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Supporting Information

A Synthetic Cycle for Heteroarene Synthesis by Nitride Insertion

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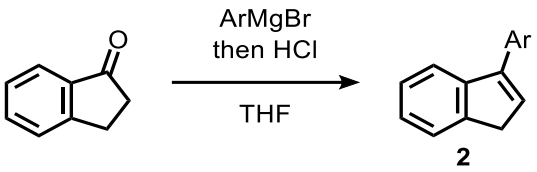
Contents

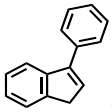
1. General Procedures

Unless noted otherwise, reactions were performed without precaution to exclude air and water. Unless otherwise noted, all reagents were used as received. [*cis*-(terpy)$OsNCl_2$]PF_6 (**1**)[1] was synthesized according to literature methods. Solvents were degassed and dried using a PPT Solvent Purification System. Reaction temperatures are reported as the temperature of the bath surrounding the flasks or vials.

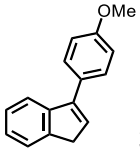
High resolution mass spectra were recorded on an Agilent 6224 TOF High Resolution Accurate MS with electrospray ionization. All mass spectra were processed with an Agilent MassHunter Operating System. Nuclear magnetic resonance spectra (1H-NMR, 13C-NMR and 19F-NMR) were recorded with Bruker spectrometers operating at 400 or 500 MHz for 1H. Chemical shifts are reported in parts per million (ppm, δ), downfield from tetramethylsilane (TMS, δ=0.00 ppm) and are referenced to residual solvent.[2] Coupling constants were reported in Hertz (Hz). Data for 1H-NMR spectra were reported as follows: chemical shift (ppm, s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, dd = doublet of doublets, td = triplet of doublets, ddd = doublet of doublet of doublets, m = multiplet, coupling constant (Hz), and integration).

2. Synthesis of indenes (2)

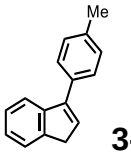




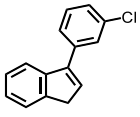
3-phenyl-1H-indene (2a): A solution of PhMgBr (13.3 mL; 3 M in Et_2O; 40 mmol) was transferred into a flame-dried round bottom flask under N_2 and cooled to 0 °C. The Grignard was diluted with 20 mL of THF. 1-indanone (2.64 g; 20 mmol) was added dropwise in THF (10 mL). The solution was allowed to warm to room temperature and stirred overnight. The reaction was quenched with HCl (15%; 9.2 mL conc. HCl + 15.8 mL H_2O) at 0 °C. The solution was allowed to warm to room temperature and stirred for 2 h. The organic layer was separated, and the aqueous layer extracted with Et_2O (3x20 mL). The organic layers were combined and washed with saturated $NaHCO_3$ (15 mL), H_2O (15 mL), and brine (15 mL). The organic layer was then dried over Na_2SO_4 and purified via column chromatography (hexanes). Clear liquid (1.4 g; 38%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.63 (ddt, *J* = 7.5, 6.1, 2.5 Hz, 3H), 7.56 (dd, *J* = 6.7, 2.5 Hz, 1H), 7.52 – 7.44 (m, 2H), 7.44 – 7.23 (m, 3H), 6.61 (q, *J* = 2.5 Hz, 1H), 3.53 (d, *J* = 2.4 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 145.34, 144.90, 144.04, 136.29, 131.07, 128.70, 127.85, 127.70, 126.29, 124.99, 124.25, 120.45, 38.31. NMR is in alignment with reported data.[3,4]



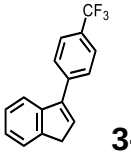
3-(4-methoxyphenyl)-1H-indene (2b): a flame dry flask was charged with Mg turnings (219 mg; 9 mmol) and purged with N_2. THF (1 mL) and dibromoethane (2 drops) were added and the mixture was stirred for 10 minutes. 4-bromoanisole (935 µL; 7.5 mmol) was added dropwise in THF (7 mL). At the conclusion of the addition, the reaction was heated to reflux using a heat gun, then allowed to cool to room temperature and stirred for 3 hours. 1-indanone (528 mg; 4 mmol) was added dropwise in THF (2.5 mL). The reaction was stirred at room temperature overnight. The reaction was quenched with HCl (15%; 9.2 mL conc. HCl + 15.8 mL H_2O) at 0 °C. The solution was allowed to warm to room temperature and stirred for 2 h. The organic layer was separated, and the aqueous layer extracted with Et_2O (3x20 mL). The organic layers were combined and washed with saturated $NaHCO_3$ (15 mL), H_2O (15 mL), and brine (15 mL). The organic layer was then dried over Na_2SO_4 and purified via column chromatography (1-5% Et_2O/hexanes). White solid (290 mg; 33%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.67 – 7.61 (m, 1H), 7.61 – 7.53 (m, 3H), 7.41 – 7.25 (m, 2H), 7.08 – 6.99 (m, 2H), 6.55 (q, *J* = 2.3 Hz, 1H), 3.89 (d, *J* = 1.5 Hz, 3H), 3.53 (d, *J* = 2.2 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 159.29, 144.94, 144.75, 144.26, 129.98, 128.94, 128.83, 126.24, 124.87, 124.20, 120.39, 114.12, 55.43, 38.19. NMR matches reported data.[4]



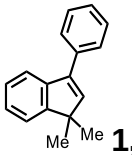
3-(*p*-tolyl)-1H-indene (2c): Synthesized using the same method as **2a** with *p*-tolylmagnesium bromide (1M in THF) instead of phenylmagnesium bromide. Low-melting white solid (831 mg; 76%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.5 Hz, 1H), 7.62 – 7.52 (m, 3H), 7.39 (td, *J* = 7.5, 1.3 Hz, 1H), 7.36 – 7.28 (m, 3H), 6.58 (t, *J* = 2.2 Hz, 1H), 3.50 (d, *J* = 2.4 Hz, 2H), 2.46 (d, *J* = 2.2 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 145.14, 144.86, 144.10, 137.26, 133.34, 130.40, 129.33, 127.65, 126.20, 124.86, 124.14, 120.41, 38.14, 21.31. NMR matches reported data.[5]



3-(3-chlorophenyl)-1H-indene (2d): Synthesized using the same method as **2b** using 1-bromo-3-chlorobenzene instead of 4-bromoanisole. Clear liquid (750 mg; 66%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (dt, *J* = 2.5, 1.1 Hz, 1H), 7.62 (ddt, *J* = 11.5, 7.3, 0.9 Hz, 2H), 7.58 – 7.52 (m, 1H), 7.46 – 7.38 (m, 3H), 7.35 (td, *J* = 7.4, 1.3 Hz, 1H), 6.66 (t, *J* = 2.2 Hz, 1H), 3.57 (d, *J* = 2.3 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 144.72, 144.07, 143.44, 138.04, 134.57, 131.97, 129.93, 127.87, 127.73, 126.39, 125.93, 125.22, 124.31, 120.21, 38.33. NMR matches reported data.[6]

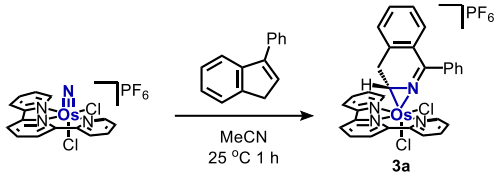


3-(4-(trifluoromethyl)phenyl)-1H-indene (2e): Synthesized using the same method as **2b** using 4-bromobenzotrifluoride instead of 4-bromoanisole. White solid (358 mg; 34%) **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.85 – 7.77 (m, 4H), 7.67 (dt, *J* = 7.8, 1.6 Hz, 2H), 7.46 (td, *J* = 7.5, 1.4 Hz, 1H), 7.41 (td, *J* = 7.4, 1.3 Hz, 1H), 6.74 (t, *J* = 2.3 Hz, 1H), 3.62 (d, *J* = 2.3 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 144.78, 144.22, 143.34, 139.87 (t, *J* = 1.5 Hz), 132.62, 129.73 (q, *J* = 32.4 Hz), 128.07, 126.47, 125.83, 125.66 (q, *J* = 3.8 Hz), 124.48 (q, J=271.7 Hz), 124.43, 120.20, 38.43. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.25. NMR matches reported data.[5]



1,1-dimethyl-3-phenylindene (2f): Synthesized using the same method as **2a** with 3,3-dimethyl-1-indanone as starting material. White low-melting solid (178 mg; 80%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.64 – 7.55 (m, 2H), 7.55 – 7.46 (m, 1H), 7.49 – 7.40 (m, 2H), 7.44 – 7.32 (m, 2H), 7.36 – 7.19 (m, 2H), 6.42 (s, 1H), 1.40 (d, *J* = 0.7 Hz, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.57, 144.14, 141.92, 141.01, 136.07, 128.66, 127.80, 127.66, 126.50, 125.49, 121.64, 120.75, 48.49, 24.85. NMR matches reported data.[7]

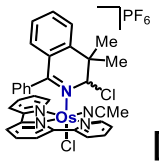
3. Reaction of [*cis*-(terpy)OsNCl$_2$]PF$_6$ with indenes



***Cis*-[(terpy)OsCl$_2$(η^2(C,N)-1-phenyl-4-hydroisoquinoline)] (3a).** An oven dried Schlenk tube was charged with **1** (130 mg; 0.2 mmol) and evacuated and backfilled with N_2 three times on a Schlenk line. A solution of **2a** (184 mg, 0.96 mmol) in MeCN (6 mL) was added, and the solution stirred for 2 hours at room temperature. After this time, the solvent was evaporated under vacuum. The residue was taken up in CH_2Cl_2 (3 mL) and the product was precipitated by addition of Et_2O (19 mL). The product was washed with copious Et_2O and dried to yield a very dark red solid (131 mg; 77%). **^{1}H NMR** (400 MHz, CD_3CN) δ 9.25 – 9.19 (m, 1H), 8.97 – 8.91 (m, 1H), 8.50 (d, *J* = 8.3 Hz, 1H), 8.39 (dd, *J* = 8.2, 0.9 Hz, 1H), 8.35 – 8.21 (m, 5H), 8.00 – 7.90 (m, 2H), 7.57 (ddd, *J* = 7.5, 5.6, 1.4 Hz, 1H), 7.54 – 7.44 (m, 3H), 7.31 (d, *J* = 7.6 Hz, 2H), 7.19 (t, *J* = 7.6 Hz, 2H), 6.84 (d, *J* = 7.7 Hz, 1H), 6.25 (dd, *J* = 10.9, 6.2 Hz, 1H), 3.04 (dd, *J* = 16.1, 6.2 Hz, 1H), 2.94 (dd, *J* = 16.1, 10.9 Hz, 1H). **HSQC** (^{13}C, 101 MHz, CD_3CN) δ 153.94, 153.67, 142.60, 142.33, 139.52, 135.21, 135.12, 131.61, 130.29, 130.20, 130.02, 129.15, 128.35, 128.18, 125.89, 125.72, 125.01, 124.75, 42.90, 30.51 **^{31}P NMR** (162 MHz, CD_3CN) δ -145 (hept, J=707 Hz). **^{19}F NMR** (376 MHz, CD_3CN) δ -65 (d, *J* = 706.2 Hz). **HRMS** (ESI-TOF) calcd for $C_{30}H_{23}Cl_2N_4Os$ $[M]^+$ 701.0915, observed 701.0889. **IR** (ATR) ν(C=N) 1601 cm^{-1}.

A standard ^{13}C NMR was unable to be obtained due to instability of **3a** in solution on the timescale required to achieve sufficient signal. As such, HSQC was used to generate a partial ^{13}C peak list.

Numerous attempts were made to crystallize **3a** in a glovebox from non-coordinating solvents, but none resulted in crystals suitable for diffraction. Recrystallization from acetone/Et_2O in air provided single crystals of the aromatized Os(III) isoquinoline (**12**), and recrystallization from MeCN/Et_2O under any atmosphere provided single crystals of **7.**

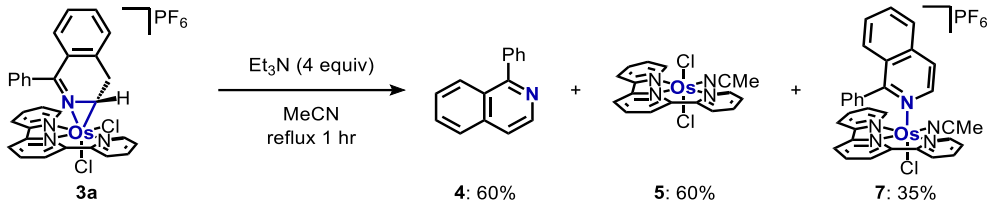


[terpyOs(Cl)(NCMe)(3-chloro-4,4-dimethyl-1-phenyl-3,4-dihydroisoquinoline)]PF$_6$ (8). A solution of **1** (65 mg; 0.1 mmol) and **2b** (110 mg; 0.5 mmol) was stirred in MeCN (5 mL) for 12 h at room temperature under N_2 in an oven dried 2 dram vial. The solvent was evaporated under vacuum and the residue was washed with Et_2O (5 x 10 mL). The resulting black solid was recrystallized from MeCN/Et_2O. Black solid (64.7 mg; 72%). Crystals suitable for X-ray diffraction were grown by vapor diffusion of Et_2O into MeCN. **^{1}H NMR** (400 MHz, CD_3CN) δ 9.10 – 9.01 (m, 1H), 8.98 (d, *J* = 5.4 Hz, 1H), 8.05 – 8.01 (m, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.90 (dd, *J* = 8.1, 3.8 Hz, 2H), 7.76 (td, *J* = 7.8, 1.5 Hz, 1H), 7.71 (td, *J* = 7.8, 1.5 Hz, 1H), 7.66 –

7.55 (m, 2H), 7.41 (td, *J* = 7.5, 1.3 Hz, 1H), 7.36 – 7.26 (m, 2H), 7.13 (t, *J* = 8.1 Hz, 1H), 6.91 (td, *J* = 7.8, 1.3 Hz, 1H), 6.85 (dt, *J* = 8.3, 6.9 Hz, 2H), 6.58 (s, 1H), 6.22 – 6.13 (m, 2H), 5.91 (dd, *J* = 8.1, 1.3 Hz, 1H), 3.25 (s, 3H), 1.60 (s, 3H), 1.08 (s, 3H). **HSQC** (^{13}C, 101 MHz, CD_3CN) δ 154.99, 154.64, 138.11, 137.76, 134.60, 134.25, 130.03, 128.97, 128.97, 128.62 (from C3,3'' on terpy, only one diastereotopic 13C shift observed in HSQC), 127.92, 126.86, 125.81, 124.75, 124.05, 124.05, 121.23, 90.99, 26.64, 23.12, 15.39, 5.54z **^{31}P NMR** (162 MHz, CD_3CN) δ -145 (hept, J=707 Hz). **^{19}F NMR** (376 MHz, CD_3CN) δ -65 (d, *J* = 706.2 Hz). **HRMS** (ESI-TOF) calcd for C34H30Cl2N5Os $[M]^+$ 770.1493, observed 770.1481. **IR** (ATR) ν(C≡N) 2259 cm^{-1}.

A standard ^{13}C NMR was unable to be obtained due to instability of **8** in solution on the timescale required to achieve sufficient signal. As such, HSQC was used to generate a partial ^{13}C peak list.

4. Procedure for release of isoquinoline (4) and terpy$OsCl_2$NCMe (5)



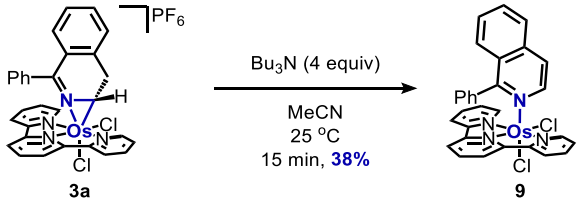
A 100 mL oven-dried Schlenk flask was charged with **3a** (141 mg; 0.17 mmol) and evacuated and backfilled with N_2 three times. MeCN (10 mL) was added followed quickly by Et_3N (123 µL; 0.9 mmol). The reaction was heated to reflux for 1 h. Et_2O (25 mL) was added and the black precipitate was filtered off. The precipitate was washed with Et_2O (3 x 10 mL) and recrystallized from CH_2Cl_2/Et_2O to yield **5** as a black solid (18.6 mg; 65%). The filtrate from the reaction was dried *in vacuo* and redissolved in a small amount (~ 5 mL) of MeCN. Et_2O (30 mL) was added to precipitate **7** as a dark purple solid (50.0 mg, 35%). The filtrate was evaporated and purified by column chromatography (0-30% EtOAc/hexanes), from which 1-phenylisoquinoline was obtained as a white solid (20.7 mg; 0.10 mmol; 60%).

1-phenylisoquinoline (**4**): White solid (20.7 mg; 0.10 mmol; 60%) **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.62 (d, *J* = 5.7 Hz, 1H), 8.11 (dq, *J* = 8.5, 1.0 Hz, 1H), 7.88 (dt, *J* = 8.2, 1.0 Hz, 1H), 7.74 – 7.66 (m, 3H), 7.65 (dd, *J* = 5.7, 0.9 Hz, 1H), 7.58 – 7.45 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.87, 142.36, 139.73, 136.97, 130.10, 130.03, 128.69, 128.45, 127.70, 127.27, 127.09, 126.83, 120.02. **HRMS** (ESI-TOF) calcd for C15H11N $[M]^+$ 205.0891, observed 205.0755. The spectral data matches what was previously reported.[8]

***trans*-(terpy)$OsCl_2$NCMe** (**5**): Black solid (54.5 mg; 60%). Crystals suitable for X-ray diffraction were grown by vapor diffusion of Et_2O into a CH_2Cl_2 solution of **5**. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.90 (d, *J* = 5.6 Hz, 2H), 8.01 (dd, *J* = 7.9, 1.3 Hz, 2H), 7.85 (d, *J* = 8.0 Hz, 2H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.34 (ddd, *J* = 7.4, 5.6, 1.5 Hz, 2H), 6.68 (t, *J* = 8.0 Hz, 1H), 3.31 (s, 3H). **HSQC** (^{13}C, 101 MHz, $CDCl_3$) δ 152.79, 134.51, 129.23, 127.12, 121.50, 117.28, 5.10. **IR** (ATR): ν(C≡N) 2249 cm^{-1}. **HRMS** (ESI-TOF) calcd for $C_{17}H_{14}Cl_2N_4Os^+$ $[M]^+$ 536.0210, observed 536.0197.

5 was also synthesized by reaction of NBu_4N_3 with [*trans*-(terpy)$OsNCl_2$]PF_6 as previously reported.[9] While no NMR data was previously reported, the sample prepared by this method matched the sample prepared by the release of isoquinoline. The limited solubility of **5** precluded sufficient signal/noise for an independent ^{13}C NMR, but a partial peak list was generated from HSQC NMR.

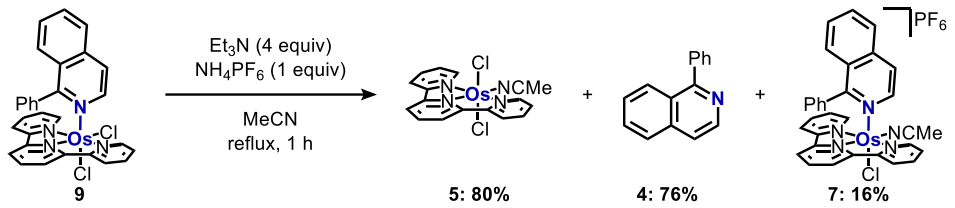
[(terpy)Os(1-phenylisoquinoline)Cl(NCMe)]PF_6 (**7**): Crystals suitable for x-ray diffraction were grown by vapor diffusion of Et2O into a saturated MeCN solution of **7** or **3a**. Purple solid (50.0 mg; 35%) **^{1}H NMR** (400 MHz, CD_3CN) δ 9.45 (d, *J* = 7.1 Hz, 1H), 9.12 (dt, *J* = 5.4, 1.2 Hz, 2H), 8.10 (dd, *J* = 8.0, 1.2 Hz, 2H), 8.04 (d, *J* = 8.1 Hz, 2H), 7.94 (d, *J* = 8.1 Hz, 1H), 7.81 (td, *J* = 7.8, 1.5 Hz, 2H), 7.73 (dddd, *J* = 9.1, 7.4, 6.2, 1.3 Hz, 3H), 7.67 (dd, *J* = 7.1, 0.9 Hz, 1H), 7.46 (tt, *J* = 7.5, 1.3 Hz, 1H), 7.37 (ddd, *J* = 8.4, 6.8, 1.2 Hz, 1H), 7.22 (t, *J* = 8.0 Hz, 1H), 7.01 – 6.93 (m, 2H), 6.59 (dd, *J* = 8.6, 1.0 Hz, 1H), 6.41 – 6.34 (m, 2H), 3.36 (s, 3H), 1.16 (s, 1H). **^{13}C NMR** (101 MHz, CD_3CN) δ 169.62, 162.67, 162.62, 153.42, 148.69, 136.91, 135.47, 134.46, 132.80, 132.21, 130.93, 130.24, 128.74, 128.40, 128.33, 127.91, 127.77, 126.66, 123.69, 121.90, 120.54, 4.98 (coordinated acetonitrile sp carbon 13C shift is not detected). **^{31}P NMR** (162 MHz, CD_3CN) δ -145 (hept, J=707 Hz). **^{19}F NMR** (376 MHz, CD_3CN) δ -65 (d, *J* = 706.2 Hz). **HRMS** (ESI-TOF) calcd for $C_{32}H_{25}ClN_5Os^+$ $[M]^+$ 706.1413, observed 706.1397. **IR** (ATR) ν(C≡N) 2259 cm^{-1}.



***Cis*-(terpy)Os(1-phenylisoquinoline)Cl_2 (9)**: A 2-dram vial was charged with **3a** (84 mg; 0.1 mmol) and evacuated and backfilled with N_2 three times. MeCN (5 mL) was added, followed by tributylamine (95 µL; 0.4 mmol). The reaction was stirred for 15 minutes, at which time Et_2O (10 mL) was added and the black solid was collected and washed with a small amount of MeCN (1 mL) and Et_2O (3 x 5 mL) and dried *in vacuo*. **9** was obtained as a black solid (56 mg; 79%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.15 (d, *J* = 7.1 Hz, 1H), 9.41 (d, *J* = 5.6 Hz, 2H), 7.68 (d, *J* = 7.9 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.53 (td, *J* = 7.5, 4.7 Hz, 3H), 7.42 (dt, *J* = 11.3, 7.6 Hz, 3H), 7.25 – 7.19 (m, 2H), 7.07 – 6.98 (m, 1H), 6.78 (t, *J* = 7.7 Hz, 2H), 6.47 (t, *J* = 7.9 Hz, 1H), 6.31 (d, *J* = 8.7 Hz, 1H), 6.12 (d, *J* = 7.4 Hz, 2H). The ^{1}H NMR displayed significant line broadening upon sitting in solution over the course of a few hours. **HSQC** (^{13}C, 101 MHz, $CDCl_3$) δ 156.01, 148.41, 135.56, 130.29, 129.93, 127.83, 127.83, 127.47, 127.12, 127.12, 127.12, 126.07, 120.79, 120.09, 117.28 **HRMS** (ESI-TOF) calcd for $C_{30}H_{22}Cl_2N_4Os^+$ $[M]^+$ 700.0836, observed 700.0802.

A standard ^{13}C NMR was unable to be obtained due to instability of **9** in solution on the timescale required to achieve sufficient signal. As such, HSQC was used to generate a partial ^{13}C peak list.

Isolation of **9** from reactions employing Et_3N were hampered by difficulty separating the Et_3NHCl impurity.



An oven-dried 2 dram vial was charged with **9** (35.8 mg; 0.05 mmol) and NH_4PF_6 (8.2 mg; 0.05 mg) and evacuated and backfilled with N_2 five times. MeCN (3 mL) and Et_3N (28 µL; 0.2 mmol) were added, and the black mixture was refluxed for one hour. Et_2O (3 mL) was added, and the black precipitate collected and washed with MeCN (1 mL) and Et_2O (15 mL). Recrystallization from DCM/Et_2O afford **5** as a black solid (22.1 mg; 80%). The filtrate and washes were combined and concentrated to ~1 mL. Et_2O (30 mL) was added, and the precipitate collected and washed with Et_2O (2 x 10 mL) to give **7** as a purple solid (6.8 mg; 16%). The filtrate and washes were collected and purified by column chromatography (0-30% EtOAc/hexanes) to give **4** as a white solid (8.0 mg; 76%).

In a separate experiment, a flame-dried NMR tube under N_2 was charged with a solution of **3a** (0.007 mmol quantified by integration against mesitylene as an internal standard) in CD_3CN. Et_3N was added, and the solution was gently shaken. After 10 minutes, the NMR displayed near quantitative conversion to a new species with broadened NMR peaks, which we assign as **9**. Heating this solution at reflux for one hour resulted in a 78% yield of **4** and an 18% yield of **7**.

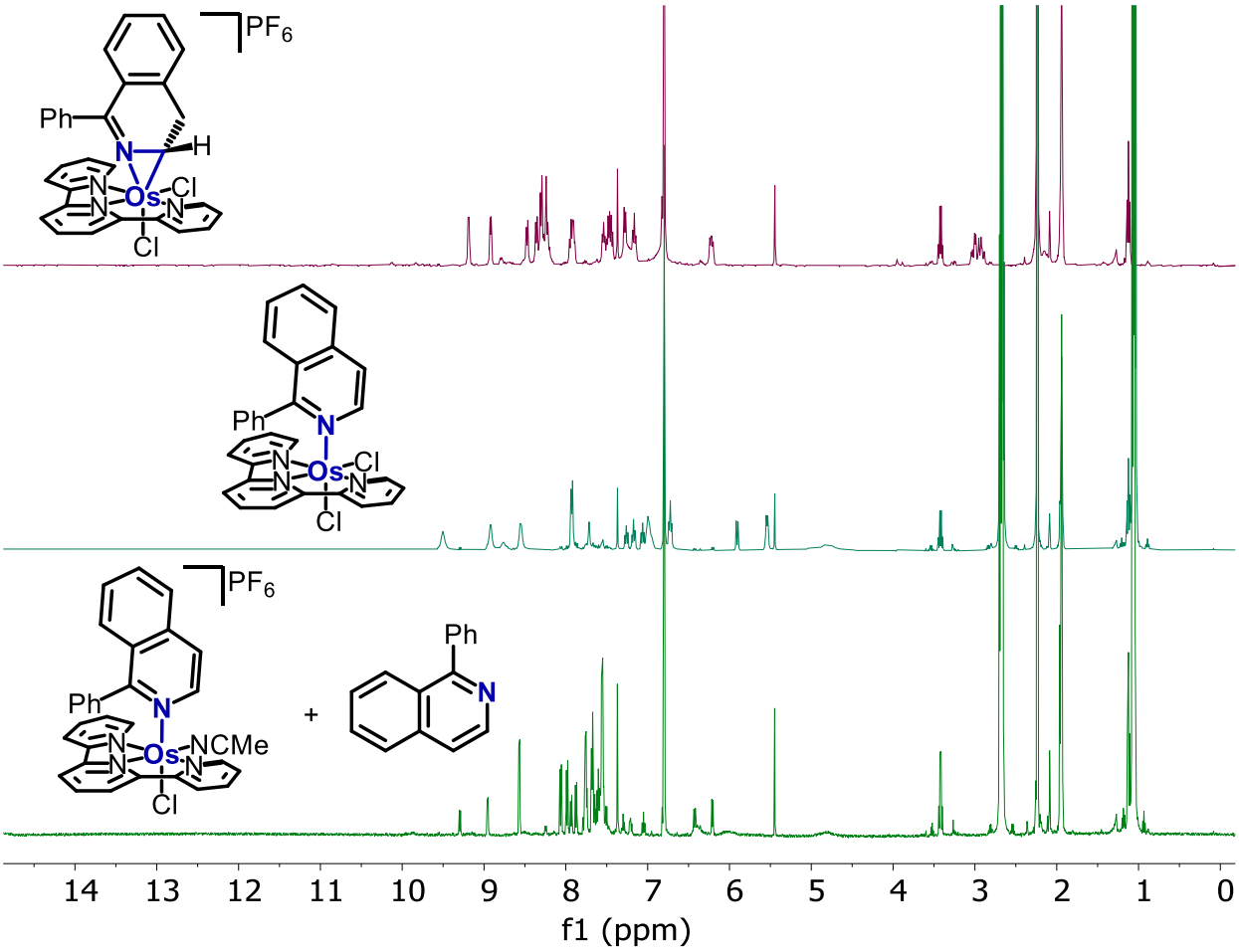


Figure S1: Representative spectra for formation of **9** from **3a** and after heating **9**

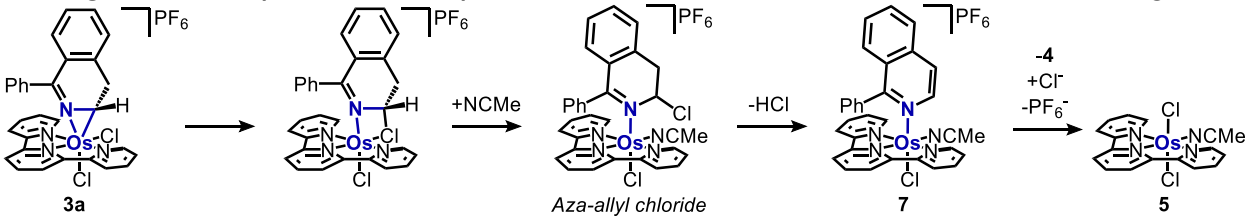
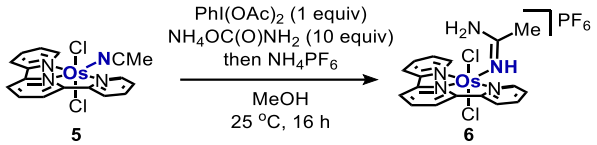


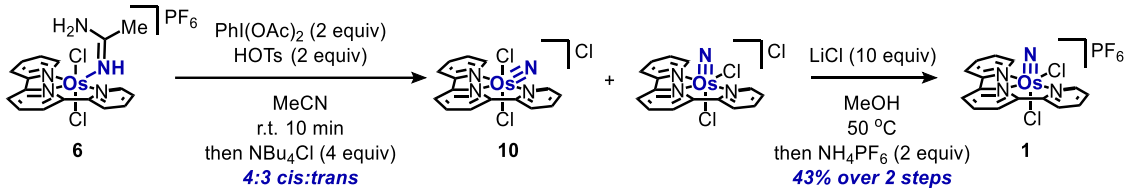
Figure S2: Alternate pathway for formation of **5** and **7** via the intermediacy of an aza-allyl chloride

5. Procedure for oxidation of 5 to 1



[*cis*-(terpy)Os(NC(OH)Me)Cl$_2$]PF$_6$ (6): To a solution of **5** (43.4 mg; 0.08 mmol) in MeOH (8 mL) was added (diacetoxy)iodobenzene (26.0 mg; 0.08 mmol). The solution was stirred at room temperature for 10 minutes, at which point ammonium carbamate (63.2 mg; 0.8 mmol) was added and the solution stirred for an additional 8 hours. Ammonium

hexafluorophosphate (20 mg; 0.12 mmol) was added, and the solution stirred at 0 °C for 15 minutes. The resulting brown solid was filtered and washed with cold MeOH (3 mL) followed by copious amounts of Et_2O and dried *in vacuo*. **6** was obtained as a brown solid (41.6 mg; 74%). **^{1}H NMR** (400 MHz, CD_3CN) δ 11.35 – 9.52 (bs), 8.30 – 7.46 (bs), 3.17 (s), 1.05 – 0.59 (bs), -2.16 – -3.00 (bs), -4.68 – -5.67 (bs), -6.37 – -7.96 (bs), -7.96 – -9.12 (bs, 2H). **^{31}P NMR** (162 MHz, CD_3CN) δ -145 (hept, J=707 Hz). **^{19}F NMR** (376 MHz, CD_3CN) δ -65 (d, *J* = 706.2 Hz). **IR** (ATR) ν(C=N) 1451 cm^{-1}, 1640 cm^{-1}, (N-H) 3476 cm^{-1}. **HRMS** (ESI-TOF) calcd for $C_{17}H_{17}Cl_2N_5Os$ 553.0476, observed 553.0453. μ_{eff} (Evans' Method) = 1.59; Diamagnetic correction -269.37 x 10^{-6} emu/mol.



[*cis*-(terpy)OsNCl$_2$]PF$_6$ (1): To a solution of **6** (33 mg, 0.049 mmol) in MeCN (3 mL) was added p-toluenesulfonic acid monohydrate (19 mg, 0.1 mmol) and (diacetoxy)iodobenzene (32 mg, 0.1 mmol). The solution was stirred at room temperature for 10 minutes. Tetrabutylammonium chloride (54 mg, 0.2 mmol) was added and the solution stirred at 0 °C for 10 minutes. The pink precipitate was filtered and washed with CH_2Cl_2 (5 mL) and dissolved in MeOH (4 mL). Lithium chloride (42 mg; 1 mmol) was added and the solution stirred at 50 °C for 15 minutes. Ammonium hexafluorophosphate (35 mg; 0.2 mmol) was added, and the solution stirred at 0 °C for 15 minutes. The orange solid was collected, washed with cold MeOH (2 mL), and Et_2O (10 mL). After drying *in vacuo*, **1** was obtained as an orange solid (trial 1: 43%; trial 2: 52%; average: 48%). **^{1}H NMR** (400 MHz, CD_3CN) δ 9.81 (dd, *J* = 5.5, 1.6 Hz, 2H), 8.89 (dd, *J* = 9.2, 6.9 Hz, 1H), 8.84 – 8.77 (m, 4H), 8.69 (td, *J* = 8.0, 1.6 Hz, 2H), 8.20 (ddd, *J* = 7.3, 5.5, 1.3 Hz, 2H). **^{13}C NMR** (101 MHz, CD_3CN) δ 160.91, 156.72, 155.70, 148.08, 145.92, 131.26, 128.16, 127.18. **^{31}P NMR** (162 MHz, CD_3CN) δ -145 (hept, J=707 Hz). **^{19}F NMR** (376 MHz, CD_3CN) δ -65 (d, *J* = 706.2 Hz). The spectral data match those previously reported.[1]

In a separate experiment, 0.007 mmol (quantified by NMR comparison to dioxane as internal standard) of **6** in 1 mL of CD_3CN was treated with p-toluenesulfonic acid monohydrate (6.8 mg; 0.04 mmol). No reaction occurred for 1 hour despite the excess of acid. After 1 hour, (diacetoxy)iodobenzene (4.3 mg; .013 mmol) was added, and an instant color change from dark brown to pink was observed. ^{1}H-NMR after 5 minutes indicated a 75% yield of [trans-terpyOsCl$_2$N]$^+$ (**10**).

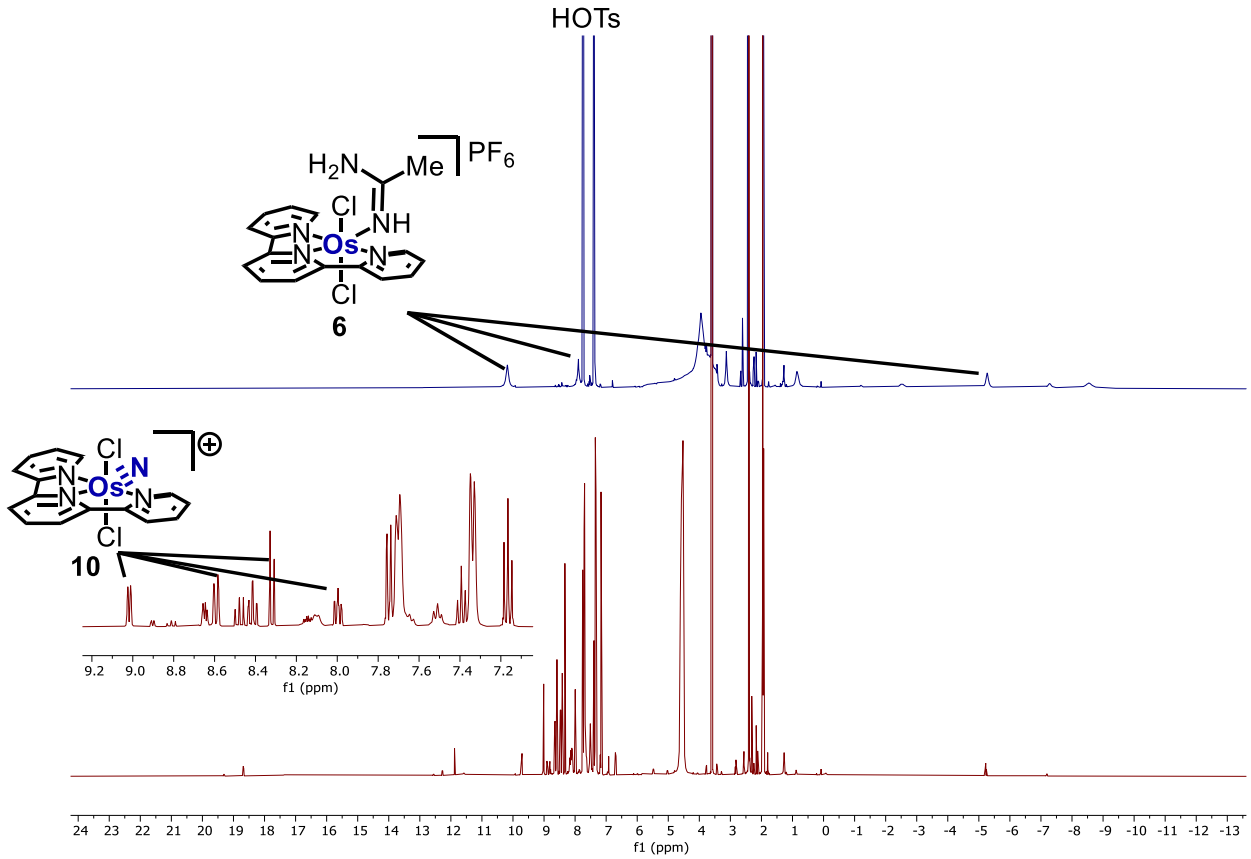
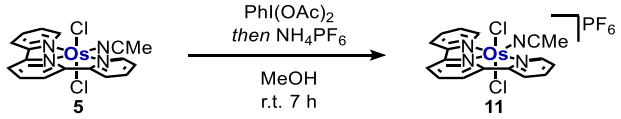


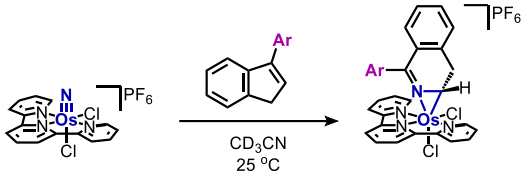
Figure S2: Representative crude ^{1}H-NMR spectra of the formation of **10** from **6**.



[*trans*-(terpy)OsCl$_2$NCMe]PF$_6$ (11): To a solution of **5** (14.6 mg; 0.027 mmol) in MeOH (2.5 mL) was added (diacetoxy)iodobenzene (39.0 mg; 0.12 mmol). The solution was stirred at room temperature for 3 hours and then filtered to remove unreacted starting material. Ammonium hexafluorophosphate (16 mg; 0.1 mmol) was added, and the solution stirred at 0 °C for 15 minutes. The resulting brown solid was filtered and washed with cold MeOH (3 mL) followed by copious amounts of Et_2O and dried in vacuo. **11** was obtained as a brown solid (4.0 mg; 22%). **^{1}H NMR** (500 MHz, CD_3CN) δ 3.09 (bs), -1.19 (bs), -7.84 (bs), -18.89 (bs), -22.31 (bs), -45.07 (bs). **^{31}P NMR** (162 MHz, CD_3CN) δ -145 (hept, J=707 Hz). **^{19}F NMR** (376 MHz, CD_3CN) δ -65 (d, *J* = 706.2 Hz). **HRMS** (ESI-TOF) calcd for $C_{17}H_{14}Cl_2N_4Os^+$ $[M]^+$ 536.0210, observed 536.0196. μ_{eff} (Evans' Method) = 1.67; Diamagnetic correction -264.6 x 10^{-6} emu/mol.

6. Hammett analysis

General procedure for determination of rate constant

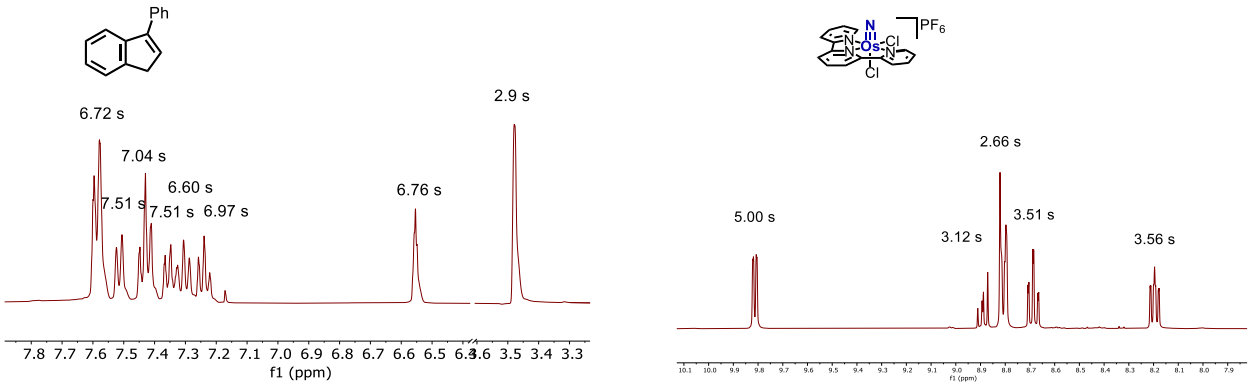


A solution of **1** in CD_3CN (0.5 mL) was syringe filtered into a septum capped, flame-dried NMR tube under N_2. Mesitylene (1.4 µL; 0.01 mmol) was added as an internal standard and the contents of the tube thoroughly mixed. The concentration of **1** was determined by integration relative to mesitylene. A solution of indene **2** (10 equiv. in 0.25 mL) was added via syringe and the reaction monitored by NMR. Observed rate constants (k_{obs}) were determined by taking the slope of a plot of $ln\left(\frac{[\mathbf{1}]_0}{[\mathbf{1}]}\right)$ vs. time. The rate constant was obtained by the following equation: $k = \frac{k_{obs}}{[\mathbf{2}]_0}$ where the concentration of **2** ($[\mathbf{2}]_0$) was determined by NMR integration relative to the internal standard at the first timepoint added to the amount of **1** that had been consumed.

$$[\mathbf{2}]_0 = [\mathbf{2}]_t + ([\mathbf{1}]_0 - [\mathbf{1}]_t)$$

Each reaction was performed in triplicate, and the average of the rate constants were used in the Hammett plot ($\log\frac{k_{X,avg}}{k_{H,avg}}$). Error was propagated using the following equation: $S_{final} = 0.434\left(\sqrt{\left(\frac{S_X}{k_{X,avg}}\right)^2 + \left(\frac{S_H}{k_{H,avg}}\right)^2}\right)$ where S_X is the standard deviation in the rate constants for a given substituent, and S_{final} is the propagated error. All Hammett parameters (σ, σ⁻, σ⁺) were obtained from tabulated results by H.C. Brown.[10,11]

T_1 values for 1 and 2a (representative indene)



Representative NMR spectra for each kinetic run

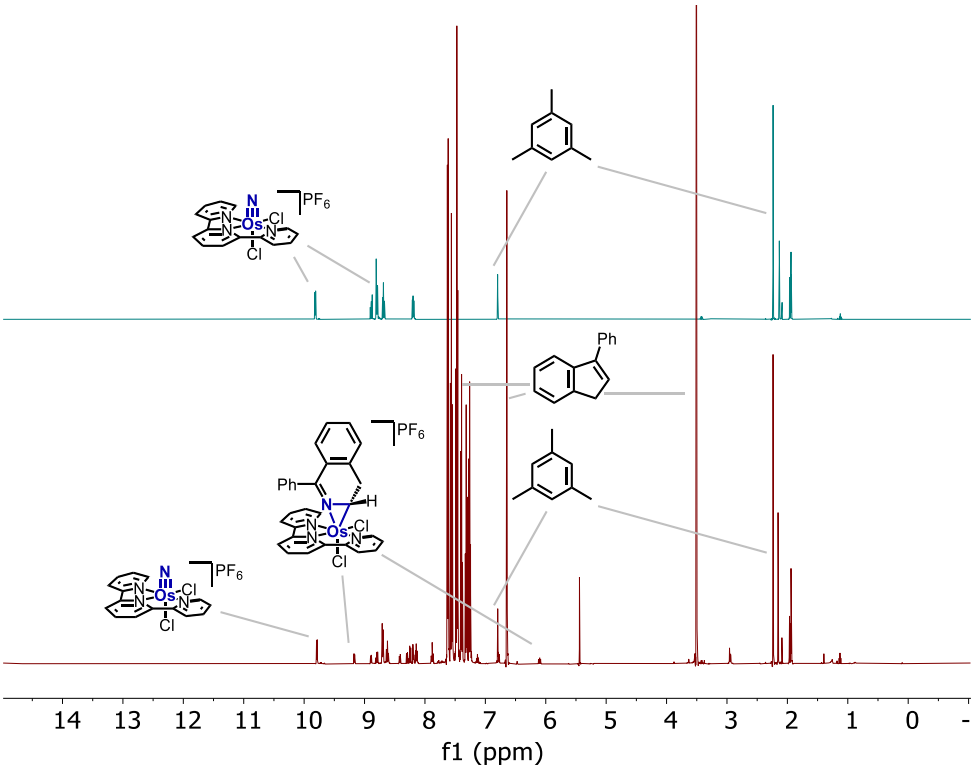


Figure S3: Representative NMR spectra for kinetics of reaction between **1** and **2a**

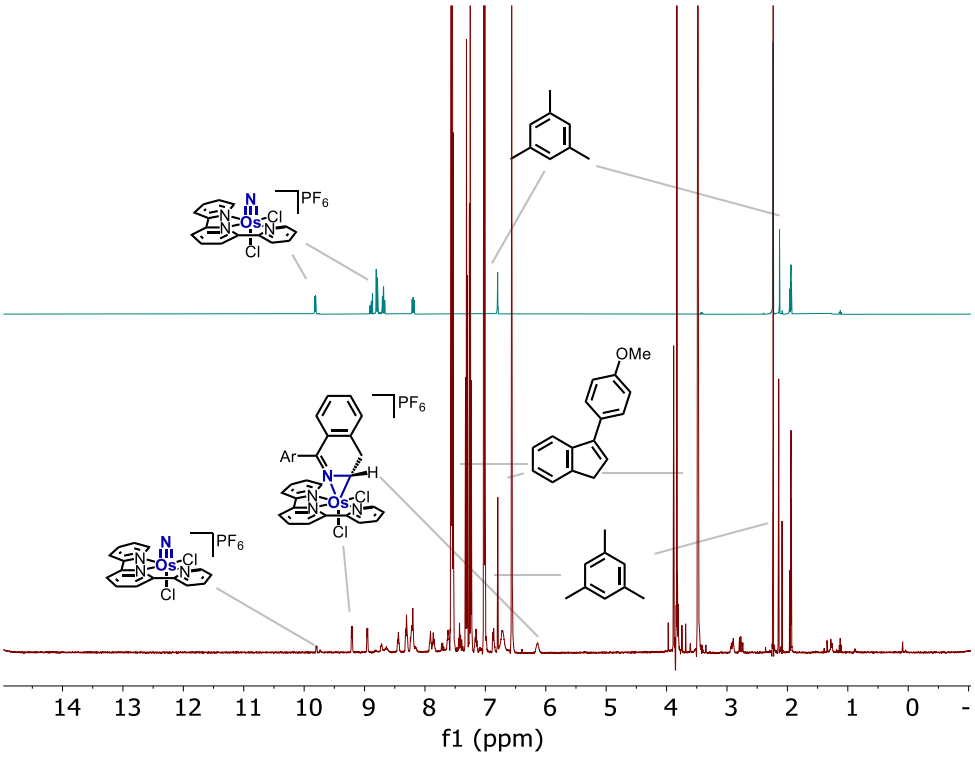


Figure S4: Representative NMR spectra for kinetics of reaction between **1** and **2b**

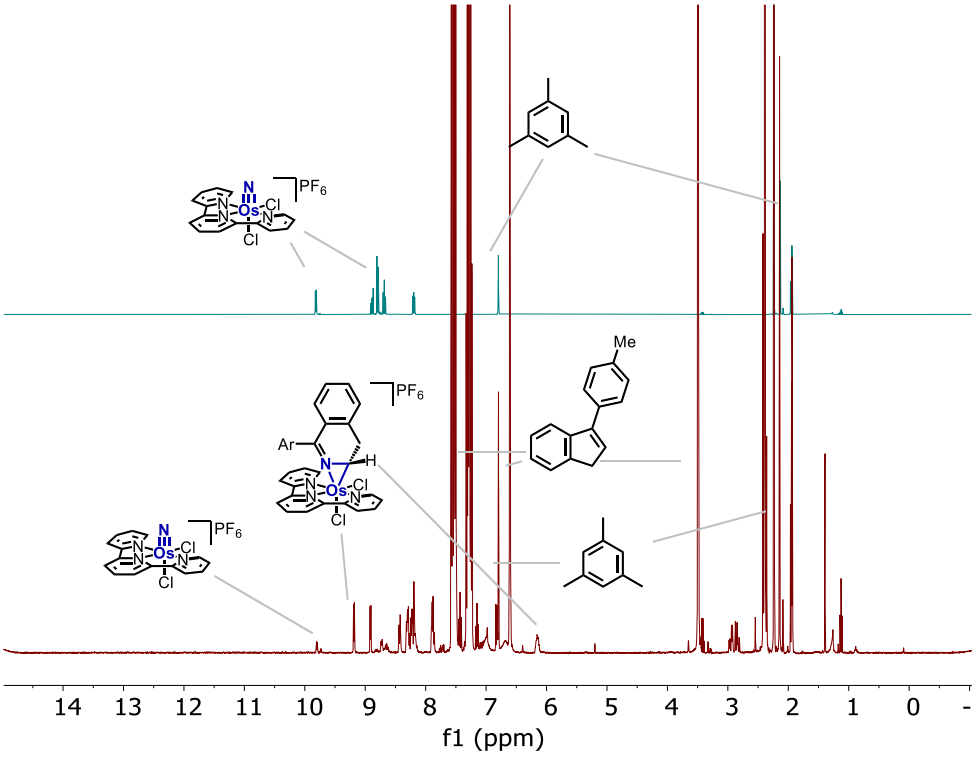


Figure S5: Representative NMR spectra for kinetics of reaction between **1** and **2c**

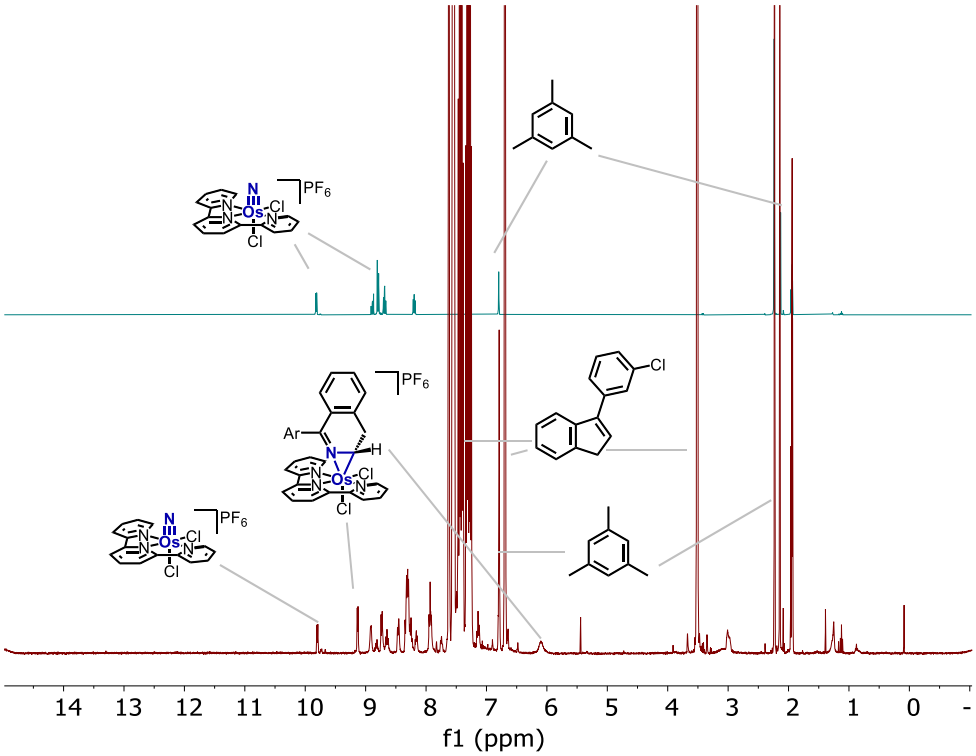


Figure S6: Representative NMR spectra for kinetics of reaction between **1** and **2d**

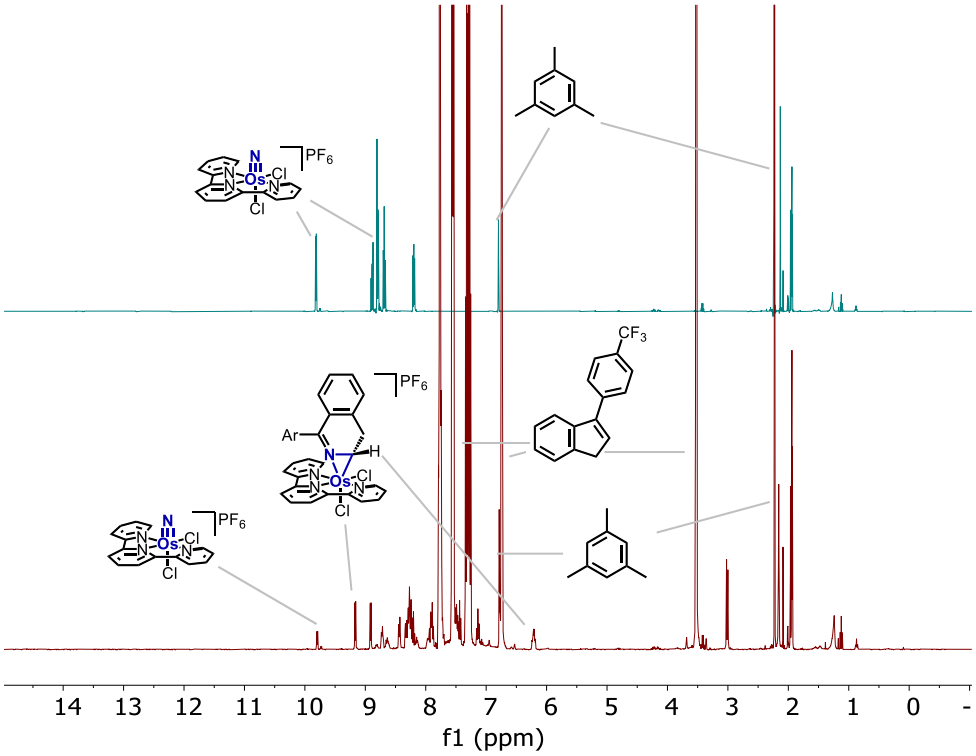


Figure S7: Representative NMR spectra for kinetics of reaction between **1** and **2e**

Representative log plots from kinetic experiments

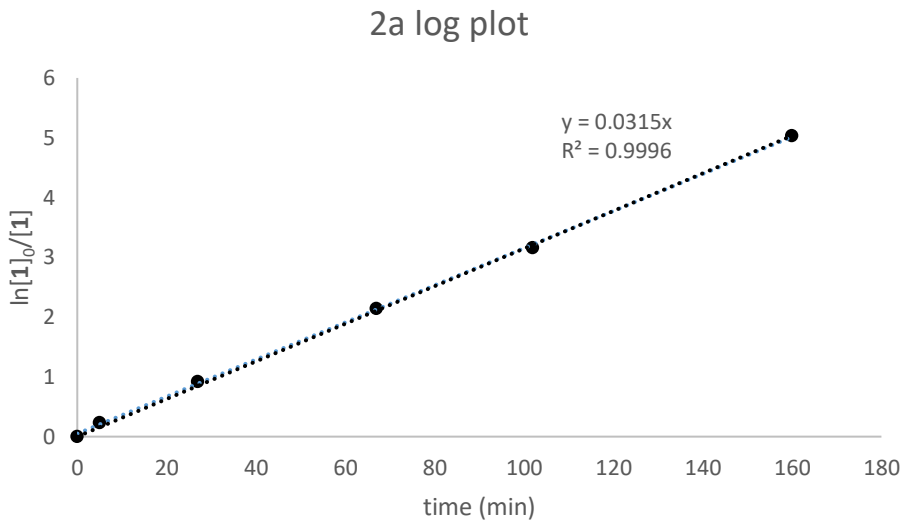


Figure S8: Representative log plot for kinetics of reaction between **1** and **2a.**

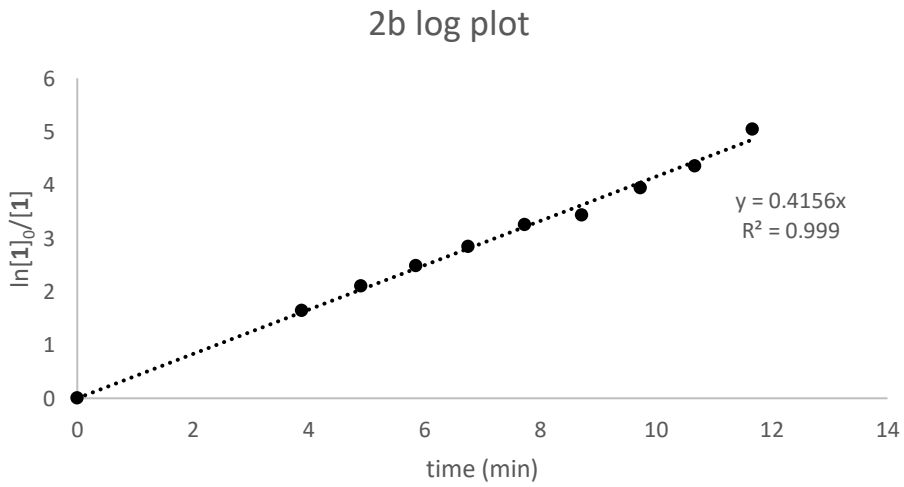


Figure S9: Representative log plot for kinetics of reaction between **1** and **2b**

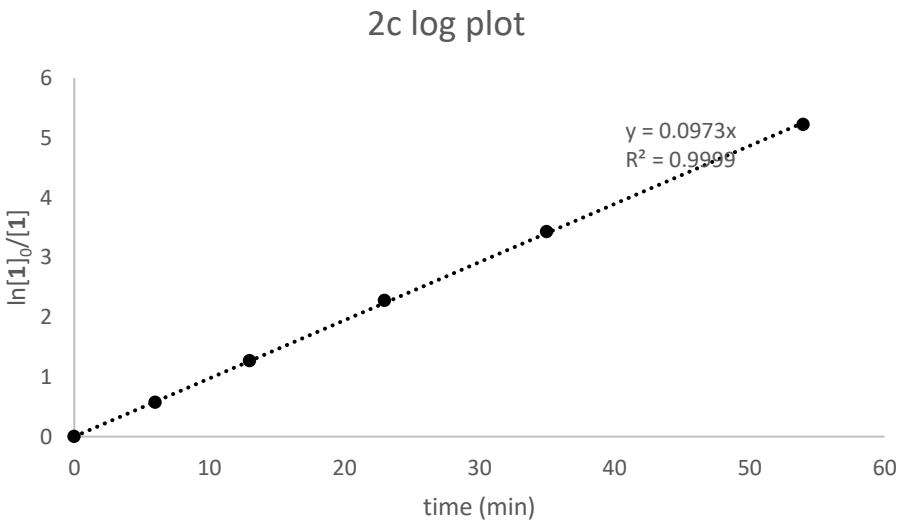


Figure S10: Representative log plot for kinetics of reaction between **1** and **2c**

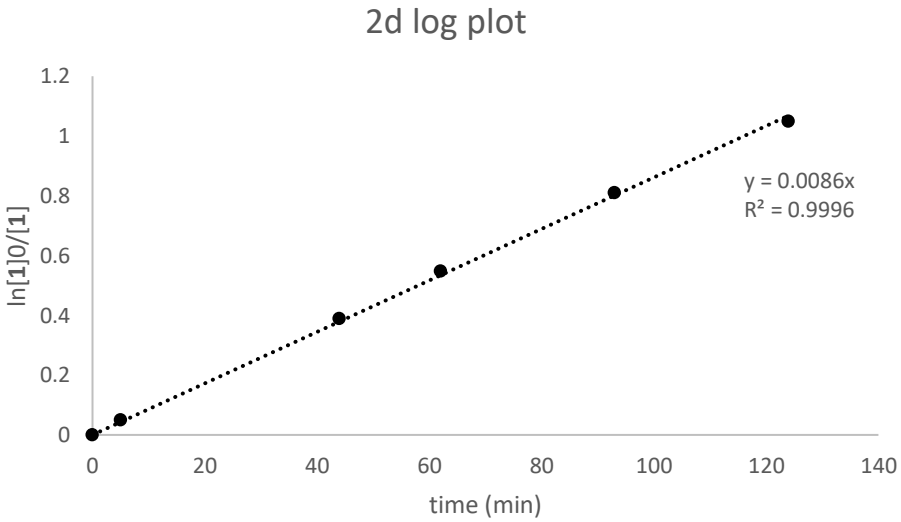


Figure S11: Representative log plot for kinetics of reaction between **1** and **2d**

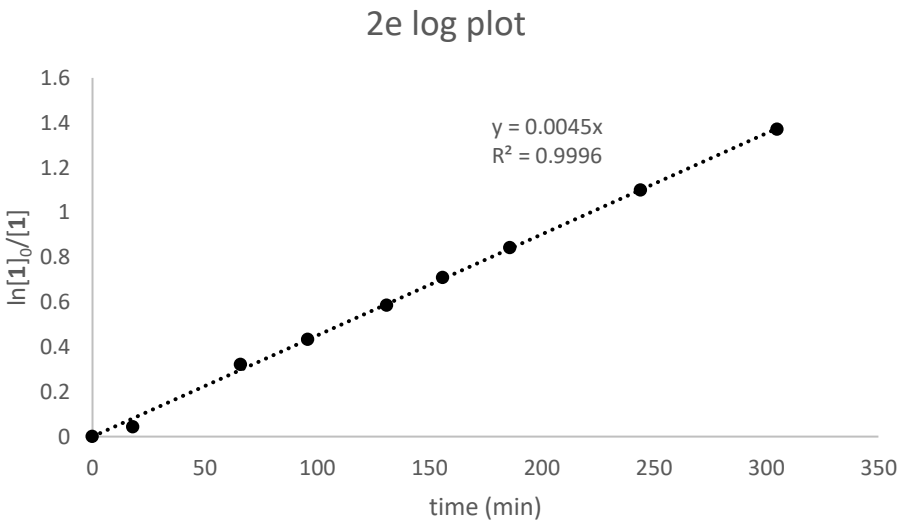


Figure S12: Representative log plot for kinetics of reaction between **1** and **2e**

Table S1: Individual rate constants and statistical analysis

 X (substituent)	σ^+	σ	σ^-	$k_{trial\ 1}$ (M^{-1} min^{-1})	$k_{trial\ 2}$ (M^{-1} min^{-1})	$k_{trial\ 3}$ (M^{-1} min^{-1})	k_{avg} (M^{-1} min^{-1})	stdev	$\log[k_X/k_H]$	error
H (**2a**)	0	0	0	0.149	0.130	0.144	0.141	0.008	0.000	0.035
p-OMe (**2b**)	-0.778	-0.268	0.27	2.781	1.840	1.560	2.060	0.522	1.164	0.113
p-Me (**2c**)	-0.311	-0.17	0.16	0.367	0.470	0.564	0.467	0.081	0.520	0.079
m-Cl (**2d**)	0.399	0.373	-0.03	0.041	0.056	0.039	0.045	0.008	-0.494	0.076
p-CF3 (**2e**)	0.612	0.54	0.05	0.018	0.013	0.018	0.016	0.002	-0.942	0.062

Table S2: Indene concentrations and calculation of k for each trial

 X (substituent)	$[\mathbf{1}]_{trial\ 1}$ (M)	$[\mathbf{1}]_{trial\ 2}$ (M)	$[\mathbf{1}]_{trial\ 3}$ (M)	$[\mathbf{2}]_{trial\ 1}$ (M)	$[\mathbf{2}]_{trial\ 2}$ (M)	$[\mathbf{2}]_{trial\ 3}$ (M)	$k_{obs,\ trial\ 1}$ (min^{-1})	$k_{obs,\ trial\ 2}$ (min^{-1})	$k_{obs,\ trial\ 3}$ (min^{-1})
H (**2a**)	0.020	0.024	0.013	0.211	0.317	0.164	0.0315	0.0413	0.0236
p-OMe (**2b**)	0.010	0.013	0.014	0.149	0.225	0.266	0.4156	0.3735	0.472
p-Me (**2c**)	0.028	0.012	0.012	0.403	0.226	0.172	0.148	0.106	0.097
m-Cl (**2d**)	0.015	0.012	0.016	0.259	0.154	0.251	0.0107	0.0086	0.0097
p-CF3 (**2e**)	0.022	0.030	0.011	0.255	0.488	0.199	0.0045	0.0064	0.0035

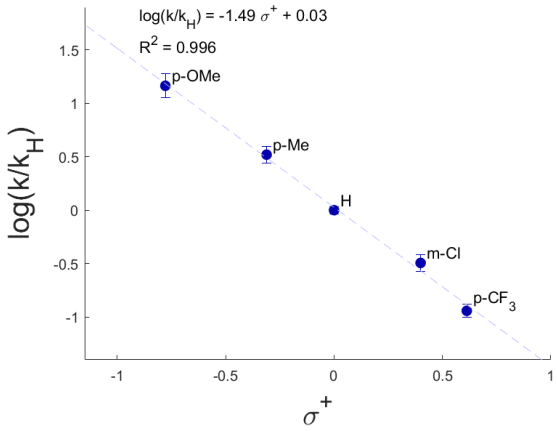


Figure S13: Correlation with sigma plus

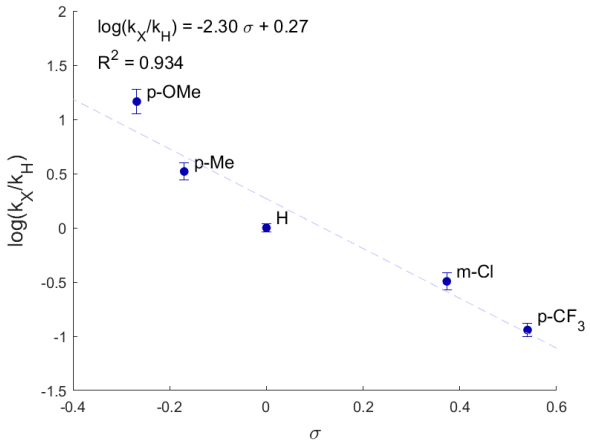


Figure S14: Correlation with sigma

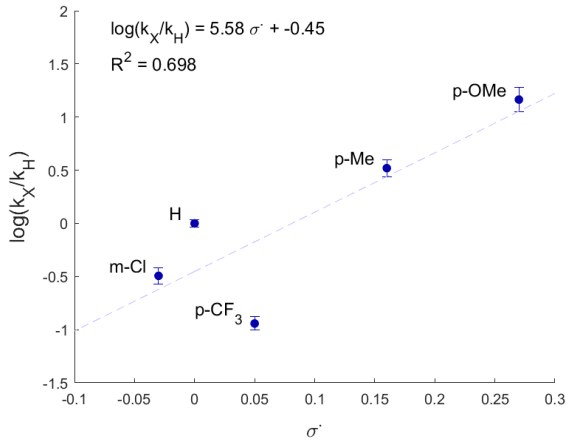


Figure S15: Correlation with sigma radical

7. Kinetics of the formation of aza-allyl chloride (8)

Procedure for kinetics: A solution of **1** in CD_3CN (0.5 mL) was syringe filtered into a septum capped, flame-dried NMR tube under N_2. Mesitylene (1.4 µL; 0.01 mmol) was added as an internal standard and the contents of the tube thoroughly mixed. The concentration of **1** was determined by integration relative to mesitylene. A solution of **2f** (~10 equiv. in 0.25 mL) was added via syringe and the reaction monitored by NMR. The concentration of **1**, the intermediate (putatively **3f**), and **8** were quantified by integration of the most downfield peaks. The kinetics were modeled as a pseudo-first order A → B → C using the following equations:

$$\mathbf{A} \xrightarrow{k_{1,obs}} \mathbf{B} \xrightarrow{k_2} \mathbf{C}$$

$$[\mathbf{1}]_t = A_0 e^{-k_{1,obs}t}$$

$$[\mathbf{3b}]_t = (yield_{\mathbf{3b}})\left(\frac{k_{1,obs}A_0}{k_2 - k_{1,obs}}\right)(e^{-k_{1,obs}t} - e^{-k_2 t})$$

$$[\mathbf{8}]_t = [\mathbf{8}]_{t-1} + (yield_{\mathbf{8}}) * [\mathbf{3b}]_{t-1} * k_2 * (t_n - t_{n-1})$$

The values of k_1, k_2, and A_0 were optimized using the Excel solver function. The yield of **3f** and **8** were estimated by hand to obtain the best fit. The final values used were 84% and 90% for **3f** and **8** respectively. The final fit was obtained with the following values:

$$k_{1,obs} = 0.0257\ s^{-1} = k_1[\mathbf{2}]_0 \rightarrow k_1 = 0.54\ M^{-1}s^{-1}$$

$$k_2 = 0.0050\ s^{-1}$$

$$A_0 = 23.87\ mM$$

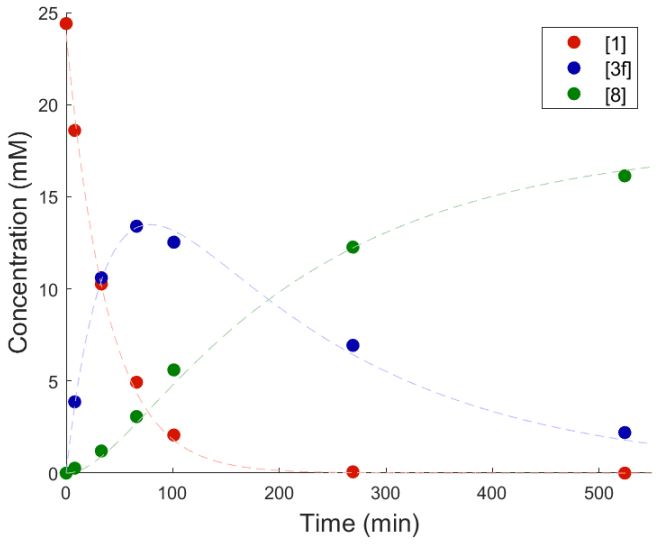


Figure S16: Plot of the intermediate buildup over time.

Representative NMR spectra of the intermediate

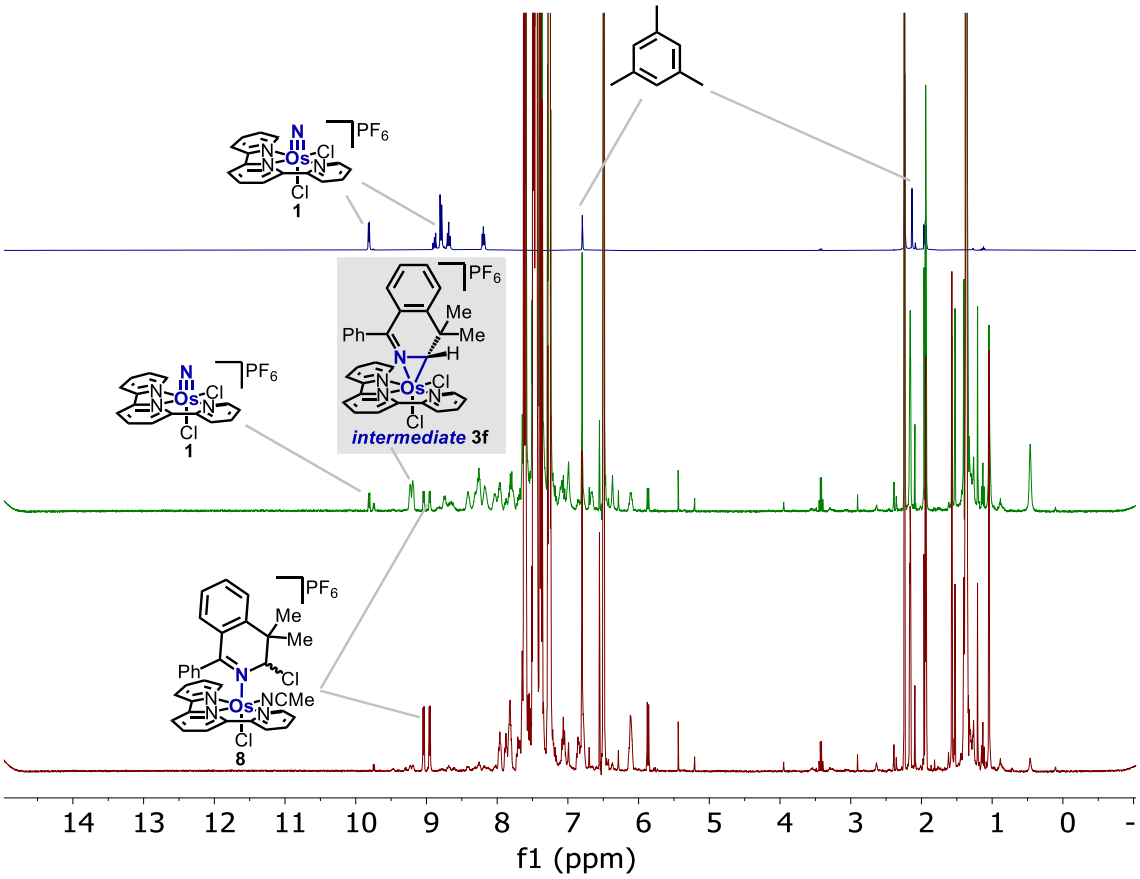


Figure S17: Representative NMR spectra from the reaction of **1** with **2f**.

Table S3: actual concentrations and approximation of k_1 for each trial.

Trial #	$[\mathbf{1}]_0$ (M)	$[\mathbf{2f}]_0$ (M)	k_{obs} ($k^*[\mathbf{2f}]$) ($min^{-1}M^{-1}$)	k_1 (min^{-1})**
1*	0.0244	0.479	0.022	0.045929
2	0.009	0.15	0.0092	0.061333
3	0.01	0.1	0.0051	0.051
4	0.009	0.028	0.0025	0.089286

*Used for the analysis of $A \rightarrow B \rightarrow C$ kinetics on previous page (Figure S16).
**approximated by $k_{obs}/[\mathbf{2f}]_0$

Log Plot demonstrating first order decay of 1

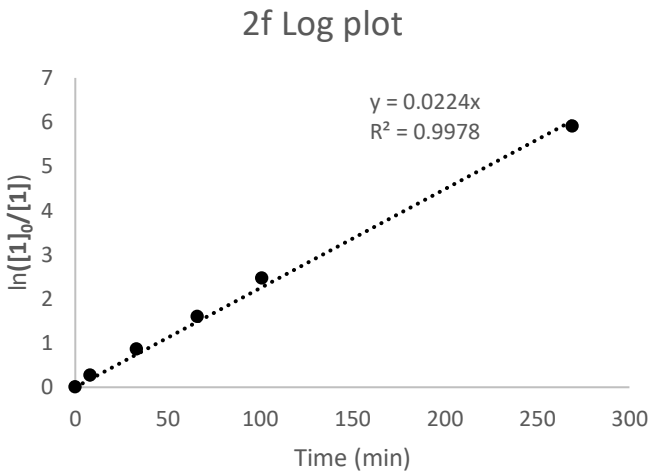
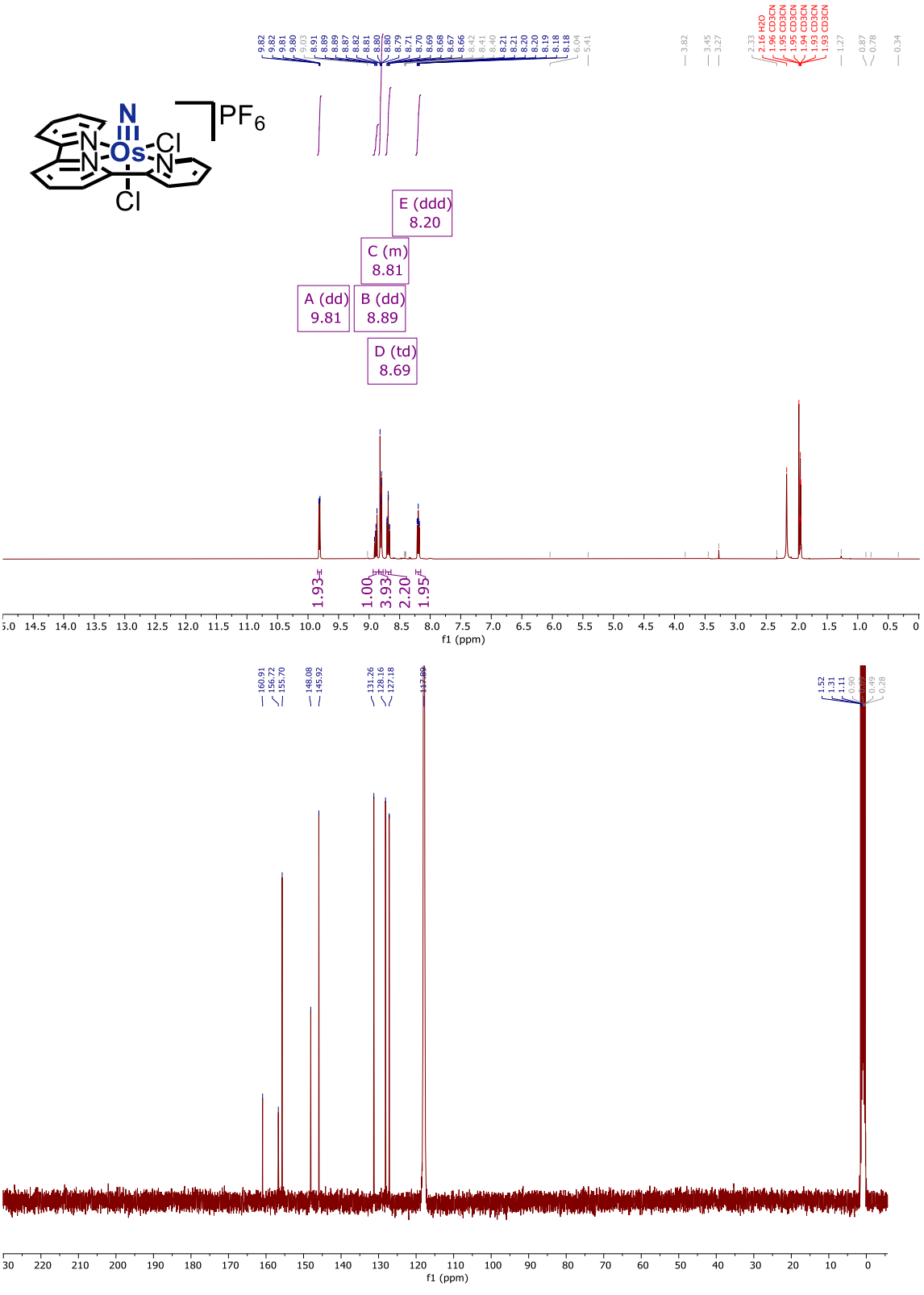
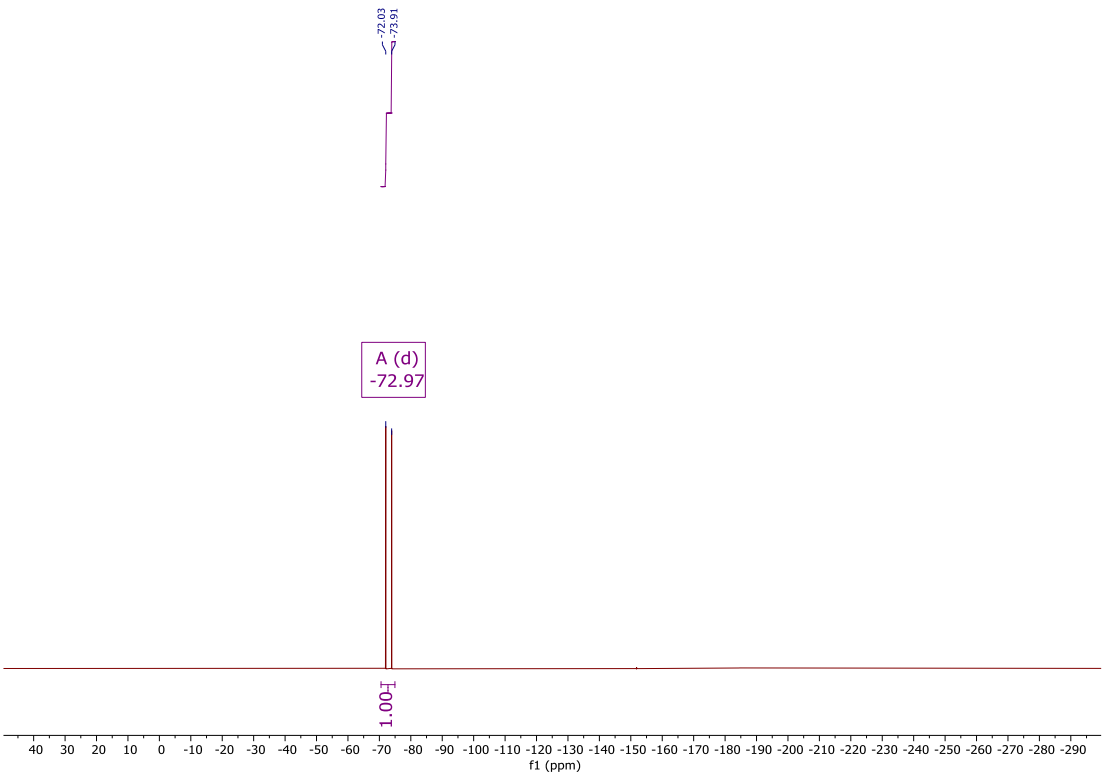


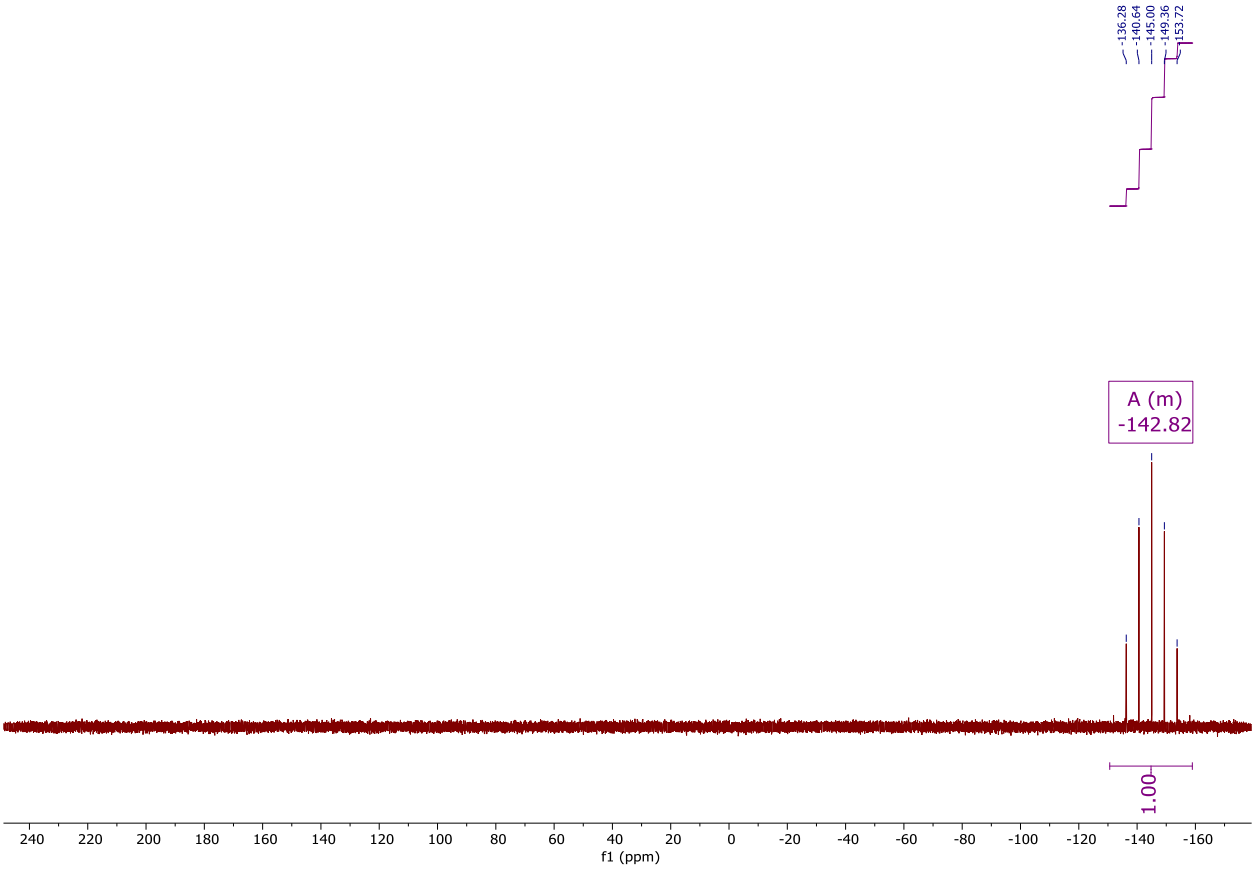
Figure S18: Representative log plot demonstrating first order decay of **1** in the presence of **2f.** $[\mathbf{2f}]_0$ = 0.479 M

8. NMR of compounds

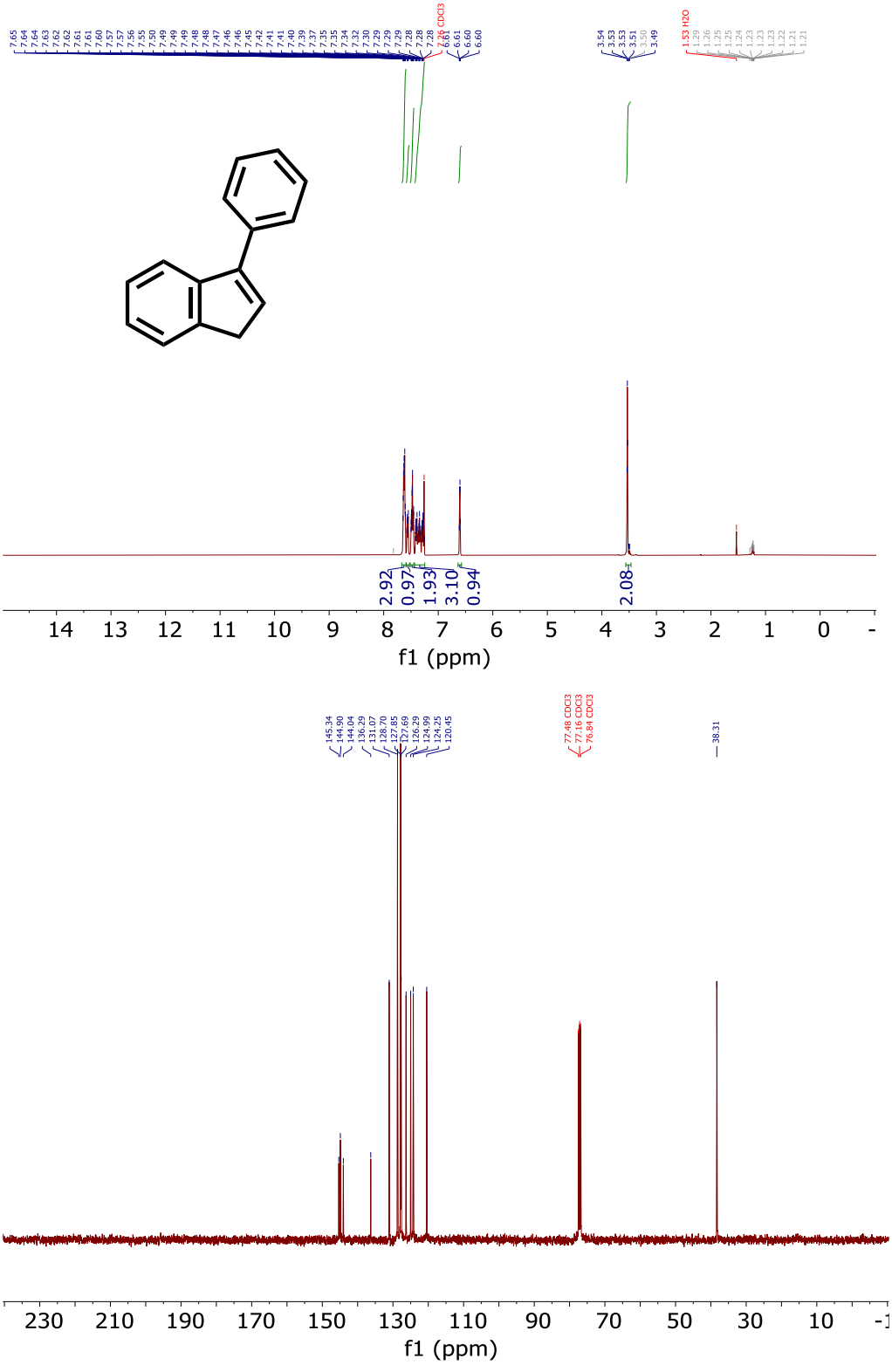
1



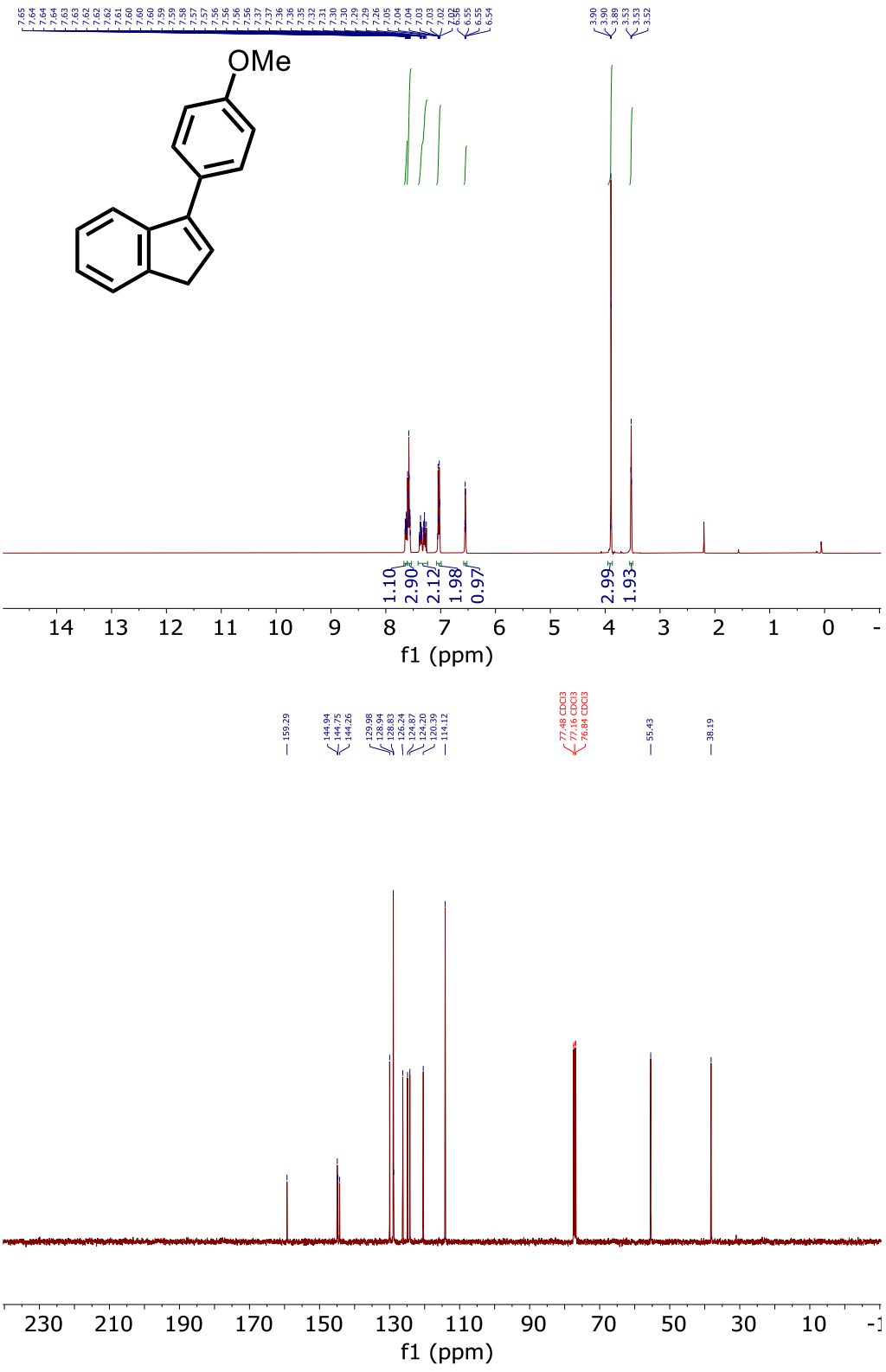

-72.03
-73.91
A (d)
-72.97
1.00
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260 -270 -280 -290
f1 (ppm)


-136.28
-140.64
-145.00
-149.36
-153.72
A (m)
-142.82
1.00
240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)

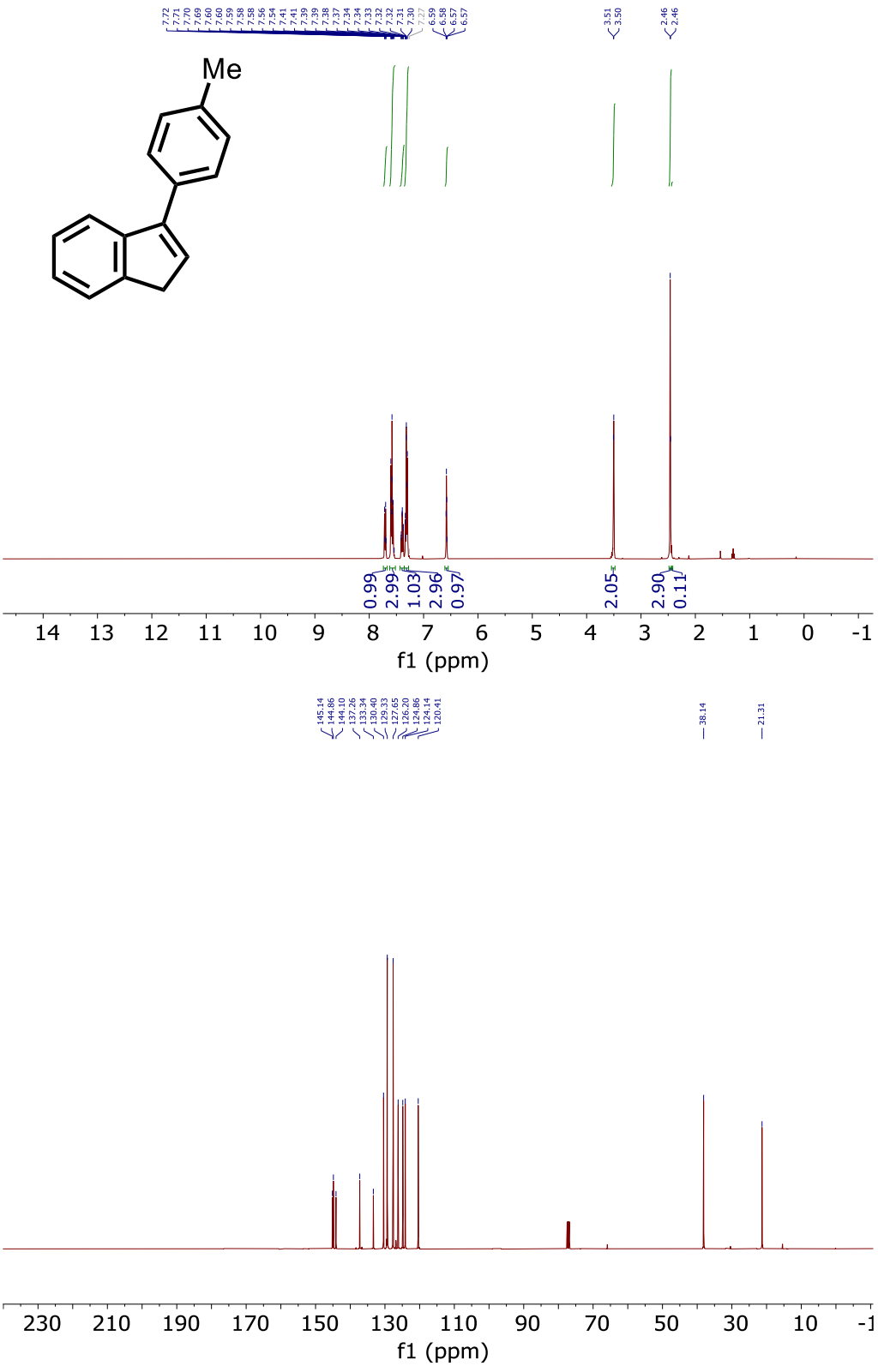
2a


7.65 7.64 7.64 7.63 7.62 7.62 7.61 7.61 7.60 7.57 7.57 7.56 7.55 7.55 7.49 7.49 7.49 7.48 7.48 7.47 7.46 7.46 7.45 7.42 7.41 7.41 7.40 7.39 7.37 7.35 7.35 7.34 7.32 7.30 7.29 7.29 7.29 7.28 7.28 7.26 CDCl3 6.61 6.60 6.60
3.54 3.53 3.53 3.51 3.50 3.49
1.53 H2O
1.29 1.26 1.25 1.25 1.24 1.23 1.23 1.23 1.22 1.21 1.21
2.92 0.97 1.93 3.10 0.94 2.08
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -
f1 (ppm)
145.34 144.90 144.04 136.29 131.07 128.70 127.85 127.69 126.29 124.99 124.25 120.45
77.48 CDCl3 77.16 CDCl3 76.84 CDCl3
38.31
230 210 190 170 150 130 110 90 70 50 30 10 -1
f1 (ppm)

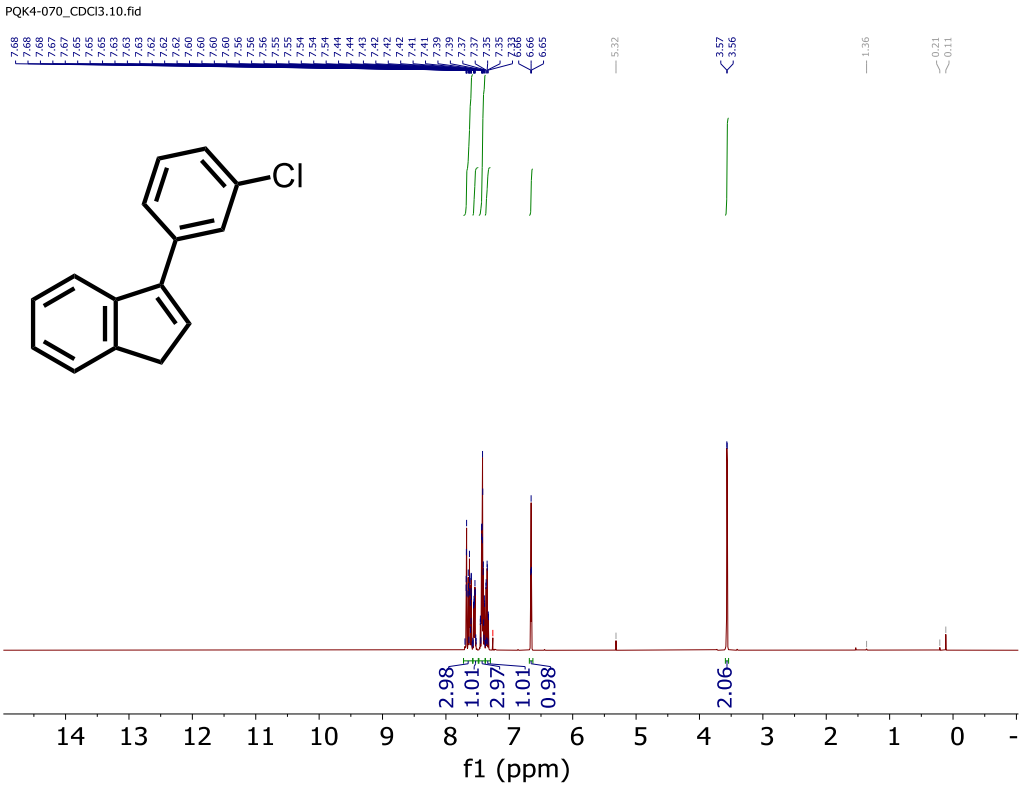
2b

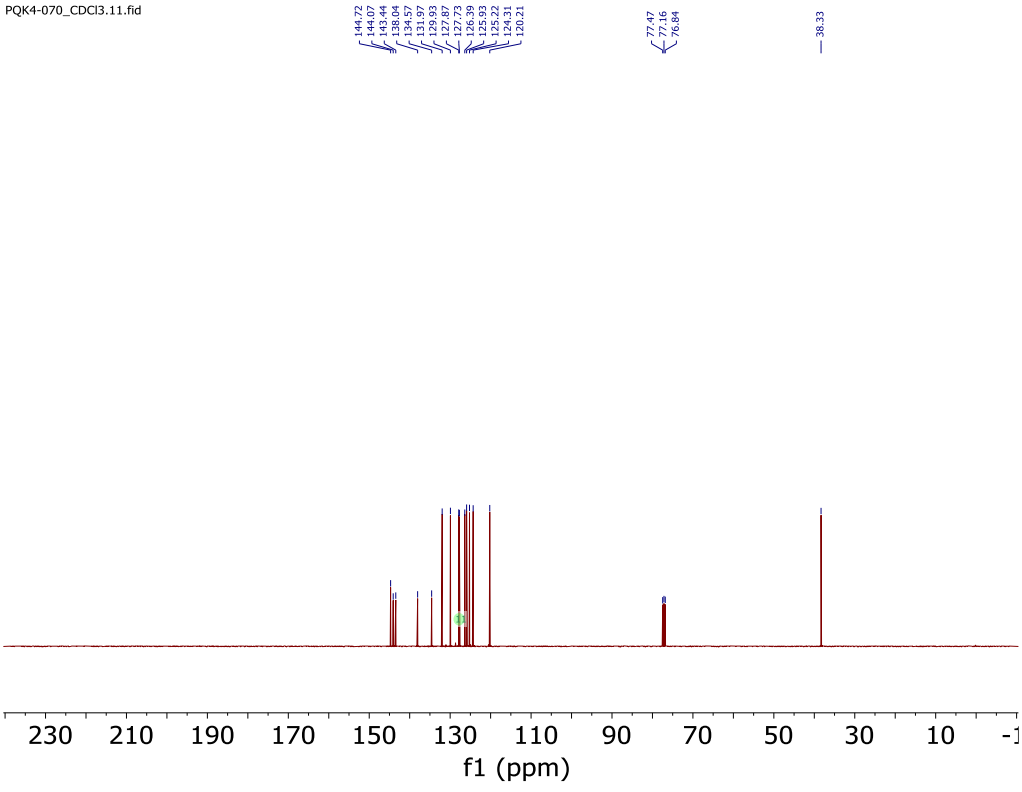

OMe
1.10
2.90
2.12
1.98
0.97
2.99
1.93
f1 (ppm)
159.29
144.94
144.75
144.26
129.98
128.94
128.83
126.24
124.87
124.20
120.39
114.12
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
55.43
38.19
f1 (ppm)

2c

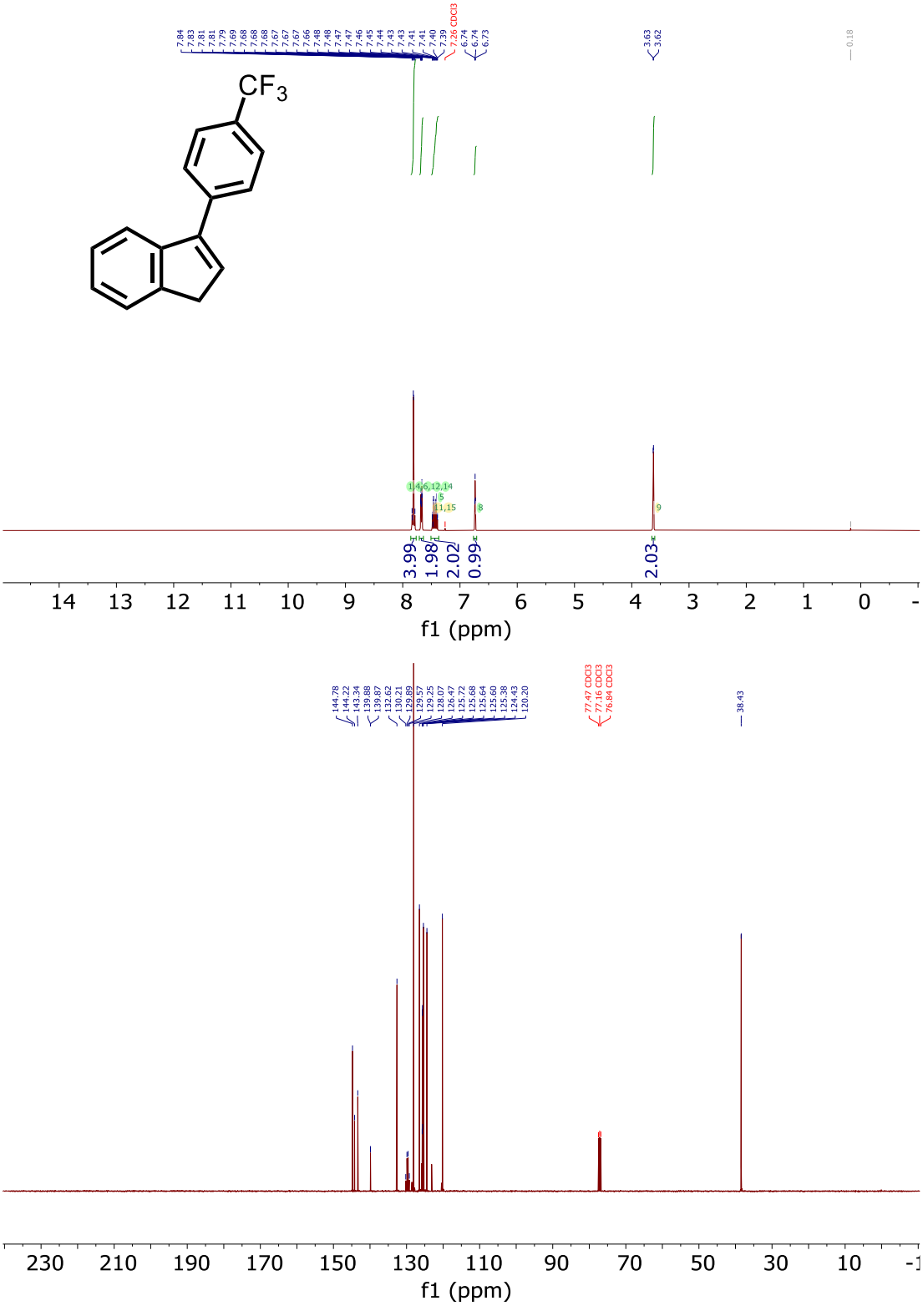

Me
7.72
7.71
7.70
7.69
7.60
7.60
7.59
7.58
7.58
7.56
7.54
7.41
7.41
7.39
7.39
7.38
7.37
7.34
7.34
7.33
7.32
7.32
7.31
7.30
7.27
6.59
6.58
6.57
6.57
3.51
3.50
2.46
2.46
0.99
2.99
1.03
2.96
0.97
2.05
2.90
0.11
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)
145.14
144.86
144.10
137.26
133.34
130.40
129.33
127.65
126.20
124.86
124.14
120.41
38.14
21.31
230 210 190 170 150 130 110 90 70 50 30 10 -1
f1 (ppm)

2d

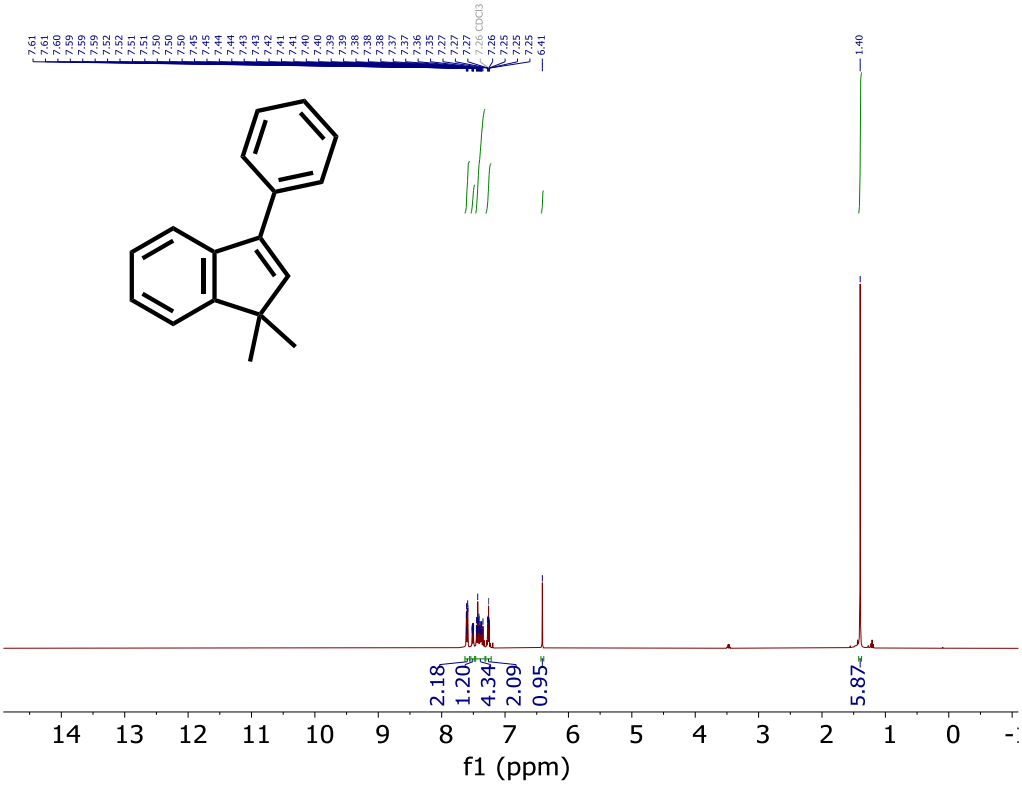

PQK4-070_CDCl3.10.fid
Cl
2.98
1.01
2.97
1.01
0.98
2.06
f1 (ppm)

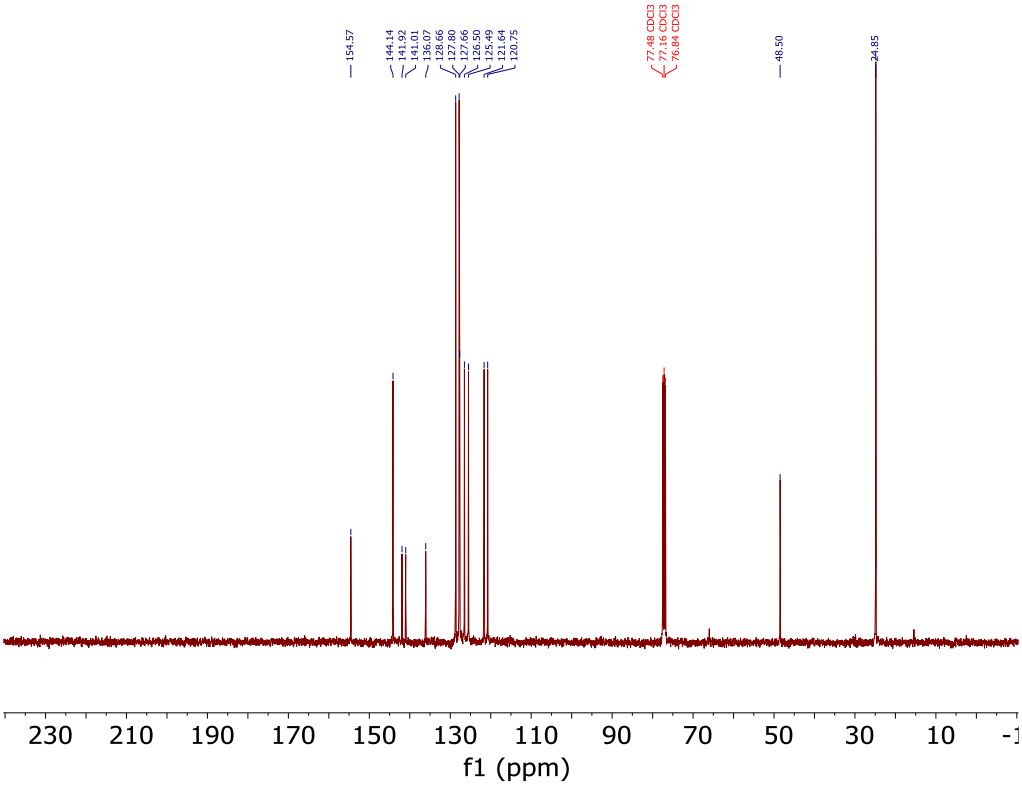

PQK4-070_CDCl3.11.fid
f1 (ppm)

2e

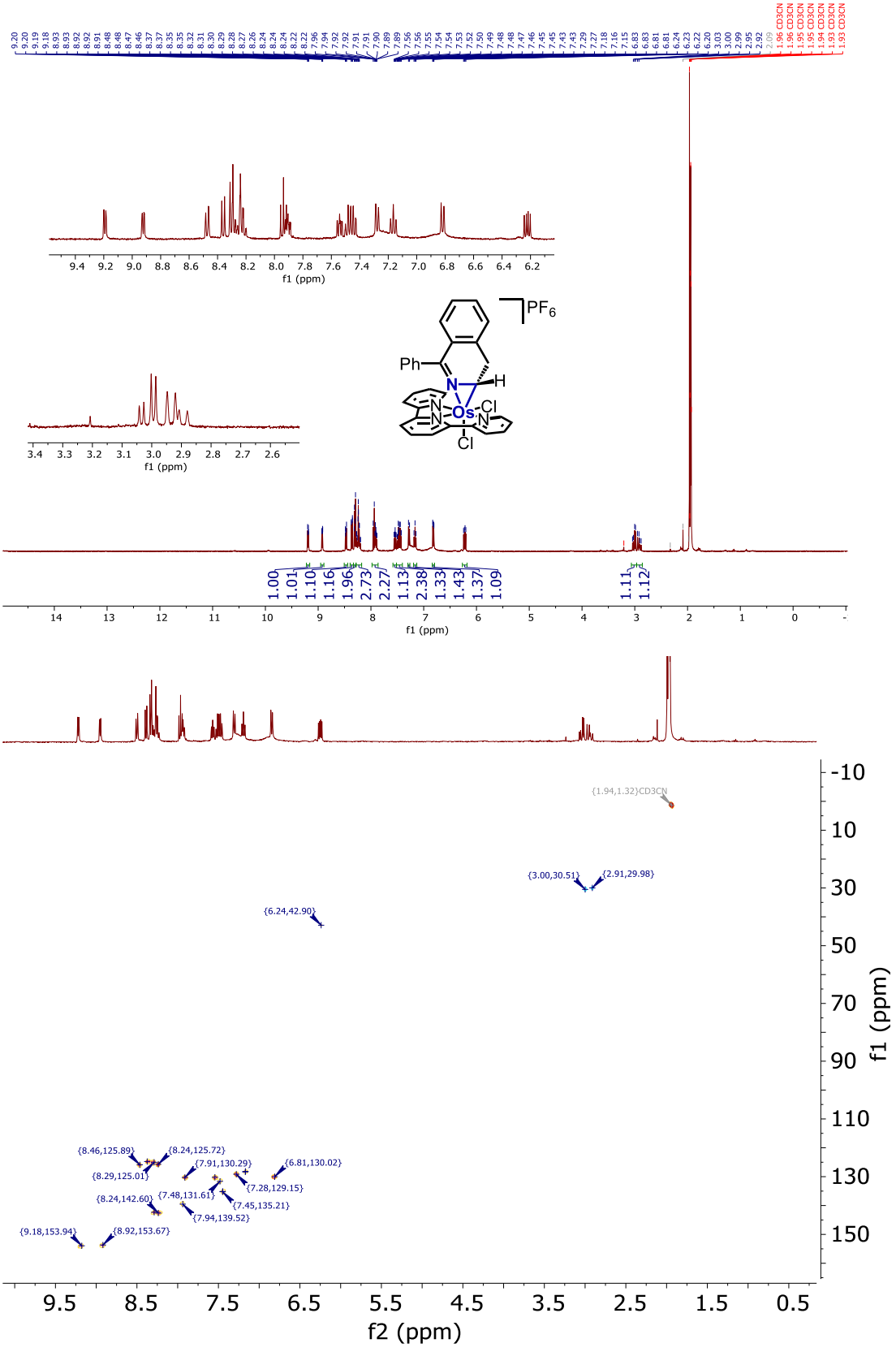


2f


7.61
7.61
7.60
7.59
7.59
7.59
7.52
7.52
7.51
7.51
7.50
7.50
7.50
7.45
7.45
7.44
7.44
7.43
7.43
7.42
7.41
7.41
7.40
7.40
7.39
7.39
7.38
7.38
7.38
7.37
7.37
7.36
7.35
7.27
7.27
7.26 CDCl3
7.26
7.25
7.25
7.25
6.41
1.40
2.18
1.20
4.34
2.09
0.95
5.87
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

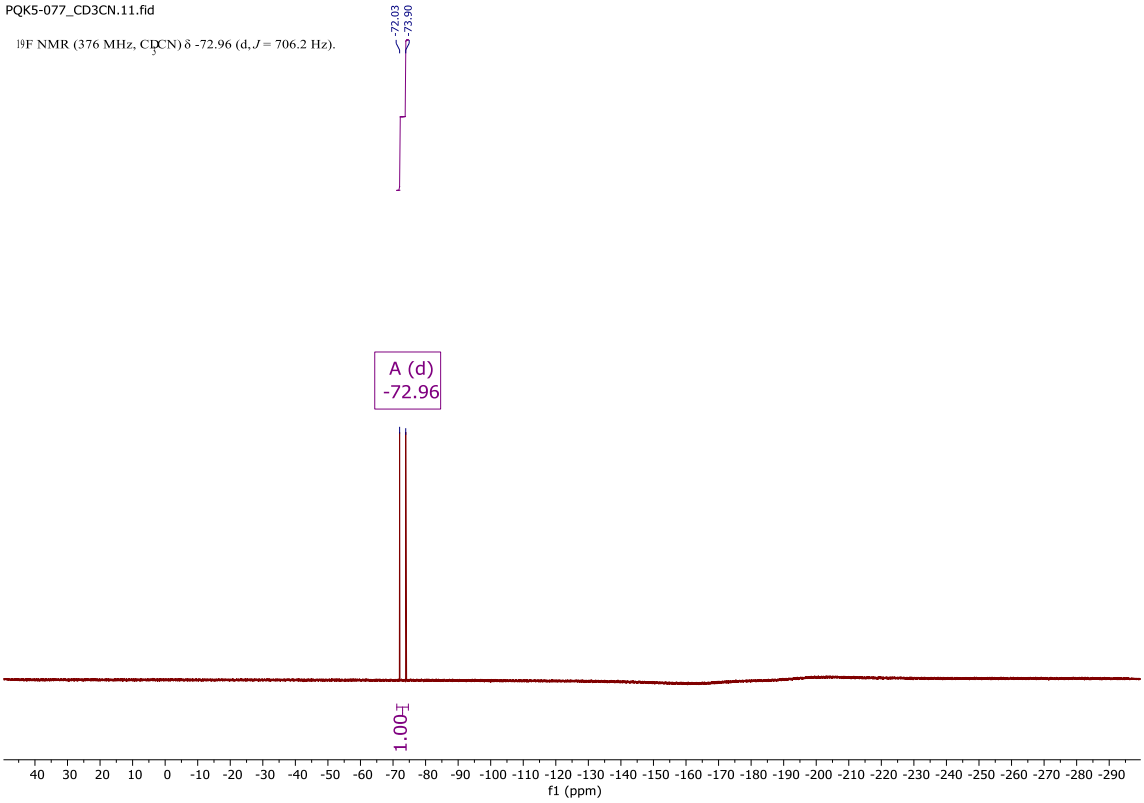

154.57
144.14
141.92
141.01
138.07
128.66
127.80
127.66
126.50
125.49
121.64
120.75
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
48.50
24.85
230 210 190 170 150 130 110 90 70 50 30 10
f1 (ppm)

3a


f1 (ppm)
f2 (ppm)
PF6
Ph
N
H
Os
Cl
{1.94,1.32}CD3CN
{3.00,30.51}
{2.91,29.98}
{6.24,42.90}
{8.46,125.89}
{8.24,125.72}
{8.29,125.01}
{7.91,130.29}
{6.81,130.02}
{7.28,129.15}
{8.24,142.60}
{7.48,131.61}
{7.45,135.21}
{7.94,139.52}
{9.18,153.94}
{8.92,153.67}

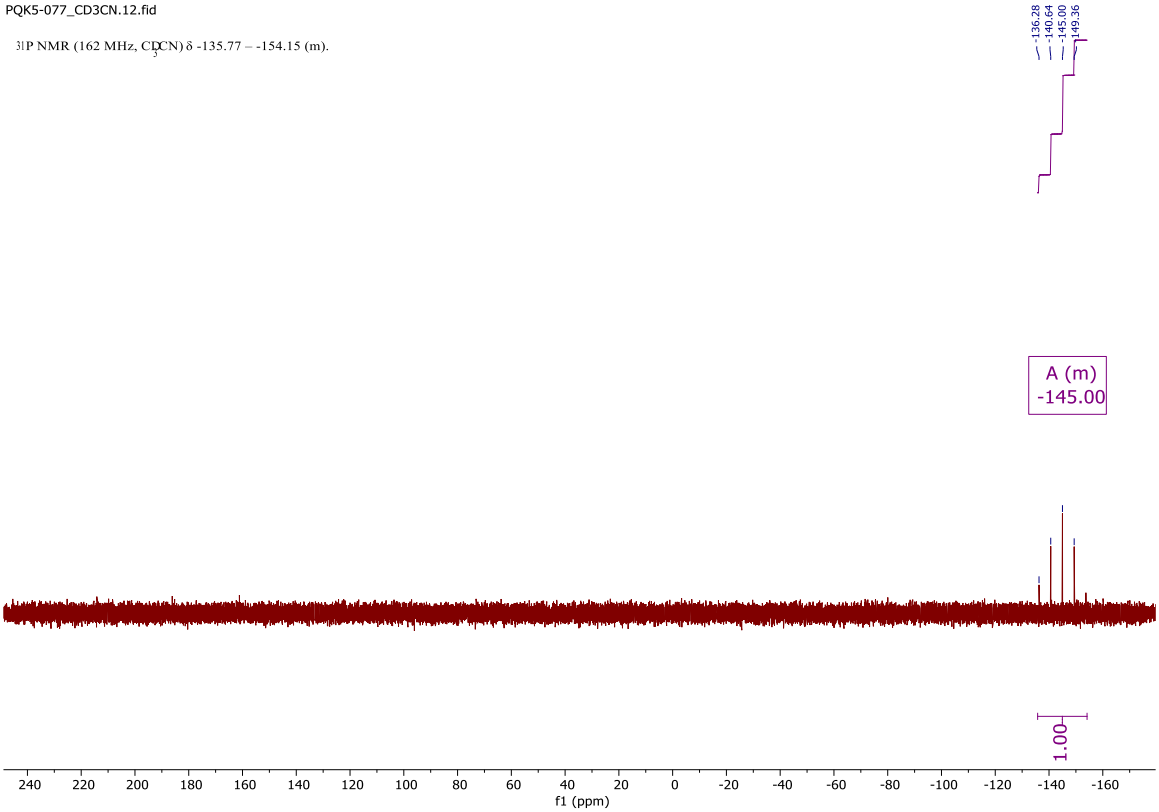
PQK5-077_CD3CN.11.fid

^{19}F NMR (376 MHz, CD_3CN) δ -72.96 (d, J = 706.2 Hz).

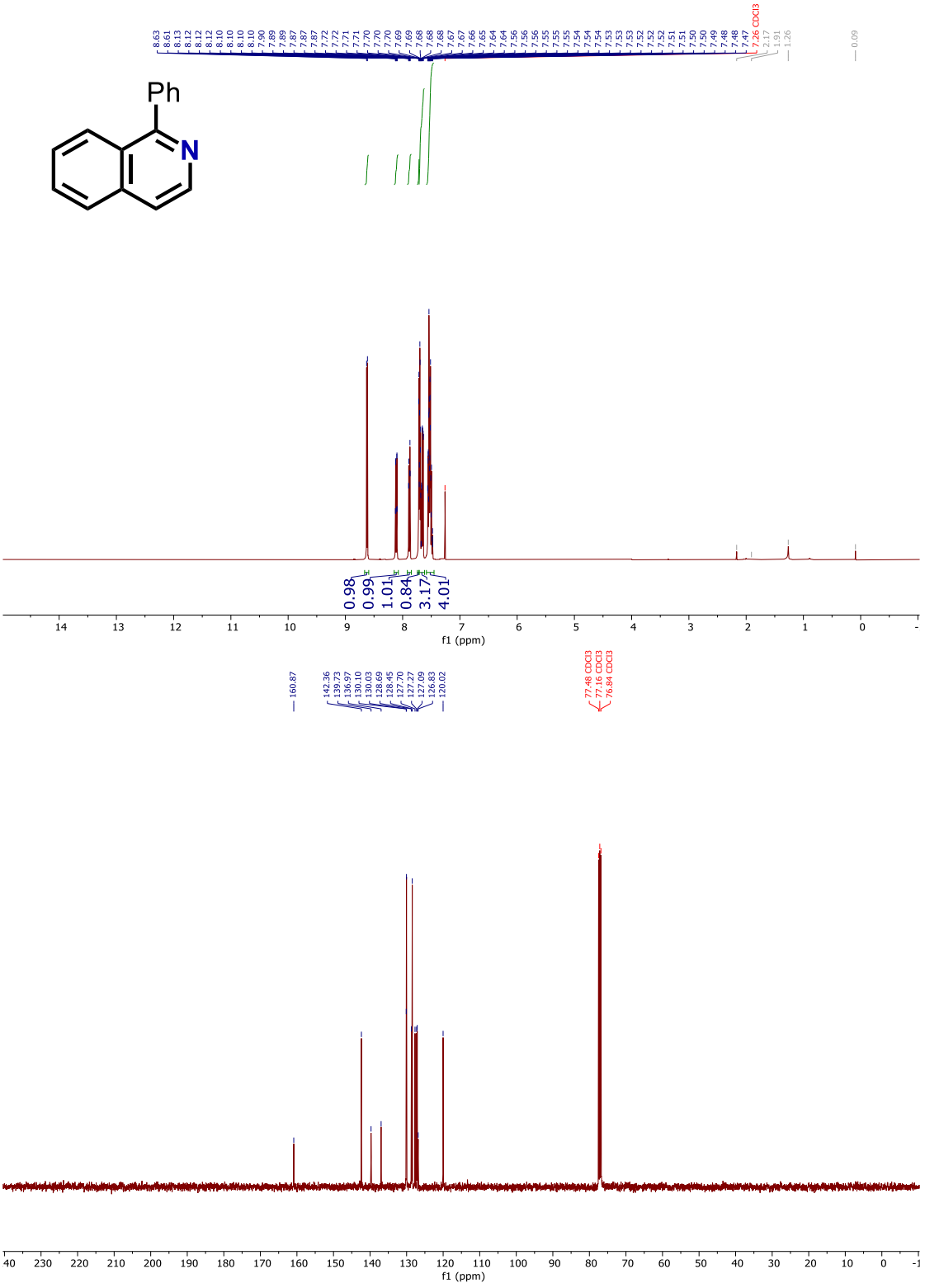


PQK5-077_CD3CN.12.fid

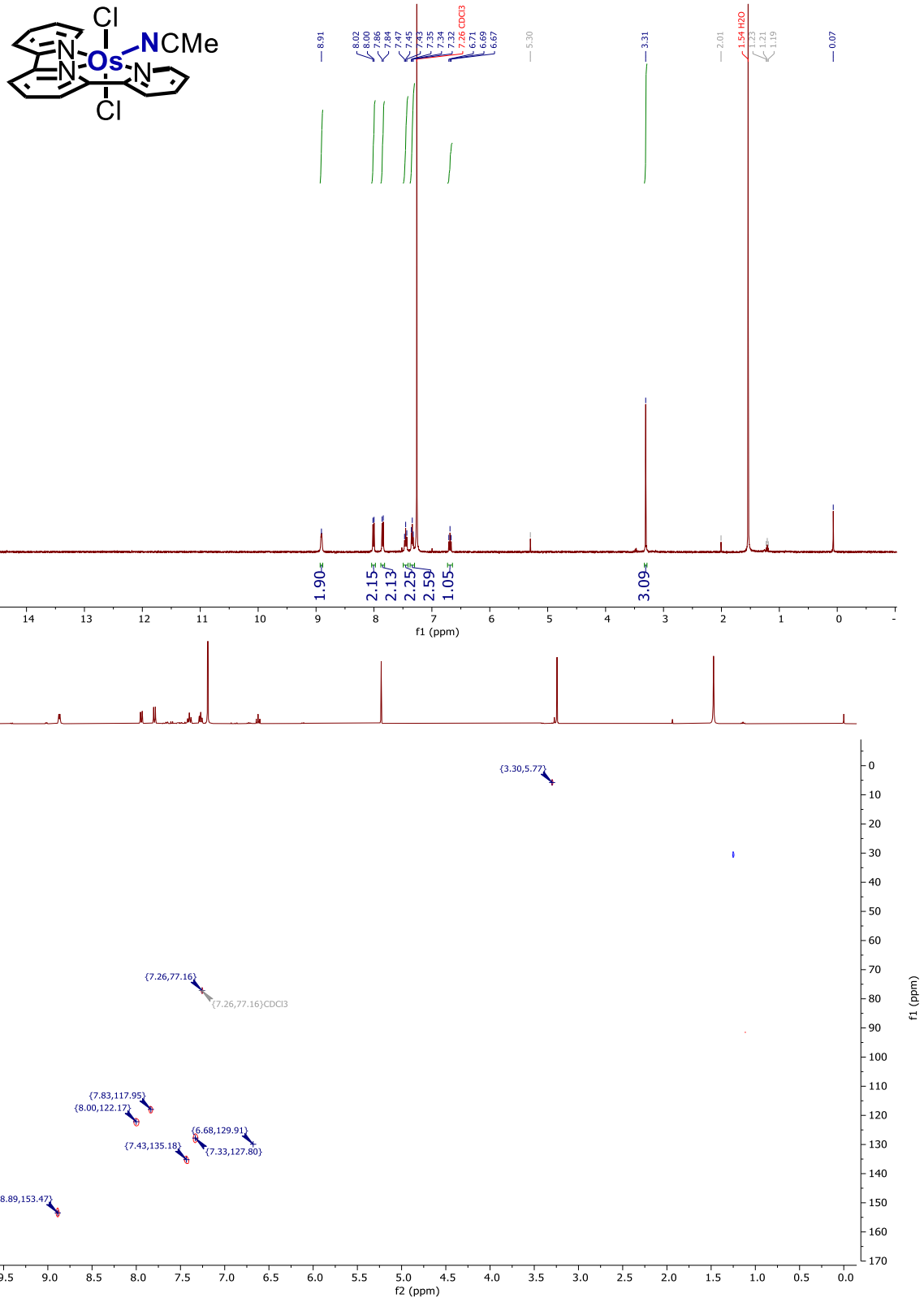
^{31}P NMR (162 MHz, CD_3CN) δ -135.77 – -154.15 (m).



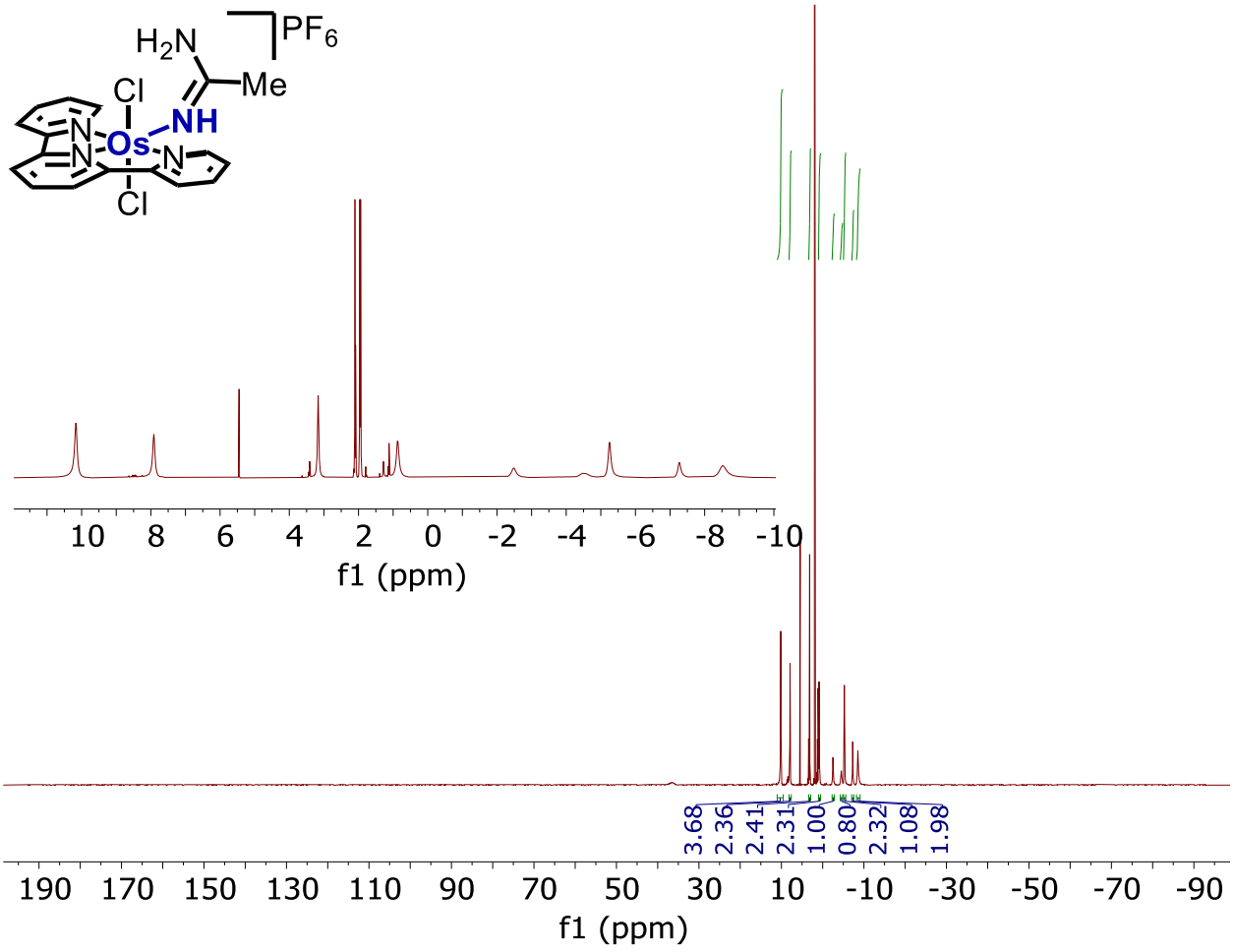
4

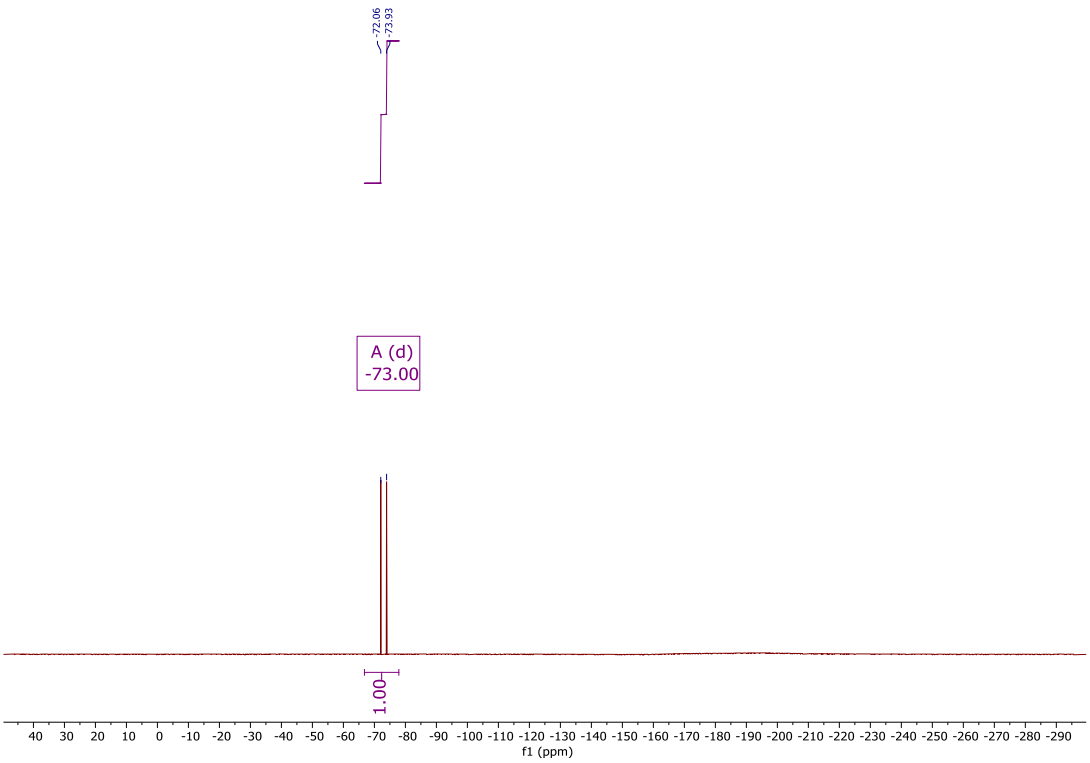


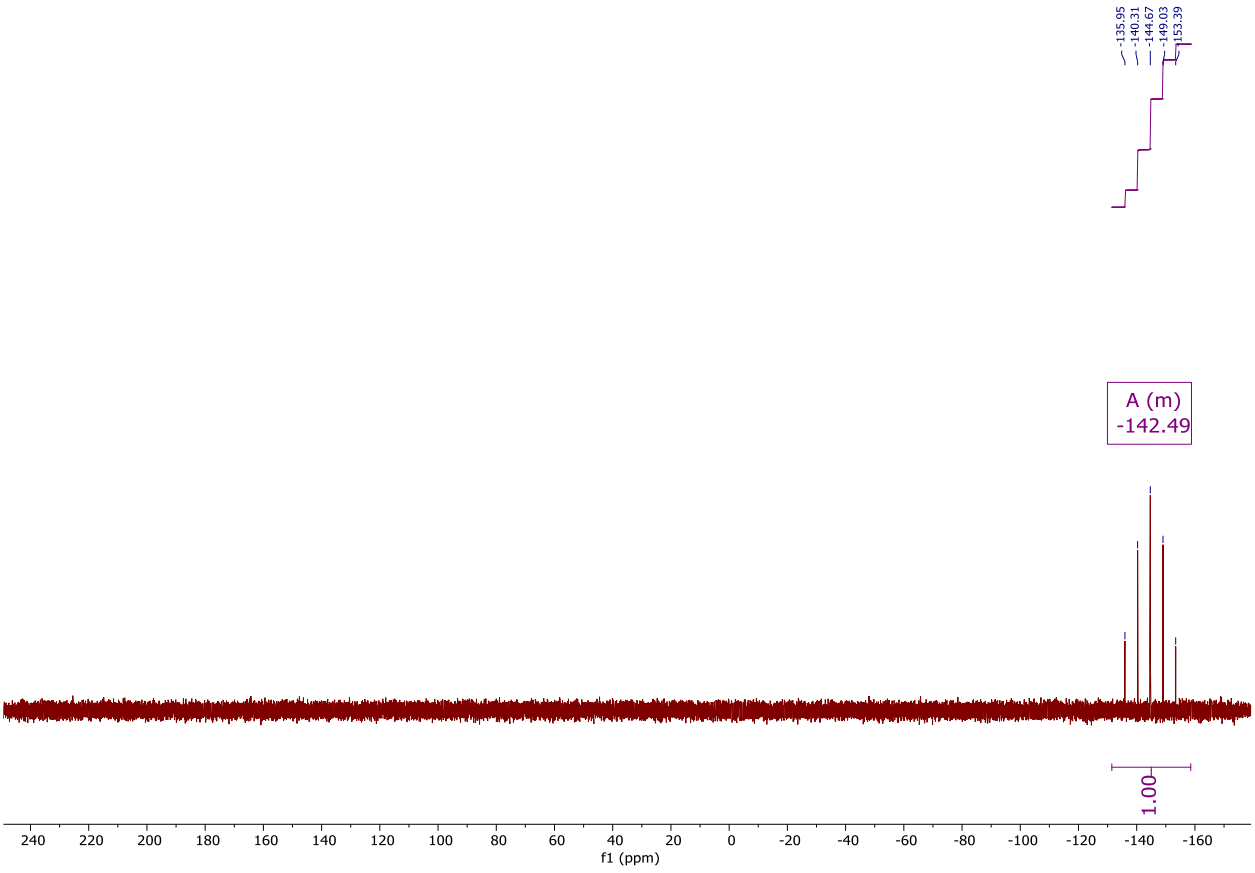
5


Cl
NCMe
Os
N
N
N
Cl
8.91
8.02
8.00
7.86
7.84
7.47
7.45
7.43
7.35
7.34
7.32
7.26 CDCl3
6.71
6.69
6.67
5.30
3.31
2.01
1.54 H2O
1.23
1.21
1.19
0.07
1.90
2.15
2.13
2.25
2.59
1.05
3.09
f1 (ppm)
{3.30,5.77}
{7.26,77.16}
{7.26,77.16}CDCl3
{7.83,117.95}
{8.00,122.17}
{6.68,129.91}
{7.43,135.18}
{7.33,127.80}
{8.89,153.47}
f2 (ppm)
f1 (ppm)

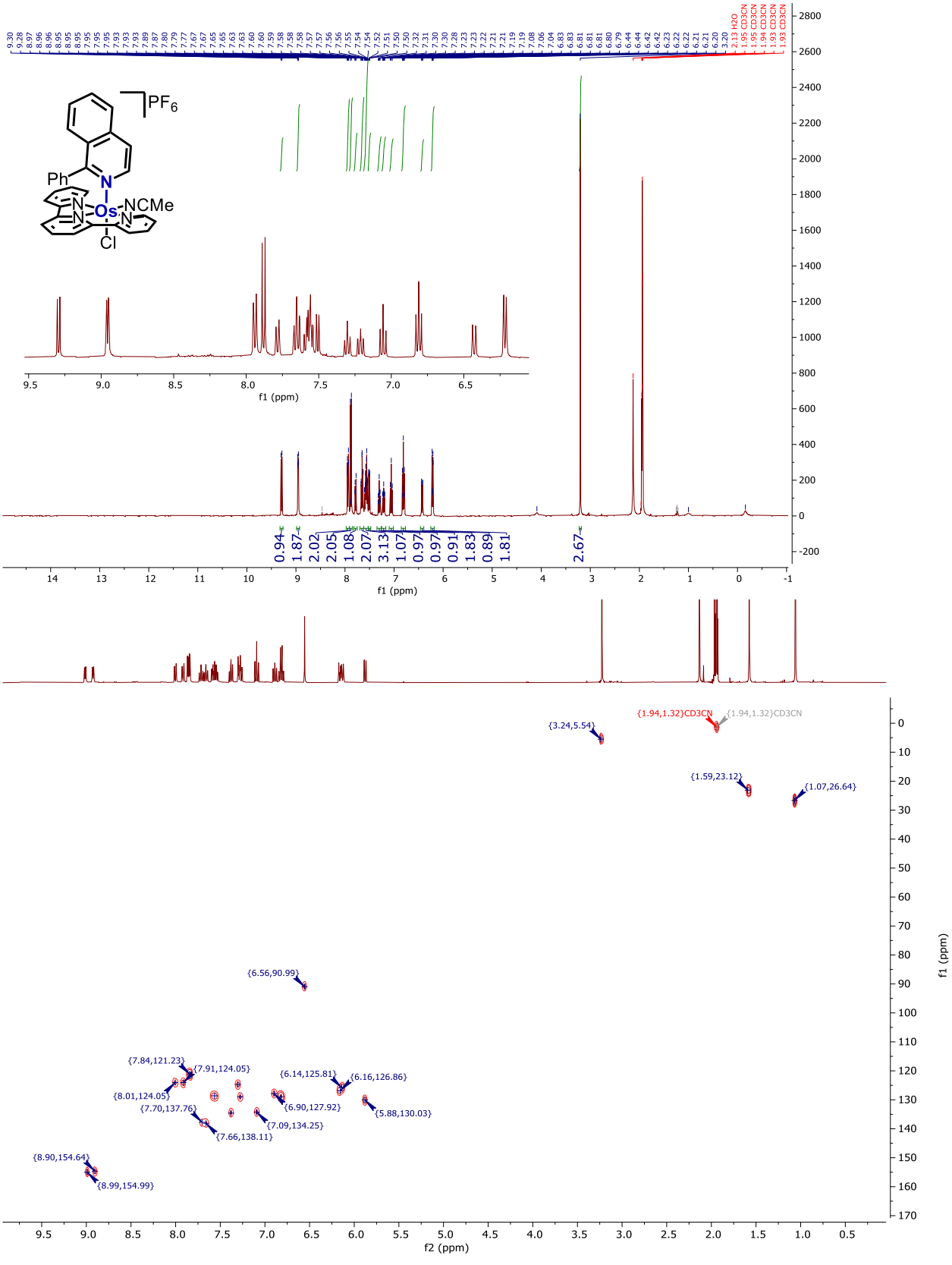
6

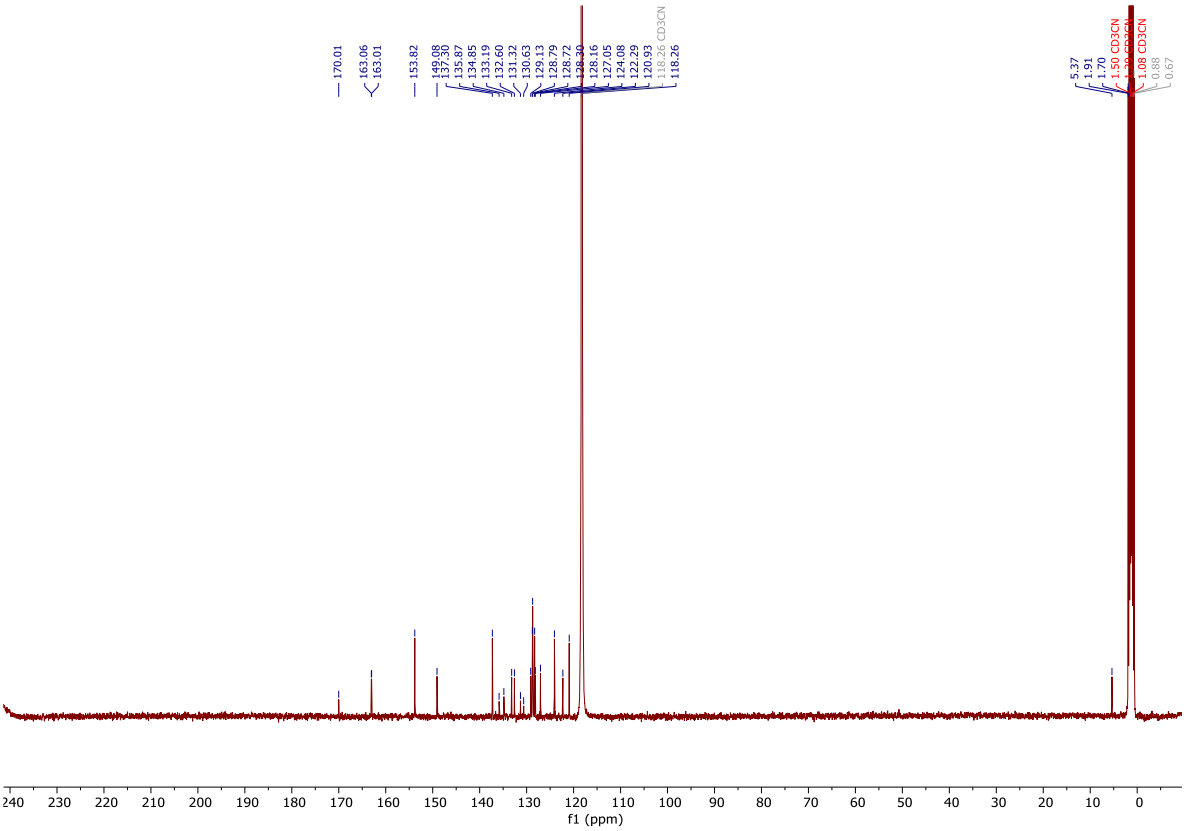

H2N
PF6
Me
Cl
NH
N
Os
N
N
Cl
10 8 6 4 2 0 -2 -4 -6 -8 -10
f1 (ppm)
3.68
2.36
2.41
2.31
1.00
0.80
2.32
1.08
1.98
190 170 150 130 110 90 70 50 30 10 -10 -30 -50 -70 -90
f1 (ppm)

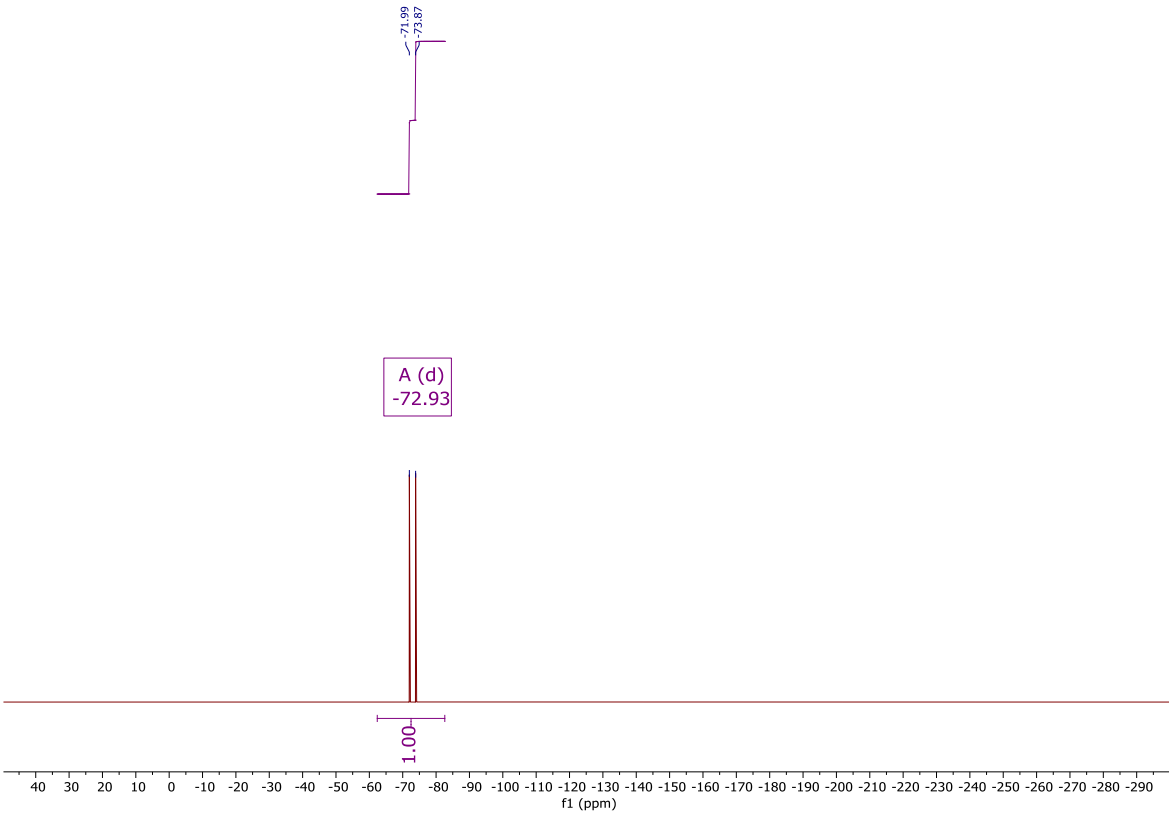

-72.06
-73.93
A (d)
-73.00
1.00
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260 -270 -280 -290
f1 (ppm)

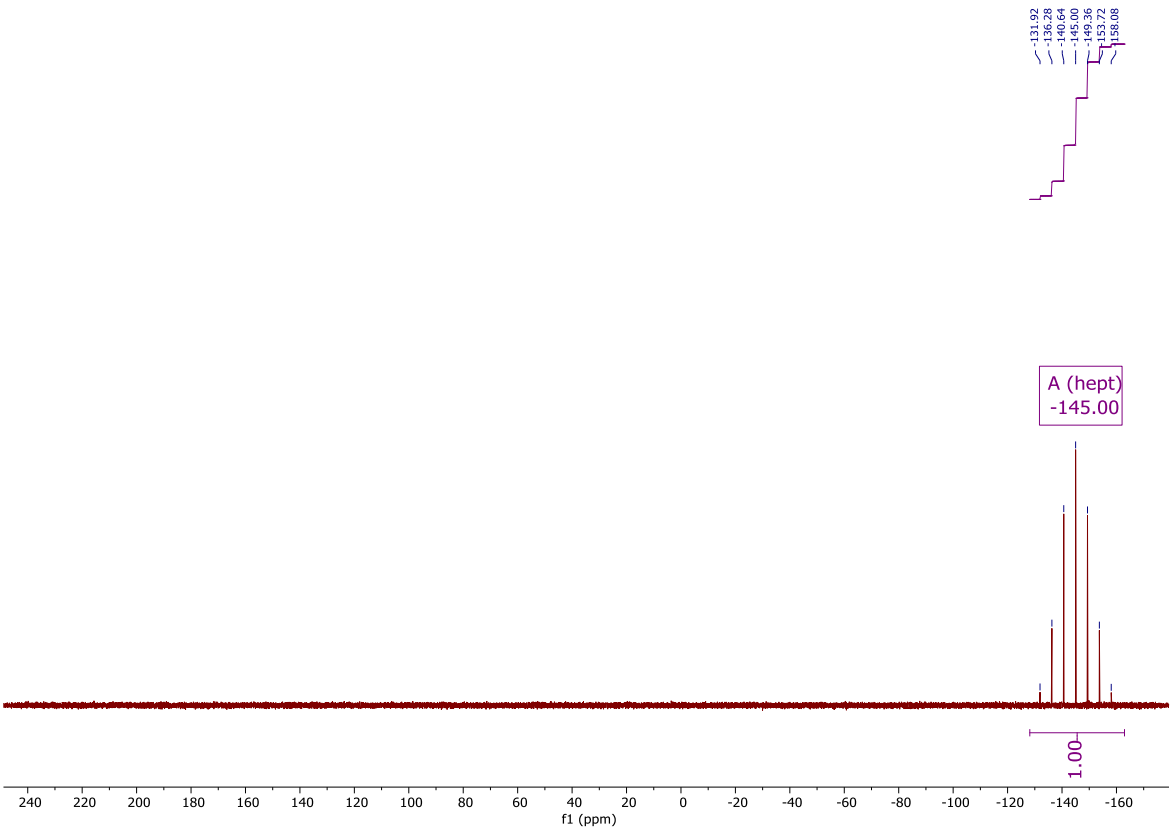

-135.95
-140.31
-144.67
-149.03
-153.39
A (m)
-142.49
1.00
240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)

7

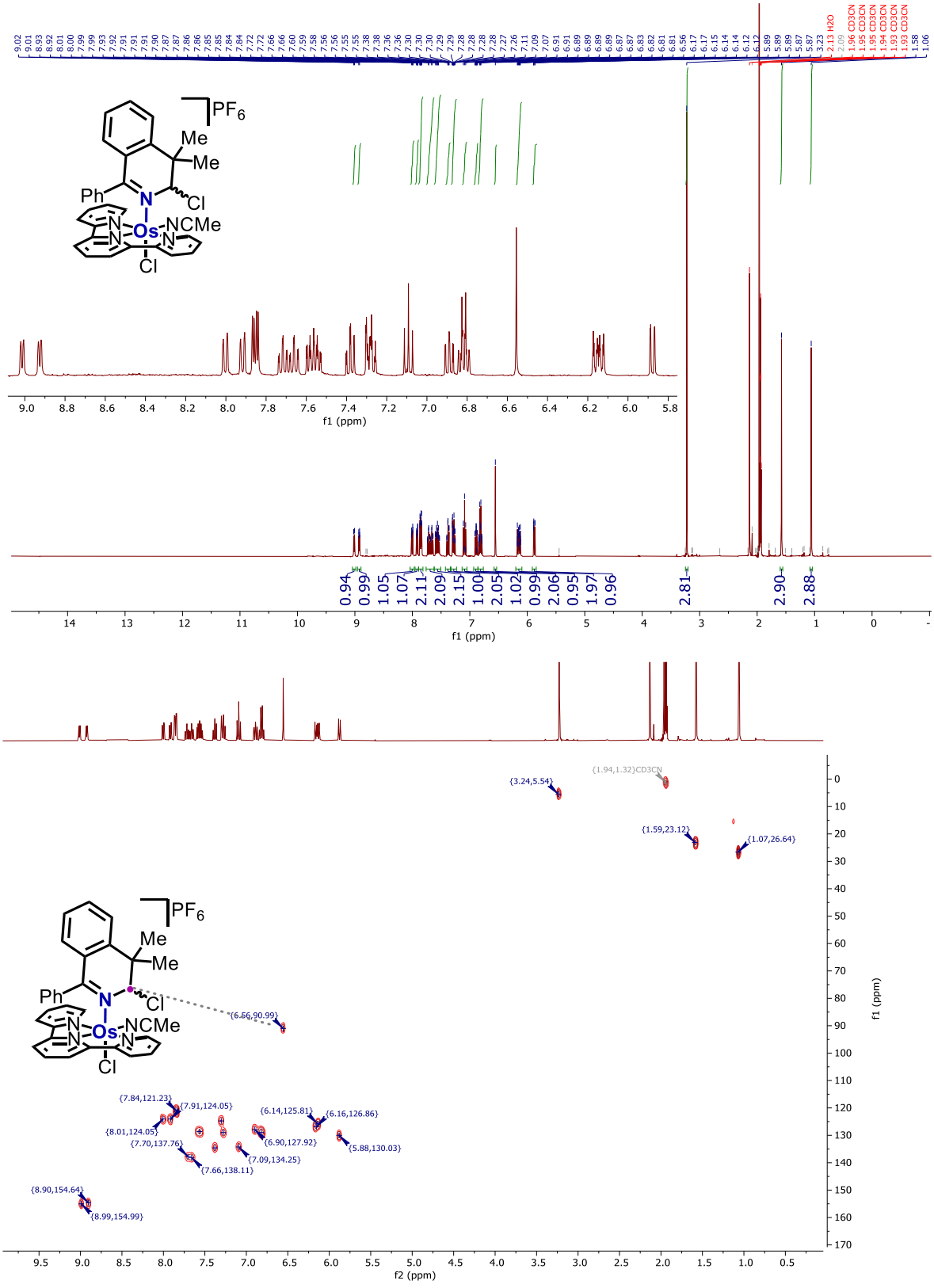

PF6
Ph
N
Os
NCMe
Cl
f1 (ppm)
0.94
1.87
2.02
2.05
1.08
2.07
3.13
1.07
0.97
0.97
0.91
1.83
0.89
1.81
2.67
{1.94,1.32}CD3CN
{1.94,1.32}CD3CN
{3.24,5.54}
{1.59,23.12}
{1.07,26.64}
{6.56,90.99}
{7.84,121.23}
{7.91,124.05}
{8.01,124.05}
{7.70,137.76}
{7.66,138.11}
{6.14,125.81}
{6.16,126.86}
{6.90,127.92}
{7.09,134.25}
{5.88,130.03}
{8.90,154.64}
{8.99,154.99}
f2 (ppm)
f1 (ppm)

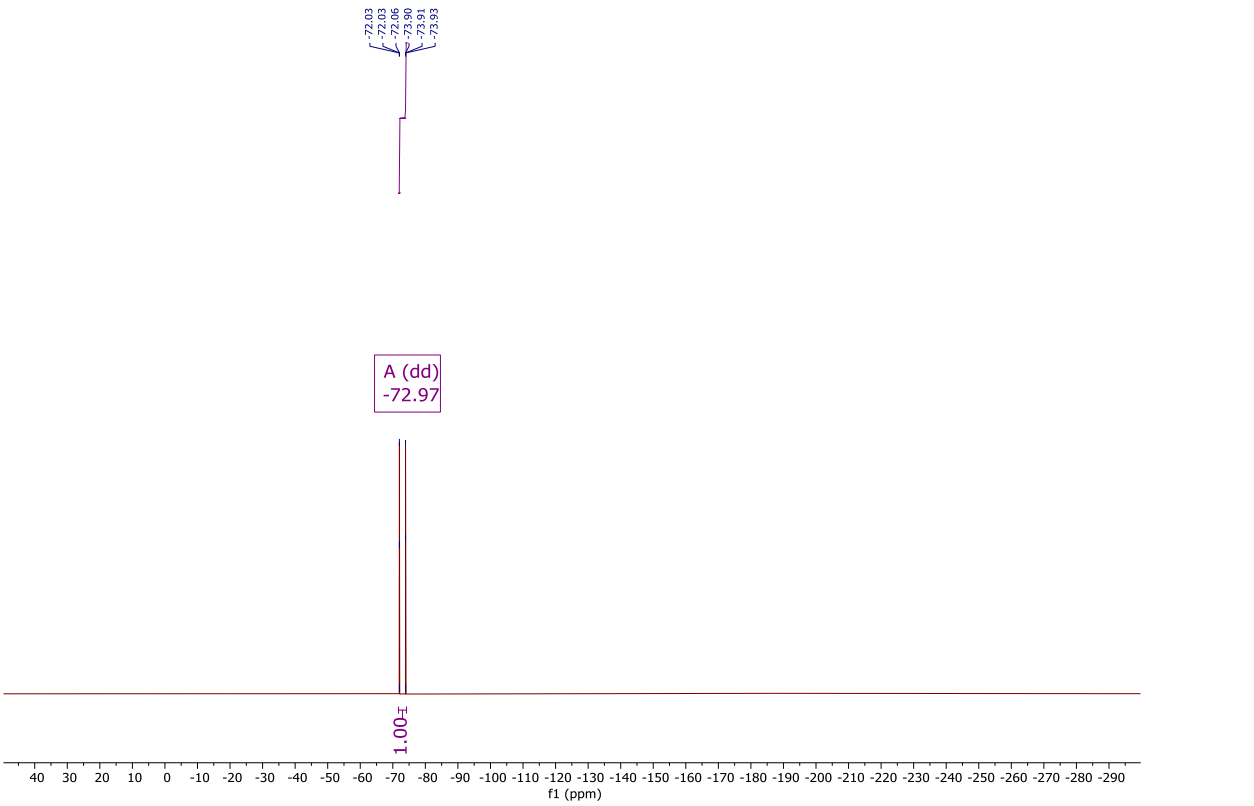

170.01
163.06
163.01
153.82
149.08
137.30
135.87
134.85
133.19
132.60
131.32
130.63
129.13
128.79
128.72
128.32
128.16
127.05
124.08
122.29
120.93
118.26 CD3CN
118.26
5.37
1.91
1.70
1.50 CD3CN
1.08 CD3CN
0.88
0.67
f1 (ppm)

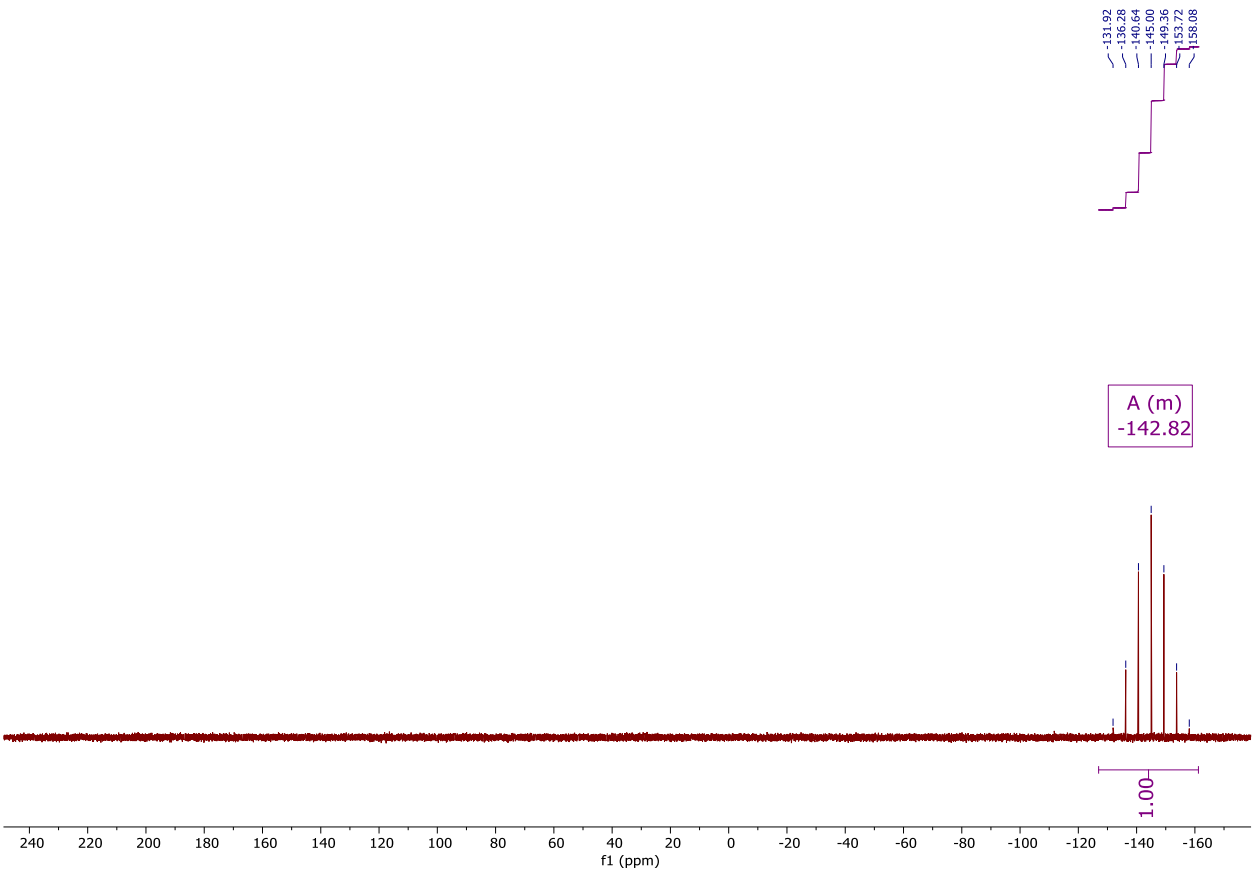

-71.99
-73.87
A (d)
-72.93
1.00
f1 (ppm)


-131.92
-136.28
-140.64
-145.00
-149.36
-153.72
-158.08
A (hept)
-145.00
1.00
240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)

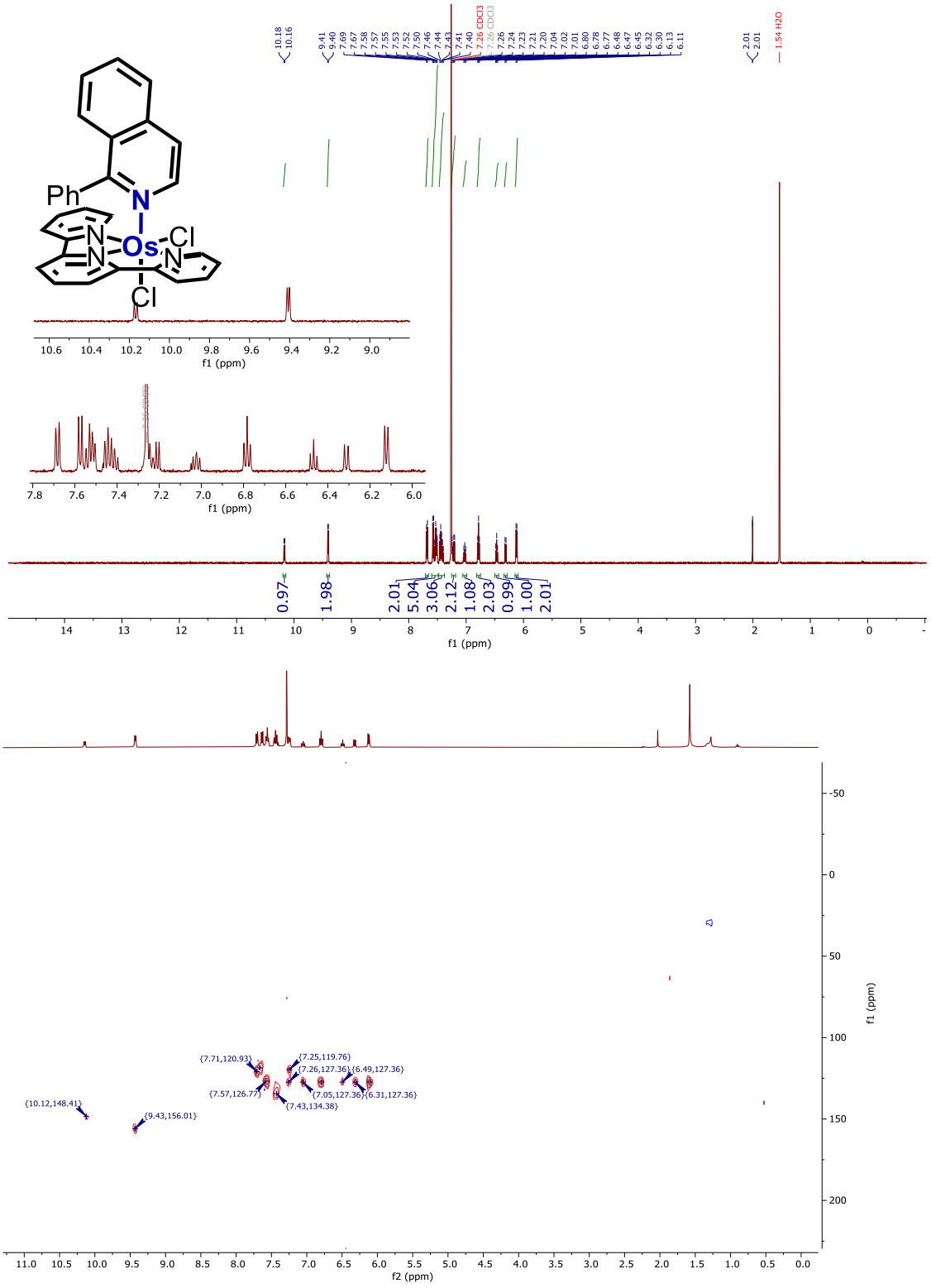
8


PF6
Me
Me
Ph
N
Cl
N
Os
NCMe
N
N
Cl
f1 (ppm)
0.94
0.99
1.05
1.07
2.11
2.09
2.15
1.00
2.05
1.02
0.99
2.06
0.95
1.97
0.96
2.81
2.90
2.88
{1.94,1.32}CD3CN
{3.24,5.54}
{1.59,23.12}
{1.07,26.64}
{6.56,90.99}
{7.84,121.23}
{7.91,124.05}
{8.01,124.05}
{7.70,137.76}
{7.66,138.11}
{6.14,125.81}
{6.16,126.86}
{6.90,127.92}
{7.09,134.25}
{5.88,130.03}
{8.90,154.64}
{8.99,154.99}
f2 (ppm)
f1 (ppm)

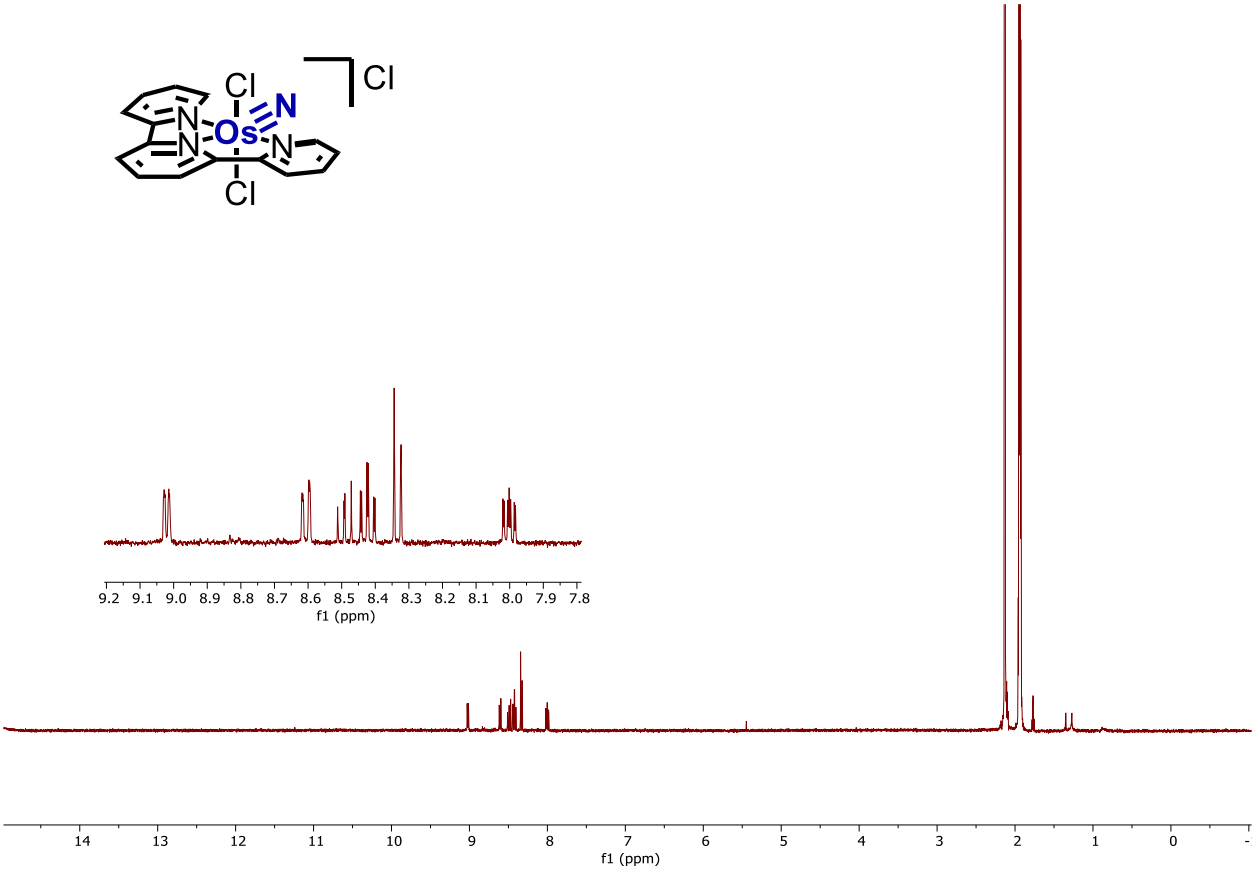

-72.03
-72.03
-72.06
-73.90
-73.91
-73.93
A (dd)
-72.97
1.00
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260 -270 -280 -290
f1 (ppm)


-131.92
-136.28
-140.64
-145.00
-149.36
-153.72
-158.08
A (m)
-142.82
1.00
240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)

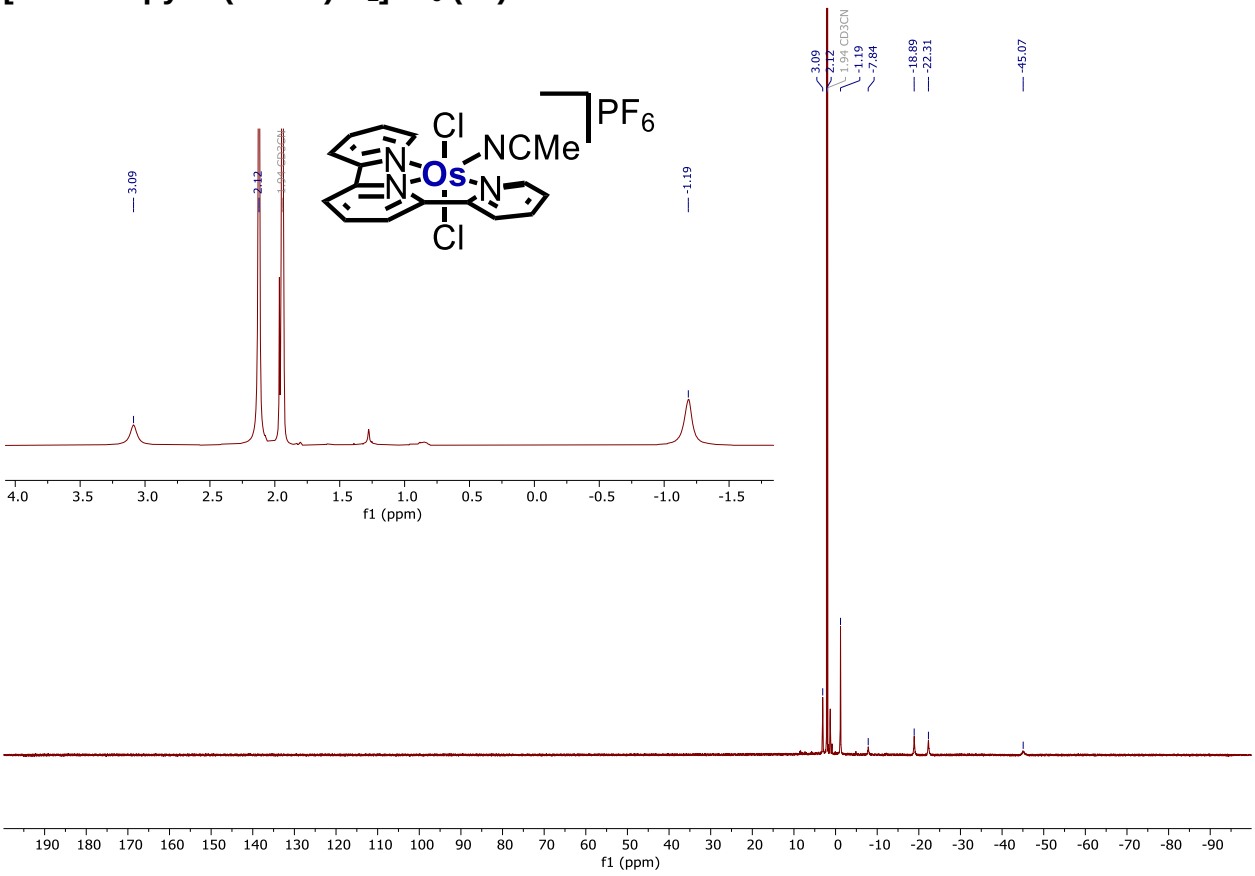
9

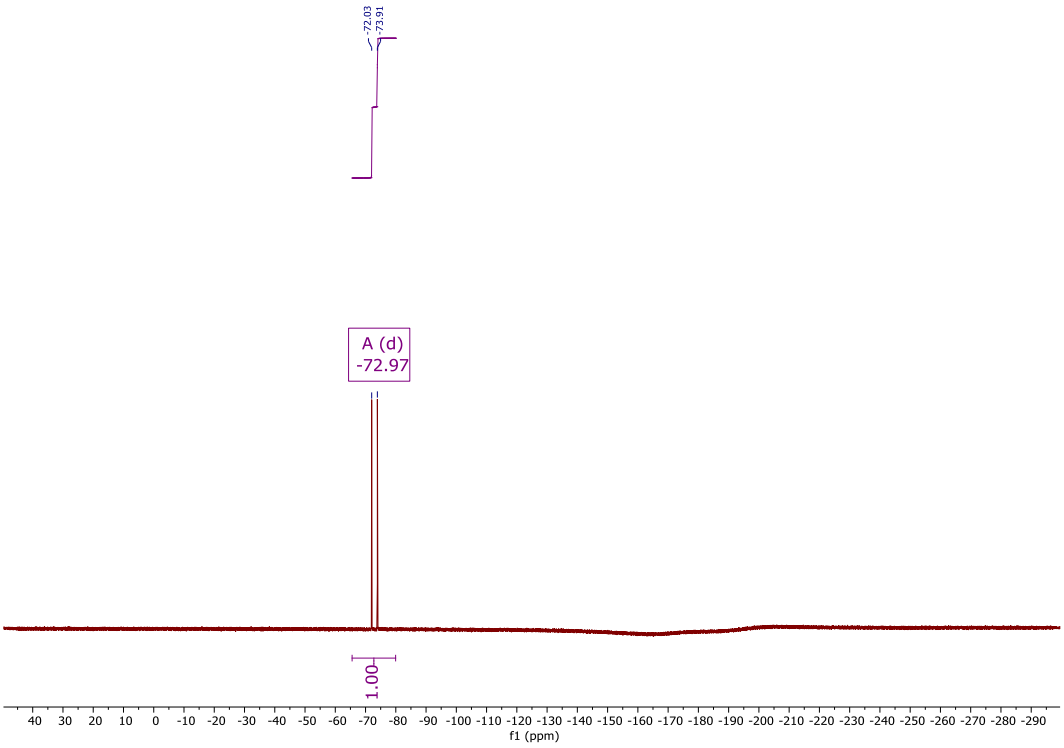

Ph
N
Os
Cl
Cl
f1 (ppm)
0.97
1.98
2.01
5.04
3.06
2.12
1.08
2.03
0.99
1.00
2.01
f2 (ppm)
f1 (ppm)
{7.71,120.93}
{7.25,119.76}
{7.26,127.36}
{6.49,127.36}
{7.57,126.77}
{7.05,127.36}
{6.31,127.36}
{7.43,134.38}
{10.12,148.41}
{9.43,156.01}

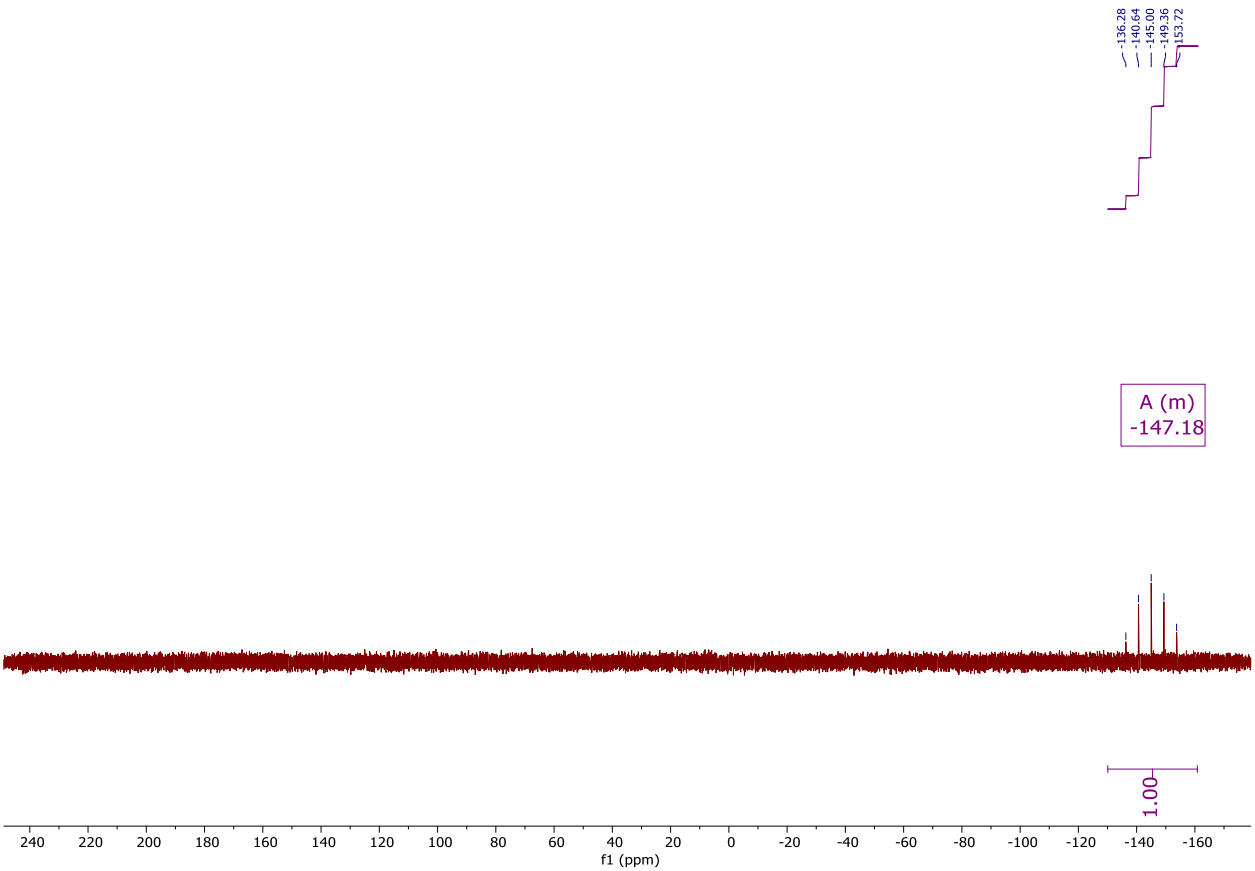
[*trans*-terpyOsNCl$_2$]Cl (10)



[*trans*-terpyOs(NCMe)Cl_2]PF_6 (11)






-136.28
-140.64
-145.00
-149.36
-153.72
A (m)
-147.18
1.00
240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160
f1 (ppm)

9. Crystallographic details

The diffraction data for **5**, **6**, and **8** were measured at 100 K on a Bruker D8 VENTURE diffractometer equipped with a microfocus Mo-target X-ray tube (λ = 0.71073 Å) and PHOTON 100 CMOS detector. Data were collected using ϕ scans. The data reduction and integration were performed with the Bruker APEX4 software package (Bruker AXS, version 2017.3-0, 2018). Data were scaled and corrected for absorption effects using the multi-scan procedure as implemented in SADABS. The structures were solved by SHELXT and refined by a full-matrix least-squares procedure using SHELXL. Crystallographic data and details of the data collection and structure refinement are listed in table S2.

Table S4. Crystallographic and refinement data for complexes

Compound	5	7	8
Empirical formula	$C_{17.5}H_{15}Cl_3N_4Os$	$C_{36}H_{35}ClF_6N_5OOsP$	$C_{36}H_{33}Cl_2F_6N_6OsP$
Formula weight	577.88	924.31	955.75
Temperature/K	100.00	100(2)	100(2)
Crystal system	triclinic	monoclinic	monoclinic
Space group	P-1	$P2_1/c$	$P2_1/n$
a/Å	8.7833(6)	10.3859(9)	13.7254(6)
b/Å	12.9573(9)	25.871(2)	20.4491(9)
c/Å	16.9575(12)	13.7021(11)	14.1861(6)
α/°	87.923(2)	90	90
β/°	89.343(2)	99.733(2)	111.9870(10)
γ/°	71.487(2)	90	90
Volume/Å^3	1828.8(2)	3628.7(5)	3692.1(3)
Z	4	4	4
ρ_{calc}g/cm^3	2.099	1.692	1.719
μ/mm^{-1}	7.420	3.700	0.904
F(000)	1100.0	1824.0	1880.0
Crystal size/mm^3	0.406 × 0.291 × 0.174	0.24 × 0.16 × 0.13	0.002 × 0.002 × 0.002
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	synchrotron (λ = 0.41328)
2Θ range for data collection/°	4.808 to 71.214	4.36 to 52.866	2.048 to 29.958
Index ranges	-14 ≤ h ≤ 14, -21 ≤ k ≤ 21, -27 ≤ l ≤ 27	-12 ≤ h ≤ 12, -32 ≤ k ≤ 31, -17 ≤ l ≤ 17	-17 ≤ h ≤ 17, -25 ≤ k ≤ 25, -17 ≤ l ≤ 17
Reflections collected	74777	61471	98580
Independent reflections	15749 [R_{int} = 0.0305, R_{sigma} = 0.0289]	7161 [R_{int} = 0.1155, R_{sigma} = 0.0979]	7396 [R_{int} = 0.0543, R_{sigma} = 0.0222]
Data/restraints/parameters	15749/0/462	7161/0/463	7396/134/486
Goodness-of-fit on F^2	1.066	1.101	1.064
Final R indexes [I>=2σ (I)]	R_1 = 0.0256, wR_2 = 0.0485	R_1 = 0.0569, wR_2 = 0.1002	R_1 = 0.0494, wR_2 = 0.1264
Final R indexes [all data]	R_1 = 0.0382, wR_2 = 0.0516	R_1 = 0.1033, wR_2 = 0.1100	R_1 = 0.0515, wR_2 = 0.1273
Largest diff. peak/hole / e Å^{-3}	1.57/-1.54	2.12/-1.49	3.07/-4.17

Compound	**6**	**terpyOs(phisq)Cl_2 PF_6 (additional attempted crystallization of 3a)**	**9**
Empirical formula	$C_{19}H_{20}Cl_2F_6N_6OsP$	$C_{30}H_{22}Cl_2F_6N_4OsP$	$C_{32}H_{26}Cl_4N_4Os$
Formula weight	738.48	844.58	798.57
Temperature/K	100(2)	100(2)	100.00
Crystal system	triclinic	monoclinic	monoclinic
Space group	P-1	$P2_1/n$	C2/c
a/Å	7.4440(4)	15.9951(16)	25.4099(19)
b/Å	13.9894(8)	13.9851(14)	14.4653(11)
c/Å	24.6751(14)	17.5090(18)	17.1632(13)
α/°	103.657(2)	90	90
β/°	91.346(2)	116.483(2)	114.790(2)
γ/°	104.576(2)	90	90
Volume/Å^3	2407.2(2)	3505.7(6)	5727.2(8)
Z	4	4	8
ρ_{calc}g/cm^3	2.038	1.600	1.852
μ/mm^{-1}	5.654	3.892	4.857
F(000)	1420.0	1636.0	3120.0
Crystal size/mm^3	0.297 × 0.113 × 0.094	0.366 × 0.224 × 0.051	0.306 × 0.127 × 0.057
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.116 to 51.482	4.63 to 51.522	4.664 to 61.248
Index ranges	$-9 \le h \le 9$, $-17 \le k \le 17$, $-30 \le l \le 30$	$-19 \le h \le 19$, $-16 \le k \le 17$, $-21 \le l \le 21$	$-36 \le h \le 36$, $-20 \le k \le 20$, $-24 \le l \le 24$
Reflections collected	59407	45508	108764
Independent reflections	9150 [R_{int} = 0.0695, R_{sigma} = 0.0495]	6679 [R_{int} = 0.1310, R_{sigma} = 0.0880]	8819 [R_{int} = 0.0544, R_{sigma} = 0.0256]
Data/restraints/parameters	9150/431/701	6679/60/397	8819/0/370
Goodness-of-fit on F^2	1.089	1.011	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0664, wR_2 = 0.1366	R_1 = 0.0726, wR_2 = 0.1675	R_1 = 0.0296, wR_2 = 0.0672
Final R indexes [all data]	R_1 = 0.0856, wR_2 = 0.1435	R_1 = 0.1206, wR_2 = 0.1960	R_1 = 0.0410, wR_2 = 0.0713
Largest diff. peak/hole / e Å^{-3}	3.28/-3.66	6.33/-1.58	1.60/-2.35

10. Computational Details

Conformational searches were conducted for all ground states using Crest as implemented in the XTB python package.[12] Conformers within 6 kcal/mol of the minimum (typically 1-50) were used as starting coordinates for geometry optimization conducted using density functional theory (DFT) in Gaussian16 (Revision A.03).[13] The lowest energy conformers are reported in the main text Fig. 2. Each structure was optimized using the polarizable continuum model (PCM)[14,15] in acetonitrile (MeCN) at the B3LYP-D3 level of theory[16,17] with the SDD basis set for osmium and the 6-31g(d) basis set for the other atoms.[18] Frequency calculations were conducted at the same level to check whether each optimized structure is an energy minimum or transition state. Single point energy calculations were conducted using PCM(MeCN) at the B3LYP-D3 level of theory with the SDD basis set for osmium and the 6-311+g(d,p) basis set for the other atoms. Transition states were verified by intrinsic reaction coordinate (IRC) calculations. Quasi-harmonic corrected free energies (Gtz) for each compound were computed using Grimme entropic corrections[17] and Head-Gordon enthalpic corrections[19] as implemented in Paton's GoodVibes python package.[20]

11. Supplemental computational figures

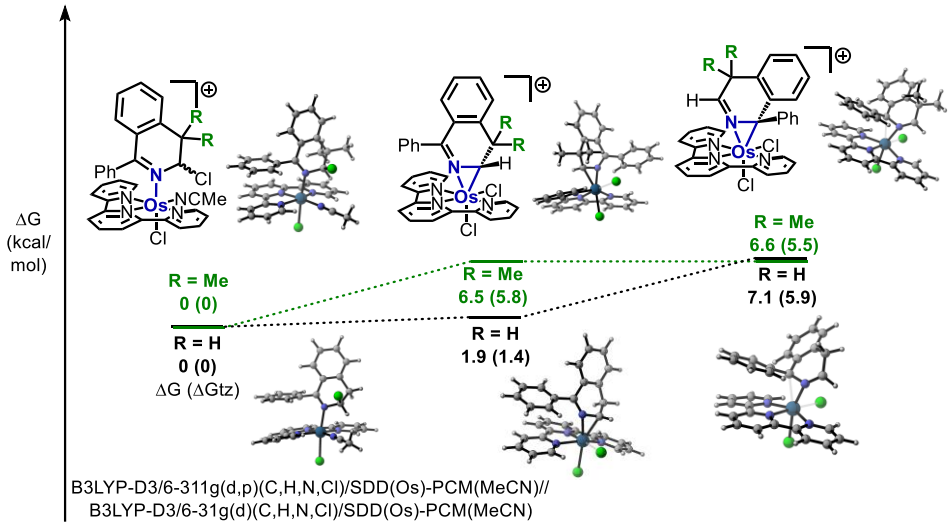


Figure S18: Stability of Aza-allyl chloride relative to azaallenium for **3a** and **3b**. Energies are referenced to the starting indene, **1**, and free MeCN.

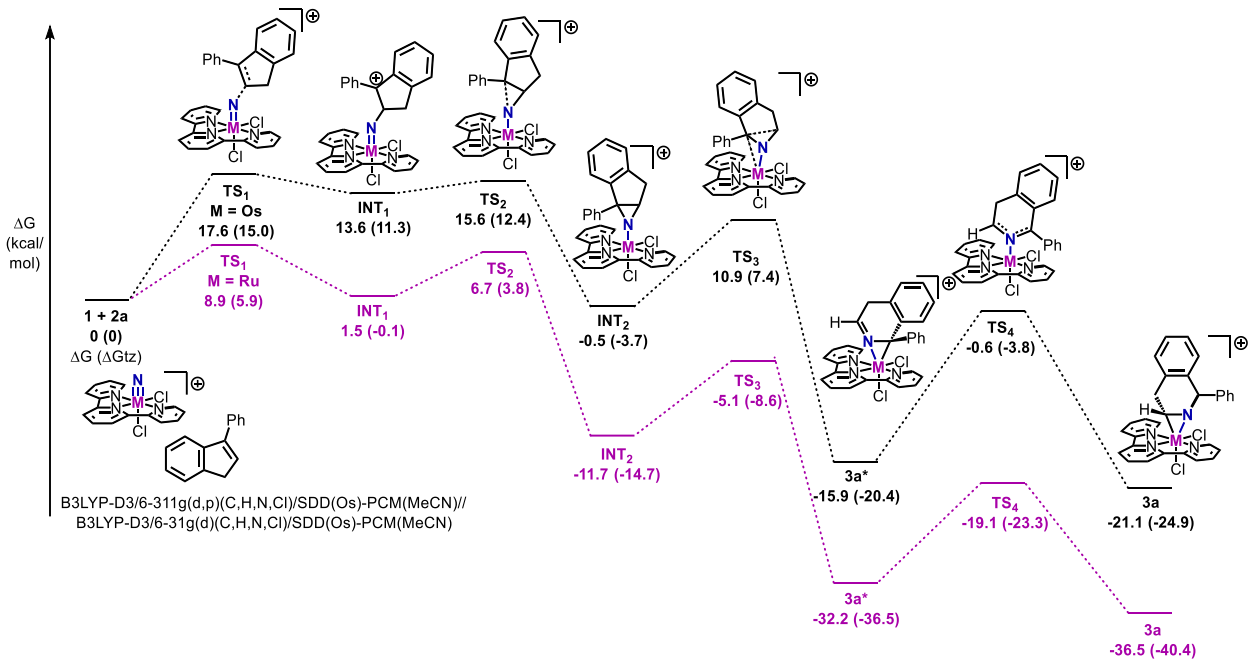


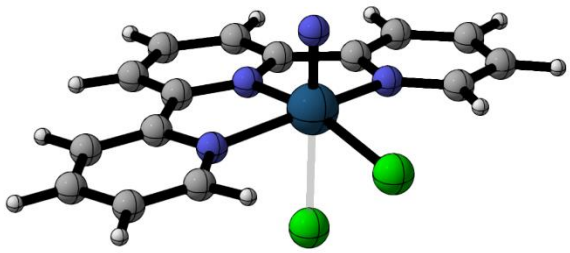
Figure S19: Energy diagram for insertion of $[(terpy)MNCl_2]^+$ (M = Os and Ru) into **2a**. DFT energy values indicate that N-atom insertion is feasible with either metal.

Table S5: Computational Energies

Structure	E	G(T)	qh-G(T)	E_SPC	G(T)_SPC	qh-G(T)_SPC
1	-1134759.102	-1134638.961	-1134639.348	-1134924.453	-1134804.312	-1134804.7
1-Ru	-1137375.821	-1137255.568	-1137255.968	-1137540.767	-1137420.515	-1137420.915
2a	-363231.7555	-363115.6826	-363115.8364	-363321.2006	-363205.1277	-363205.2815
g16_2a_freq	-363231.7555	-363115.6826	-363115.8364	N/A	N/A	N/A
2f	-412577.1619	-412427.6258	-412427.8298	-412679.619	-412530.0836	-412530.2869
3a-isom	-1498025.194	-1497770.584	-1497770.805	-1498284.757	-1498030.146	-1498030.368
3a-isom-Ru	-1500657.932	-1500403.462	-1500403.666	-1500916.917	-1500662.447	-1500662.651
3a	-1498030.759	-1497776.05	-1497776.121	-1498289.937	-1498035.227	-1498035.298
3a-Ru	-1500662.644	-1500407.794	-1500407.856	-1500921.367	-1500666.518	-1500666.579
3f-isom	-1547369.781	-1547081.204	-1547081.53	-1547642.875	-1547354.298	-1547354.624
3f	-1547369.719	-1547081.255	-1547081.239	-1547642.8	-1547354.336	-1547354.32
8	-1630699.4	-1630384.632	-1630384.385	-1630998.351	-1630683.583	-1630683.337
8-no-Me	-1581354.901	-1581074.462	-1581074.126	-1581640.311	-1581359.871	-1581359.535
INT1	-1497993.418	-1497741.019	-1497740.945	-1498251.194	-1497998.795	-1497998.721
INT1-Ru	-1500621.517	-1500369.736	-1500369.512	-1500879.002	-1500627.222	-1500626.997
INT2	-1498009.903	-1497756.997	-1497756.804	-1498268.158	-1498015.253	-1498015.06
INT2-Ru	-1500636.445	-1500382.926	-1500382.903	-1500894.419	-1500640.9	-1500640.878
MeCN	-83310.36266	-83296.82352	-83296.82917	-83336.7469	-83323.20777	-83323.21279
TS1	-1497989.856	-1497738.115	-1497738.026	-1498248.393	-1497996.652	-1497996.562
TS1-Ru	-1500614.257	-1500362.36	-1500362.291	-1500872.258	-1500620.361	-1500620.292
TS2	-1497991.099	-1497739.013	-1497738.851	-1498249.871	-1497997.785	-1497997.623

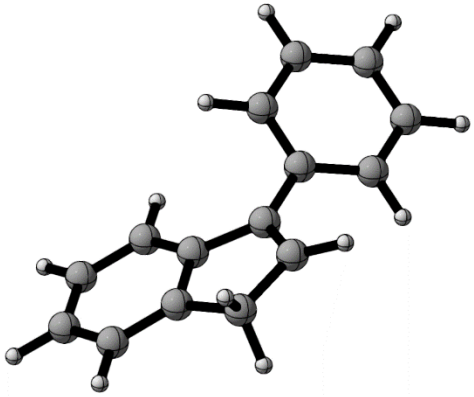
TS2-Ru	-1500617.309	-1500364.569	-1500364.487	-1500875.217	-1500622.477	-1500622.395
TS3	-1497995.808	-1497743.65	-1497743.558	-1498254.882	-1498002.725	-1498002.632
TS3-Ru	-1500628.781	-1500376.373	-1500376.304	-1500887.281	-1500634.873	-1500634.804
TS4	-1498008.311	-1497754.699	-1497754.751	-1498267.331	-1498013.719	-1498013.771
TS4-Ru	-1500642.957	-1500390.383	-1500390.118	-1500902.363	-1500649.788	-1500649.524

12. DFT coordinates



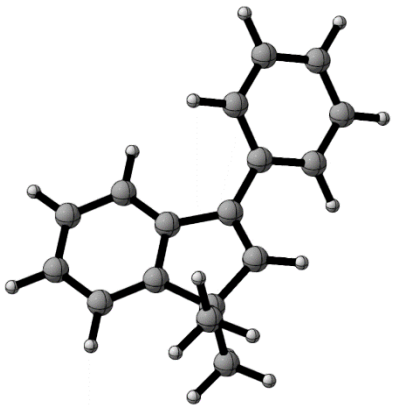
1

Os	0.00005	-0.68679	-0.33435
C	3.04010	-1.21868	-0.00128
C	2.35707	1.03927	-0.07905
C	4.37681	-0.84333	0.10944
H	2.71921	-2.25314	-0.01377
C	3.67615	1.46261	0.02622
C	4.69610	0.51180	0.11895
H	5.14075	-1.60796	0.18413
H	3.91086	2.51949	0.04230
C	1.19770	1.95635	-0.12374
C	-1.19786	1.95625	-0.12391
C	1.21785	3.34740	-0.03945
C	-1.21815	3.34729	-0.03962
C	-0.00018	4.03213	-0.01327
H	2.15294	3.88988	0.01730
H	-2.15330	3.88967	0.01704
C	-3.03999	-1.21894	-0.00145
C	-2.35716	1.03906	-0.07930
C	-4.37673	-0.84369	0.10941
H	-2.71903	-2.25338	-0.01387
C	-3.67626	1.46230	0.02604
C	-4.69612	0.51141	0.11891
H	-5.14058	-1.60838	0.18427
H	-3.91106	2.51915	0.04215
N	-0.00005	1.33538	-0.19828
N	-2.06603	-0.30291	-0.09828
N	2.06606	-0.30272	-0.09804
N	-0.00001	-0.85503	-1.97976
Cl	-0.00049	-0.36237	2.24772
Cl	0.00054	-3.05252	0.16816
H	-0.00024	5.11448	0.05042
H	-5.72801	0.83436	0.20198
H	5.72797	0.83484	0.20184



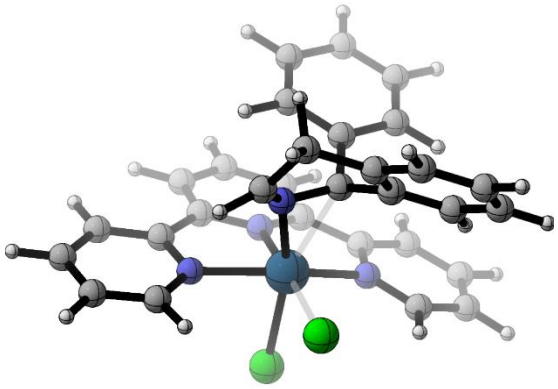
2a

C	-1.15507	-0.10353	0.02024
C	-2.28459	0.73404	-0.10680
C	-3.56951	0.21515	-0.01113
C	-3.73023	-1.15840	0.21866
C	-2.61288	-1.98891	0.36118
C	-1.31692	-1.46955	0.26789
C	0.06004	0.73200	-0.10613
C	-0.32056	2.01945	-0.28992
H	-4.43799	0.86224	-0.10817
H	-4.72914	-1.57966	0.29335
H	-2.75201	-3.04999	0.55095
H	-0.45678	-2.11923	0.39695
H	0.35506	2.85506	-0.43582
C	-1.82039	2.15558	-0.31511
C	1.45086	0.24151	-0.04485
C	1.83196	-0.95225	-0.68309
C	2.43605	0.97934	0.63501
C	3.15594	-1.39156	-0.64385
H	1.09173	-1.52474	-1.23373
C	3.75952	0.54116	0.67240
H	2.15122	1.89416	1.14742
C	4.12477	-0.64805	0.03485
H	3.43122	-2.31366	-1.14877
H	4.50487	1.12443	1.20656
H	5.15465	-0.99265	0.06834
H	-2.17709	2.57903	-1.26531
H	-2.18957	2.82927	0.47209



2f

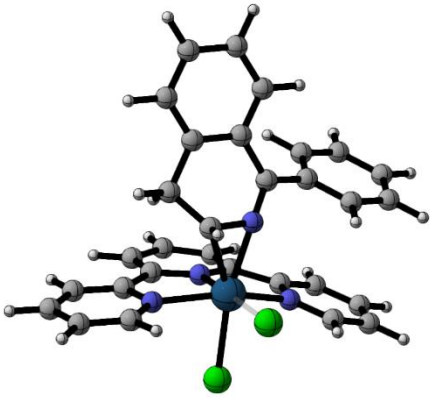
C	0.71502	0.66941	0.06451
C	1.98528	0.06089	-0.00606
C	3.14294	0.82240	0.08046
C	3.03224	2.21103	0.24499
C	1.77366	2.81509	0.33203
C	0.60408	2.04985	0.24694
C	-0.31204	-0.39292	-0.03702
C	0.31909	-1.58407	-0.15174
H	4.12211	0.35238	0.02684
H	3.92974	2.82006	0.31197
H	1.70097	3.89051	0.47135
H	-0.36799	2.52570	0.33277
H	-0.17112	-2.54605	-0.26491
C	1.82762	-1.44461	-0.15102
C	-1.77255	-0.18210	-0.01729
C	-2.36517	0.88511	-0.71551
C	-2.60927	-1.06851	0.68369
C	-3.74997	1.05797	-0.71353
H	-1.73904	1.56697	-1.28297
C	-3.99322	-0.89664	0.68400
H	-2.16213	-1.88674	1.24153
C	-4.56951	0.16941	-0.01288
H	-4.18895	1.88552	-1.26440
H	-4.62190	-1.59076	1.23540
H	-5.64728	0.30699	-0.00835
C	2.43458	-1.95920	-1.47551
H	3.51938	-1.80285	-1.48537
H	2.24370	-3.03205	-1.59361
H	2.00297	-1.43431	-2.33416
C	2.45821	-2.19622	1.04336
H	2.26902	-3.27267	0.96119
H	3.54310	-2.04117	1.06369
H	2.04165	-1.84291	1.99242



3a-isomer

Os	-0.42315	-0.50322	-0.67989
C	-2.51181	-2.73286	-0.12209
C	-3.03532	-0.56898	0.64693
C	-3.68410	-3.25078	0.41924
H	-1.79341	-3.33811	-0.66348
C	-4.21897	-1.03919	1.21375
C	-4.54332	-2.39089	1.10305
H	-3.90781	-4.30501	0.30545
H	-4.88430	-0.35883	1.73087
C	-2.62711	0.85065	0.63420
C	-0.98693	2.31422	-0.27868
C	-3.33928	1.93466	1.14871
C	-1.66555	3.42398	0.22396
C	-2.83432	3.22206	0.95998
H	-4.27210	1.78538	1.67817
H	-1.29860	4.42641	0.04289
C	1.65693	0.99076	-2.43817
C	0.19767	2.32332	-1.16023
C	2.27600	2.11503	-2.97273
H	1.94147	-0.02156	-2.69956
C	0.78642	3.48296	-1.66445
C	1.83984	3.37846	-2.56964
H	3.08250	1.99410	-3.68650
H	0.42018	4.45547	-1.35940
N	-1.45196	1.07160	-0.00234
N	0.66350	1.09332	-1.54060
N	-2.19259	-1.43488	0.00063
N	0.27452	-1.24498	1.07834
Cl	-1.66369	-0.27150	-2.75846
Cl	0.76972	-2.44400	-1.66325
C	4.88980	-0.92902	-0.08219
C	5.14004	-2.05050	0.71082
C	4.12614	-2.57989	1.51327
C	3.62805	-0.33337	-0.07111

C	2.60906	-0.85991	0.72707
C	2.85939	-1.99494	1.52678
H	4.31888	-3.45482	2.12792
H	3.44145	0.53104	-0.69551
H	5.67247	-0.51700	-0.71185
H	6.12012	-2.51800	0.70219
C	1.24022	-0.26984	0.88482
C	0.43904	-2.36037	1.68912
C	1.74171	-2.56557	2.39763
H	1.89009	-3.62853	2.60160
H	1.72103	-2.05512	3.37306
H	-0.31589	-3.13347	1.58901
C	1.08821	0.98699	1.67246
C	0.06116	1.10640	2.62814
C	-0.12182	2.29510	3.32809
C	0.71477	3.39010	3.08607
C	1.74894	3.27545	2.15524
C	1.94044	2.08235	1.45805
H	2.40971	4.11585	1.96527
H	2.75051	2.01329	0.74269
H	-0.92306	2.36931	4.05711
H	0.56457	4.32108	3.62432
H	-0.60297	0.26842	2.81166
H	-5.46205	-2.76400	1.54274
H	-3.36813	4.07394	1.36589
H	2.30575	4.27479	-2.96461



3a

Os	0.88782	-0.65461	-0.60236
C	3.77513	0.45323	-0.82840
C	2.79589	0.50640	1.31079
C	4.94553	1.02889	-0.34666
H	3.63543	0.17994	-1.86764
C	3.94514	1.09034	1.84297
C	5.02745	1.35710	1.00730
H	5.76837	1.21701	-1.02642
H	3.99567	1.32737	2.89864
C	1.61417	0.12197	2.10623
C	-0.42691	-1.09119	1.94328
C	1.43738	0.27868	3.48196
C	-0.64665	-0.94649	3.31250
C	0.28214	-0.23306	4.07391
H	2.18605	0.77958	4.08318
H	-1.51218	-1.39466	3.78421
C	-1.24690	-2.84154	-1.16513
C	-1.19122	-1.94758	1.01094
C	-2.27574	-3.71235	-0.82122
H	-0.81131	-2.80273	-2.15649
C	-2.24384	-2.77312	1.39822
C	-2.78933	-3.66344	0.47338
H	-2.66952	-4.39795	-1.56227
H	-2.62425	-2.73664	2.41132
N	0.64854	-0.48826	1.37660
N	-0.73042	-1.97985	-0.27743
N	2.72877	0.20910	-0.02374
N	-0.56451	0.78159	-0.96937
Cl	2.20252	-2.67086	-0.21393
Cl	1.16156	-1.01857	-3.04782
C	-2.72098	5.00761	-0.46373
C	-1.47708	5.63120	-0.33511
C	-0.30268	4.87067	-0.28755
C	-2.79396	3.61862	-0.54252
C	-1.61942	2.84953	-0.49426
C	-0.35952	3.48269	-0.37007
H	0.66044	5.36276	-0.18625
H	-3.75469	3.12782	-0.65463
H	-3.62878	5.60066	-0.50921
H	-1.41673	6.71396	-0.27689
C	-1.65135	1.38008	-0.56223
C	0.65559	1.41091	-1.15986
C	0.88306	2.61011	-0.26820
H	1.78175	3.15323	-0.56840
H	1.01161	2.31946	0.78109
H	0.94864	1.52751	-2.20429
C	-2.85955	0.61210	-0.21864
C	-3.55083	0.87430	0.97745
C	-4.69443	0.14379	1.29326
C	-5.17649	-0.82192	0.40397
C	-4.50545	-1.06672	-0.79737
C	-3.34389	-0.36147	-1.10580
H	-4.88089	-1.81298	-1.49043
H	-2.81747	-0.54179	-2.03734

H	-5.21279	0.33270	2.22825
H	-6.07503	-1.38152	0.64616
H	-3.17744	1.63199	1.65915
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H	0.12195	-0.10766	5.13883
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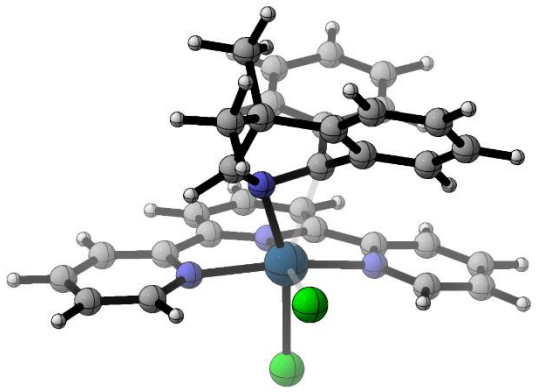

3f-isomer

Os	-0.47022	-0.35342	-0.84171
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C	-2.31103	-4.30540	-0.21514
H	-0.71525	-3.44022	-1.42285
C	-3.46636	-2.67712	1.13450
C	-3.29963	-3.99788	0.71938
H	-2.15870	-5.31862	-0.56816
H	-4.24064	-2.42226	1.84770
C	-2.76776	-0.24722	0.92558
C	-1.93027	1.88629	0.28432
C	-3.72532	0.35046	1.74545
C	-2.87052	2.52269	1.09413
C	-3.75288	1.74246	1.84326
H	-4.44141	-0.25093	2.29155
H	-2.92226	3.60317	1.13940
C	0.62886	2.14669	-2.32060
C	-0.98500	2.52799	-0.65079
C	0.71037	3.50519	-2.60495
H	1.21146	1.39749	-2.84328
C	-0.93769	3.90069	-0.89363
C	-0.07692	4.39419	-1.87125
H	1.38076	3.85023	-3.38346
H	-1.57203	4.57512	-0.33182
N	-1.86887	0.53228	0.27795
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Cl	-2.02876	-0.20716	-2.70106
Cl	1.16224	-1.44749	-2.35825
C	4.64346	1.24374	-0.76859
C	5.41840	0.16284	-0.34947
C	4.82599	-0.90127	0.33525
C	3.27763	1.26273	-0.48927
C	2.67891	0.20229	0.19724
C	3.45559	-0.90638	0.60897
H	5.44645	-1.73252	0.65050
H	2.67910	2.09945	-0.82529
H	5.09481	2.06912	-1.31051
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C	1.38745	-2.18041	0.86343
C	2.80115	-2.07585	1.38052
H	0.93677	-3.13417	0.60481
C	0.76950	1.09521	1.68791
C	-0.07489	0.61311	2.70729
C	-0.56354	1.46832	3.68974
C	-0.22290	2.82533	3.67411
C	0.62803	3.31013	2.67970
C	1.12659	2.45304	1.69784
H	0.90602	4.35956	2.66132
H	1.78773	2.85170	0.93921
H	-1.21707	1.07677	4.46331
H	-0.61304	3.49500	4.43453
H	-0.35681	-0.43433	2.72123
H	-3.94199	-4.77528	1.11881
H	-4.48204	2.22233	2.48624
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H	2.92225	-4.23306	1.60724
H	3.57989	-3.64403	0.06258
C	2.80149	-1.76155	2.90335
H	2.29071	-0.81971	3.11879
H	2.30838	-2.56431	3.46119
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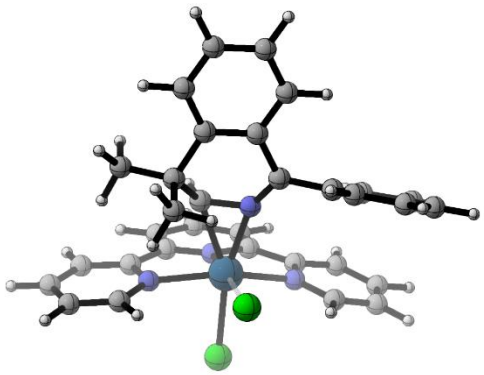

3f

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H	2.34955	1.40145	-2.57759
C	4.46753	1.31325	0.61241
C	4.91799	2.08873	-0.45611
H	4.50170	2.70370	-2.49381
H	5.04910	1.24967	1.52368
C	2.75685	-0.33116	1.51263
C	1.09193	-2.00394	1.84427
C	3.36272	-0.66392	2.72450
C	1.66801	-2.36515	3.06330
C	2.79274	-1.66892	3.50891
H	4.26673	-0.16413	3.04976
H	1.26205	-3.18082	3.64864
C	-1.20010	-2.83905	-0.88499
C	0.00116	-2.70264	1.13485
C	-1.79739	-4.03290	-0.49183
H	-1.40243	-2.36383	-1.83710
C	-0.60078	-3.87321	1.59238
C	-1.50627	-4.54545	0.77049
H	-2.49264	-4.52778	-1.15938
H	-0.34896	-4.27103	2.56778
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N	-0.86603	0.53760	0.29264
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C	-3.67139	2.59799	1.26031
C	-2.40272	2.25592	0.76482
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H	-0.88749	5.28962	1.08139
H	-4.44595	1.84075	1.31633
H	-4.90729	4.15419	2.08551
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C	-0.02359	2.85489	0.03273
H	0.64632	1.34157	1.46106
C	-3.19830	-0.06466	-0.02142
C	-3.34829	-1.25379	0.70452
C	-4.40610	-2.11703	0.41570
C	-5.30438	-1.80671	-0.60717
C	-5.15710	-0.61962	-1.33314
C	-4.11992	0.26034	-1.03028
H	-5.85541	-0.37543	-2.12790
H	-4.01090	1.19191	-1.57707
H	-4.51977	-3.03453	0.98468
H	-6.12136	-2.48458	-0.83618
H	-2.64862	-1.48951	1.50039
H	5.84690	2.64187	-0.36937
H	3.24738	-1.93253	4.45721
H	-1.97103	-5.46281	1.11541
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H	2.09219	3.32889	0.12473
H	1.05495	4.74370	0.25758
H	1.23257	3.65075	1.64416
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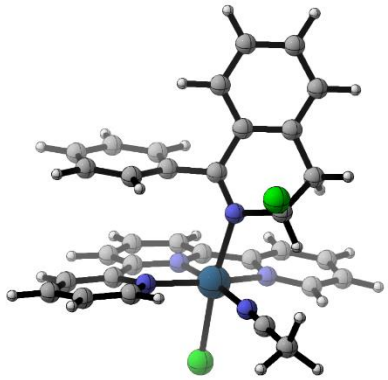

8-no-Me

Os	0.82358	-0.96494	-0.05911

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H	1.85972	-0.61986	-3.03186
C	3.30038	0.99877	-3.10980
H	3.51831	0.86780	-4.16380
C	3.93975	1.97924	-2.34886
H	4.67614	2.63789	-2.79668
C	3.61144	2.10724	-1.00226
H	4.08257	2.87115	-0.39577
C	2.65773	1.26038	-0.43783
C	2.20073	1.35666	0.95924
C	2.60846	2.28760	1.91395
H	3.34290	3.04474	1.66918
C	2.05015	2.23674	3.19215
H	2.34896	2.96229	3.94058
C	1.12322	1.24517	3.51742
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C	0.75407	0.31873	2.54106
C	-0.09498	-0.87429	2.72659
C	-0.75849	-1.17350	3.91697
H	-0.71952	-0.47863	4.74740
C	-1.46549	-2.36817	4.03497
H	-1.98820	-2.60465	4.95554
C	-1.47656	-3.25550	2.95870
H	-1.99609	-4.20555	3.01070
C	-0.80794	-2.90124	1.79171
H	-0.78543	-3.55595	0.92836
C	-0.74881	2.99815	0.84812
H	-1.35282	2.68992	1.69602
C	0.00547	4.16791	0.90858
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C	0.75748	4.57572	-0.19862
H	1.33732	5.49285	-0.15324
C	0.75808	3.80590	-1.36352
H	1.33797	4.11871	-2.22626
C	0.02644	2.61796	-1.41869
H	0.02575	2.01357	-2.31981
C	-0.72268	2.20546	-0.30959
C	-1.61192	1.02417	-0.43777
C	-3.06061	1.29649	-0.46370
C	-3.56201	2.59873	-0.65620
H	-2.88039	3.42099	-0.83849
C	-4.93370	2.83436	-0.62623
H	-5.31020	3.84054	-0.78237
C	-5.82179	1.77860	-0.39807
H	-6.89180	1.96260	-0.37323
C	-5.33542	0.48102	-0.21779
H	-6.02277	-0.34505	-0.05801
C	-3.96610	0.23498	-0.25911
C	-3.37546	-1.13280	-0.09855
C	-2.08107	-1.24480	-0.87621
H	-1.62172	-2.21001	-0.72083
C	0.49335	-3.26621	-2.27215
C	0.36810	-4.28365	-3.30560
H	0.30079	-5.27714	-2.85167
H	1.23590	-4.25305	-3.97178
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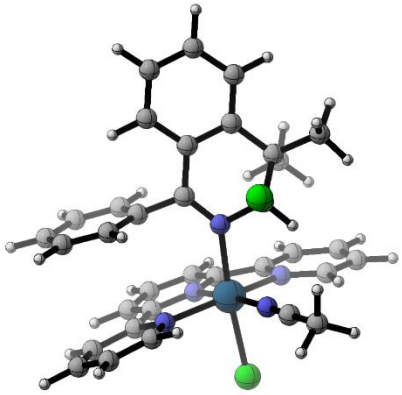
H	-3.12761	-1.32465	0.95697
H	-4.06498	-1.92010	-0.41373



8

Os	-0.77739	-0.95577	0.41351
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C	-2.34487	0.80906	2.42338
H	-1.69755	0.33752	3.15296
C	-3.36141	1.68247	2.79500
H	-3.51472	1.90857	3.84430
C	-4.16675	2.24182	1.80314
H	-4.97144	2.92284	2.05860
C	-3.91756	1.91888	0.47139

H	-4.52507	2.34775	-0.31618
C	-2.87967	1.04435	0.15313
C	-2.53368	0.65099	-1.22408
C	-3.12330	1.10831	-2.40276
H	-3.92259	1.83833	-2.37307
C	-2.65648	0.62530	-3.62565
H	-3.09194	0.98685	-4.55066
C	-1.65074	-0.34330	-3.66353
H	-1.32149	-0.75217	-4.61107
C	-1.10612	-0.79870	-2.46246
C	-0.18071	-1.93510	-2.28391
C	0.32110	-2.69779	-3.33876
H	0.11131	-2.41084	-4.36228
C	1.07617	-3.83834	-3.07214
H	1.46936	-4.43526	-3.88795
C	1.29848	-4.20657	-1.74490
H	1.85945	-5.09819	-1.48883
C	0.79518	-3.39657	-0.73263
H	0.94754	-3.63142	0.31448
C	-0.19554	2.79536	-1.51574
H	0.28124	2.30505	-2.35958
C	-1.14558	3.79566	-1.72735
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H	-2.47214	5.22387	-0.80524
C	-1.38557	4.07882	0.66444
H	-1.84525	4.57536	1.51326
C	-0.45171	3.06574	0.88013
H	-0.17077	2.78310	1.88971
C	0.13757	2.41274	-0.21129
C	1.25423	1.46143	0.03403
C	2.61190	2.01879	-0.10845
C	2.81564	3.41144	-0.16508
H	1.97396	4.08587	-0.06406
C	4.09525	3.93108	-0.33672
H	4.24092	5.00631	-0.36941
C	5.18427	3.06665	-0.46796
H	6.18475	3.46638	-0.60505
C	4.99321	1.68268	-0.41698
H	5.84832	1.02336	-0.51770
C	3.72012	1.15032	-0.22713
C	3.43183	-0.33699	-0.19885
C	4.62197	-1.19651	0.26260
H	5.41226	-1.18860	-0.49342
H	4.30399	-2.23661	0.39363
H	5.04103	-0.83910	1.20580
C	3.03473	-0.78538	-1.63322
H	2.15912	-0.24822	-2.00481
H	2.82834	-1.85814	-1.66173
H	3.87095	-0.58101	-2.30803
C	2.23092	-0.55385	0.73520
H	1.97650	-1.60495	0.78664
C	0.13573	-2.26195	3.19531
C	0.55522	-2.83762	4.46439
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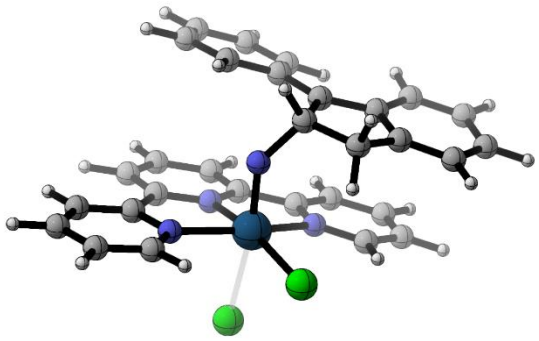

INT1

Os	0.74733	-0.99875	0.12903
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C	3.25806	0.48143	-0.17743
C	4.81264	-1.33640	-1.55821
H	3.02694	-2.57399	-1.40588
C	4.56103	0.82539	-0.53160
C	5.34641	-0.09155	-1.23072
H	5.39014	-2.07578	-2.10109
H	4.96232	1.79559	-0.26485
C	2.36032	1.36862	0.59336
C	0.18807	1.43939	1.59267
C	2.64374	2.64840	1.07510
C	0.43423	2.71577	2.09199
C	1.66823	3.31411	1.81769
H	3.59901	3.11889	0.87999
H	-0.31144	3.24410	2.67160
C	-2.05595	-1.46178	1.41075
C	-1.03364	0.61952	1.78780
C	-3.16431	-1.09703	2.16822
H	-1.96493	-2.43209	0.93924
C	-2.12401	1.04121	2.54239
C	-3.20652	0.17897	2.72507
H	-3.97947	-1.79882	2.29532

H	-2.13241	2.02756	2.98948
N	1.14998	0.83410	0.86239
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N	2.74589	-0.74608	-0.51219
N	0.25768	-0.35761	-1.48603
Cl	1.72205	-1.69069	2.37386
Cl	0.39320	-3.36661	-0.31564
C	-5.30221	-0.02097	-0.31648
C	-5.27841	-1.39294	-0.62090
C	-4.17765	-1.96064	-1.26877
C	-4.22039	0.79495	-0.61709
C	-3.08402	0.23131	-1.24800
C	-3.10616	-1.14597	-1.60920
H	-4.17038	-3.01535	-1.52650
H	-4.28325	1.85154	-0.39711
H	-6.17669	0.40741	0.16265
H	-6.13322	-2.01258	-0.36746
C	-1.83600	0.80968	-1.66654
C	-1.00654	-0.24625	-2.32813
C	-1.87506	-1.51854	-2.37387
H	-1.36010	-2.38822	-1.95531
H	-2.12036	-1.75745	-3.41525
H	-0.65012	0.03642	-3.32090
C	-1.28691	2.12270	-1.46545
C	-0.07651	2.47884	-2.12781
C	0.52268	3.71535	-1.91175
C	-0.06599	4.63946	-1.04611
C	-1.25775	4.31338	-0.38206
C	-1.85403	3.07839	-0.57866
H	-1.70472	5.01960	0.31030
H	-2.72928	2.82964	0.00328
H	1.44565	3.96042	-2.42749
H	0.39982	5.60623	-0.88196
H	0.38043	1.79440	-2.83011
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H	6.36146	0.16730	-1.51207
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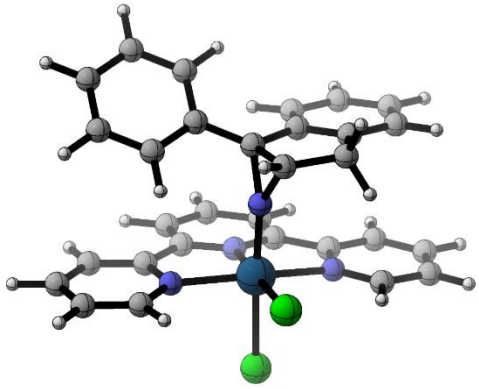

INT2

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C	4.34365	-1.87282	-0.29736
H	2.63502	-2.43567	-1.52726
C	3.73616	-0.57405	1.64122
C	4.71558	-1.18184	0.85694
H	5.07810	-2.35917	-0.92840
H	4.01027	-0.04022	2.54285
C	1.27741	-0.09007	2.02318
C	-1.10411	0.03528	2.02932
C	1.33858	0.58276	3.24544
C	-1.08607	0.70064	3.25339
C	0.14671	0.98457	3.84869
H	2.28974	0.78057	3.72356
H	-2.00759	0.99628	3.73874
C	-3.07368	-1.51850	-0.65454
C	-2.29889	-0.37563	1.25690
C	-4.39909	-1.27871	-0.30515
H	-2.78570	-2.06456	-1.54524
C	-3.60639	-0.11047	1.65044
C	-4.66481	-0.56352	0.86093
H	-5.19660	-1.64555	-0.94037
H	-3.80267	0.44738	2.55707
N	0.07091	-0.30543	1.44908
N	-2.05825	-1.07205	0.09987
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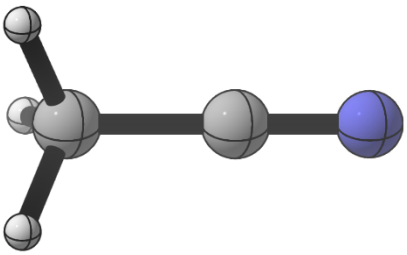
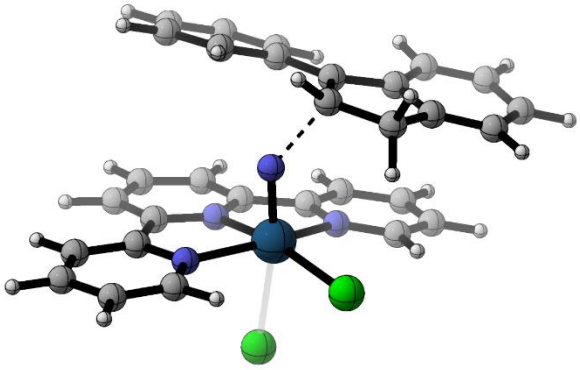
Cl	-0.11881	-2.38952	-2.49919
C	-2.68918	3.31480	0.95999
C	-3.75895	2.98240	0.12032
C	-3.53761	2.31943	-1.09263
C	-1.37846	2.98889	0.59983

C	-1.16091	2.34712	-0.61901
C	-2.23331	2.00095	-1.46097
H	-4.37237	2.04922	-1.73252
H	-0.54997	3.22059	1.26105
H	-2.87697	3.81833	1.90338
H	-4.77322	3.23210	0.41720
C	0.13623	1.83207	-1.18802
C	-0.27496	1.07756	-2.45582
C	-1.76836	1.27324	-2.70652
H	-2.26714	0.30820	-2.84593
H	-1.92748	1.86374	-3.61576
H	0.41707	0.92794	-3.28075
C	1.47132	2.45691	-0.96096
C	1.58187	3.79434	-0.55664
C	2.83968	4.36485	-0.35025
C	3.99862	3.61051	-0.54664
C	3.89487	2.28262	-0.97020
C	2.64076	1.71164	-1.18005
H	4.78810	1.68723	-1.13523
H	2.56867	0.68439	-1.52063
H	2.91011	5.40189	-0.03519
H	4.97498	4.05514	-0.37770
H	0.69036	4.39474	-0.41191
H	0.17531	1.50944	4.79688
H	5.75836	-1.11682	1.14782
H	-5.68672	-0.35506	1.15863



MeCN

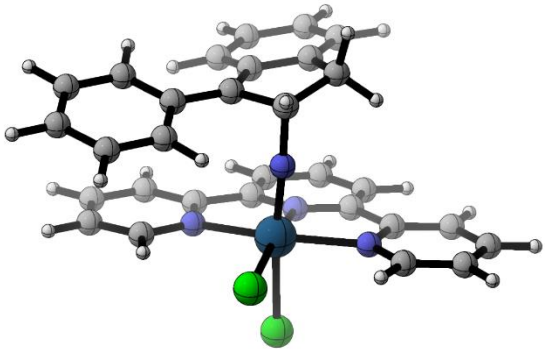
C	0.27927	0.00001	-0.00008
N	1.44033	-0.00000	0.00003
C	-1.18125	-0.00000	0.00002
H	-1.55675	-0.92530	0.44712
H	-1.55675	0.84984	0.57781
H	-1.55693	0.07546	-1.02477



TS1

Os	0.77037	-0.97536	0.07898
C	3.56285	-1.62107	-1.17153
C	3.31060	0.48415	-0.15679
C	4.88326	-1.33789	-1.51618
H	3.08368	-2.56261	-1.41317
C	4.62229	0.82071	-0.48081
C	5.41592	-0.09884	-1.16886
H	5.46846	-2.07831	-2.04894
H	5.02597	1.78537	-0.19861
C	2.40414	1.36983	0.60880
C	0.22852	1.43680	1.60129
C	2.68924	2.64301	1.10345
C	0.47676	2.70804	2.11425
C	1.71116	3.30586	1.84720
H	3.64783	3.11122	0.91992
H	-0.26792	3.23027	2.70056
C	-2.00077	-1.47465	1.40570
C	-0.98590	0.61056	1.80130
C	-3.09013	-1.13659	2.20180
H	-1.91411	-2.43327	0.91089
C	-2.05990	1.00551	2.59164
C	-3.12739	0.12674	2.78594
H	-3.89533	-1.84805	2.33506
H	-2.06567	1.98161	3.06039
N	1.18848	0.84046	0.86361
N	-0.98793	-0.62049	1.19396
N	2.80117	-0.73661	-0.51580
N	0.32407	-0.33771	-1.47176
Cl	1.79299	-1.70651	2.32627
Cl	0.40937	-3.33060	-0.38721
C	-5.33594	-0.04421	-0.09763
C	-5.33997	-1.41051	-0.41170
C	-4.28786	-1.97144	-1.14378
C	-4.27310	0.77514	-0.47119

C	-3.19217	0.21874	-1.18522
C	-3.24298	-1.15329	-1.55087
H	-4.30017	-3.02366	-1.41300
H	-4.32012	1.83012	-0.23749
H	-6.17087	0.38462	0.44795
H	-6.17475	-2.03207	-0.10191
C	-1.96869	0.80168	-1.72620
C	-1.26879	-0.21641	-2.44333
C	-2.06442	-1.50266	-2.41150
H	-1.48014	-2.34372	-2.01968
H	-2.37730	-1.77980	-3.42641
H	-0.72432	0.01700	-3.34793
C	-1.39664	2.12353	-1.52656
C	-0.24047	2.50596	-2.25603
C	0.38803	3.72614	-2.02406
C	-0.11784	4.60856	-1.06668
C	-1.25656	4.25337	-0.33528
C	-1.88091	3.03115	-0.55371
H	-1.64672	4.92325	0.42490
H	-2.71674	2.76214	0.07533
H	1.27149	3.98960	-2.59760
H	0.37160	5.56098	-0.88717
H	0.15938	1.85446	-3.02273
H	1.91536	4.29904	2.23124
H	6.43875	0.15499	-1.42533
H	-3.97153	0.42798	3.39643



TS2

Os	-0.60107	-1.05997	0.17543
C	2.21799	-1.46578	1.37464
C	1.10556	0.53545	1.91401
C	3.34040	-1.07884	2.09787
H	2.16141	-2.40779	0.84552
C	2.20701	0.97281	2.64623
C	3.34065	0.16486	2.72844
H	4.19840	-1.73848	2.14262
H	2.18254	1.93312	3.14660
C	-0.14916	1.30044	1.78777
C	-2.32077	1.19755	0.78227
C	-0.46504	2.51874	2.39241
C	-2.67172	2.40849	1.37234
C	-1.72930	3.06330	2.17333
H	0.25211	3.03130	3.02029
H	-3.65273	2.84066	1.22201
C	-3.32027	-1.67070	-1.28617
C	-3.17555	0.34299	-0.08262
C	-4.62412	-1.38085	-1.68854
H	-2.80524	-2.58004	-1.57401
C	-4.47122	0.68505	-0.45755
C	-5.20270	-0.18672	-1.26867
H	-5.16090	-2.08239	-2.31642
H	-4.91127	1.61759	-0.12656
N	-1.07675	0.71142	1.00241
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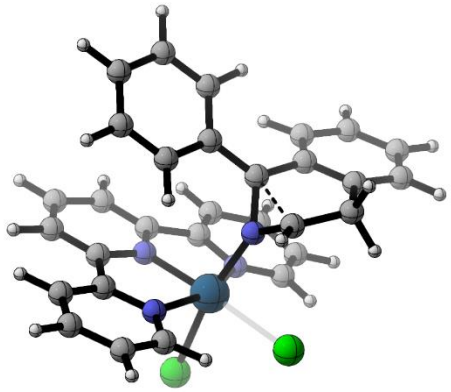
N	1.13828	-0.67411	1.26082
N	-0.03528	-0.38126	-1.39339
Cl	-1.60322	-1.93014	2.24079
Cl	-0.17933	-3.37589	-0.48596
C	1.27334	4.26588	-0.05741
C	0.09609	4.66424	-0.69945
C	-0.52553	3.81902	-1.63014
C	1.85037	3.02383	-0.32795
C	1.24933	2.18023	-1.27662
C	0.05427	2.59257	-1.91598
H	-1.44755	4.12052	-2.11890
H	2.72951	2.71462	0.22310
H	1.73519	4.91878	0.67701
H	-0.34803	5.62712	-0.46568
C	1.62012	0.84783	-1.74906
C	0.46538	0.31874	-2.52852
C	-0.42849	1.53505	-2.88395
H	-1.49196	1.30009	-2.79240
H	-0.23398	1.82132	-3.92427
H	0.64339	-0.36187	-3.36695
C	2.82456	0.07397	-1.52663
C	2.84326	-1.31724	-1.79934
C	3.98193	-2.07688	-1.55839
C	5.14390	-1.47523	-1.06184
C	5.15762	-0.09691	-0.82982
C	4.01798	0.66951	-1.05716
H	6.06089	0.38636	-0.46934
H	4.06706	1.73970	-0.90567

H	3.95975	-3.14585	-1.74913
H	6.03036	-2.07205	-0.86960
H	1.94492	-1.82089	-2.13937
H	-1.98908	4.00995	2.63381
H	4.20751	0.50212	3.28608
H	-6.21361	0.07203	-1.56475



TS3

Os	0.61976	-1.04603	0.12119
C	3.21188	-1.40864	-1.56591
C	3.15473	0.40188	-0.06175
C	4.48304	-1.05056	-2.00640
H	2.67603	-2.26914	-1.94924
C	4.42573	0.80054	-0.46474
C	5.09610	0.06879	-1.44688
H	4.97407	-1.64450	-2.76848
H	4.89047	1.67376	-0.02384
C	2.35109	1.11382	0.95930
C	0.24167	1.06997	2.06923
C	2.73837	2.23020	1.69585
C	0.58631	2.20145	2.81136
C	1.83830	2.78159	2.61236
H	3.71896	2.66984	1.56289
H	-0.09903	2.61274	3.54202
C	-2.11099	-1.65896	1.44493
C	-0.99104	0.27222	2.18505
C	-3.19119	-1.39748	2.27974
H	-2.07358	-2.51595	0.78288
C	-2.04774	0.57886	3.04341
C	-3.15862	-0.26024	3.08812
H	-4.04217	-2.06838	2.28080
H	-2.00472	1.46431	3.66596
N	1.11304	0.58902	1.14708
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N	2.56200	-0.70124	-0.62667
N	-0.53949	-0.26379	-1.20434
Cl	1.60975	-2.37247	1.91585
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C	-5.41943	-0.32508	-0.88274
C	-4.57499	-0.91257	-1.82824
C	-3.64493	1.18079	-0.19569
C	-2.80218	0.60288	-1.15690
C	-3.27068	-0.44428	-1.96593
H	-4.92924	-1.72564	-2.45521
H	-3.27594	1.94060	0.48290
H	-5.60195	1.14657	0.68500
H	-6.43928	-0.68153	-0.77488
C	-1.35331	0.88867	-1.28281
C	-0.87269	-0.54924	-2.50168
C	-2.24943	-0.96381	-2.93038
H	-2.24707	-2.06264	-2.97551
H	-2.42940	-0.60899	-3.95293
H	-0.04135	-0.68552	-3.19044
C	-0.73411	2.20928	-1.24079
C	0.66060	2.34643	-1.42345
C	1.26522	3.59565	-1.39543
C	0.49218	4.74472	-1.19322
C	-0.89440	4.63162	-1.05968
C	-1.50740	3.38205	-1.09588
H	-1.50473	5.52079	-0.93616
H	-2.58554	3.32257	-1.02686
H	2.33927	3.67364	-1.53414
H	0.96527	5.72146	-1.16288
H	1.26049	1.46682	-1.61846
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H	6.08652	0.37445	-1.76676
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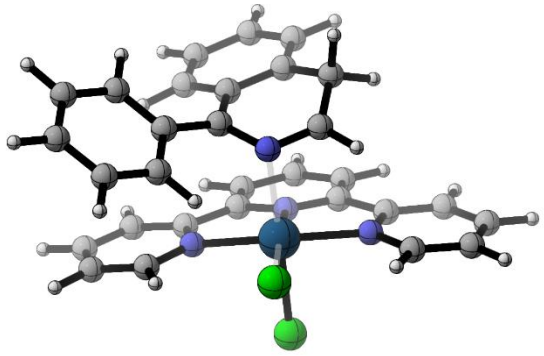

TS4

Os	-0.58693	-1.00793	0.18204
C	2.14744	-1.50214	1.59551
C	1.08773	0.55516	2.00065
C	3.21364	-1.16231	2.42413
H	2.08143	-2.46021	1.09587
C	2.13280	0.94669	2.83548
C	3.21170	0.08621	3.04217
H	4.02277	-1.86832	2.57181
H	2.10682	1.91374	3.32306
C	-0.12161	1.36706	1.75641
C	-2.24645	1.30696	0.67120
C	-0.42202	2.60981	2.31088
C	-2.57280	2.55416	1.20304
C	-1.64499	3.21281	2.01055
H	0.28295	3.10574	2.96656
H	-3.53805	3.00302	1.00296
C	-3.33144	-1.68564	-1.13170
C	-3.12687	0.42175	-0.11152
C	-4.65613	-1.43536	-1.47348
H	-2.82798	-2.61457	-1.37454
C	-4.44852	0.72677	-0.44062
C	-5.22001	-0.20571	-1.13052
H	-5.22556	-2.19235	-2.00076
H	-4.87371	1.68093	-0.15332
N	-1.01311	0.77525	0.91178
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N	1.12526	-0.66201	1.36071
N	0.38977	-0.32292	-1.79310
Cl	-1.55681	-1.93885	2.16021
Cl	-0.15222	-3.31514	-0.67021
C	1.59234	4.05320	-0.11927
C	0.47344	4.59715	-0.76180
C	-0.31034	3.80992	-1.60953
C	1.93179	2.72492	-0.32782
C	1.15916	1.91835	-1.19690
C	0.01508	2.47489	-1.82792
H	-1.18424	4.23481	-2.09366
H	2.75546	2.28882	0.22306
H	2.18017	4.65981	0.56131
H	0.20026	5.63333	-0.58888
C	1.43588	0.51567	-1.42421
C	-0.65037	0.16394	-2.40837
C	-0.80712	1.60435	-2.74189
H	-1.87134	1.86674	-2.71334
H	-0.50369	1.74785	-3.79366
H	-1.41548	-0.54336	-2.70851
C	2.74647	-0.09023	-1.39855
C	2.86690	-1.50475	-1.39064
C	4.11803	-2.10467	-1.40688
C	5.27571	-1.31883	-1.44641
C	5.17527	0.07708	-1.49573
C	3.92978	0.68939	-1.47930
H	6.07069	0.68593	-1.56698
H	3.87032	1.76458	-1.58879
H	4.19368	-3.18718	-1.38147
H	6.25319	-1.79160	-1.45584
H	1.97095	-2.11260	-1.34534
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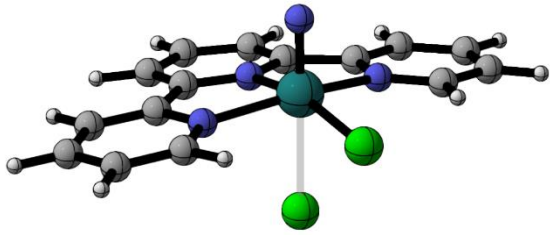
H	-6.24811	0.02416	-1.38911



1-Ru

Ru	0.00000	-0.77980	-0.39969
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C	4.36547	-0.95948	0.04685
H	2.70804	-2.36289	-0.11347
C	3.67350	1.34902	0.00380
C	4.68986	0.39394	0.08413
H	5.12583	-1.72870	0.11108
H	3.91006	2.40502	0.04179
C	1.19598	1.84649	-0.14677
C	-1.19599	1.84648	-0.14677
C	1.21692	3.23725	-0.04600
C	-1.21693	3.23725	-0.04601
C	-0.00001	3.92270	-0.01109
H	2.15328	3.77724	0.01496
H	-2.15329	3.77723	0.01495
C	-3.02745	-1.32832	-0.07930
C	-2.35322	0.93046	-0.11602
C	-4.36547	-0.95949	0.04685
H	-2.70804	-2.36290	-0.11348

C	-3.67350	1.34901	0.00381
C	-4.68986	0.39393	0.08413
H	-5.12582	-1.72871	0.11107
H	-3.91006	2.40501	0.04180
N	-0.00000	1.22700	-0.22585
N	-2.05902	-0.40725	-0.16160
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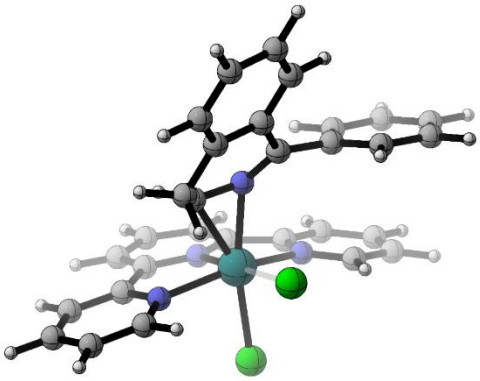
N	-0.00000	-0.92876	-2.00631
Cl	-0.00001	-0.50288	2.18807
Cl	0.00002	-3.13547	0.05004
H	-0.00001	5.00425	0.06484
H	-5.72237	0.71157	0.17928
H	5.72237	0.71159	0.17927



3a-Ru

Ru	-0.81288	-0.07708	0.58558
C	-2.82386	2.20848	1.21952
C	-3.37328	0.77793	-0.55964
C	-3.99396	2.94279	1.04062
H	-2.10181	2.43851	1.99470
C	-4.55539	1.48085	-0.78826
C	-4.86584	2.57689	0.01648
H	-4.20529	3.78180	1.69343
H	-5.23044	1.17266	-1.57738
C	-2.97674	-0.44175	-1.29510
C	-1.40109	-2.22227	-1.23614
C	-3.67793	-1.06437	-2.33067
C	-2.06673	-2.87657	-2.27379
C	-3.19658	-2.27426	-2.83246
H	-4.58292	-0.62562	-2.73245
H	-1.72518	-3.83892	-2.63484
C	1.09348	-2.35100	1.43734
C	-0.28414	-2.75163	-0.42268
C	1.62627	-3.63538	1.36766
H	1.39621	-1.63145	2.18816
C	0.23031	-4.04055	-0.55275
C	1.19372	-4.48599	0.35261
H	2.37258	-3.94616	2.08888
H	-0.12820	-4.69680	-1.33628
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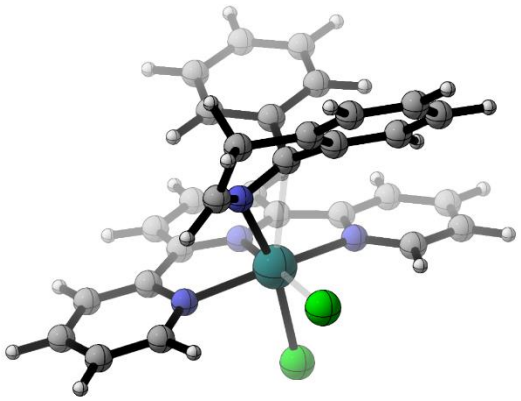
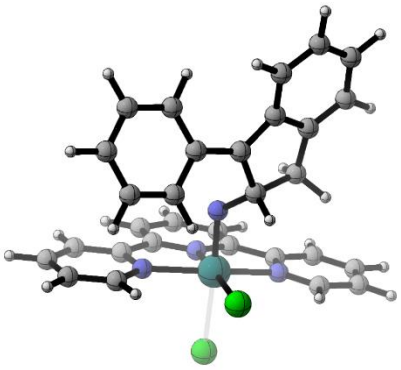
C	3.35607	4.81812	-0.96081
C	2.00975	4.55054	-0.69305
C	3.83001	2.45637	-1.05281
C	2.47839	2.17752	-0.76630
C	1.55279	3.23807	-0.60666
H	1.30972	5.37054	-0.56111
H	4.52578	1.63965	-1.20878
H	5.30720	3.98491	-1.36975
H	3.69141	5.84822	-1.03711
C	1.99829	0.81029	-0.59458
C	-0.24763	1.54427	-0.76299
C	0.09816	2.93739	-0.29518
H	-0.05107	3.04725	0.78518
H	-0.56062	3.65738	-0.78836
H	-0.92746	1.46518	-1.61021
C	2.90763	-0.32202	-0.37755
C	2.78325	-1.45915	-1.19573
C	3.66541	-2.52539	-1.04276
C	4.65590	-2.47862	-0.05704
C	4.77516	-1.35529	0.76762
C	3.91826	-0.26972	0.59833
H	5.53915	-1.32250	1.53812
H	4.00680	0.60645	1.23220
H	3.57333	-3.39608	-1.68432
H	5.33449	-3.31697	0.06896
H	2.01231	-1.48411	-1.95863
H	-5.78282	3.13094	-0.15321
H	-3.72141	-2.76656	-3.64368
H	1.59671	-5.48911	0.26337



3a-isomer-Ru

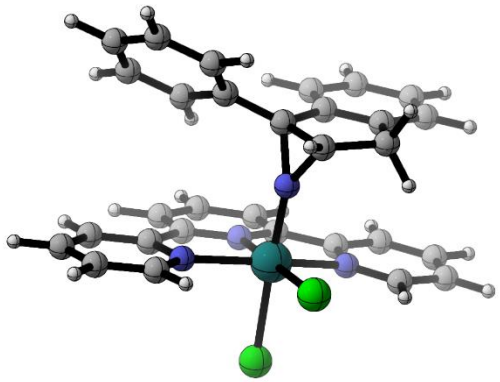
Ru	0.46772	-0.57962	0.77044
C	2.52408	-2.82456	0.20104
C	3.08776	-0.65743	-0.50629
C	3.70577	-3.34539	-0.32077
H	1.79139	-3.43791	0.71421
C	4.28180	-1.12518	-1.05399
C	4.59085	-2.48234	-0.96507
H	3.91597	-4.40396	-0.22099
H	4.96655	-0.43984	-1.53842
C	2.69397	0.76683	-0.47279
C	1.03783	2.22423	0.40986
C	3.42985	1.85297	-0.95048
C	1.73811	3.33925	-0.05272
C	2.92946	3.14064	-0.75236
H	4.37453	1.70516	-1.45890
H	1.36979	4.34103	0.12912
C	-1.71503	0.88989	2.41266
C	-0.18543	2.22817	1.23867
C	-2.34848	2.01128	2.94147
H	-2.02958	-0.12231	2.63899
C	-0.78638	3.38609	1.73212
C	-1.88365	3.27710	2.58422
H	-3.18993	1.88440	3.61289
H	-0.39668	4.35997	1.46207
N	1.50950	0.98735	0.13783
N	-0.67911	0.99671	1.56841
N	2.21878	-1.52368	0.09735
N	-0.26400	-1.26161	-1.03022
Cl	1.64769	-0.36660	2.86305
Cl	-0.78789	-2.50599	1.67584
C	-4.89629	-0.75350	0.00022
C	-5.15805	-1.93637	-0.69475
C	-4.14151	-2.56388	-1.41899
C	-3.62213	-0.19002	-0.03633
C	-2.59682	-0.81464	-0.75725
C	-2.85777	-2.02026	-1.44727
H	-4.34444	-3.48613	-1.95564
H	-3.42889	0.71981	0.51624
H	-5.68119	-0.26815	0.57167
H	-6.15015	-2.37670	-0.66773
C	-1.22360	-0.28217	-0.95592
C	-0.44680	-2.43091	-1.52946
C	-1.73816	-2.69906	-2.22946
H	-1.89720	-3.77658	-2.31487
H	-1.69915	-2.30249	-3.25626
H	0.29579	-3.19996	-1.34672
C	-0.96757	0.97883	-1.67393
C	0.13472	1.06909	-2.55161
C	0.40955	2.25340	-3.22424
C	-0.40317	3.37647	-3.02988
C	-1.50817	3.29408	-2.17962
C	-1.79730	2.10441	-1.51441
H	-2.14954	4.15721	-2.03140
H	-2.66316	2.06185	-0.86745
H	1.26332	2.30488	-3.89257
H	-0.17947	4.30584	-3.54467
H	0.77661	0.20710	-2.69704
H	5.51703	-2.85575	-1.38874
H	3.48153	3.99538	-1.12702
H	-2.35999	4.17081	2.97283



INT1-Ru

Ru	1.19075	0.03599	-0.69651
C	1.22546	3.12447	-0.78577
C	2.03468	2.10712	1.16581
C	1.45376	4.39614	-0.26589
H	0.81565	2.96704	-1.77679
C	2.28507	3.35447	1.73746
C	1.98659	4.51058	1.01721

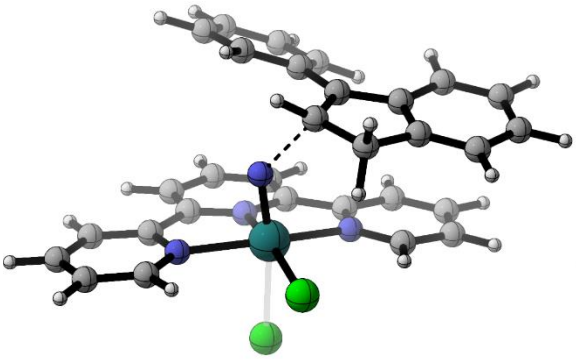
H	1.21060	5.26990	-0.85959
H	2.71112	3.42462	2.73108
C	2.35252	0.82235	1.82105
C	2.31464	-1.52846	1.44847
C	2.94482	0.63753	3.07475
C	2.90434	-1.75958	2.69083
C	3.21162	-0.66229	3.50215
H	3.19715	1.48352	3.70206
H	3.12478	-2.76509	3.02717
C	1.06923	-2.91982	-1.70959
C	1.93945	-2.55102	0.43853
C	1.24268	-4.29763	-1.58833
H	0.65545	-2.46010	-2.60024
C	2.13069	-3.91912	0.61850
C	1.77475	-4.80133	-0.40367
H	0.96221	-4.94940	-2.40766
H	2.55432	-4.29763	1.54076
N	2.05594	-0.25805	1.07298
N	1.39563	-2.07567	-0.72323
N	1.49923	2.01233	-0.09002
N	-0.44490	0.05433	0.12065
Cl	3.55663	0.07113	-1.61819
Cl	0.28537	0.35788	-2.96077
C	-5.95932	-1.92014	0.91305
C	-5.30265	-3.16191	1.05097
C	-3.93340	-3.30064	0.80714
C	-5.25159	-0.78969	0.54833
C	-3.85410	-0.90759	0.33301
C	-3.21029	-2.17330	0.44125
H	-3.45063	-4.26839	0.89534
H	-5.76227	0.15239	0.38939
H	-7.03026	-1.86157	1.07530
H	-5.88271	-4.03523	1.33396
C	-2.90240	0.06691	-0.06282
C	-1.60675	-0.61510	-0.44570
C	-1.75427	-2.06654	0.10963
H	-1.13709	-2.18178	1.00902
H	-1.43219	-2.82451	-0.60762
H	-1.56920	-0.65918	-1.54985
C	-3.04017	1.48991	-0.09246
C	-2.20643	2.25781	-0.94938
C	-2.32332	3.64036	-0.98096
C	-3.23295	4.28743	-0.13549
C	-4.03783	3.54823	0.74206
C	-3.95402	2.16382	0.76041
H	-4.71977	4.05703	1.41532
H	-4.53814	1.60144	1.47876
H	-1.70437	4.21996	-1.65786
H	-3.30757	5.37055	-0.15172
H	-1.51219	1.75954	-1.61763
H	3.66926	-0.82546	4.47170
H	2.17353	5.48569	1.45421
H	1.91924	-5.86836	-0.27202



INT2-Ru

Ru	-0.01962	-1.31111	-0.49422
C	2.97450	-1.84848	-0.94320
C	2.35125	-1.00987	1.16525
C	4.31994	-1.84564	-0.58515
H	2.62751	-2.17303	-1.91742
C	3.68223	-0.98630	1.57360
C	4.67582	-1.40684	0.68946
H	5.06446	-2.17870	-1.29874
H	3.94311	-0.63983	2.56599
C	1.21811	-0.58775	2.01108
C	-1.15039	-0.35112	1.98081
C	1.27032	-0.15046	3.33674
C	-1.14465	0.10187	3.30056
C	0.07815	0.20665	3.96856
H	2.21250	-0.08986	3.86695
H	-2.06723	0.35946	3.80514
C	-3.10211	-1.46132	-0.91792
C	-2.33864	-0.59775	1.13200
C	-4.42849	-1.21613	-0.56885
H	-2.81643	-1.90320	-1.86572
C	-3.64476	-0.32762	1.52973
C	-4.69907	-0.63587	0.66818
H	-5.22145	-1.47252	-1.26151
H	-3.84188	0.12236	2.49451
N	0.02461	-0.64464	1.38502
N	-2.09232	-1.15057	-0.09553
N	2.02169	-1.43750	-0.09352

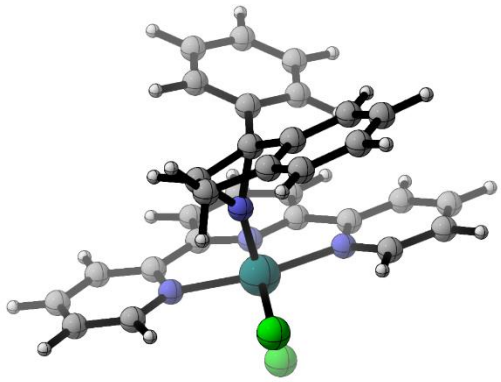
N	0.03973	0.38792	-1.19538
Cl	-0.21238	-3.54695	0.41309
Cl	-0.13693	-2.16254	-2.78628
C	-2.58242	3.27416	1.24896
C	-3.66965	3.01796	0.40477
C	-3.47712	2.43291	-0.85189
C	-1.28353	2.93636	0.85755
C	-1.09760	2.34797	-0.39234
C	-2.18619	2.09625	-1.24891
H	-4.32245	2.23802	-1.50502
H	-0.44500	3.13554	1.51537
H	-2.74660	3.73543	2.21797
H	-4.67372	3.27561	0.72818
C	0.17862	1.83721	-1.01828
C	-0.26090	1.20999	-2.33323
C	-1.75022	1.46980	-2.55663
H	-2.27452	0.53726	-2.78636
H	-1.89182	2.14794	-3.40564
H	0.40561	1.07853	-3.18139
C	1.54900	2.36572	-0.74106
C	2.34221	2.85005	-1.78869
C	3.63665	3.30876	-1.53576
C	4.14999	3.28219	-0.23658
C	3.36073	2.80442	0.81328
C	2.06666	2.34961	0.56217
H	3.75121	2.77928	1.82628
H	1.46581	1.97557	1.38250
H	4.24266	3.68408	-2.35500
H	5.15970	3.63211	-0.04288
H	1.94818	2.87484	-2.80003
H	0.09932	0.55647	4.99461
H	5.71591	-1.38920	0.99656
H	-5.71988	-0.42273	0.96632



TS1-Ru

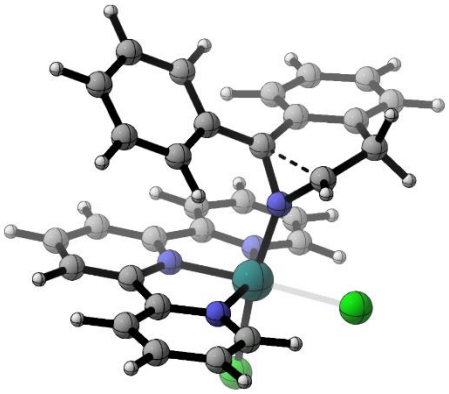
Ru	0.82621	-1.09261	0.05578
C	3.57954	-1.74542	-1.26011
C	3.40304	0.29647	-0.11521
C	4.90697	-1.48442	-1.59881
H	3.07156	-2.65598	-1.55681
C	4.72399	0.61103	-0.42645
C	5.48250	-0.28842	-1.17771
H	5.46371	-2.20845	-2.18227
H	5.16215	1.54091	-0.08526
C	2.52818	1.15867	0.70975
C	0.36886	1.23032	1.72276
C	2.86203	2.38488	1.28794
C	0.66611	2.45113	2.32784
C	1.91654	3.02546	2.09087
H	3.83451	2.83199	1.12622
H	-0.05425	2.95026	2.96297
C	-1.95559	-1.57773	1.34754
C	-0.87326	0.43936	1.87295
C	-3.04297	-1.24695	2.15196
H	-1.90117	-2.51083	0.80108
C	-1.94121	0.82901	2.67551
C	-3.04194	-0.01976	2.80851
H	-3.87527	-1.93465	2.23405
H	-1.91819	1.77776	3.19729
N	1.29849	0.65489	0.93648
N	-0.91162	-0.75203	1.19820
N	2.85463	-0.88069	-0.54298
N	0.39129	-0.38270	-1.42165
Cl	1.85503	-1.97365	2.26211
Cl	0.40721	-3.39043	-0.54534
C	-5.29523	0.25041	-0.03723
C	-5.42873	-1.11262	-0.34214
C	-4.44118	-1.77942	-1.07490
C	-4.16699	0.96459	-0.43192
C	-3.15321	0.29855	-1.14877
C	-3.32451	-1.06810	-1.49348
H	-4.55522	-2.82871	-1.33063
H	-4.10657	2.02329	-0.21498
H	-6.08266	0.75787	0.51118
H	-6.31585	-1.64995	-0.02051
C	-1.89816	0.77031	-1.72160
C	-1.29763	-0.30739	-2.42712
C	-2.17726	-1.53081	-2.34470
H	-1.64552	-2.39205	-1.92140
H	-2.51052	-1.83143	-3.34663
H	-0.69479	-0.15529	-3.31142
C	-1.23610	2.05408	-1.54983

C	-0.17362	2.42366	-2.41233
C	0.53888	3.60152	-2.20756
C	0.21611	4.44117	-1.13813
C	-0.82642	4.09274	-0.27236
C	-1.54047	2.91702	-0.47118
H	-1.06935	4.72961	0.57247
H	-2.29649	2.63908	0.25018
H	1.34438	3.86560	-2.88579
H	0.77424	5.35840	-0.97662
H	0.07535	1.80094	-3.26318
H	2.16005	3.97951	2.54499
H	6.51185	-0.05261	-1.42543
H	-3.88239	0.27666	3.42642



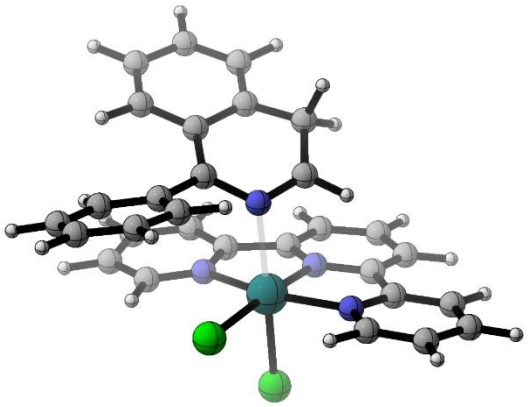
TS2-Ru

Ru	-0.66140	-1.12392	0.33380
C	2.15229	-1.20547	1.59596
C	0.90444	0.75967	1.89434
C	3.22506	-0.67779	2.31061
H	2.17633	-2.19811	1.16464
C	1.94350	1.33539	2.62131
C	3.11929	0.61191	2.82605
H	4.12104	-1.27217	2.44422
H	1.84317	2.33849	3.01694
C	-0.37621	1.44285	1.61455
C	-2.48032	1.11264	0.53316
C	-0.76768	2.71395	2.03861
C	-2.90849	2.37765	0.93542
C	-2.03760	3.17213	1.68537
H	-0.10594	3.33484	2.62841
H	-3.89607	2.74025	0.68017
C	-3.27405	-2.05898	-1.12690
C	-3.26055	0.11009	-0.23389
C	-4.56588	-1.88661	-1.62633
H	-2.71706	-2.98040	-1.25552
C	-4.54736	0.34231	-0.71388
C	-5.20662	-0.66858	-1.41732
H	-5.04553	-2.69510	-2.16580
H	-5.03299	1.29593	-0.54611
N	-1.23631	0.71738	0.87332
N	-2.64656	-1.09149	-0.45264
N	1.03051	-0.50434	1.38267
N	-0.09059	-0.63698	-1.30081
Cl	-1.69300	-1.69613	2.47659
Cl	-0.12541	-3.46954	0.04447
C	1.44804	4.05129	-0.29674
C	0.26054	4.45147	-0.92005
C	-0.43114	3.57470	-1.76807
C	1.96499	2.77194	-0.50275
C	1.29325	1.89494	-1.37018
C	0.09229	2.31079	-1.99435
H	-1.36018	3.88124	-2.23940
H	2.85212	2.46235	0.03401
H	1.96287	4.73333	0.37272
H	-0.13746	5.44445	-0.73458
C	1.59459	0.52139	-1.76219
C	0.40641	-0.01459	-2.47958
C	-0.46504	1.21390	-2.87129
H	-1.53133	1.02444	-2.72578
H	-0.30381	1.42574	-3.93447
H	0.53813	-0.73540	-3.29323
C	2.78333	-0.27370	-1.52274
C	2.74026	-1.68354	-1.65458
C	3.86283	-2.45821	-1.38462
C	5.06644	-1.85233	-1.00836
C	5.13921	-0.45879	-0.92089
C	4.01548	0.32294	-1.17115
H	6.07569	0.02302	-0.65661
H	4.10629	1.40036	-1.13226
H	3.79638	-3.53915	-1.46322
H	5.94139	-2.45965	-0.79732
H	1.81099	-2.18338	-1.90562
H	-2.35552	4.15935	2.00193
H	3.93812	1.05535	3.38216
H	-6.20913	-0.49906	-1.79524



TS3-Ru

Ru	0.63666	-1.19430	0.09625
C	3.23990	-1.57611	-1.54373
C	3.20469	0.17898	0.01905
C	4.53317	-1.24448	-1.94262
H	2.68878	-2.40491	-1.97323
C	4.49670	0.55360	-0.33956
C	5.16727	-0.16510	-1.33133
H	5.02289	-1.82702	-2.71434
H	4.97721	1.39574	0.14300
C	2.39948	0.87403	1.05022
C	0.27648	0.83223	2.12163
C	2.80049	1.95530	1.83381
C	0.63004	1.92533	2.91592
C	1.89739	2.48631	2.75795
H	3.79050	2.38145	1.73046
H	-0.05885	2.32384	3.65025
C	-2.14593	-1.78320	1.31627
C	-0.98125	0.06152	2.18121
C	-3.23259	-1.53646	2.15099
H	-2.12758	-2.60344	0.60786
C	-2.03846	0.35403	3.04309
C	-3.17561	-0.45200	3.02553
H	-4.10397	-2.17867	2.10080
H	-1.97731	1.20087	3.71590
N	1.15333	0.37312	1.20172
N	-1.05525	-1.00474	1.32992
N	2.59311	-0.88210	-0.59585
N	-0.44607	-0.29401	-1.19134
Cl	1.52242	-2.61556	1.84998
Cl	0.10553	-3.20023	-1.25505
C	-4.80279	0.83273	-0.03336
C	-5.32162	-0.15393	-0.87746
C	-4.51321	-0.74555	-1.85209
C	-3.47621	1.24978	-0.15713
C	-2.67475	0.67139	-1.14983
C	-3.19244	-0.32574	-1.98669
H	-4.90752	-1.52251	-2.50038
H	-3.06913	1.97222	0.54030
H	-5.42653	1.26981	0.74025
H	-6.35488	-0.46953	-0.77001
C	-1.20654	0.89051	-1.28898
C	-0.80137	-0.46045	-2.50323
C	-2.18391	-0.85076	-2.96149
H	-2.19314	-1.94745	-3.02876
H	-2.34352	-0.46482	-3.97530
H	0.02390	-0.57138	-3.20596
C	-0.53065	2.18609	-1.19764
C	0.86866	2.26551	-1.37144
C	1.52949	3.48421	-1.28940
C	0.80723	4.65779	-1.04762
C	-0.58416	4.60274	-0.92482
C	-1.25200	3.38395	-1.00838
H	-1.15455	5.51335	-0.77065
H	-2.33185	3.36909	-0.94205
H	2.60692	3.51857	-1.41805
H	1.32322	5.61053	-0.97822
H	1.43040	1.36862	-1.59953
H	2.18960	3.33405	3.36762
H	6.17406	0.11941	-1.61800
H	-4.00796	-0.22958	3.68439



TS4-Ru

Ru	-0.91316	-0.61384	0.54486
C	1.61445	-0.06486	2.26417
C	0.41486	1.80077	1.51705
C	2.57131	0.74342	2.87493
H	1.66515	-1.14716	2.29290
C	1.35073	2.66063	2.09135
C	2.44752	2.12777	2.76837

H	3.39728	0.28715	3.40907	C	2.49076	0.82641	-1.37266
H	1.22478	3.73402	2.01463	C	1.80564	1.90806	-2.00125
C	-0.82050	2.25867	0.84637	H	1.89704	3.95524	-2.63581
C	-2.77505	1.43987	-0.23931	H	4.44951	0.17906	-0.67653
C	-1.29273	3.56907	0.75948	H	5.51215	2.36107	-0.92870
C	-3.28794	2.73547	-0.33697	H	4.23190	4.28177	-1.86379
C	-2.53170	3.80000	0.15660	C	1.76191	-0.39287	-1.11476
H	-0.71998	4.39377	1.16590	C	-0.20847	0.46245	-2.04200
H	-4.25721	2.91600	-0.78554	C	0.44765	1.66835	-2.57830
C	-3.18823	-2.13133	-0.93096	H	-0.22881	2.52404	-2.44164
C	-3.41285	0.19243	-0.71569	H	0.51711	1.55832	-3.67594
C	-4.41887	-2.23042	-1.57657	H	-1.25882	0.30420	-2.26195
H	-2.56808	-2.99653	-0.72493	C	2.35580	-1.66583	-0.74611
C	-4.65079	0.15306	-1.35746	C	1.84363	-2.81607	-1.39397
C	-5.16120	-1.07014	-1.79096	C	2.45265	-4.05570	-1.22165
H	-4.78007	-3.20110	-1.89745	C	3.52750	-4.18998	-0.34299
H	-5.21202	1.06576	-1.51855	C	3.99572	-3.07540	0.36810
N	-1.55492	1.24907	0.32066	C	3.43148	-1.82564	0.16026
N	-2.69151	-0.95745	-0.51052	H	4.79913	-3.18649	1.08923
N	0.57890	0.44152	1.57817	H	3.77251	-0.98859	0.75508
N	0.37834	-0.42721	-1.28799	H	2.07053	-4.91897	-1.75691
Cl	-2.21636	-0.59786	2.57613	H	3.98988	-5.16082	-0.19243
Cl	-0.26235	-2.93303	0.93436	H	1.00368	-2.71231	-2.06999
C	4.47032	2.23766	-1.20467	H	3.18472	2.78697	3.21405
C	3.75177	3.31597	-1.74209	H	-2.91448	4.81196	0.08359
C	2.43478	3.13880	-2.16365	H	-6.12401	-1.11143	-2.28921
C	3.86142	1.00545	-1.04460				

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