibbs Free Energy=	0.797269
Sum of electronic and zero-point Energies=	-2531.545405
Sum of electronic and thermal Energies=	-2531.495716
Sum of electronic and thermal Enthalpies=	-2531.494772
Sum of electronic and thermal Free Energies=	-2531.629226

Cartesian coordinates:

C	0.101750	-0.784015	0.149775	C	-7.243525	1.112809	5.158227
C	-0.058263	-0.308344	1.456786	C	-6.798777	0.053387	5.953021
C	1.000407	-0.418705	2.393536	C	-7.058992	-2.348716	2.717583
C	2.118566	-1.246948	2.049508	C	-8.272541	-1.631744	2.138506
C	2.243321	-1.750152	0.778841	C	-9.548790	-2.485868	2.311364
C	1.240703	-1.495649	-0.173910	C	-9.372392	-3.870625	1.685687
N	-1.277045	0.314928	1.839152	C	-8.125945	-4.592276	2.259396
C	-1.578996	0.282812	3.206438	C	-6.862499	-3.752288	2.088107
C	-0.496867	0.424200	4.126679	C	-1.737425	1.504812	1.053759
C	0.831534	0.262916	3.666609	C	-0.904983	2.791830	1.266047
C	-0.763434	0.692448	5.492904	C	0.443828	2.876562	0.581583
C	-2.089479	0.866848	5.899369	C	0.047818	0.740735	7.812176
C	-3.131444	0.611097	5.014096	O	3.302972	1.218853	2.682441
C	-2.895253	0.189496	3.688467	C	4.546007	1.662442	2.100606
C	1.870420	0.781699	4.497761	O	2.988963	-1.514094	3.054050
C	1.582788	0.996071	5.883498	C	4.061641	-2.427649	2.836686
N	0.295519	0.796624	6.359213	H	-0.858986	0.181265	7.995383
C	2.617934	1.386150	6.771550	H	-3.460074	-0.054620	0.868039
C	3.868868	1.664315	6.269737	H	-5.726138	-1.439050	0.388961
C	4.152670	1.585797	4.891751	H	-4.139501	0.753091	5.369796
C	3.156711	1.189791	4.016824	H	-2.334685	1.228212	6.891574
N	-4.002898	-0.377260	2.956992	H	-0.688245	-0.652984	-0.574369
C	-5.042511	-1.074922	3.555378	H	1.359820	-1.887449	-1.173749
N	-5.812862	-1.530041	2.565227	H	3.079001	-2.364631	0.496806
C	-5.280344	-1.181366	1.330133	H	5.127856	1.890142	4.544680
C	-4.144001	-0.463145	1.567853	H	4.656937	1.983530	6.941319
Au	-5.435848	-1.495732	5.526455	H	2.409664	1.541608	7.833194
C	-4.254778	-3.241927	5.755539	H	-0.047345	1.741294	8.240570
C	-4.421513	-3.795086	7.053922	H	0.877294	0.225366	8.315161
C	-3.745152	-4.977651	7.408720	H	-2.751084	1.720403	1.373516
C	-2.886903	-5.596762	6.493387	H	-1.748006	1.232768	0.007774
C	-2.721107	-5.059098	5.221347	H	-1.537057	3.610210	0.886843
C	-3.392487	-3.876839	4.858396	H	-0.812701	2.983443	2.345545
C	-5.349213	-3.100713	7.971989	H	1.177222	2.164407	0.975254
N	-5.907658	-1.977858	7.434633	H	0.863020	3.878309	0.681432
C	-6.818106	-1.189816	8.076538	H	0.364962	2.676109	-0.495599
C	-7.164325	-1.542801	9.373200	H	3.700647	-3.409265	2.539491
C	-6.611785	-2.661633	9.967205	H	4.585162	-2.511325	3.792911
C	-5.705851	-3.469394	9.267729	H	4.751900	-2.037919	2.060632
C	-7.302918	-0.051791	7.263221	H	4.760293	2.689855	2.387952
C	-8.206624	0.876490	7.773198	H	4.420047	1.602751	1.026807
C	-8.637299	1.928184	6.960216	H	5.386587	0.995905	2.413162
C	-8.147140	2.058178	5.656213	H	-7.183920	-2.468113	3.791819

H	-6.630737	-3.643507	1.027528	H	-6.886906	-2.953436	10.972859
H	-6.000080	-4.250250	2.549960	H	-7.894160	-0.932361	9.932259
H	-7.991884	-5.565102	1.783373	H	-3.242148	-3.476856	3.860601
H	-8.293583	-4.808971	3.324986	H	-2.077890	-5.535811	4.518268
H	-9.262126	-3.792570	0.600049	H	-2.382833	-6.493844	6.783523
H	-10.272542	-4.477211	1.870698	H	-6.866901	1.244898	4.131846
H	-10.380907	-1.965613	1.859415	H	-8.498346	2.876963	5.027503
H	-9.766183	-2.565205	3.370930	H	-9.359332	2.654292	7.332798
H	-8.123381	-1.424274	1.072638	H	-8.609156	0.799061	8.769218
H	-8.405592	-0.660397	2.626234	H	-3.876884	-5.393109	8.394562
H	-5.281014	-4.335417	9.731127				

(*aS*)-(*P*)-**6**



Geometry optimization, B3LYP/6-311G, gas phase**

SCF Done: E(RB3LYP) = -2532.44612423

Zero-point correction=	0.881488	(Hartree/Particle)
Thermal correction to Energy=	0.932072	
Thermal correction to Enthalpy=	0.933016	
Thermal correction to Gibbs Free Energy=	0.795196	
Sum of electronic and zero-point Energies=	-2531.564637	
Sum of electronic and thermal Energies=	-2531.514053	
Sum of electronic and thermal Enthalpies=	-2531.513109	
Sum of electronic and thermal Free Energies=	-2531.650928	

Cartesian coordinates:

C	2.959025	-1.659775	-1.677179	N	-1.239734	-2.081933	1.748071
C	2.775119	-0.325263	-1.285903	C	-1.578596	-1.596332	2.967276
C	3.679106	0.278675	-0.366186	C	-1.347528	-2.405094	4.080237
C	4.659157	-0.552067	0.272229	C	-0.791650	-3.667602	3.894110
C	4.811970	-1.872134	-0.119974	C	-0.468426	-4.130702	2.620948
C	3.973923	-2.401853	-1.105601	C	-2.184357	-0.254560	2.933589
N	1.701904	0.421311	-1.784456	C	-2.656040	0.387649	4.083890
C	1.242865	1.504721	-1.052143	C	-3.274192	1.630660	3.989290
C	2.186521	2.182209	-0.206942	C	-3.429596	2.234182	2.744843
C	3.503765	1.671438	-0.069317	C	-2.952759	1.602258	1.591201
C	1.822027	3.373031	0.489281	C	-2.320740	0.366171	1.661546
C	0.519359	3.872490	0.357828	C	-3.991962	-0.782161	-2.312344
C	-0.387093	3.191257	-0.425807	C	-5.281848	-0.135096	-1.784528
C	-0.066720	2.018735	-1.115377	C	-6.412593	-1.173277	-1.704375
C	4.511945	2.593175	0.357656	C	-6.633910	-1.876084	-3.049805
C	4.110626	3.742157	1.105245	C	-5.334738	-2.500694	-3.575237
N	2.756815	3.983522	1.292970	C	-4.204558	-1.461809	-3.671381
C	5.074094	4.616203	1.634123	C	1.274917	0.234843	-3.200181
C	6.408070	4.404586	1.347789	C	1.702239	1.397484	-4.107180
C	6.829280	3.361701	0.516905	C	3.217304	1.537129	-4.278213
C	5.899064	2.474210	0.002260	C	2.322324	4.990510	2.273925
N	-1.148806	1.411503	-1.848414	O	6.195699	1.516021	-0.890020
C	-1.883919	0.325024	-1.469197	C	7.540079	1.394789	-1.376211
N	-2.885822	0.218536	-2.365369	O	5.341531	0.012135	1.282434
C	-2.805584	1.246162	-3.295657	C	6.286598	-0.771922	2.021191
C	-1.725798	1.993109	-2.976928	H	1.329864	4.731053	2.633481
Au	-1.569700	-0.881599	0.133458	H	-1.309117	2.868921	-3.442578
C	-0.801310	-2.594860	-0.844471	H	-3.515010	1.358273	-4.095985
C	-0.469949	-3.606743	0.097730	H	-1.397327	3.571807	-0.510491
C	0.020967	-4.842549	-0.338232	H	0.216514	4.788639	0.840541
C	0.177223	-5.096055	-1.697698	H	2.270168	-2.138049	-2.356234
C	-0.160692	-4.116765	-2.627651	H	4.092461	-3.439973	-1.392499
C	-0.643570	-2.875494	-2.197853	H	5.552053	-2.505662	0.346292
C	-0.706459	-3.307101	1.521390	H	7.874920	3.277449	0.260489

H	7.146491	5.094526	1.738591
H	4.787291	5.483012	2.208564
H	2.305916	5.994806	1.842496
H	2.998711	4.972732	3.124439
H	0.200695	0.080873	-3.243563
H	1.740622	-0.679645	-3.553553
H	1.236592	1.219004	-5.082205
H	1.279596	2.336800	-3.735974
H	3.721878	1.735095	-3.329100
H	3.451061	2.362472	-4.953412
H	3.651754	0.628737	-4.704317
H	5.796179	-1.621565	2.503247
H	6.687312	-0.103056	2.778876
H	7.095571	-1.124226	1.375797
H	7.854834	2.311662	-1.880571
H	7.515527	0.574179	-2.088818
H	8.231652	1.157170	-0.563900
H	-3.650503	-1.534624	-1.597473
H	-4.476175	-0.713337	-4.424511
H	-3.275491	-1.933878	-4.003399
H	-5.495059	-2.948095	-4.559132
H	-5.021927	-3.315671	-2.911353
H	-7.012424	-1.152178	-3.781720
H	-7.404156	-2.644552	-2.948988
H	-7.329977	-0.680978	-1.372653
H	-6.166120	-1.917579	-0.937301
H	-5.578701	0.678498	-2.457463
H	-5.097425	0.309543	-0.802277
H	-0.048289	-5.117467	2.486903
H	-0.614390	-4.303658	4.753395
H	-1.604692	-2.059962	5.071649
H	-0.908300	-2.134893	-2.944153
H	-0.059523	-4.320561	-3.688116
H	0.544799	-6.059838	-2.028545
H	-3.099728	2.086941	0.632644
H	-3.930721	3.192784	2.668168
H	-3.646076	2.117620	4.882482
H	-2.559063	-0.080768	5.056452
H	0.268946	-5.620220	0.374855

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