Supplementary Information

For

Reshaping aromatic framework: expansion of aromatic system drives metallabenzenoids to metallapentalenes

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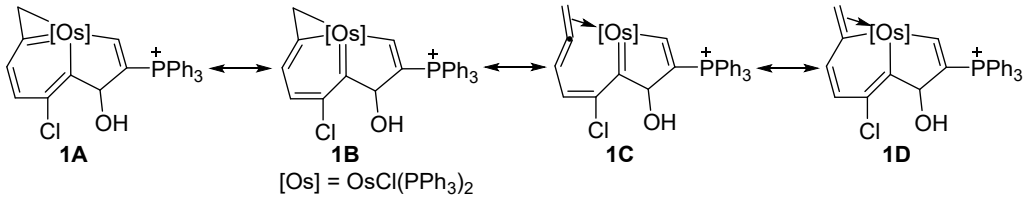
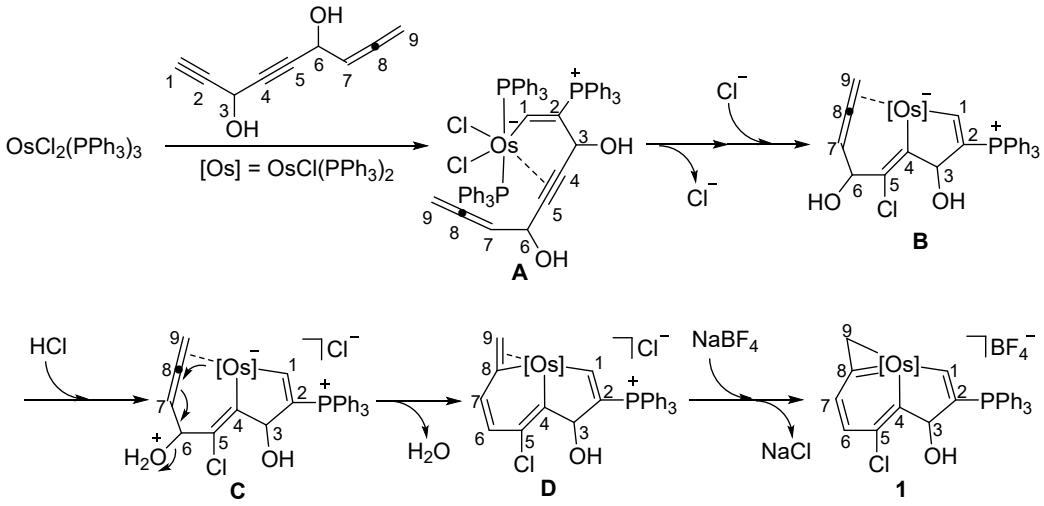


Scheme S2. A proposed mechanism for the formation of complex 1.



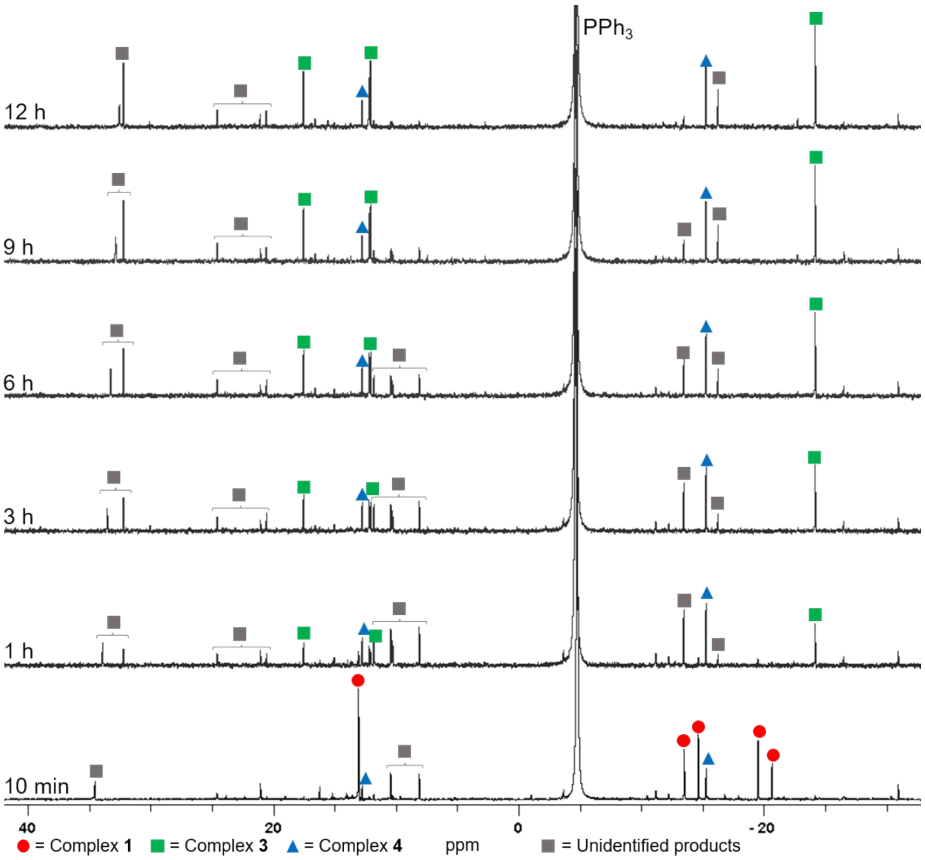


Figure S1. Stacked *in-situ* $^{31}P\{^{1}H\}$ NMR spectra (242.9 MHz, CD_2Cl_2) of the conversion from **1** to **3** at variant times. As time goes on, **1** gradually decreased while **3** and **4** increased with some unidentified products. The broad peak at about -4.69 ppm belongs to triphenylphosphine.

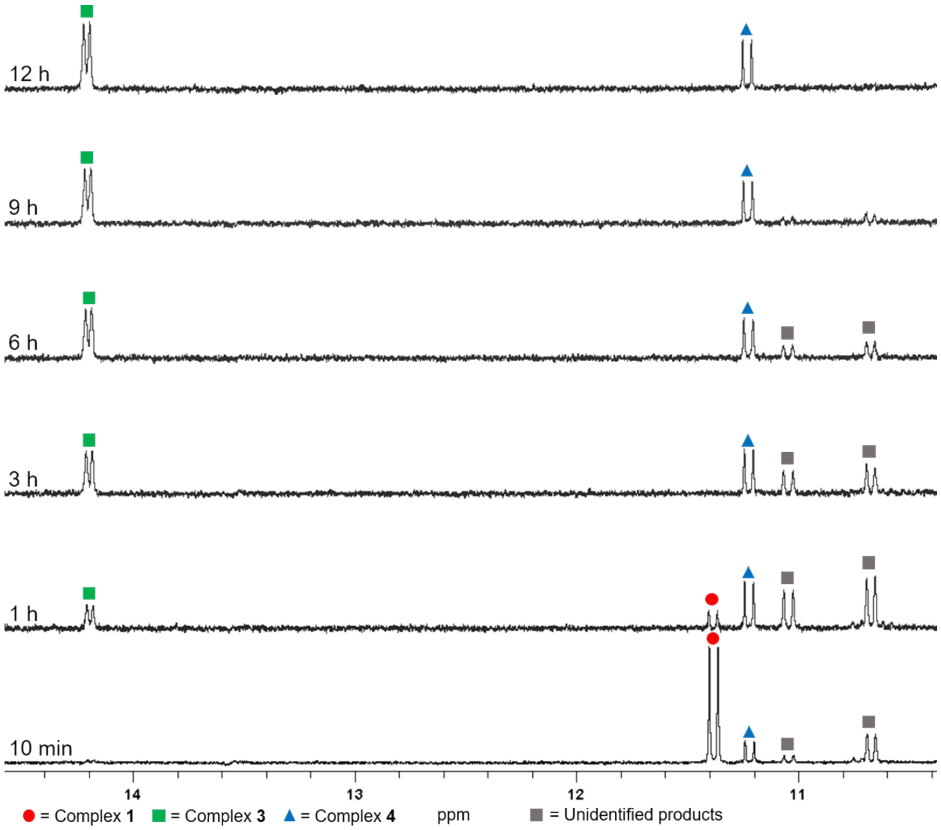


Figure S2. Stacked *in-situ* ^{1}H NMR spectra (600.1 MHz, CD_2Cl_2) of the conversion from **1** to **3** at different times in 12 hours.

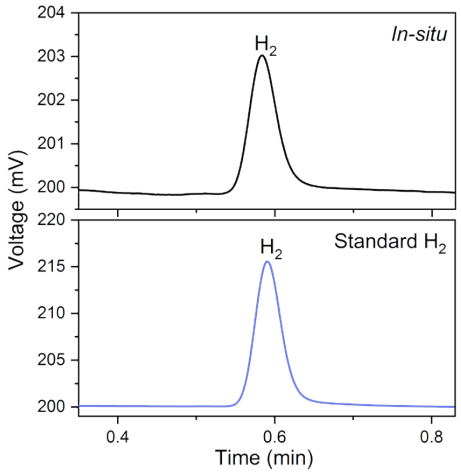


Figure S3. GC chromatograms of the *in-situ* atmosphere in the formation of **3** and standard gas of H_2 obtained from thermal conductivity detector (TCD). Carrier gas: nitrogen. The peak of the *in-situ* atmosphere was identified as H_2 (0.58 min). The gas product for GC-TCD analysis was sampled from the atmosphere of an *in-situ* reacting tube which contained complex **1** (50 mg), PPh_3 (105 mg), and HCl•Et_2O (2.0 M, 0.1 mL) in CH_2Cl_2 (0.5 mL).

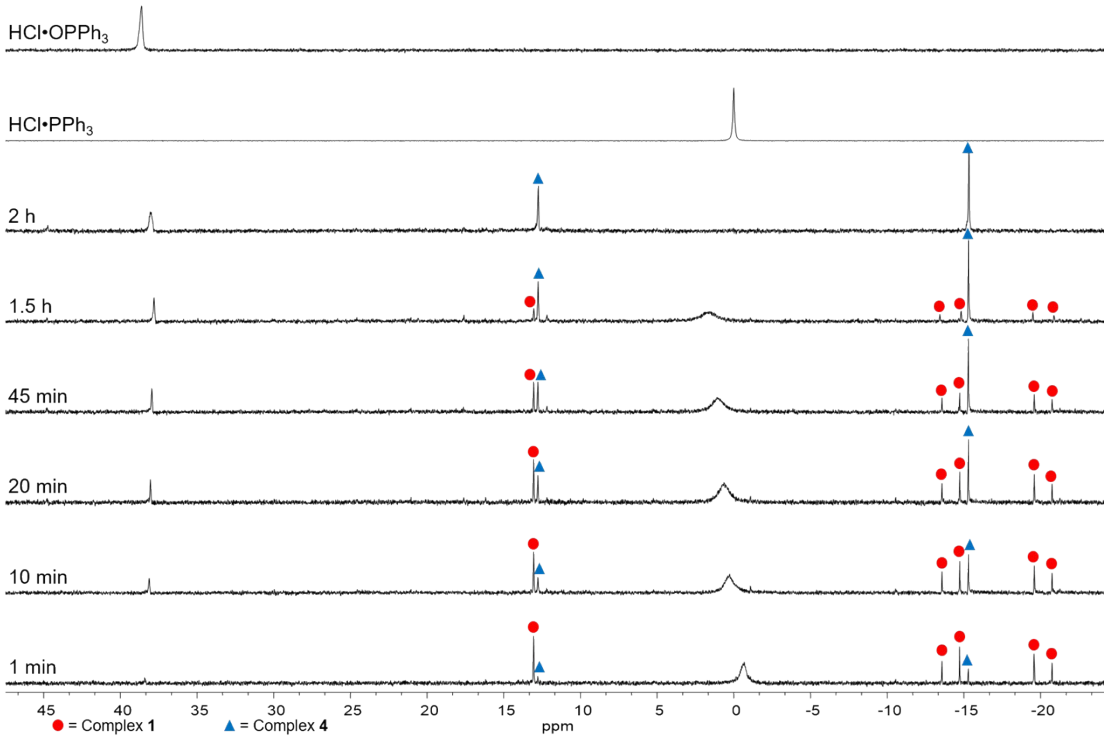


Figure S4. Stacked *in-situ* $^{31}P\{^{1}H\}$ NMR spectra (242.9 MHz, CD_2Cl_2) of the conversion from **1** to **4** at different times in 2 hours. As time goes on, **1** gradually decreased while **4** and byproduct HCl•$OPPh_3$ increased. The broad peaks at about -0.01 and 38.62 ppm belong to triphenylphosphine hydrochloride (HCl•PPh_3) and triphenylphosphine oxide hydrochloride (HCl•$OPPh_3$), respectively.

Table S1. The transformation of metallaindenol **1** to metallapentalene **3** and metallaindene **4** using different amounts of acid.[a]

Entry	Equivalent of HCl•Et_2O	Yield (**1**/**3**/**4**) (%)
1	1 eq.	68 (26/24/18)
2	2 eq.	72 (19/32/21)
3	3 eq.	59 (0/36/23)
4	4 eq.	73 (0/48/25)
5	5 eq.	77 (0/52/25)
6	6 eq.	76 (0/50/26)
7	7 eq.	72 (0/42/30)
8	8 eq.	67 (0/35/32)
9	9 eq.	63 (0/26/37)
10	10 eq.	61 (0/15/46)

[a]Reaction conditions: **1** (0.16 mmol), PPh_3 (1.60 mmol), 0.08/0.16/0.24/0.32/0.40/0.48/0.56/0.64/0.72/0.80 mL HCl•Et_2O (2.0 M), CH_2Cl_2 (4.0 mL), 25 °C, 12 hours, under nitrogen atmosphere.

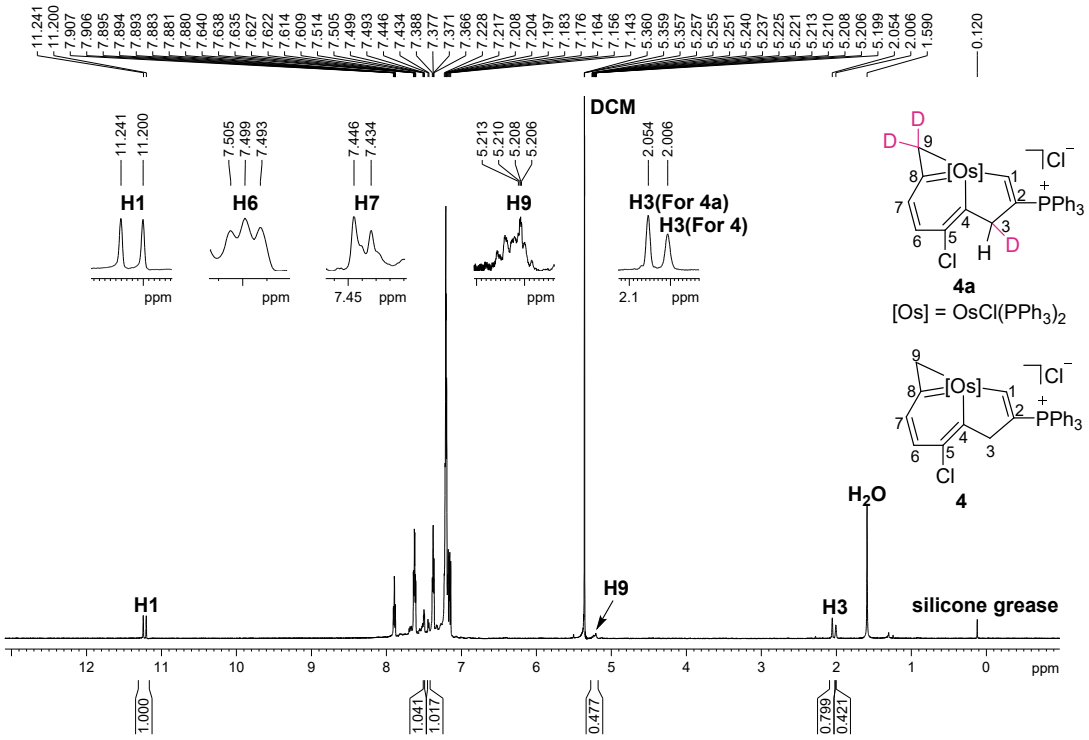


Figure S5. ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectra for complex **4a**.

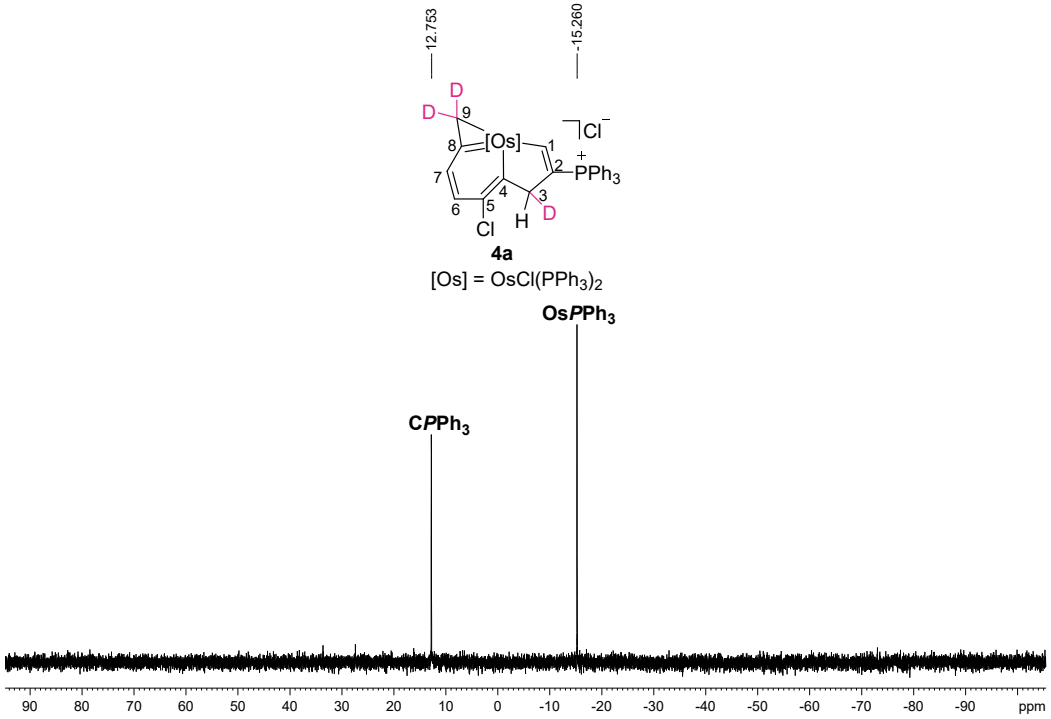
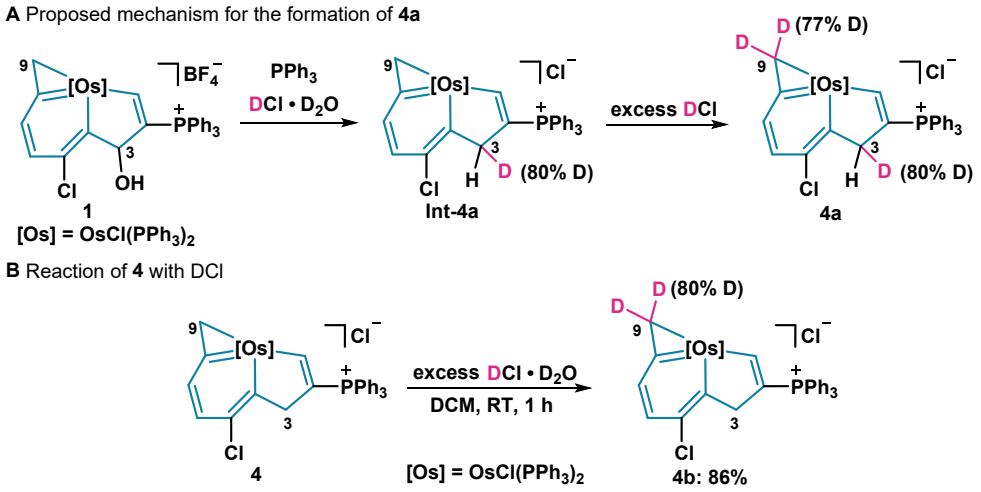


Figure S6. $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectra for complex **4a**.

Scheme S3. A possible mechanism for the formation of complex 4a.



The formation mechanism of **4a** was proposed *via* an intermediate **Int-4a**, and then protons on C9 of **Int-4a** underwent a H/D exchange due to their acidity (Scheme S3A). To prove this, the reaction of **4** with excess DCl•D_2O was performed and **4b** was isolated in a high yield (Scheme S3B). The ^{1}H NMR spectra showed deuterium was only found on C9 position (Figure S7).

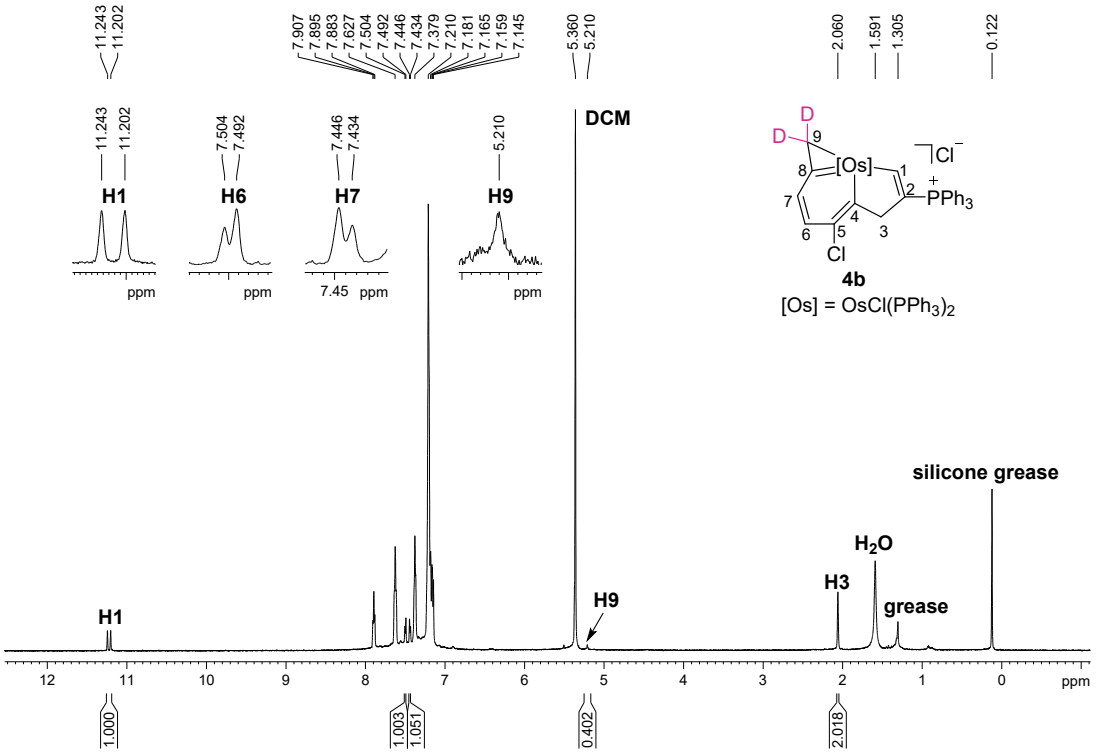


Figure S7. ^{1}H NMR spectra (600.1 MHz, CD_2Cl_2) of complex **4b**.

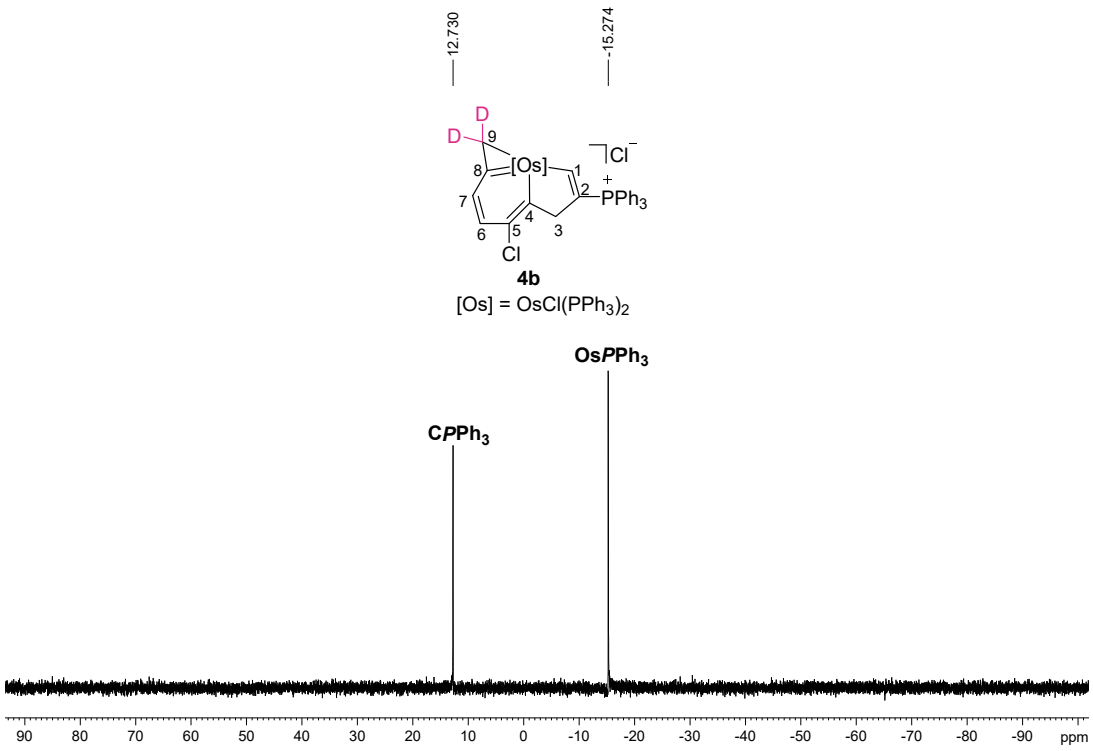


Figure S8. $^{31}P\{^{1}H\}$ NMR spectra (242.9 MHz, CD_2Cl_2) of complex **4b**.

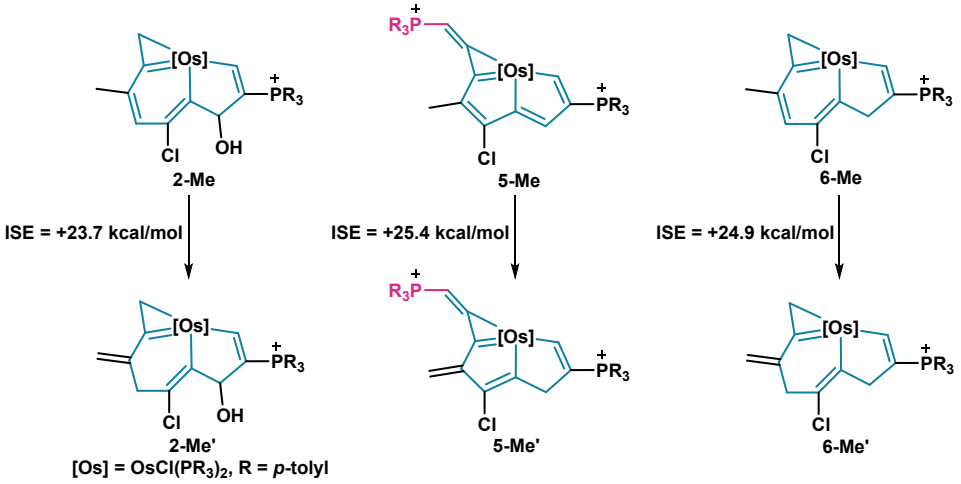


Figure S9. The isomerization stabilization energy (ISE) for **2-Me**, **5-Me**, and **6-Me**.

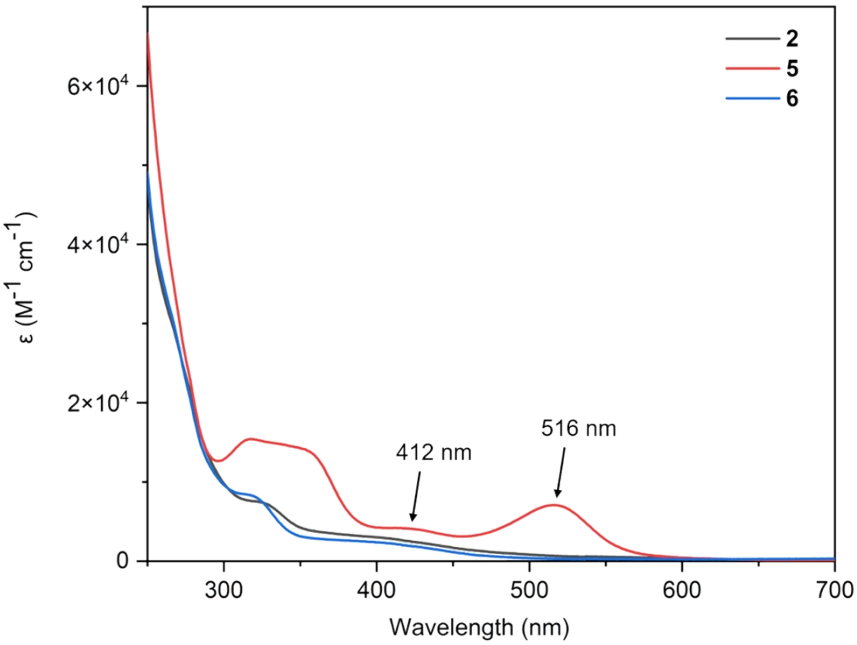


Figure S10. UV–Vis absorption spectra for complexes **2**, **5**, and **6** in DCM (1.0×10^{-5} M, RT). Complex **5** has two peaks at 516 nm (log ε = 3.85, ε: molar extinction coefficient in $L \cdot mol^{-1} \cdot cm^{-1}$) and 412 nm (log ε = 3.62) in the visible region.

Table S2. Experimental and calculated absorption spectral data for complexes **3** and **5**.

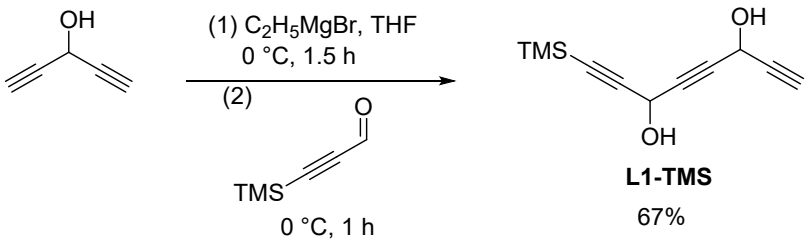
Complexes	Experimental (nm)	Calculated (nm)	f	Excitation	Percentage (%)
3	511	491	0.0867	HOMO–2→LUMO HOMO–1→LUMO HOMO→LUMO	16.8 58.9 16.8
3	408	437	0.0963	HOMO–4→LUMO HOMO–2→LUMO HOMO–1→LUMO	19.0 57.3 18.7
5	516	501	0.0627	HOMO–2→LUMO HOMO–1→LUMO HOMO→LUMO	26.3 47.6 22.1
5	412	444	0.1254	HOMO–6→LUMO HOMO–2→LUMO HOMO–1→LUMO	8.4 60.5 24.2

2. Experimental Procedures

General procedures

All synthesis reactions were applied under an inert atmosphere (N_2) with standard Schlenk techniques, except for otherwise stated. Reagents were purchased commercially without further purification. The synthesis of $OsCl_2(PR_3)_3$ (R = Ph, *p*-tolyl) was according to reported procedure.[1] The solvents (tetrahydrofuran, hexane, and diethyl ether) were distilled from sodium/benzophenone and dichloromethane was distilled from calcium hydride under N_2 before applied. Column chromatography was performed on silica gel (200−300 mesh) in air. The NMR experiments were performed on a Bruker Advance III 500 MHz spectrometer or a Bruker Ascend III 600 MHz spectrometer at 298 K. The ^{1}H and $^{13}C\{^{1}H\}$ NMR chemical shifts (δ) are calibrated to tetramethylsilane, and the $^{31}P\{^{1}H\}$ NMR chemical shifts are calibrated to 85% H_3PO_4. Two-dimensional NMR spectra are abbreviated as heteronuclear single quantum coherence (HSQC) and heteronuclear multiple bond coherence (HMBC). The absolute values of the coupling constants are in Hertz (Hz). Singlet (s), doublet (d), triplet (t), multiplet (m), and broad (br) are used to described multiplicities. High resolution mass spectra (HRMS) were tested on a Bruker En Apex Ultra 7.0T FTICR-MS. Elemental analyses were recorded on a Vario EL III elemental analyzer. Infrared spectra (IR) experiments were carried on a Nicolet iS50 FT-IR. Gas chromatography was performed with a thermal conductivity detector (TCD, column: TDX-01).

Synthesis pathway for compound L

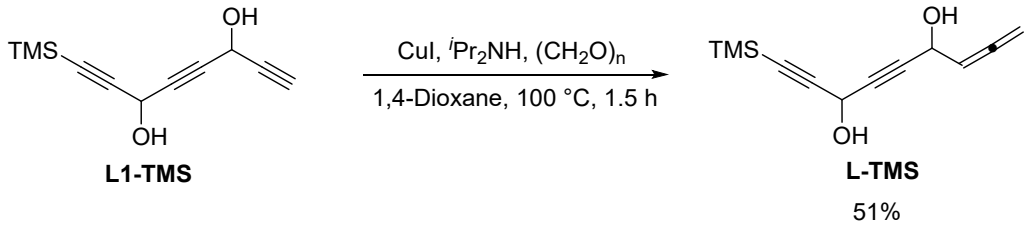


Preparation and characterization of L1-TMS

The solution of 1,4-pentadiyn-3-ol (1.92 g, 24 mmol) in tetrahydrofuran (100 mL) was cooling to 0 °C. Then ethylmagnesium bromide (48 mL, 1.0 M in tetrahydrofuran,

48 mmol) was added dropwise over 1 hour. After the reaction solution was stirred for 30 min, trimethylsilylpropynal (3.54 mL, 24 mmol) was added to the solution slowly. After 1 hour, saturated aqueous ammonium chloride (100 mL) was added and the mixture was extracted with diethyl ether (3 × 50 mL). The extract was dried using magnesium sulphate and concentrated under reduced pressure to brown oil. The residue was chromatographed with dichloromethane/diethyl ether (20/1, v/v) to give **L1-TMS** as a yellow oil. Yield: 3.27 g, 67%.

^{1}H NMR (500.2 MHz, $CDCl_3$): δ = 5.22 (s, 1H), 5.21 (s, 1H), 3.62 (br, 2H), 2.64 (m, 1H), and 0.21 ppm (s, 9H). $^{13}C\{^{1}H\}$ NMR (125.7 MHz, $CDCl_3$): δ = 101.44, 90.52, 81.91, 81.45, 80.64, 73.75, 52.53, 51.98, and 0.00 ppm. IR (thin film): 3292 (br), 2960 (s), 2900 (s), 2178 (s), 2124 (s), 1252(s), 1036 (s), and 845 (s) cm^{-1}.

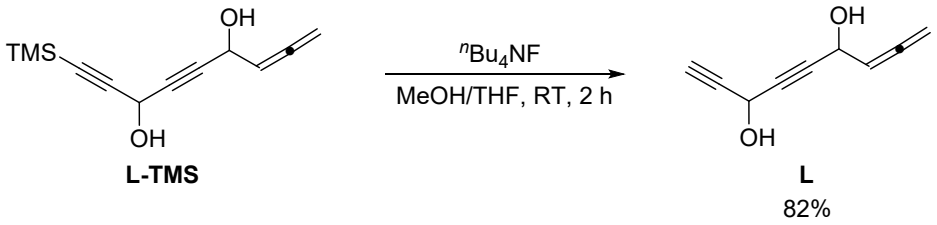


Preparation and characterization of compound L-TMS

A mixture of cuprous iodide (1.52 g, 8 mmol) and polyformaldehyde (0.72 g, 24 mmol) was dissolved in 1,4-dioxane (60 mL) at 100 °C, then diisopropylamine (4.45 mL, 32 mmol) was added to the suspension. After stirred for 5 min, **L1-TMS** (3.27g, 16 mmol, dissolved in 15 mL 1,4-dioxane) was added to the suspension and stirred for 1.5 hours to give a brownish red suspension. Water (30 mL) was added to the solution filtered from the suspension, and the organic part was extracted with diethyl ether (3 × 50 mL). Then the organic part was dried over magnesium sulphate and concentrated under reduced pressure. The residue was chromatographed with petroleum ether/ethyl acetate (2/1, v/v) to afford **L-TMS** as a brown oil. Yield: 1.80 g, 51%.

^{1}H NMR (500.2 MHz, $CDCl_3$): δ = 5.21 (ddd, $J_{H\text{-}H}$ = 14.1 Hz, $J_{H\text{-}H}$ = 7.7 Hz, $J_{H\text{-}H}$ = 1.5 Hz, 1H), 4.98 (s, 1H), 4.80 (s, 2H), 4.79 (s, 1H), 2.69 (br, 2H), and 0.00 ppm (s, 9H). $^{13}C\{^{1}H\}$ NMR (125.7 MHz, $CDCl_3$): δ = 208.09, 101.82, 92.85, 90.12, 83.83, 83.00, 79.32, 60.74, 52.78, and -0.02 ppm. IR (thin film): 3316 (br), 2960 (s), 2899 (s),

2178 (s), 1957 (s), 1250(s), 1037(s), and 844 (s) cm^{-1}.

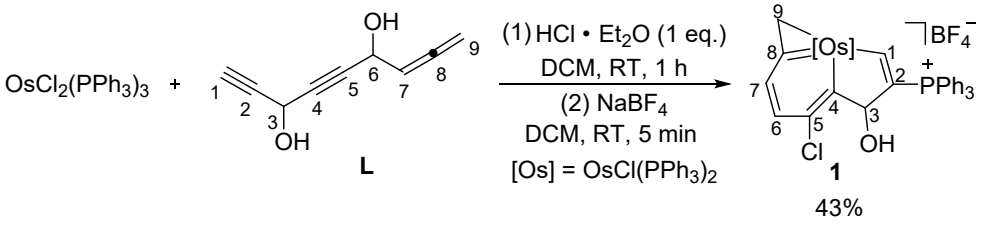


Preparation and characterization of compound L

The solution of **L-TMS** (1.80 g, 8.18 mmol) in tetrahydrofuran (40 mL) and methanol (40 mL) was added tetrabutylammonium fluoride (12 mL, 1.0 M in tetrahydrofuran, 12.0 mmol) at room temperature and stirred for 2 hours. Saturated aqueous ammonium chloride (100 mL) was added to the solution and the organic part was extracted with diethyl ether (3 × 50 mL) and dichloromethane (3 × 50 mL). Then the organic part was dried over magnesium sulphate and concentrated under reduced pressure. The residue was chromatographed with petroleum ether/ethyl acetate (1/1, v/v) to afford **L** as a brown oil. Yield: 0.99 g, 82%.

^{1}H NMR (500.2 MHz, $CDCl_3$): δ = 5.40 (m, 1H), 5.20 (s, 1H), 4.99 (m, 3H), 4.08 (br, 2H), and 2.60 ppm (d, $J_{H\text{-}H}$ = 2.3 Hz, 1H). ^{13}C{^{1}H} NMR (125.7 MHz, $CDCl_3$): δ = 207.87, 92.30, 83.68, 82.40, 80.71, 78.86, 73.01, 60.34, and 51.60 ppm. IR (thin film): 3289 (br), 2920 (s), 2850 (s), 2121 (s), 1956 (s), 1023 (s), and 852 (s) cm^{-1}.

Synthesis pathway for complex 1



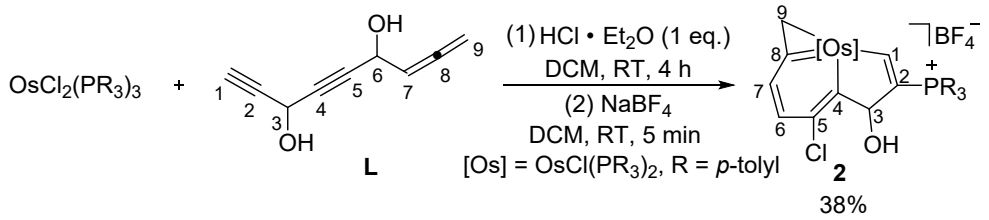
Preparation and characterization of complex 1

L (160 mg, 1.08 mmol), dissolved in 5 mL dichloromethane, was added to a solution of $OsCl_2(PPh_3)_3$ (1.00 g, 0.95 mmol) in dichloromethane (15 mL). Then hydrogen chloride (0.48 mL, 2.0 M in diethyl ether, 0.96 mmol) was added to the solution in the following. After stirring for 1 h at RT, sodium tetrafluoroborate (521 mg, 4.75 mmol)

was added to the solution for 5 min. The solution was then evaporated under vacuum to approximately 3 mL and purified by flash chromatography on silica gel (eluent: dichloromethane/acetone, 20/1) to afford a brown solid. The solid was dissolved in dichloromethane (1 mL), and diethyl ether (20 mL) was added to give a yellow precipitate. The precipitate was isolated by filtration to yield complex **1** (523 mg, 43%) as a yellow solid.

^{1}H NMR with ^{1}H-^{13}C HSQC (600.1 MHz, CD_2Cl_2): δ = 11.39 (d, $J_{P\text{-}H}$ = 23.3 Hz, 1H, H1), 7.89 (d, $J_{P\text{-}H}$ = 7.5 Hz, 1H, H6), 7.49 (d, $J_{P\text{-}H}$ = 7.6 Hz, 1H, H7), 5.43 (m, 1H, H9a), 5.10 (m, 1H, H9b), 4.61 (d, $J_{P\text{-}H}$ = 4.5 Hz, 1H, H3), 2.48 (d, $J_{P\text{-}H}$ = 4.5 Hz, 1H, OH), and 7.87−7.10 ppm (45H, other aromatic protons). ^{31}P{^{1}H} NMR (242.9 MHz, CD_2Cl_2): δ = 13.02 (s, C*P*Ph$_3$), −14.18 (d, $J_{P\text{-}P}$ = 284.4 Hz, Os*P*Ph$_3$), and −20.22 ppm (d, $J_{P\text{-}P}$ = 284.4 Hz, Os*P*Ph$_3$). ^{13}C{^{1}H} NMR with ^{1}H-^{13}C HMBC and ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2): δ = 236.47 (dt, $J_{P\text{-}C}$ = 20.5 Hz, $J_{P\text{-}C}$ = 6.7 Hz, C4), 234.98 (s, C8), 209.04 (s, C1), 153.08 (s, C6), 131.84 (s, C5), 117.99 (d, $J_{P\text{-}C}$ = 68.5 Hz, C2), 116.38 (s, C7), 96.48 (d, $J_{P\text{-}C}$ = 23.4 Hz, C3), and 34.37 ppm (s, C9). HRMS (ESI): *m/z* calcd for $[C_{63}H_{52}Cl_2OOsP_3]^+$, 1179.2217; found, 1179.2185. Anal. calcd (%) for $C_{63}H_{52}BCl_2F_4OOsP_3$: C 59.77, H 4.14; found: C 59.79, H 4.51.

Synthesis pathway for complex 2



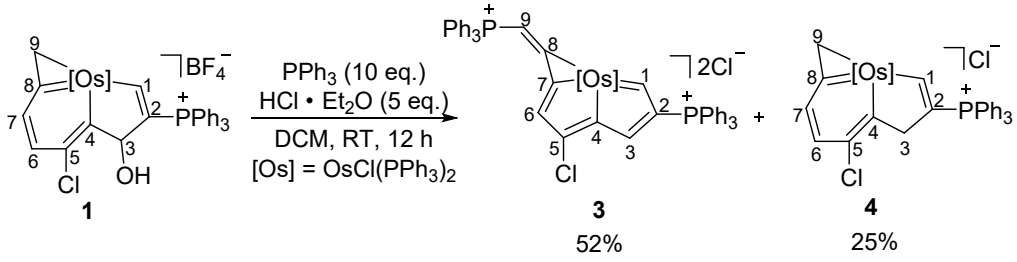
Preparation and characterization of complex 2

L (144 mg, 0.97 mmol), dissolved in 5 mL dichloromethane, was added to a solution of $OsCl_2(PR_3)_3$ (R = *p*-tolyl, 1.00 g, 0.85 mmol) in dichloromethane (15 mL). Then hydrogen chloride (0.43 mL, 2.0 M in diethyl ether, 0.85 mmol) was added to the solution in the following. After stirring for 4 h at RT, sodium tetrafluoroborate (466 mg, 4.25 mmol) was added to the solution for 5 min. The solution was then evaporated under vacuum to approximately 3 mL and purified by flash

chromatography on silica gel (eluent: dichloromethane/acetone, 20/1) to afford a brown solid. The solid was dissolved in dichloromethane (1 mL), and diethyl ether (20 mL) was added to give a yellow precipitate. The precipitate was isolated by filtration to yield complex **2** (449 mg, 38%) as a yellow solid.

^{1}H NMR with ^{1}H-^{13}C HSQC (600.1 MHz, CD_2Cl_2): δ = 11.22 (d, $J_{P\text{-}H}$ = 23.1 Hz, 1H, H1), 7.85 (d, $J_{P\text{-}H}$ = 7.6 Hz, 1H, H6), 7.40 (d, $J_{P\text{-}H}$ = 7.7 Hz, 1H, H7), 5.24 (m, 1H, H9a), 4.87 (m, 1H, H9b), 4.54 (d, $J_{P\text{-}H}$ = 4.9 Hz, 1H, H3), 2.51 (s, 9H, CP(Ph-CH_3)$_3$), 2.27 (d, $J_{P\text{-}H}$ = 4.7 Hz, 19H, Os[P(Ph-CH_3)$_3$]$_2$ and OH), and 7.41−6.81 ppm (36H, other aromatic protons). ^{31}P{^{1}H} NMR (242.9 MHz, CD_2Cl_2): δ = 12.40 (s, C*P*(Ph-CH_3)$_3$), −14.97 (d, $J_{P\text{-}P}$ = 276.9 Hz, Os*P*(Ph-CH_3)$_3$), and −21.11 ppm (d, $J_{P\text{-}P}$ = 276.9 Hz, Os*P*(Ph-CH_3)$_3$). ^{13}C{^{1}H} NMR with ^{1}H-^{13}C HMBC and ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2): δ = 236.27 (dt, $J_{P\text{-}C}$ = 20.1 Hz, $J_{P\text{-}C}$ = 5.9 Hz, C4), 234.52 (s, C8), 208.75 (s, C1), 152.35 (s, C6), 131.81 (s, C5), 118.33 (d, $J_{P\text{-}C}$ = 71.9 Hz, C2), 116.17 (s, C7), 96.41 (d, $J_{P\text{-}C}$ = 23.9 Hz, C3), 34.77 (s, C9), 21.53 (s, CP(Ph-CH_3)$_3$), and 20.95 ppm (d, $J_{P\text{-}C}$ = 6.8 Hz, Os[P(Ph-CH_3)$_3$]$_2$). HRMS (ESI): *m/z* calcd for $[C_{72}H_{70}Cl_2OOsP_3]^+$, 1305.3613; found, 1305.3582.

Synthesis pathway for complexes 3 and 4

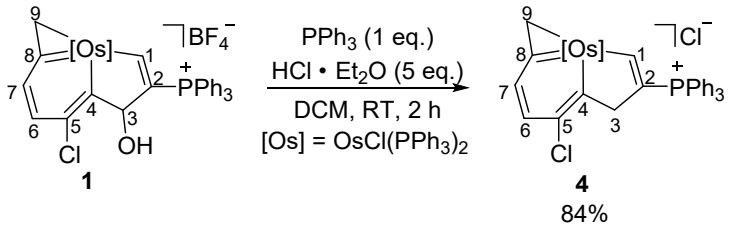


Preparation and characterization of complexes 3 and 4

Hydrochloric acid (0.40 mL, 2.0 M in diethyl ether, 0.80 mmol) was added at RT to the solution in dichloromethane (4 mL) of complex **1** (200 mg, 0.16 mmol) and triphenylphosphine (419 mg, 1.60 mmol), then stirred for 12 h to obtain a brown solution. The solution was evaporated under vacuum to approximately 2 mL. Then the solution was purified by flash chromatography on silica gel (eluent: dichloromethane/methanol, 5/1) to afford a red solid. The solid was dissolved in

dichloromethane (1 mL) and diethyl ether (20 mL) was added to yield a red precipitate which was collected by filtration to yield complex **3** (120 mg, 52%) as a red solid. Another composition was purified by flash chromatography on silica gel (eluent: dichloromethane/methanol, 20/1) to afford a brown solid. The solid was dissolved in dichloromethane (1 mL), and diethyl ether (20 mL) was added to give a brown precipitate which was obtained by filtration to yield complex **4** (48 mg, 25%) as a brown solid.

Reaction of 1 with acid and one equivalent of PPh_3

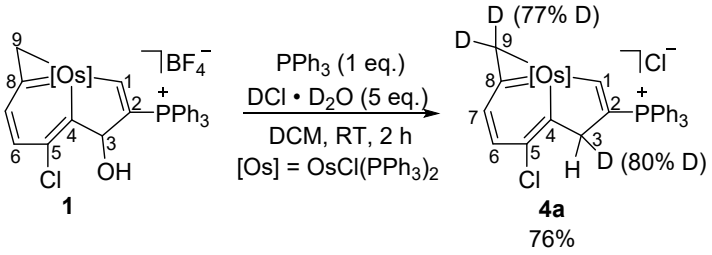


Complex **1** (200 mg, 0.16 mmol) and triphenylphosphine (42 mg, 0.16 mmol) were dissolved in dichloromethane (4 mL), then hydrochloric acid (0.40 mL, 2.0 M in diethyl ether, 0.80 mmol) was added to the solution at RT. After being stirred for 2 h, the solution was evaporated under vacuum to approximately 2 mL and purified by flash chromatography on silica gel (eluent: dichloromethane/methanol, 20/1) to afford a brown solid. The solid was dissolved in dichloromethane (1 mL), and diethyl ether (20 mL) was added to give a brown precipitate which was obtained by filtration to yield complex **4** as a brown solid. Yield: 161 mg, 84%.

Complex **3**: ^{1}H NMR with ^{1}H-^{13}C HSQC (600.1 MHz, CD_2Cl_2): δ = 14.18 (d, $J_{P\text{-}H}$ = 16.1 Hz, 1H, H1), 8.81 (s, 1H, H3), 7.00 (d, $J_{P\text{-}H}$ = 28.1 Hz, 1H, H9), 6.21 (s, 1H, H6), and 8.02−7.05 ppm (60H, other aromatic protons). ^{31}P{^{1}H} NMR (242.9 MHz, CD_2Cl_2): δ = 17.53 (s, C*P*Ph$_3$), 12.07 (s, C*P*Ph$_3$), and −24.17 ppm (s, Os*P*Ph$_3$). ^{13}C{^{1}H} NMR with ^{1}H-^{13}C HMBC and ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2): δ = 236.77 (s, C1), 191.34 (d, $J_{P\text{-}C}$ = 24.0 Hz, C4), 191.03 (m, C7), 160.52 (s, C5), 159.90 (t, $J_{P\text{-}C}$ = 4.5 Hz, C8), 149.42 (d, $J_{P\text{-}C}$ = 21.9 Hz, C3), 144.20 (d, $J_{P\text{-}C}$ = 68.9 Hz, C2), 143.30 (s, C6), and 93.00 ppm (d, $J_{P\text{-}C}$ = 81.3 Hz, C9). HRMS (ESI): *m/z* calcd for $[C_{81}H_{64}Cl_2OsP_4]^{2+}$, 711.1470; found, 711.1470. Anal. calcd (%) for $C_{81}H_{64}Cl_4OsP_4$: C 65.15, H 4.32; found: C 65.26, H 4.44.

Complex **4**: ^{1}H NMR with ^{1}H-^{13}C HSQC (600.1 MHz, CD_2Cl_2): δ = 11.22 (d, $J_{P\text{-}H}$ = 24.1 Hz, 1H, H1), 7.51 (d, $J_{P\text{-}H}$ = 7.5 Hz, 1H, H6), 7.44 (d, $J_{P\text{-}H}$ = 7.5 Hz, 1H, H7), 5.24 (t, $J_{P\text{-}H}$ = 9.3 Hz, 2H, H9), 2.06 (s, 2H, H3), and 7.92−7.15 ppm (45H, other aromatic protons). ^{31}P{^{1}H} NMR (242.9 MHz, CD_2Cl_2): δ = 12.75 (s, C*P*Ph$_3$) and −15.32 ppm (s, Os*P*Ph$_3$). ^{13}C{^{1}H} NMR with ^{1}H-^{13}C HMBC and ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2): δ = 251.15 (dt, $J_{P\text{-}C}$ = 21.1 Hz, $J_{P\text{-}C}$ = 6.3 Hz, C4), 232.83 (s, C8), 208.57 (d, $J_{P\text{-}C}$ = 4.7 Hz, C1), 153.30 (s, C6), 129.89 (s, C5), 113.83 (d, $J_{P\text{-}C}$ = 68.7 Hz, C2), 113.40 (s, C7), 68.77 (d, $J_{P\text{-}C}$ = 26.9 Hz, C3), and 36.56 ppm (s, C9). HRMS (ESI): *m/z* calcd for $[C_{63}H_{52}Cl_2OsP_3]^+$, 1163.2268; found, 1163.2201. Anal. calcd (%) for $C_{63}H_{52}Cl_3OsP_3$: C 63.13, H 4.37; found: C 63.06, H 4.68.

Synthesis pathway for complex 4a



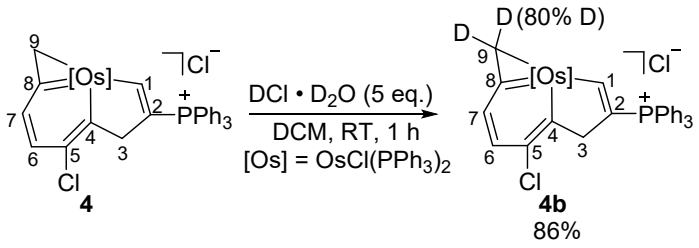
Preparation and characterization of complex 4a

Complex **1** (200 mg, 0.16 mmol) and triphenylphosphine (42 mg, 0.16 mmol) were dissolved in dichloromethane (4 mL), then deuterium chloride (0.07 mL, 35% in deuterium-oxide, 0.80 mmol) was added to the solution at RT. After being stirred for 2 h, the solution was evaporated under vacuum to approximately 2 mL and then purified by flash chromatography on silica gel (eluent: dichloromethane/methanol, 20/1) to afford a brown solid. The solid was dissolved in dichloromethane (1 mL), and diethyl ether (20 mL) was added to give a brown precipitate which was obtained by filtration to yield complex **4a** as a brown solid. Yield: 146 mg, 76%.

^{1}H NMR with ^{1}H-^{13}C HSQC (600.1 MHz, CD_2Cl_2): δ = 11.22 (d, $J_{P\text{-}H}$ = 24.1 Hz, 1H, H1), 7.50 (d, $J_{P\text{-}H}$ = 7.5 Hz, 1H, H6), 7.44 (d, $J_{P\text{-}H}$ = 7.5 Hz, 1H, H7), 5.22 (m, 0.46H, H9), 2.05 (s, 0.80H, H3), and 7.90−7.14 ppm (45H, other aromatic protons). ^{31}P{^{1}H} NMR (242.9 MHz, CD_2Cl_2): δ = 12.75 (s, C*P*Ph$_3$) and −15.26 ppm (s, Os*P*Ph$_3$).

HRMS (ESI): *m/z* calcd for $[C_{63}H_{50}D_2Cl_2OsP_3]^+$, 1165.2379; found, 1165.2383.

Synthesis pathway for complex 4b

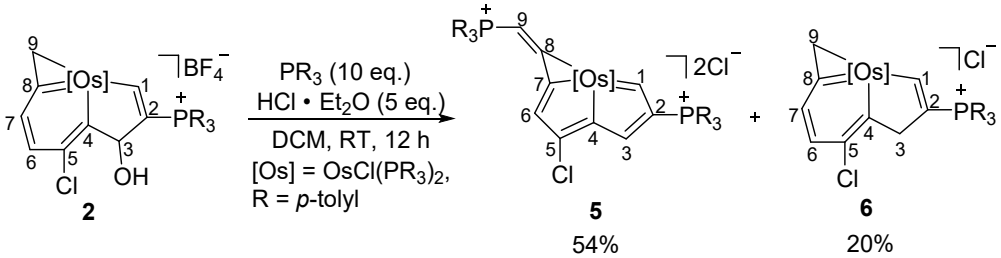


Preparation and characterization of complex 4b

Complex **4** (200 mg, 0.17 mmol) was dissolved in dichloromethane (4 mL), then deuterium chloride (0.07 mL, 35% in deuterium-oxide, 0.85 mmol) was added to the solution at RT. After being stirred for 1 h, the solution was evaporated under vacuum to approximately 2 mL and then purified by flash chromatography on silica gel (eluent: dichloromethane/methanol, 20/1) to afford a brown solid. The solid was dissolved in dichloromethane (1 mL), and diethyl ether (20 mL) was added to give a brown precipitate which was obtained by filtration to yield complex **4b** as a brown solid. Yield: 175 mg, 86%.

^{1}H NMR with ^{1}H-^{13}C HSQC (600.1 MHz, CD_2Cl_2): δ = 11.22 (d, $J_{P\text{-}H}$ = 24.4 Hz, 1H, H1), 7.50 (d, $J_{P\text{-}H}$ = 7.3 Hz, 1H, H6), 7.44 (d, $J_{P\text{-}H}$ = 7.2 Hz, 1H, H7), 5.21 (m, 0.40H, H9), 2.06 (s, 2H, H3), and 7.91−7.15 ppm (45H, other aromatic protons). ^{31}P{^{1}H} NMR (242.9 MHz, CD_2Cl_2): δ = 12.73 (s, C*P*Ph$_3$) and −15.27 ppm (s, Os*P*Ph$_3$). HRMS (ESI): *m/z* calcd for $[C_{63}H_{50}D_2Cl_2OsP_3]^+$, 1165.2379; found, 1165.2331.

Synthesis pathway for complexes 5 and 6

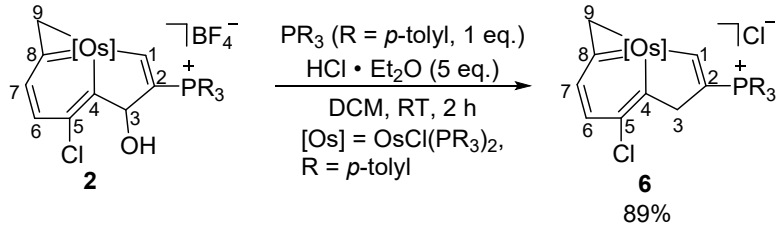


Preparation and characterization of complexes 5 and 6

Hydrochloric acid (0.35 mL, 2.0 M in diethyl ether, 0.70 mmol) was added at RT to

the solution in dichloromethane (4 mL) of complex **2** (200 mg, 0.14 mmol) and tri(*p*-tolyl)phosphine (429 mg, 1.40 mmol), then stirred for 12 h to obtain a brown solution. The solution was evaporated under vacuum to approximately 2 mL. Then the solution was purified by flash chromatography on silica gel (eluent: dichloromethane/methanol, 5/1) to afford a red solid. The solid was dissolved in dichloromethane (1 mL) and diethyl ether (20 mL) was added to yield a red precipitate which was collected by filtration to yield complex **5** (125 mg, 54%) as a red solid. Another composition was purified by flash chromatography on silica gel (eluent: dichloromethane/methanol, 20/1) to afford a brown solid. The solid was dissolved in dichloromethane (1 mL), and diethyl ether (20 mL) was added to give a brown precipitate which was obtained by filtration to yield complex **6** (37 mg, 20%) as a brown solid.

Reaction of 2 with acid and one equivalent of tri(*p*-tolyl)phosphine



Complex **2** (200 mg, 0.14 mmol) and tri(*p*-tolyl)phosphine (43 mg, 0.14 mmol) were dissolved in dichloromethane (4 mL), then hydrochloric acid (0.35 mL, 2.0 M in diethyl ether, 0.70 mmol) was added to the solution at RT. After being stirred for 2 h, the solution was evaporated under vacuum to approximately 2 mL and purified by flash chromatography on silica gel (eluent: dichloromethane/methanol, 20/1) to afford a brown solid. The solid was dissolved in dichloromethane (1 mL), and diethyl ether (20 mL) was added to give a brown precipitate which was obtained by filtration to yield complex **6** as a brown solid. Yield: 166 mg, 89%.

Complex **5**: ^{1}H NMR with ^{1}H-^{13}C HSQC (600.1 MHz, CD_2Cl_2): δ = 14.05 (d, $J_{P\text{-}H}$ = 16.1 Hz, 1H, H1), 8.63 (t, $J_{P\text{-}H}$ = 2.8 Hz, 1H, H3), 6.78 (d, $J_{P\text{-}H}$ = 20.6 Hz, 1H, H9), 6.25 (s, 1H, H6), 2.56 (s, 9H, CP(Ph-CH_3)$_3$), 2.50 (s, 9H, CP(Ph-CH_3)$_3$), 2.20 (s, 18H, Os[P(Ph-CH_3)$_3$]$_2$), and 7.45−6.76 ppm (48H, other aromatic protons). ^{31}P{^{1}H} NMR (242.9 MHz, CD_2Cl_2): δ = 16.80 (s, C*P*(Ph-CH_3)$_3$), 11.16 (s, C*P*(Ph-CH_3)$_3$), and −26.15 ppm (s, Os*P*(Ph-CH_3)$_3$). ^{13}C{^{1}H} NMR with ^{1}H-^{13}C HMBC and ^{1}H-^{13}C

HSQC (150.9 MHz, CD_2Cl_2): δ = 236.68 (s, C1), 191.65 (d, $J_{P\text{-}C}$ = 24.2 Hz, C4), 190.20 (m, C7), 159.69 (m, C8), 159.38 (s, C5), 149.04 (d, $J_{P\text{-}C}$ = 22.3 Hz, C3), 144.86 (d, $J_{P\text{-}C}$ = 70.4 Hz, C2), 142.94 (s, C6), 93.08 (d, $J_{P\text{-}C}$ = 83.2 Hz, C9), 21.75 (s, CP(Ph-CH_3)$_3$), 21.65 (s, CP(Ph-CH_3)$_3$), and 21.04 ppm (s, Os[P(Ph-CH_3)$_3$]$_2$). HRMS (ESI): *m/z* calcd for $[C_{93}H_{88}Cl_2OsP_4]^{2+}$, 795.2404; found, 795.2370.

Complex **6**: ^{1}H NMR with ^{1}H-^{13}C HSQC (600.1 MHz, CD_2Cl_2): δ = 11.05 (d, $J_{P\text{-}H}$ = 24.1 Hz, 1H, H1), 7.41 (d, $J_{P\text{-}H}$ = 7.3 Hz, 1H, H6), 7.31 (d, $J_{P\text{-}H}$ = 7.3 Hz, 1H, H7), 5.11 (t, $J_{P\text{-}H}$ = 9.4 Hz, 2H, H9), 1.91 (s, 2H, H3), 2.53 (s, 9H, CP(Ph-CH_3)$_3$), 2.29 (s, 18H, Os[P(Ph-CH_3)$_3$]$_2$), and 7.34−6.91 ppm (36H, other aromatic protons). ^{31}P{^{1}H} NMR (242.9 MHz, CD_2Cl_2): δ = 11.84 (s, C*P*(Ph-CH_3)$_3$) and −16.38 ppm (s, Os*P*(Ph-CH_3)$_3$). ^{13}C{^{1}H} NMR with ^{1}H-^{13}C HMBC and ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2): δ = 250.56 (dt, $J_{P\text{-}C}$ = 21.1 Hz, $J_{P\text{-}C}$ = 6.4 Hz, C4), 232.35 (s, C8), 207.68 (m, C1), 152.36 (s, C6), 129.72 (s, C5), 113.69 (d, $J_{P\text{-}C}$ = 72.1 Hz, C2), 112.73 (s, C7), 68.39 (d, $J_{P\text{-}C}$ = 26.4 Hz, C3), 36.16 (s, C9), 21.59 (s, CP(Ph-CH_3)$_3$), and 20.98 ppm (s, Os[P(Ph-CH_3)$_3$]$_2$). HRMS (ESI): *m/z* calcd for $[C_{72}H_{70}Cl_2OsP_3]^+$, 1289.3663; found, 1289.3662.

3. NMR and ESI-MS Spectra

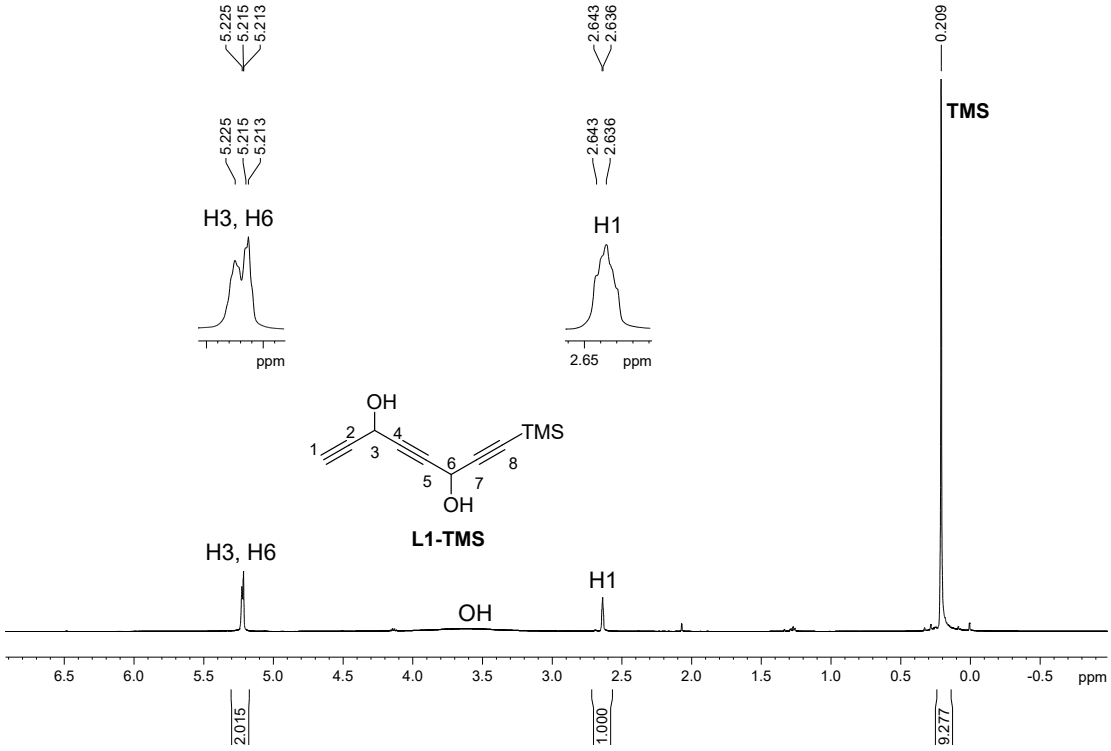


Figure S11. The ^{1}H NMR (500.2 MHz, $CDCl_3$) spectra for compound **L1-TMS**.

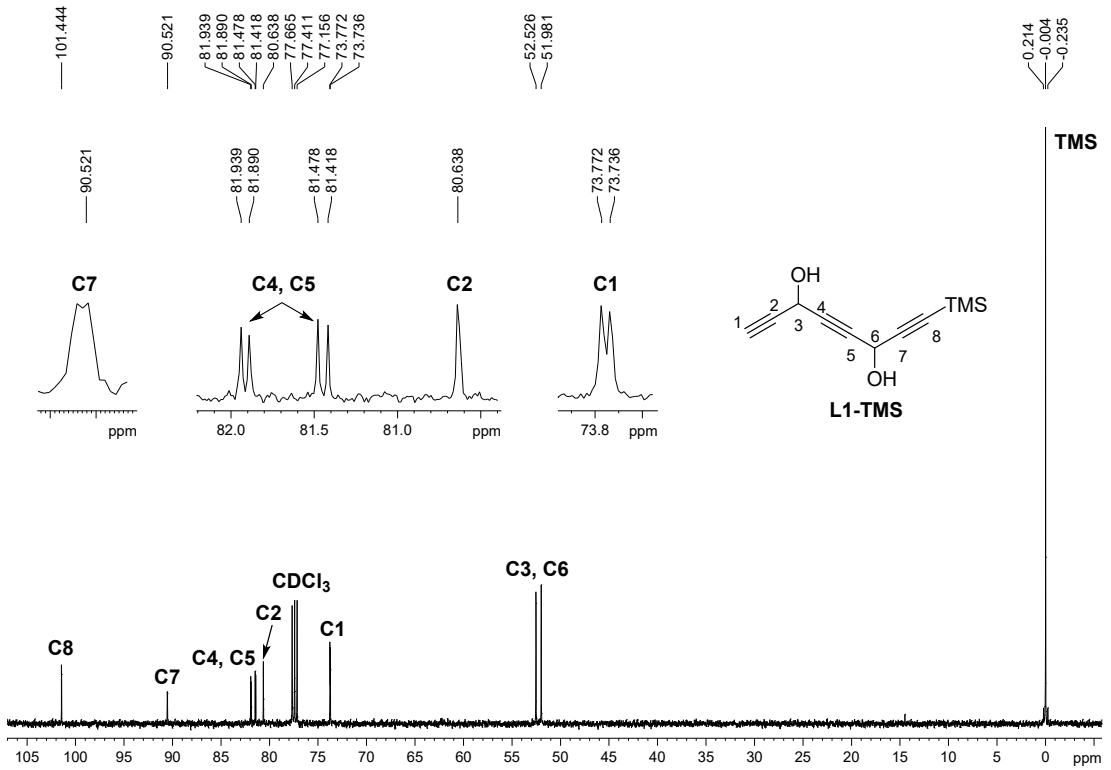


Figure S12. The $^{13}C\{^{1}H\}$ NMR (125.7 MHz, $CDCl_3$) spectra for compound **L1-TMS**.

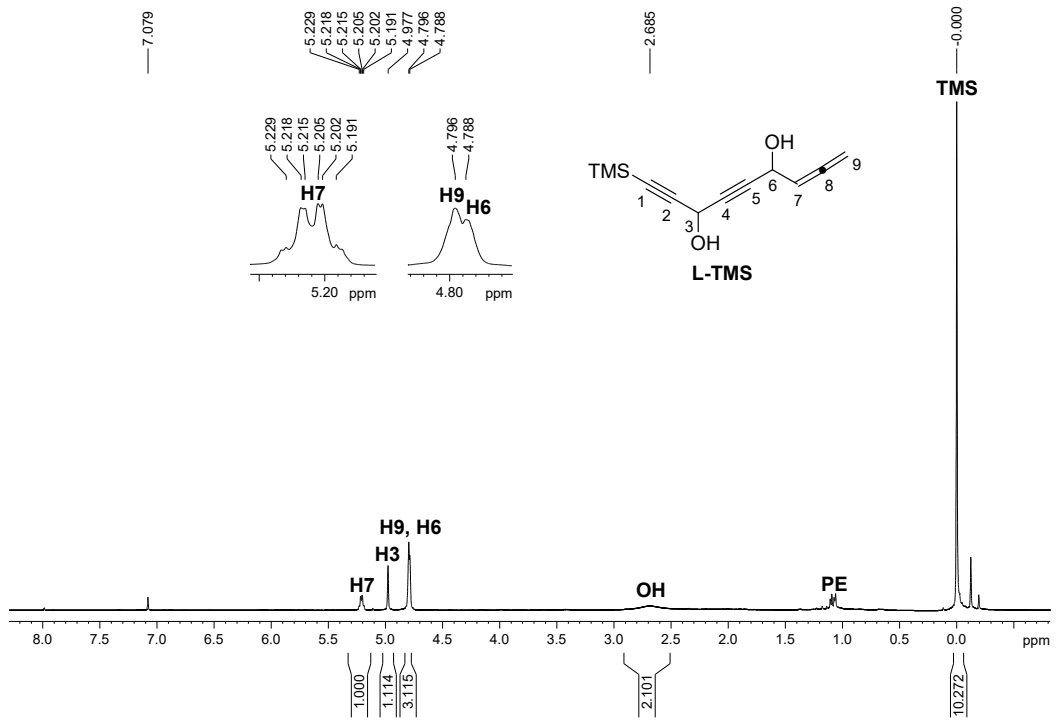


Figure S13. ^{1}H NMR (500.2 MHz, $CDCl_3$) spectra for **L-TMS**.

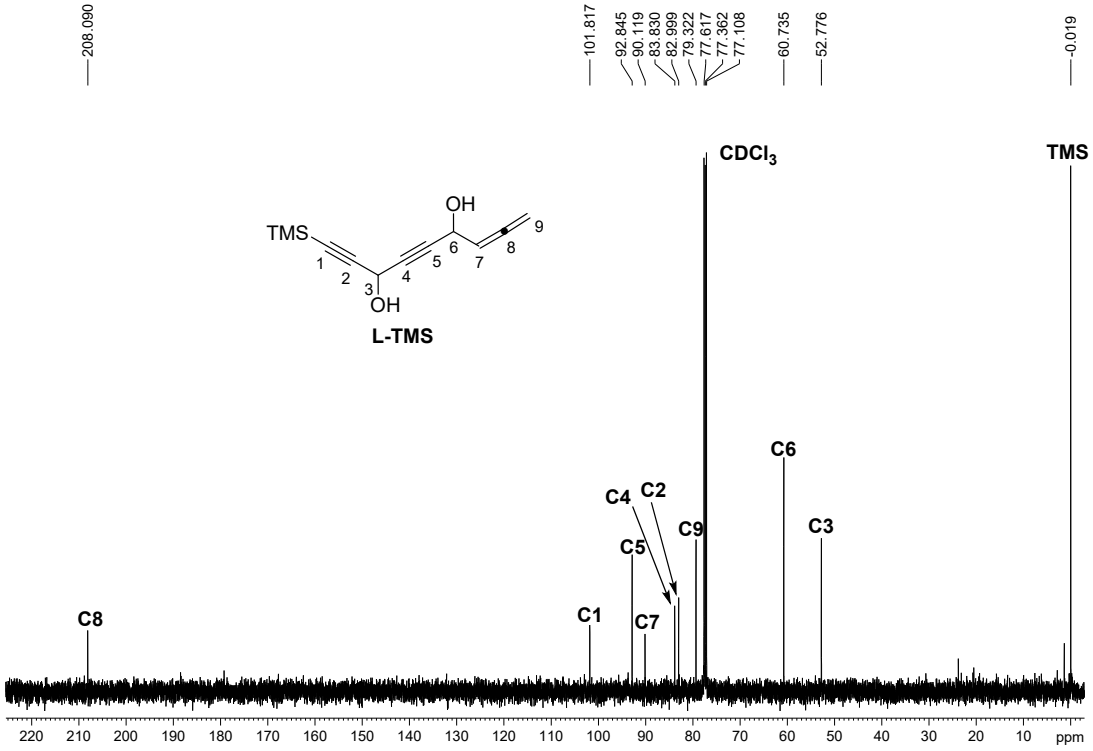


Figure S14. $^{13}C\{^{1}H\}$ NMR (125.7 MHz, $CDCl_3$) spectra for **L-TMS**.

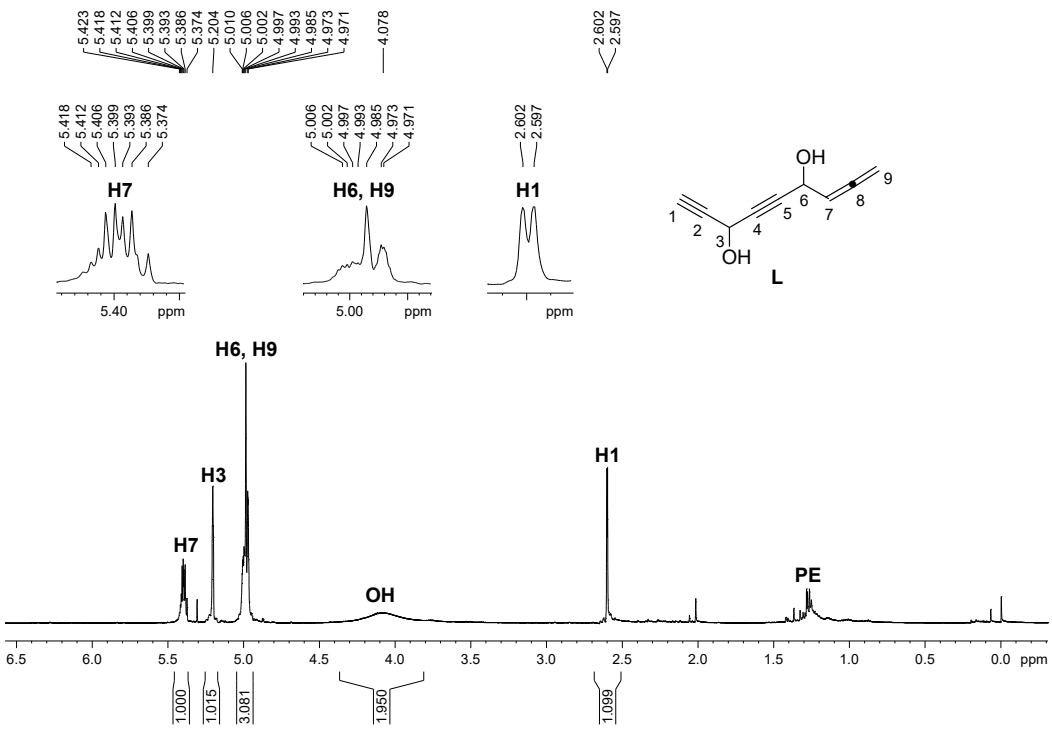


Figure S15. ^{1}H NMR (500.2 MHz, $CDCl_3$) spectra for **L**.

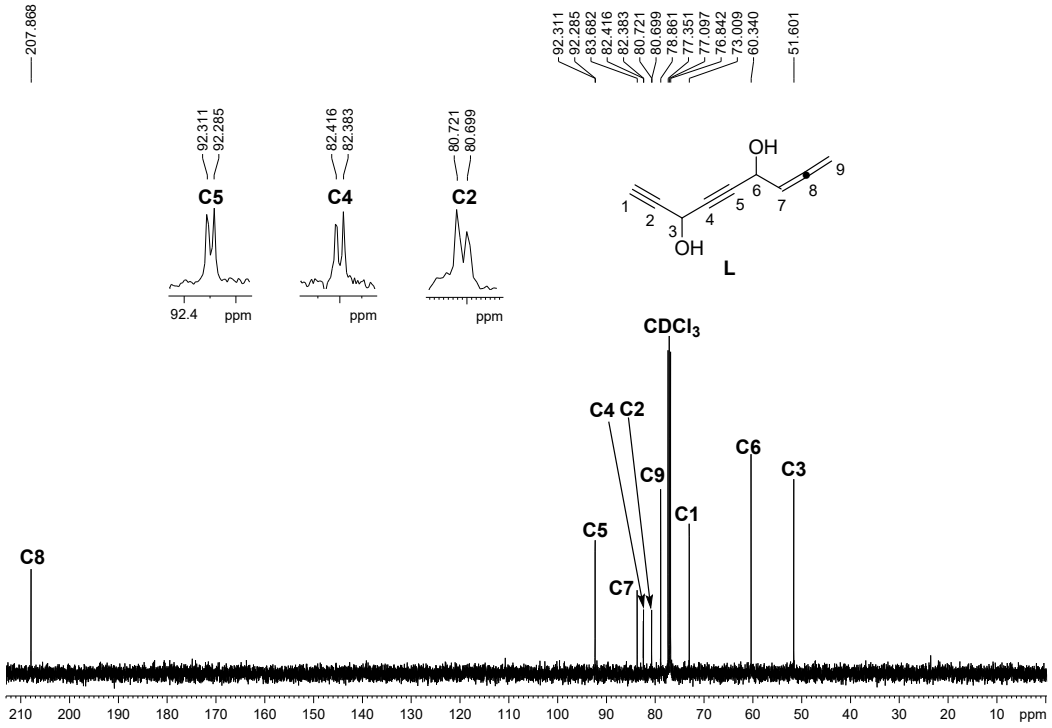


Figure S16. $^{13}C\{^{1}H\}$ NMR (125.7 MHz, $CDCl_3$) spectra for **L**.

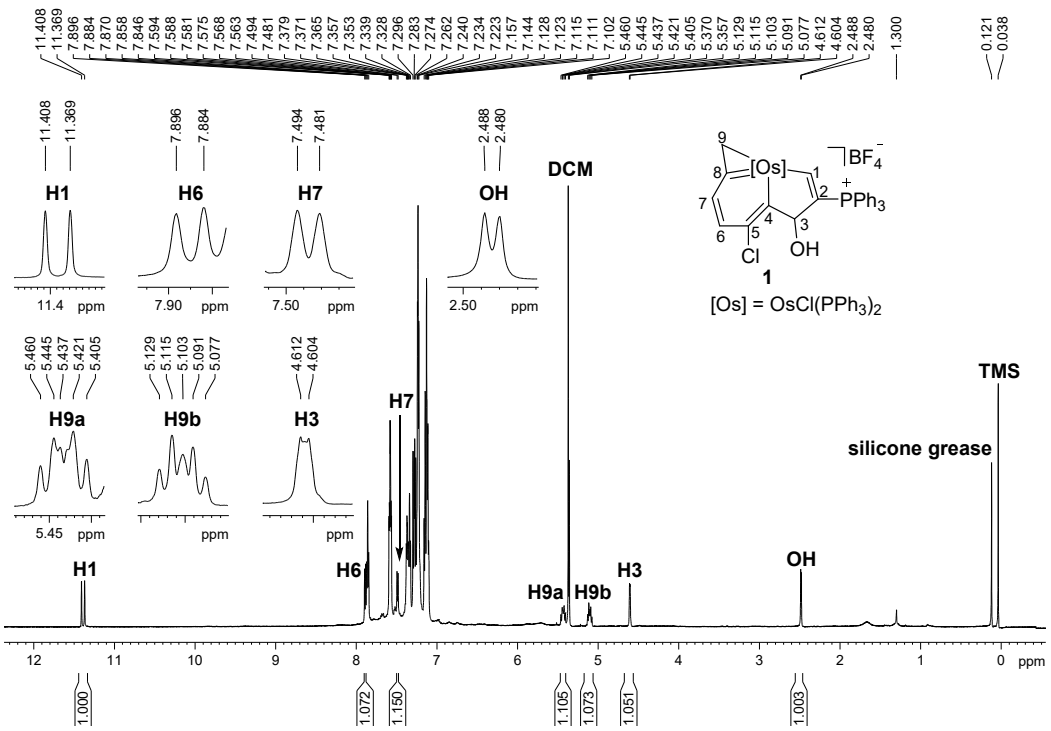


Figure S17. ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectra for complex **1**.

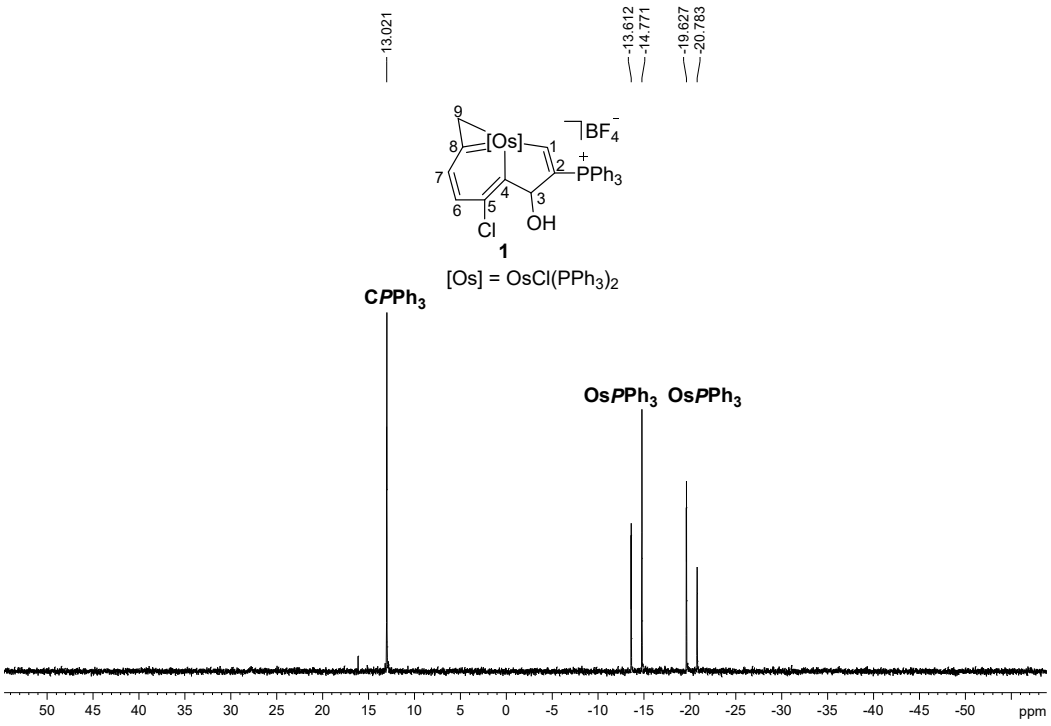


Figure S18. $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectra for complex **1**.

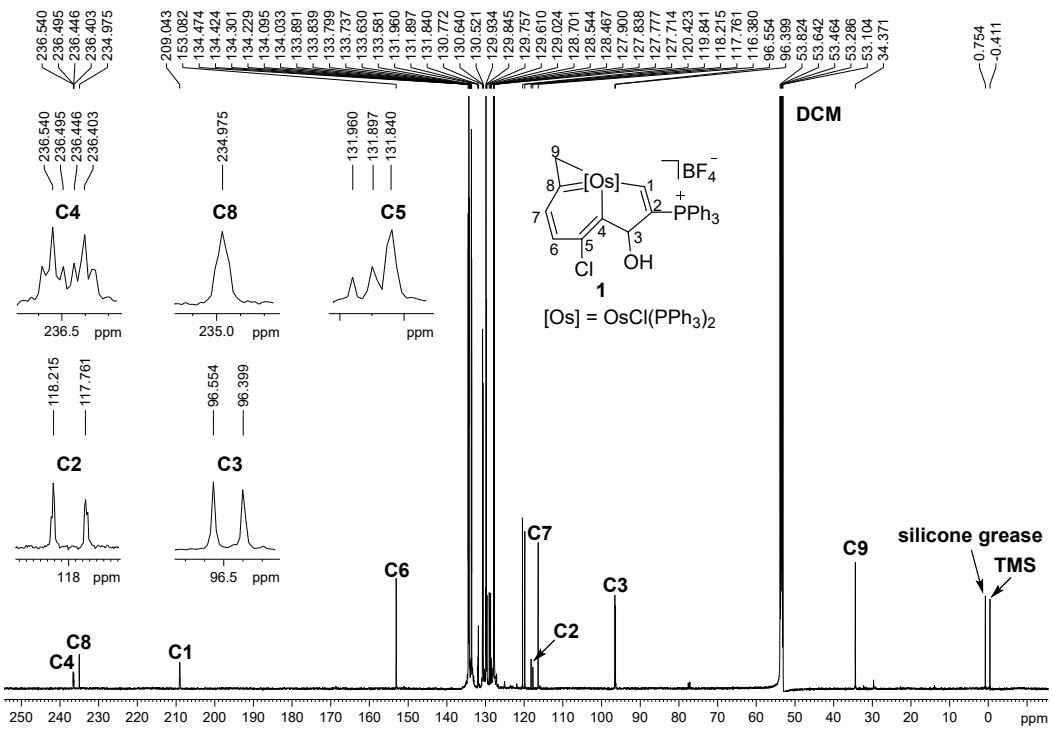


Figure S19. $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectra for complex **1**.

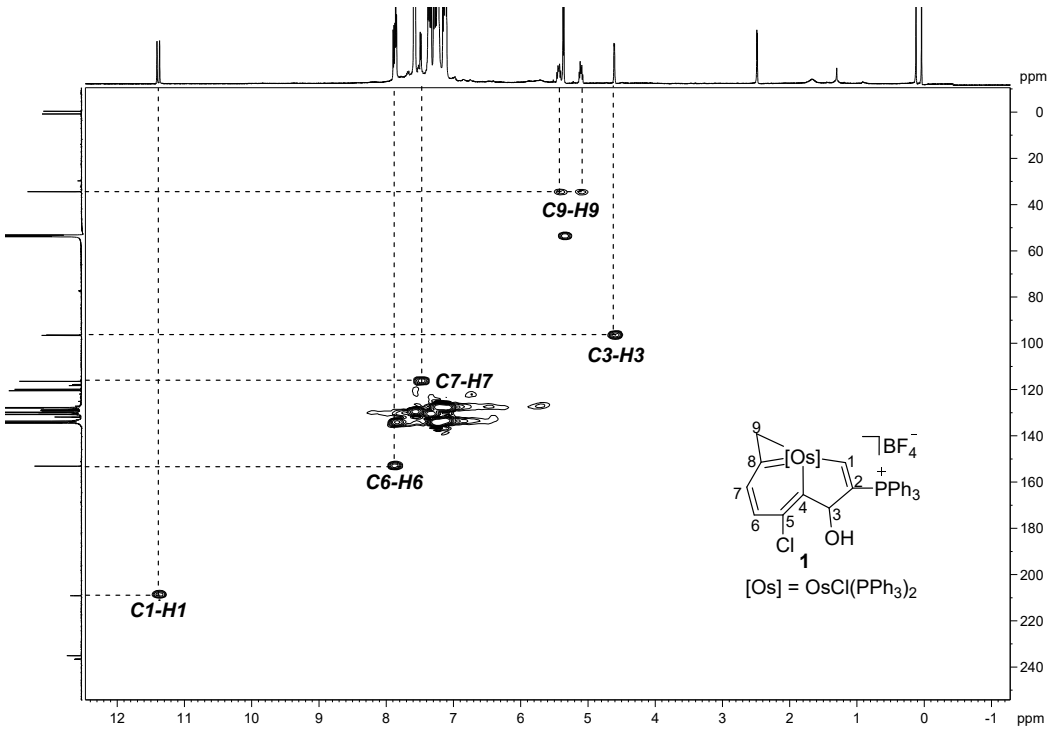


Figure S20. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectra for complex **1**.

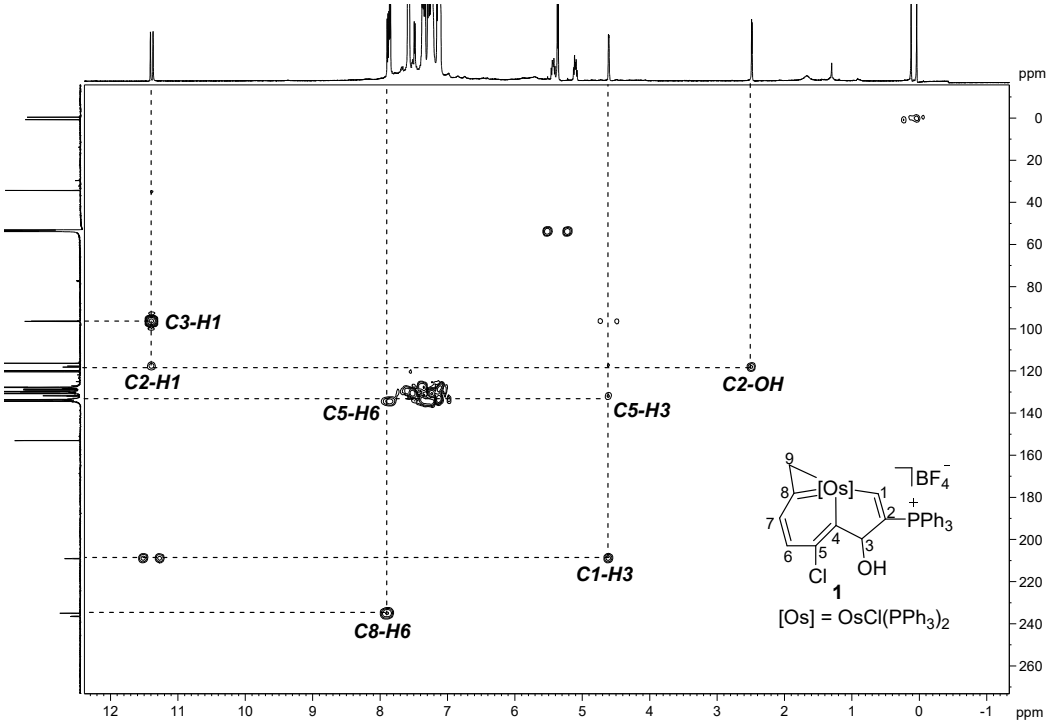


Figure S21. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectra for complex **1**.

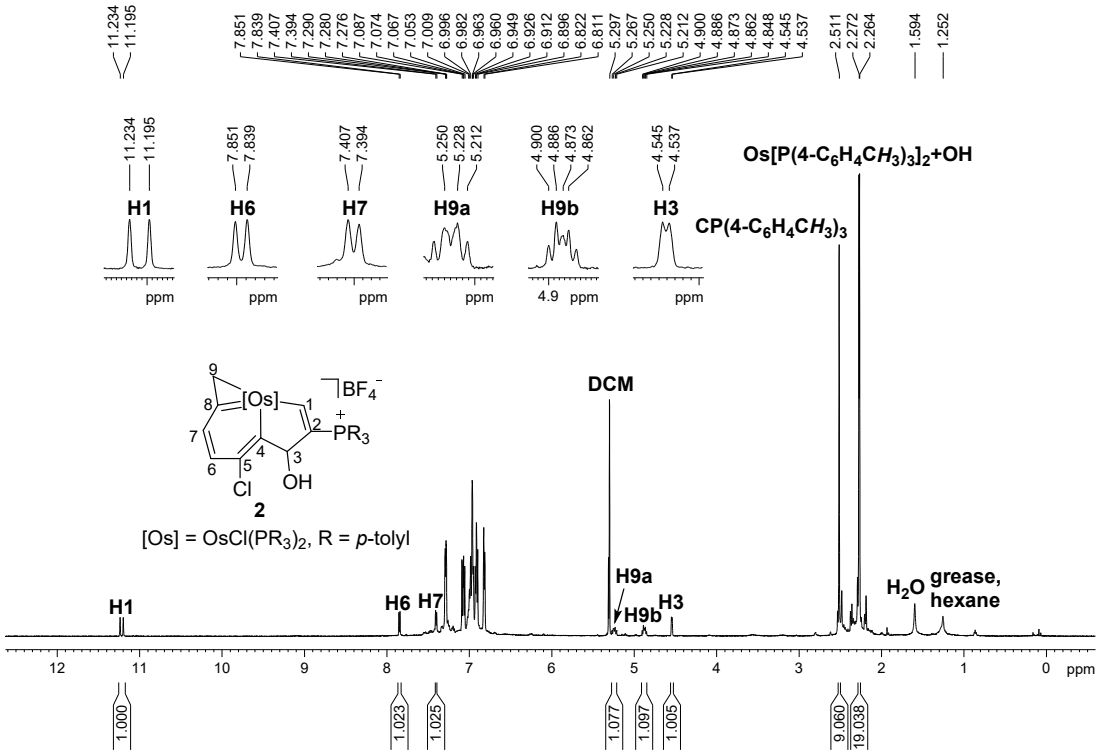


Figure S22. ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectra for complex **2**.

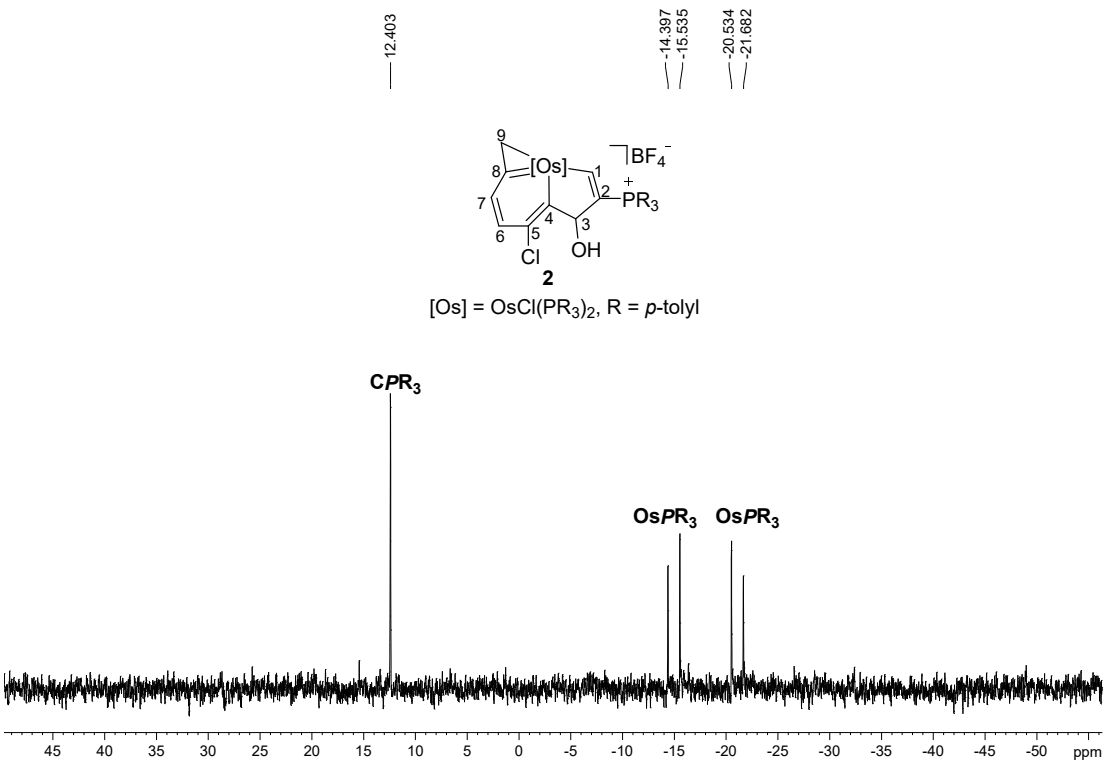


Figure S23. $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectra for complex **2**.

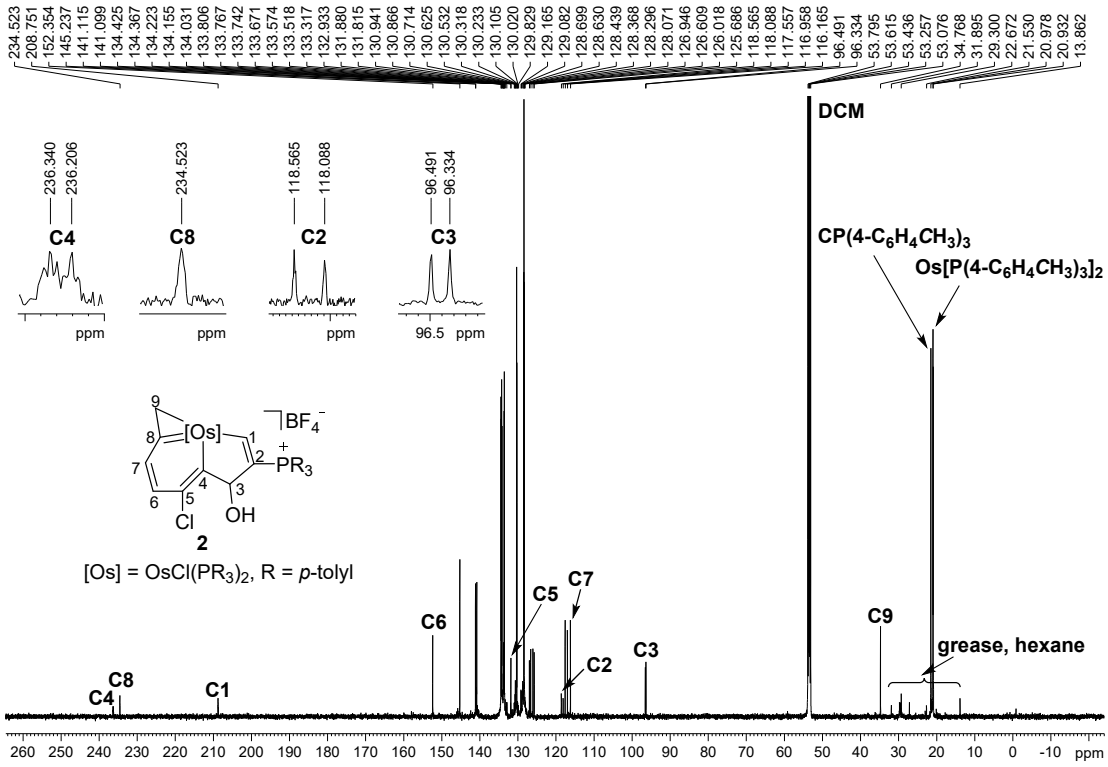


Figure S24. $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectra for complex **2**.

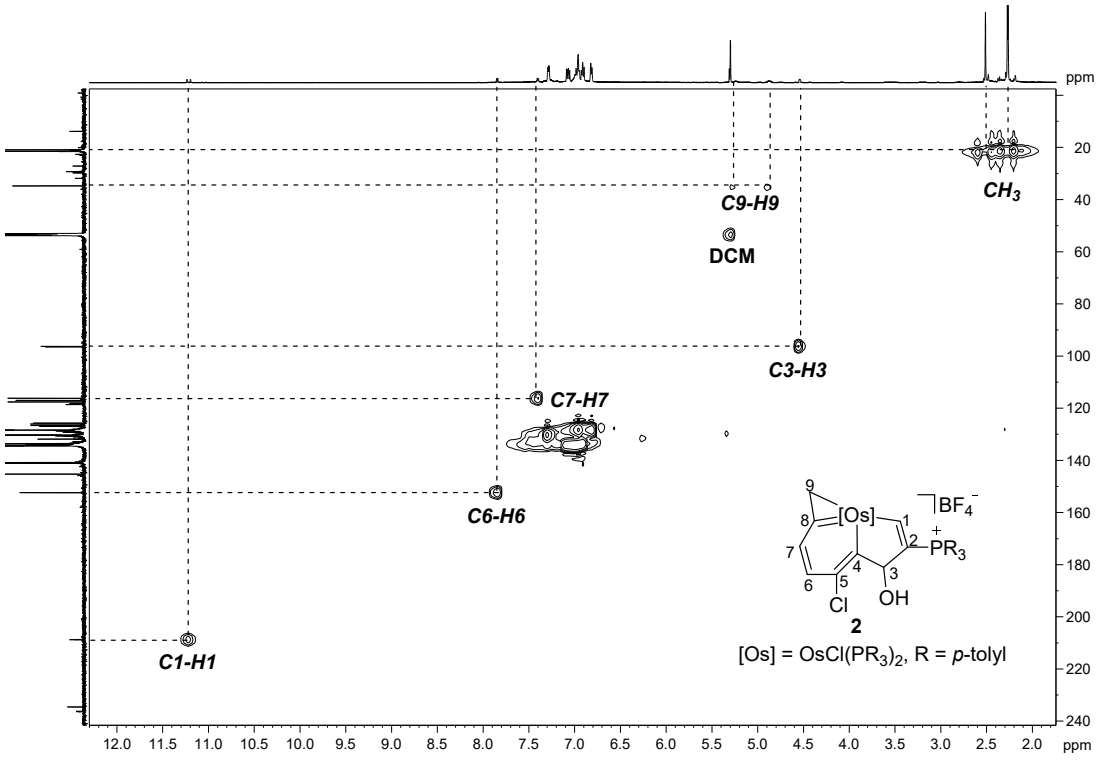


Figure S25. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectra for complex **2**.

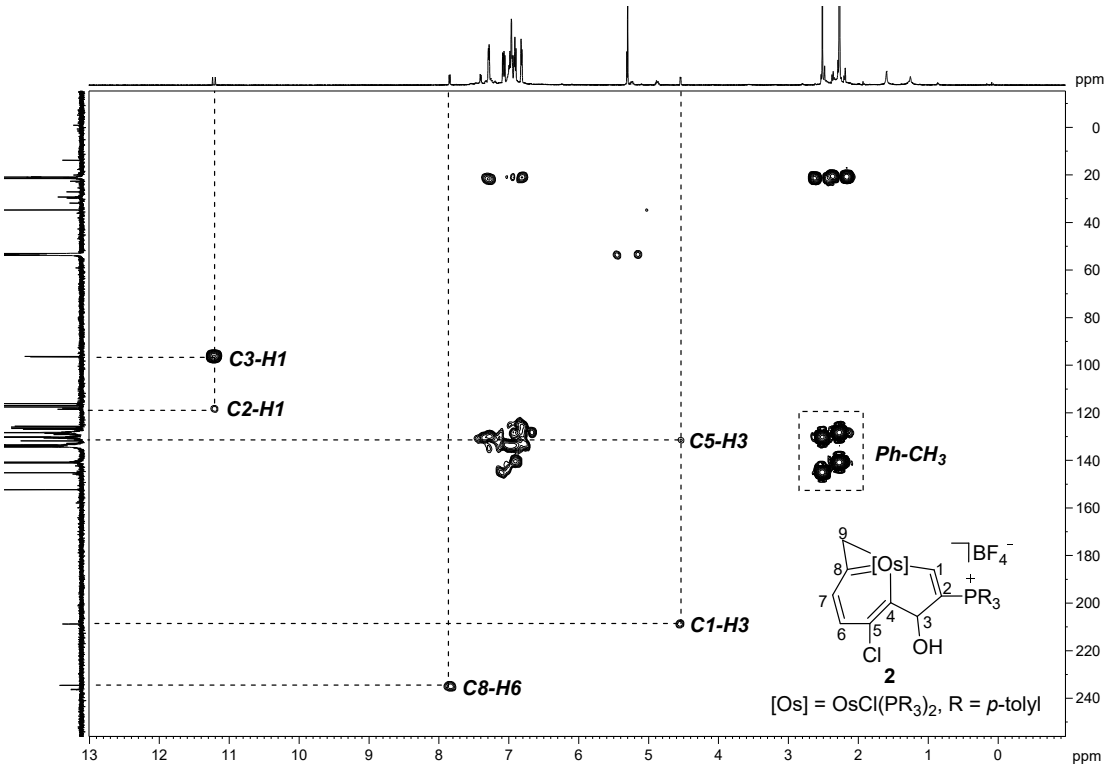


Figure S26. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectra for complex **2**.

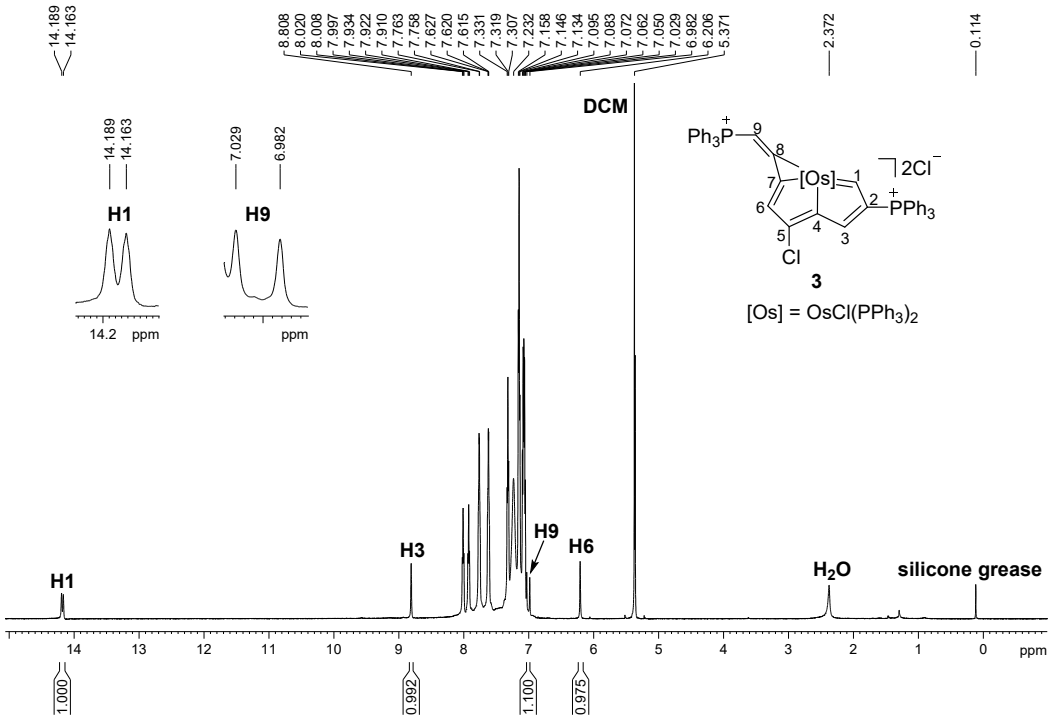


Figure S27. ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectra for complex **3**.

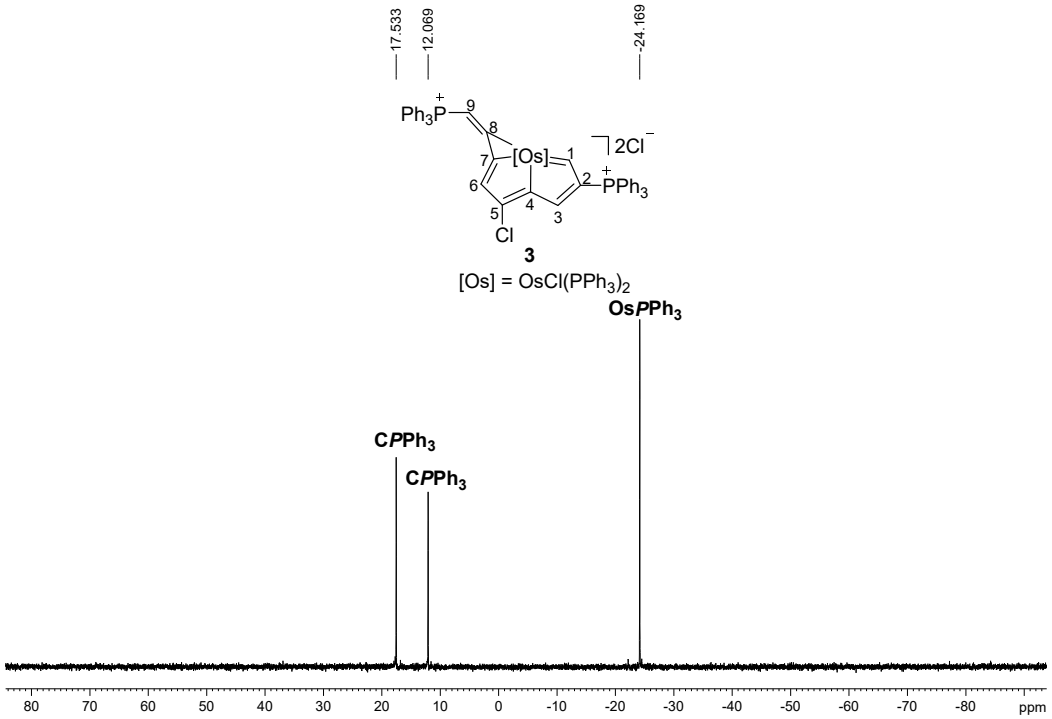


Figure S28. $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectra for complex **3**.

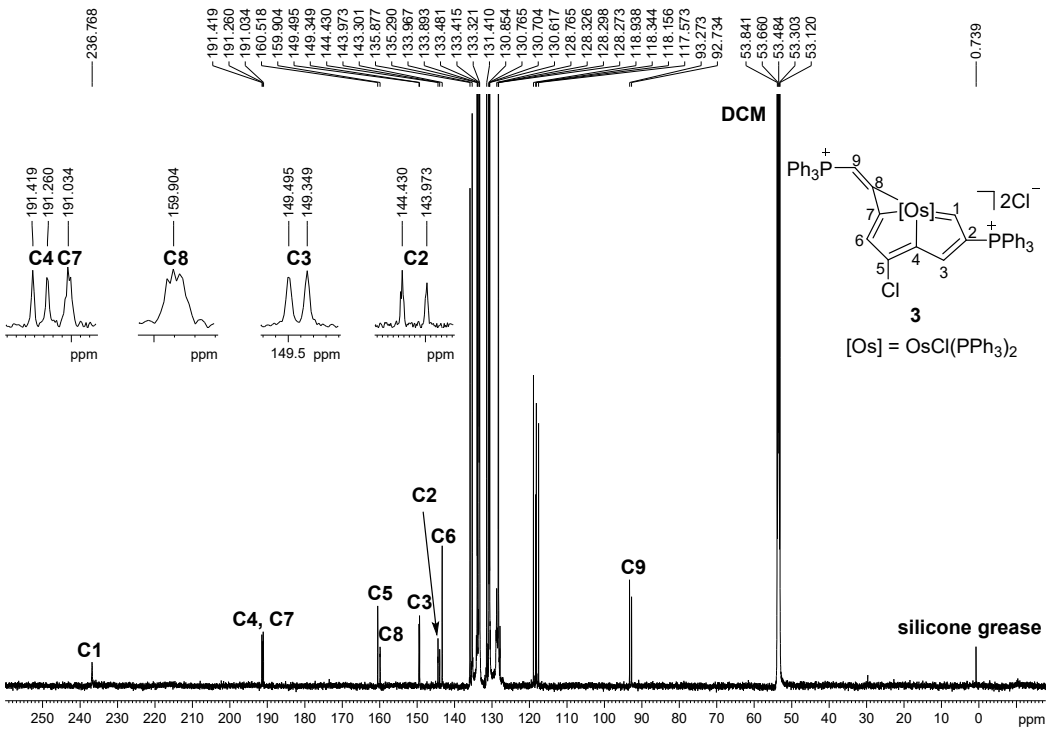


Figure S29. $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectra for complex **3**.

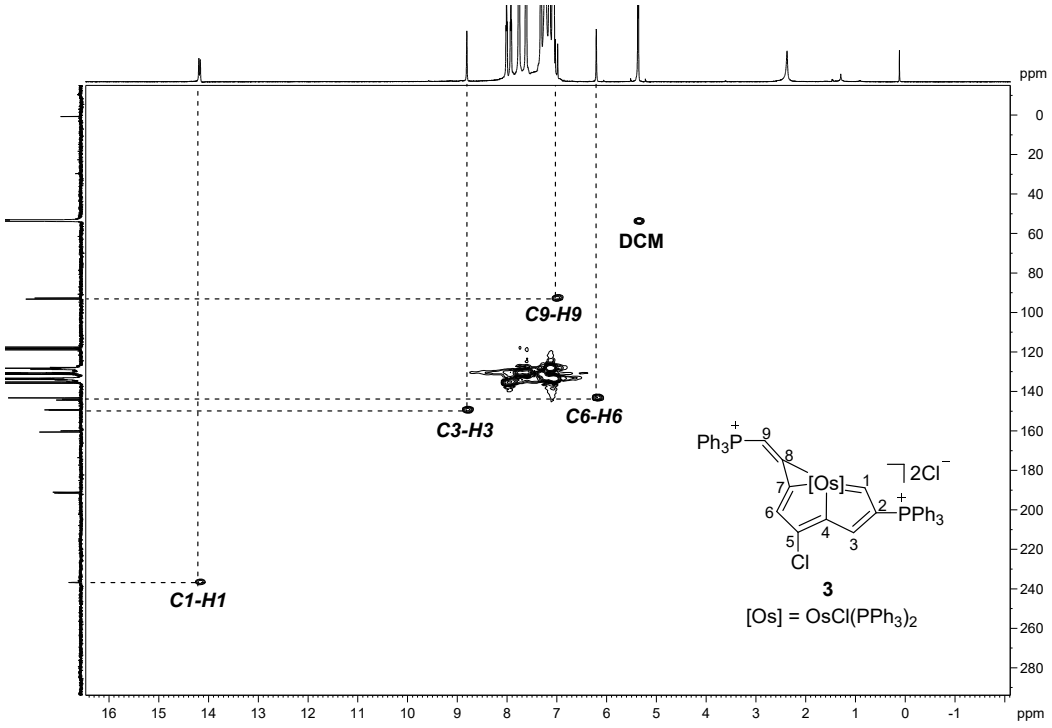


Figure S30. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectra for complex **3**.

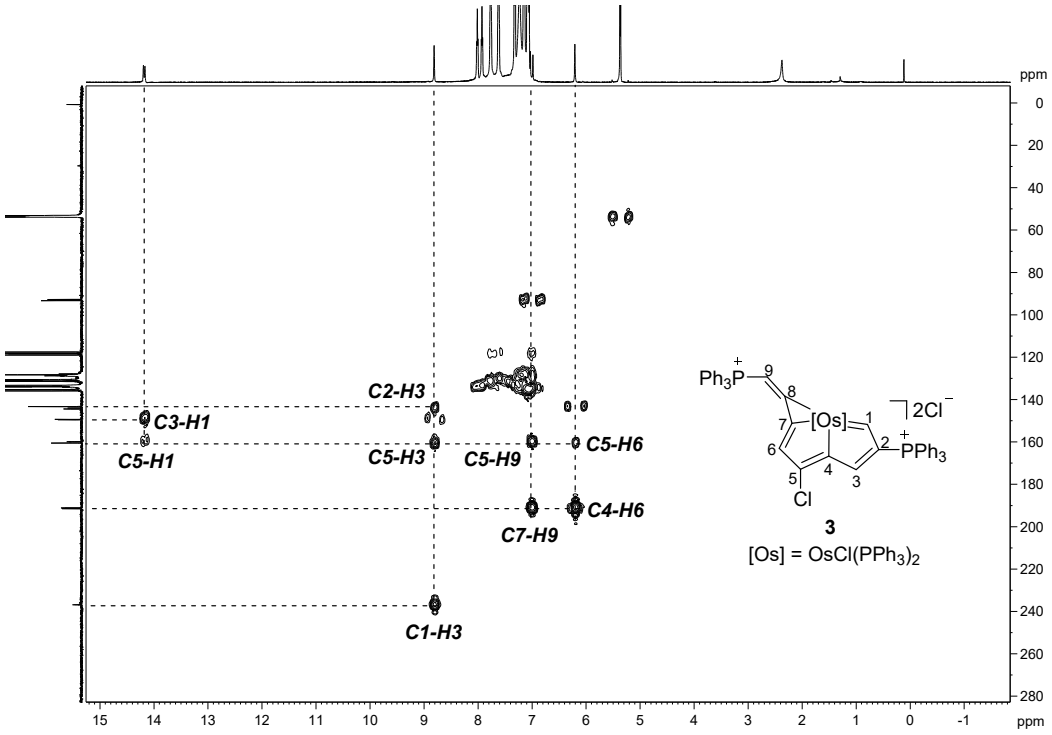


Figure S31. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectra for complex **3**.

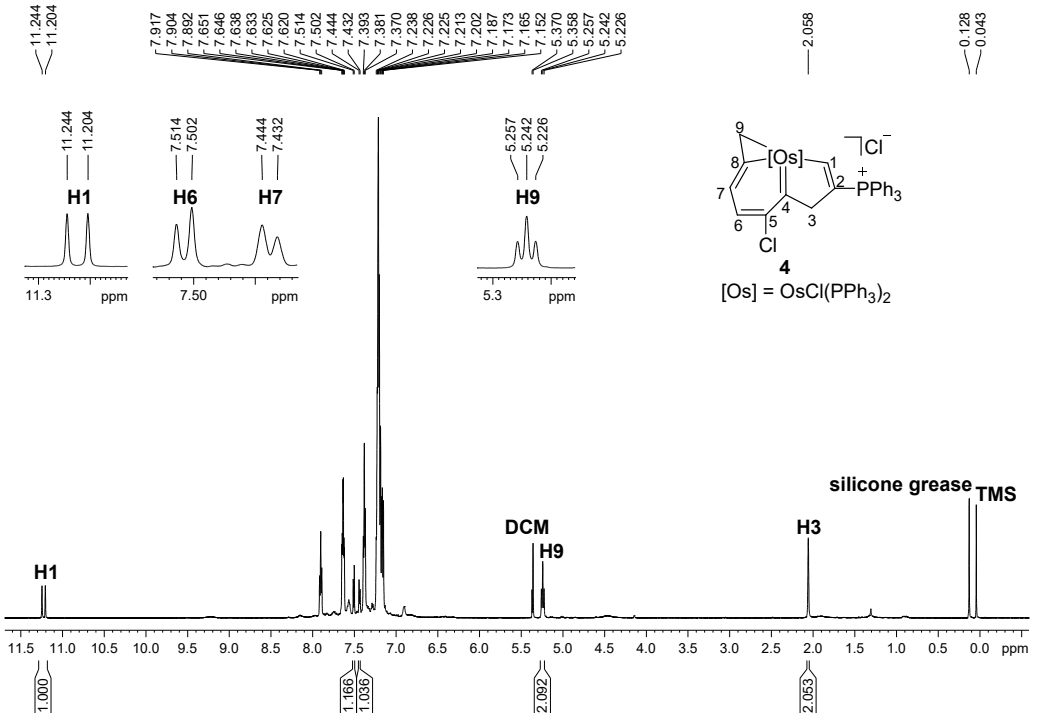


Figure S32. ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectra for complex **4**.

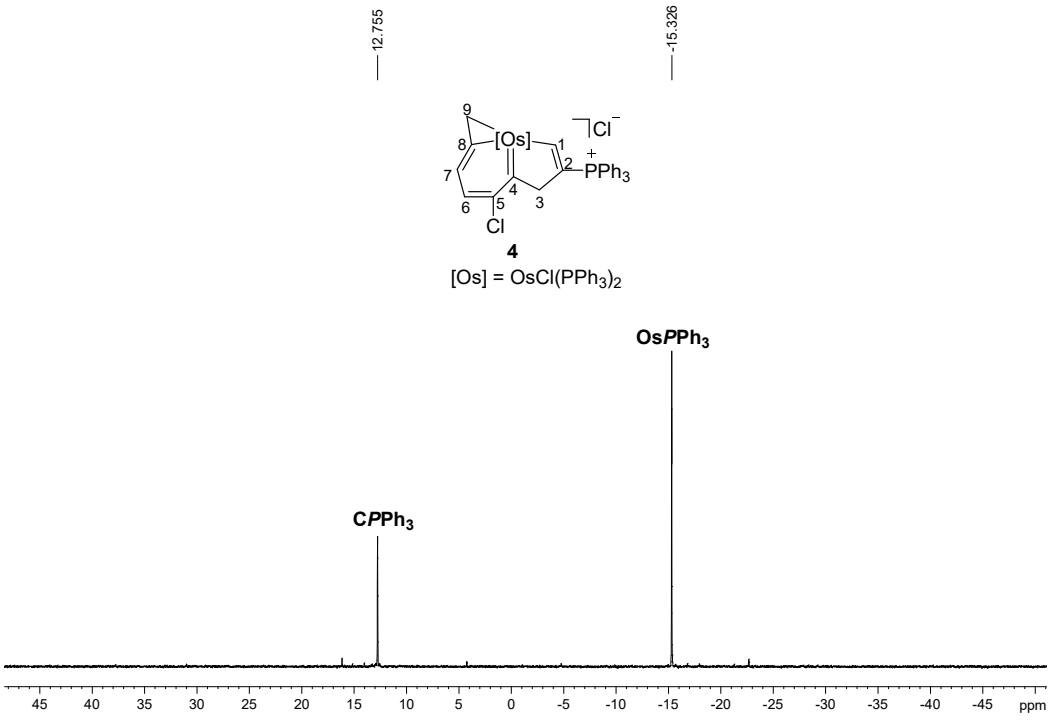


Figure S33. $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectra for complex **4**.

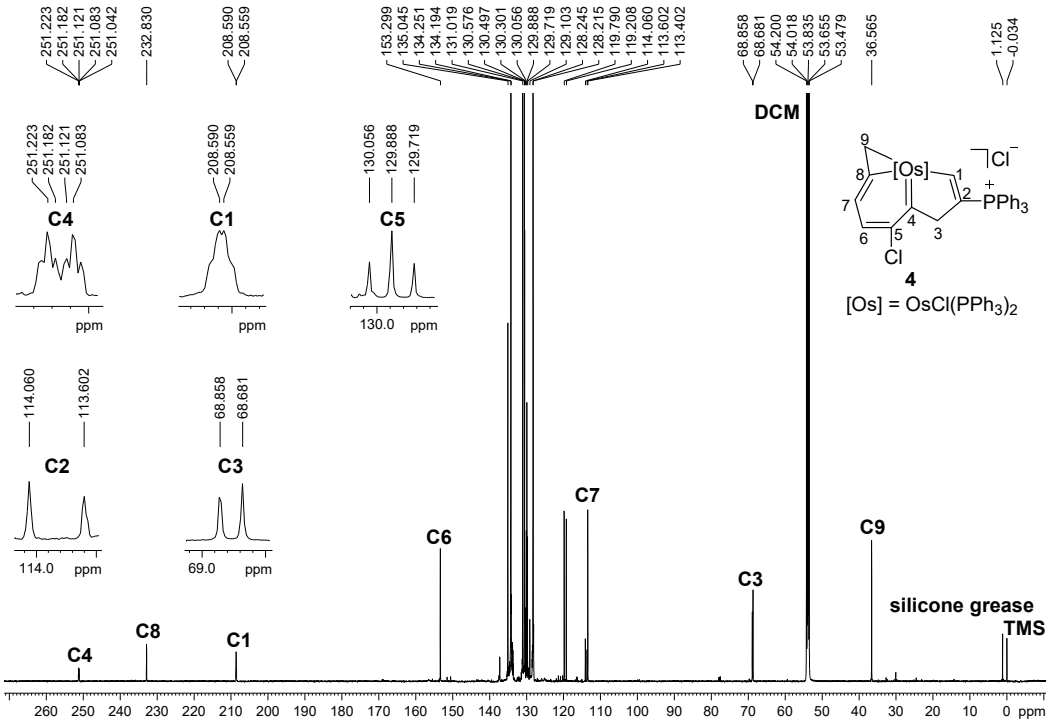


Figure S34. $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectra for complex **4**.

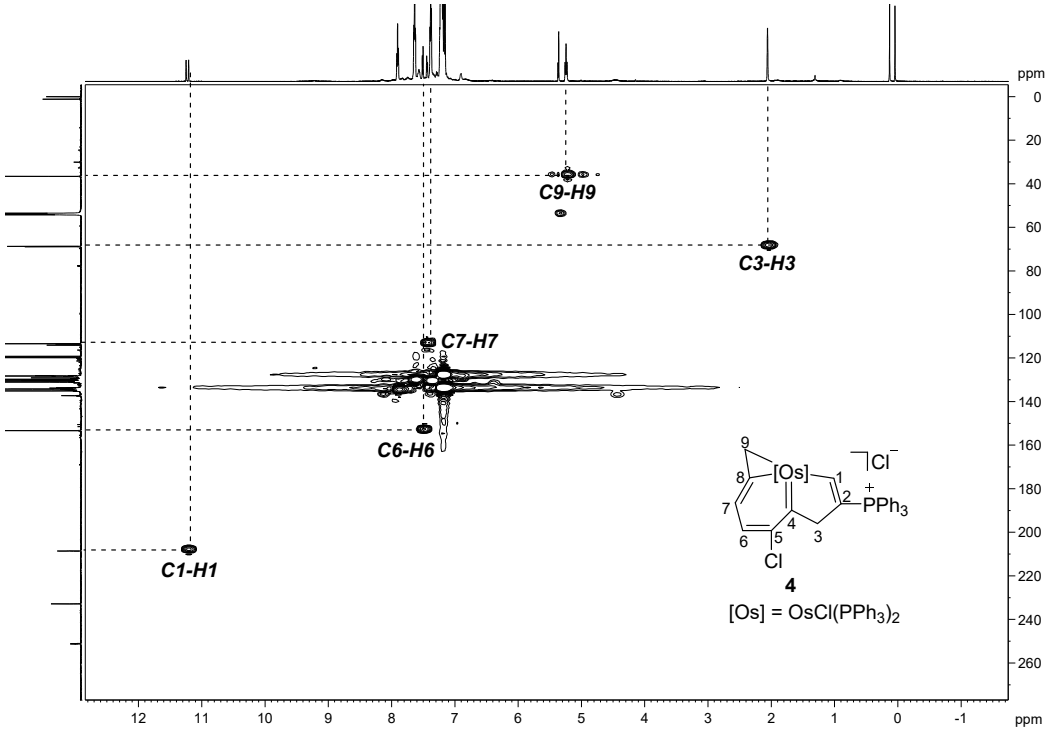


Figure S35. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectra for complex **4**.

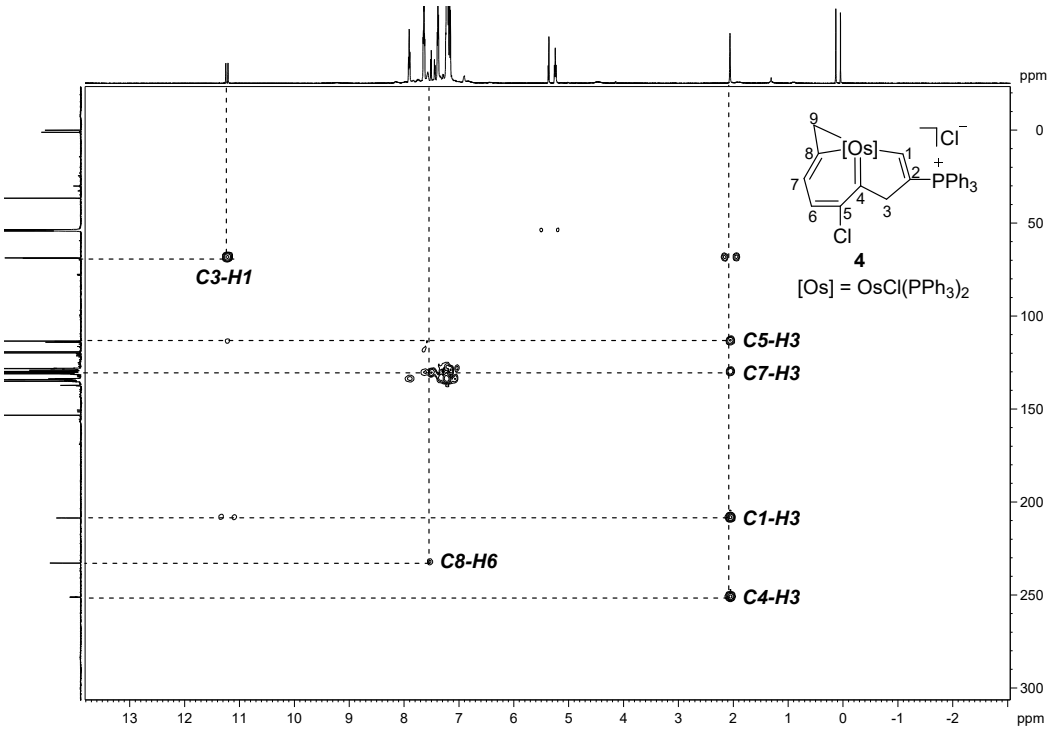


Figure S36. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectra for complex **4**.

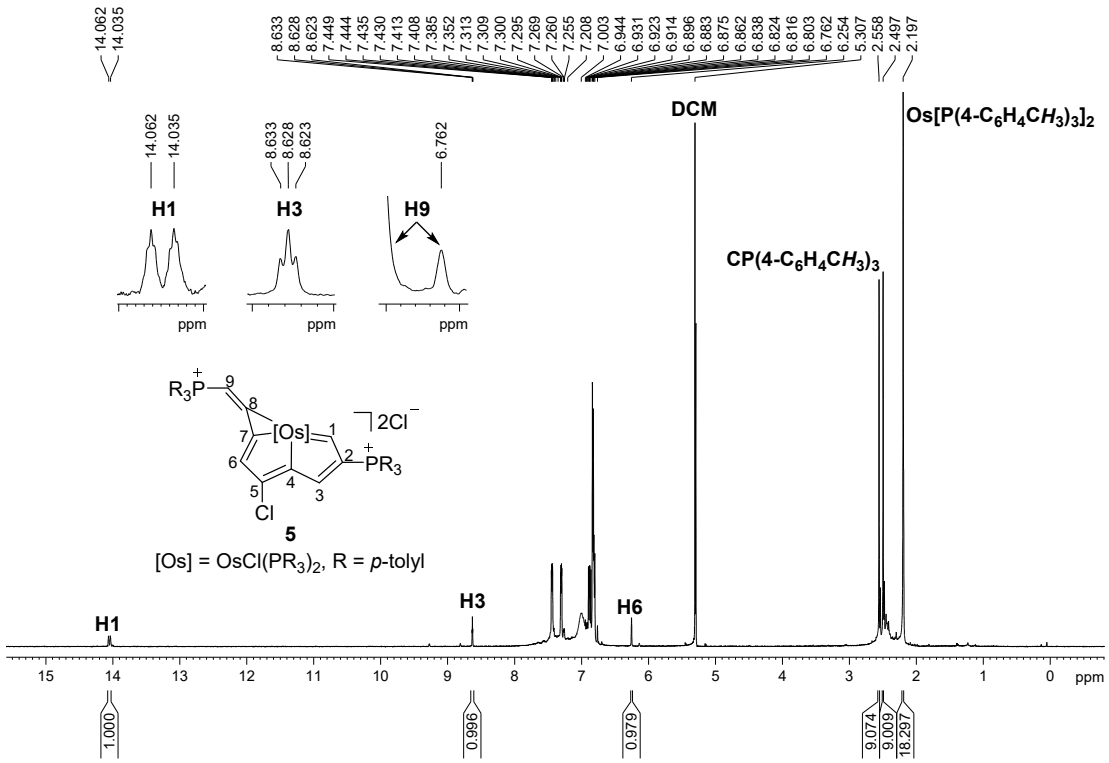


Figure S37. ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectra for complex **5**.

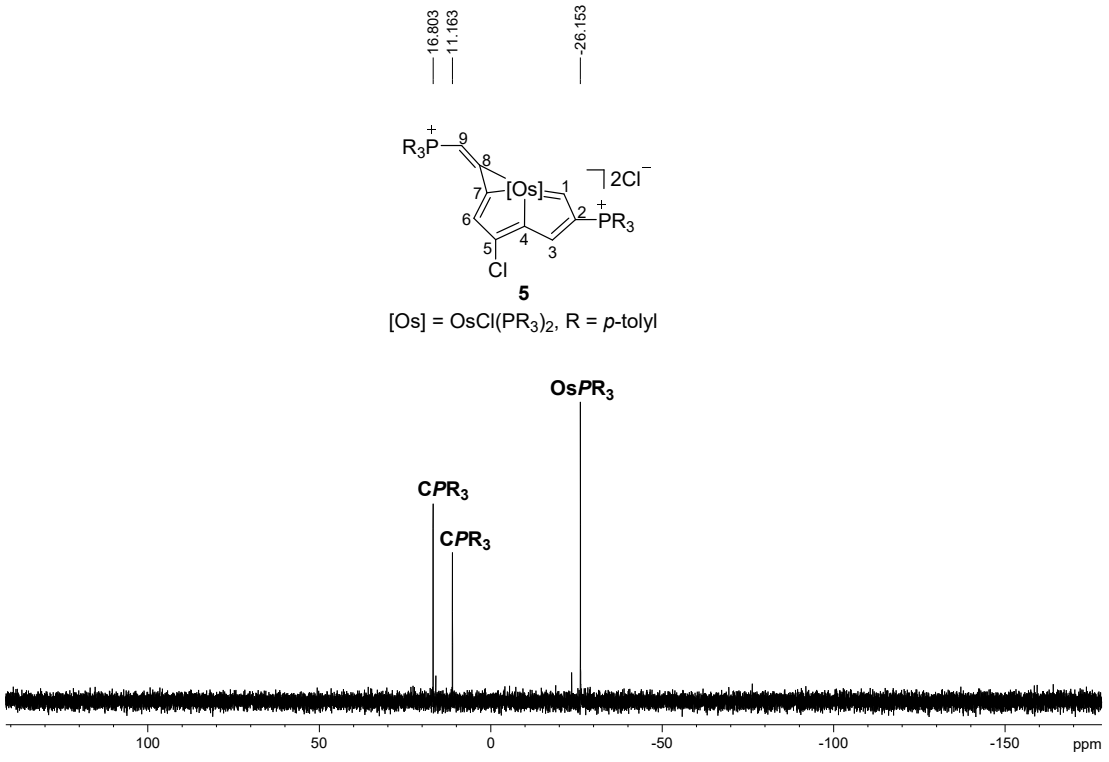


Figure S38. $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectra for complex **5**.

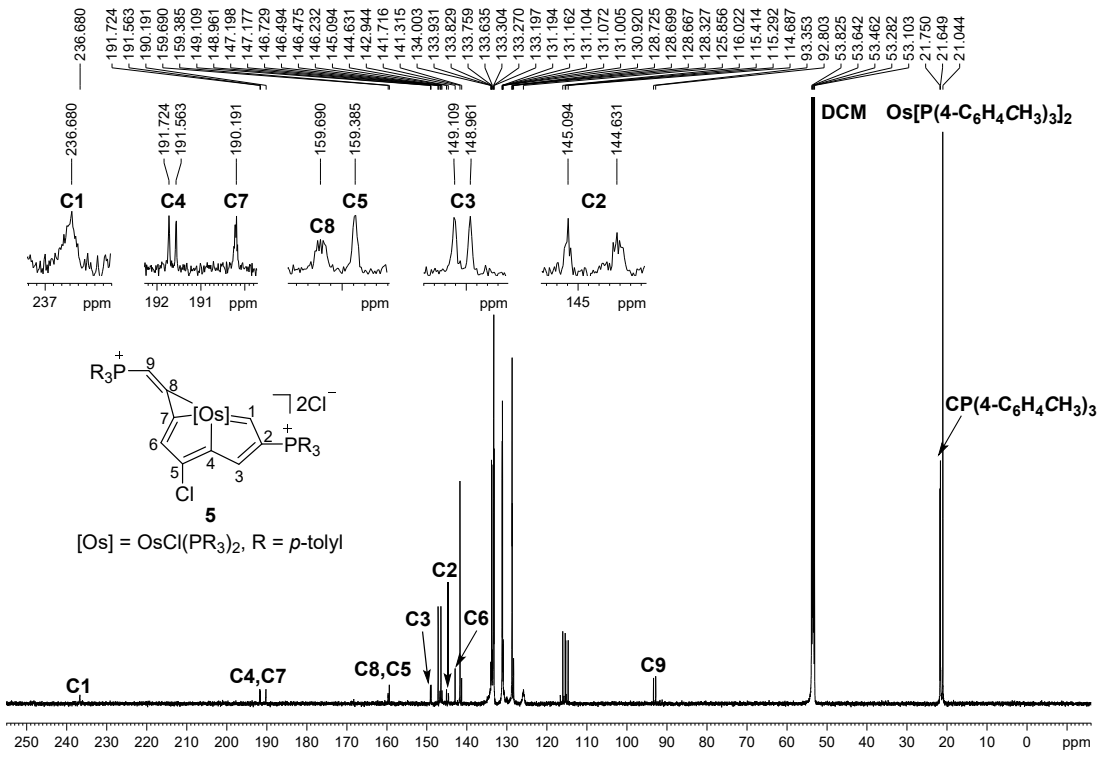


Figure S39. $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectra for complex **5**.

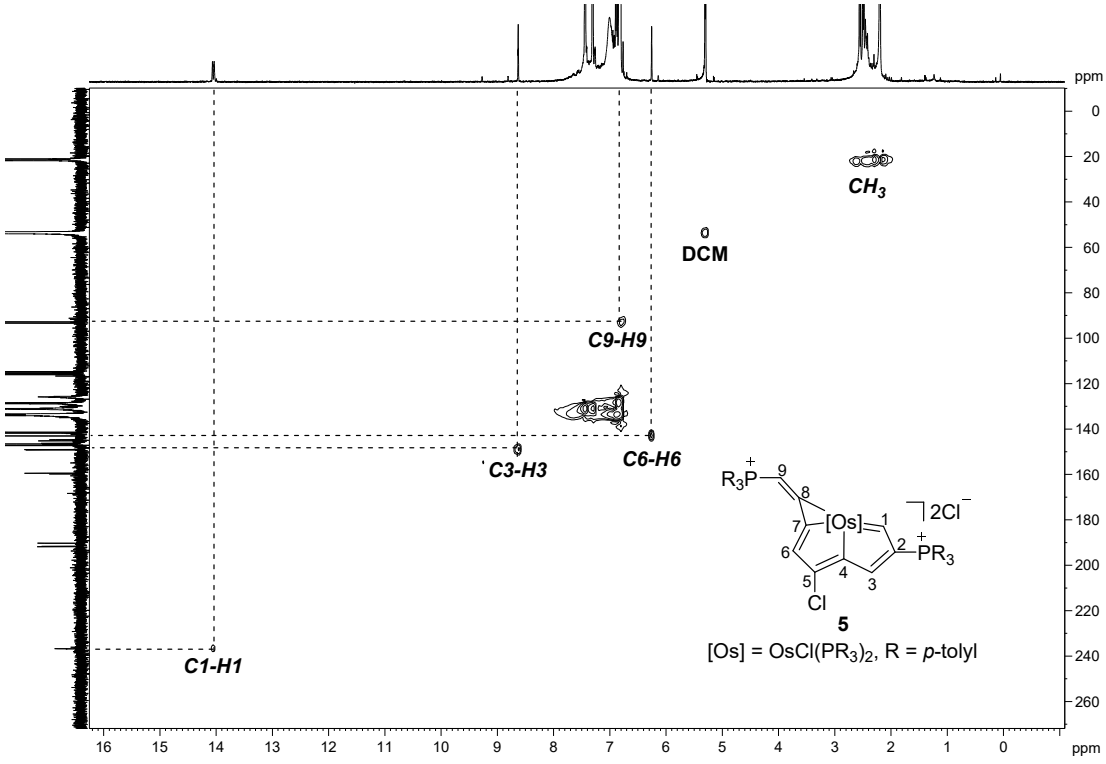


Figure S40. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectra for complex **5**.

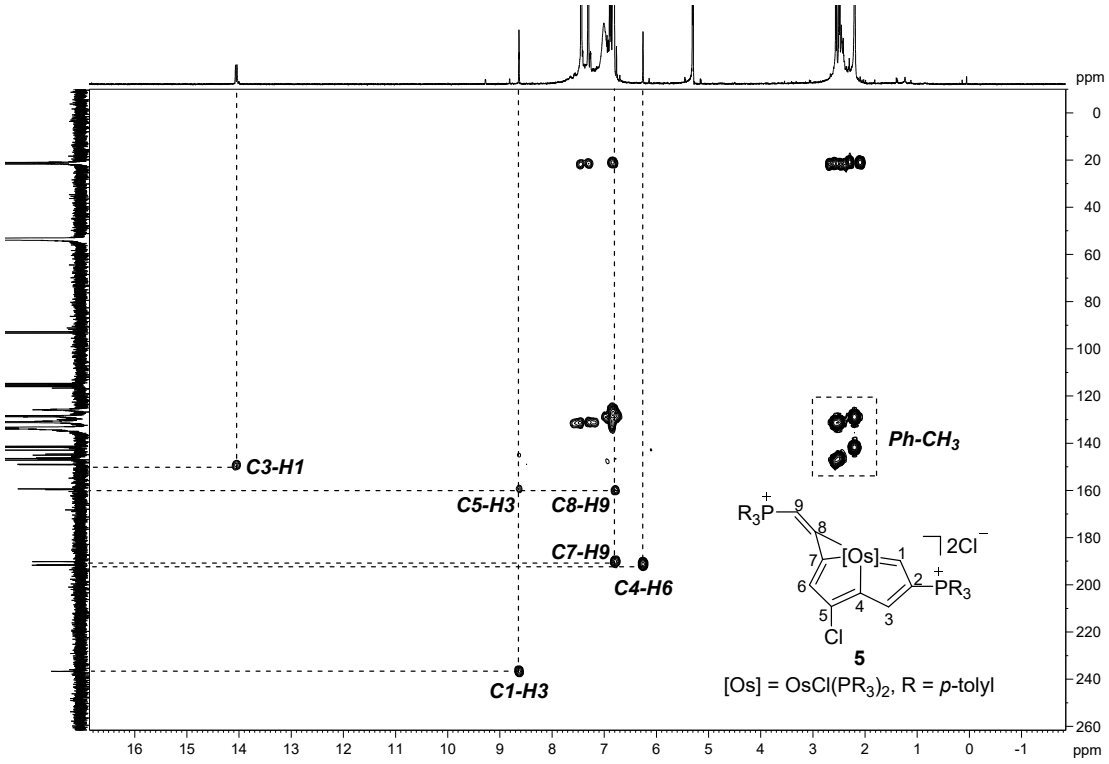


Figure S41. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectra for complex **5**.

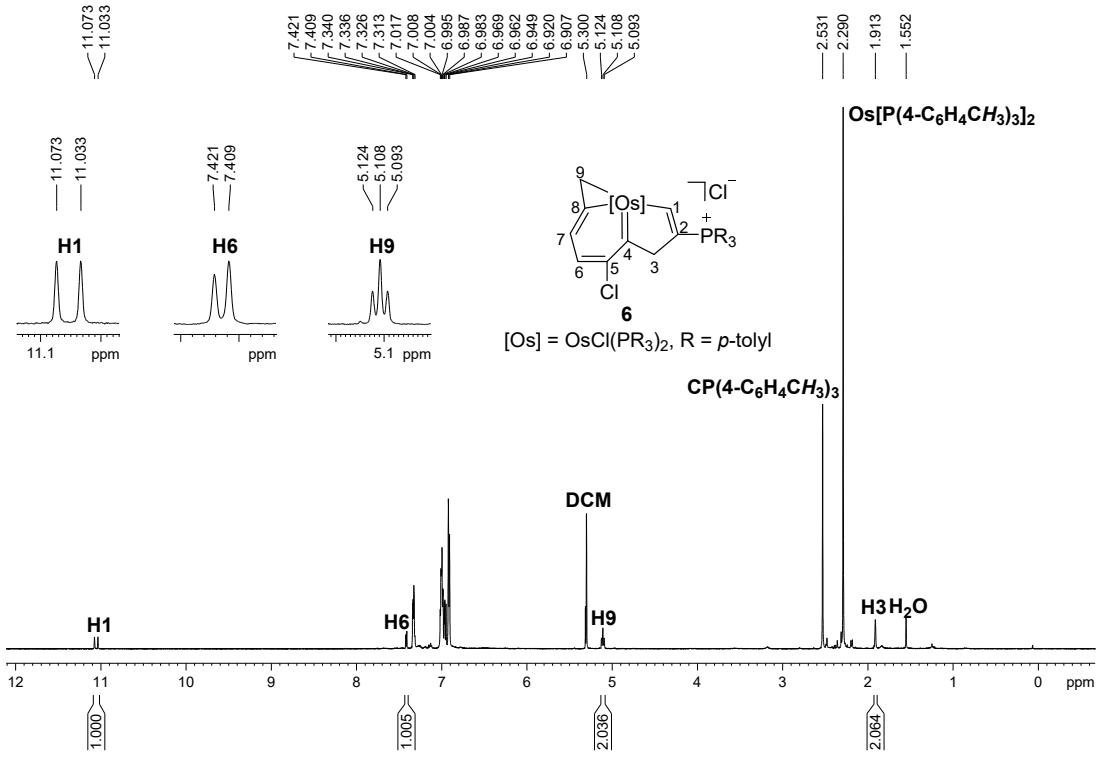


Figure S42. ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectra for complex **6**.

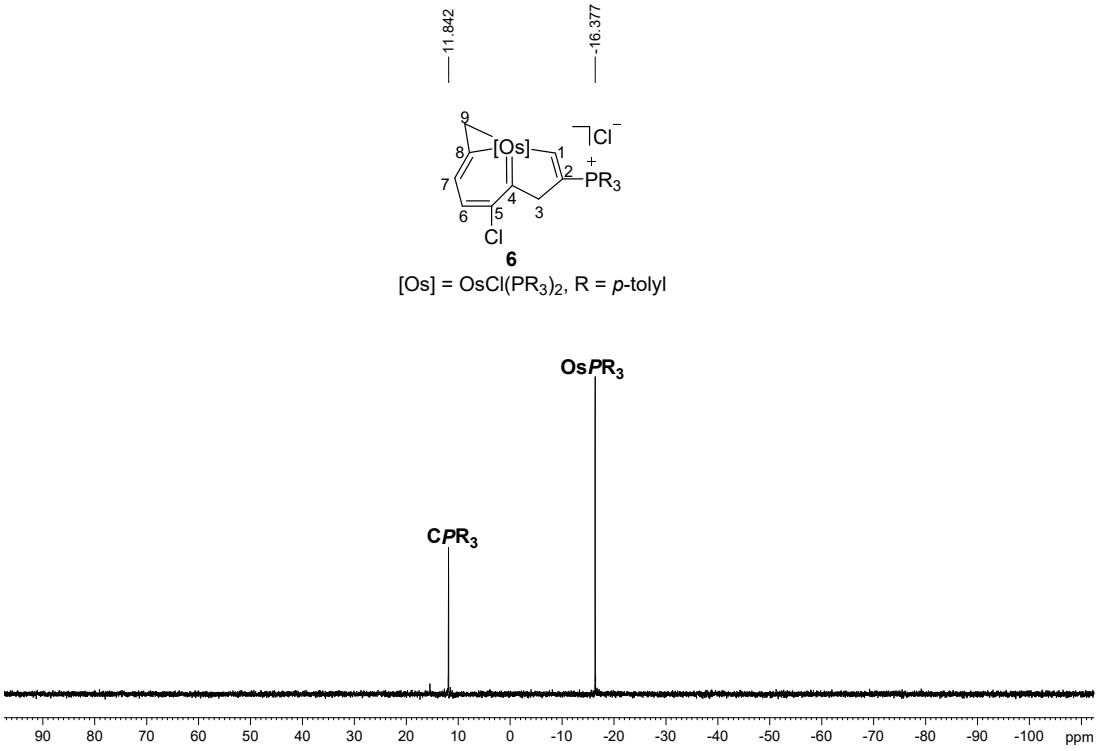


Figure S43. $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectra for complex **6**.

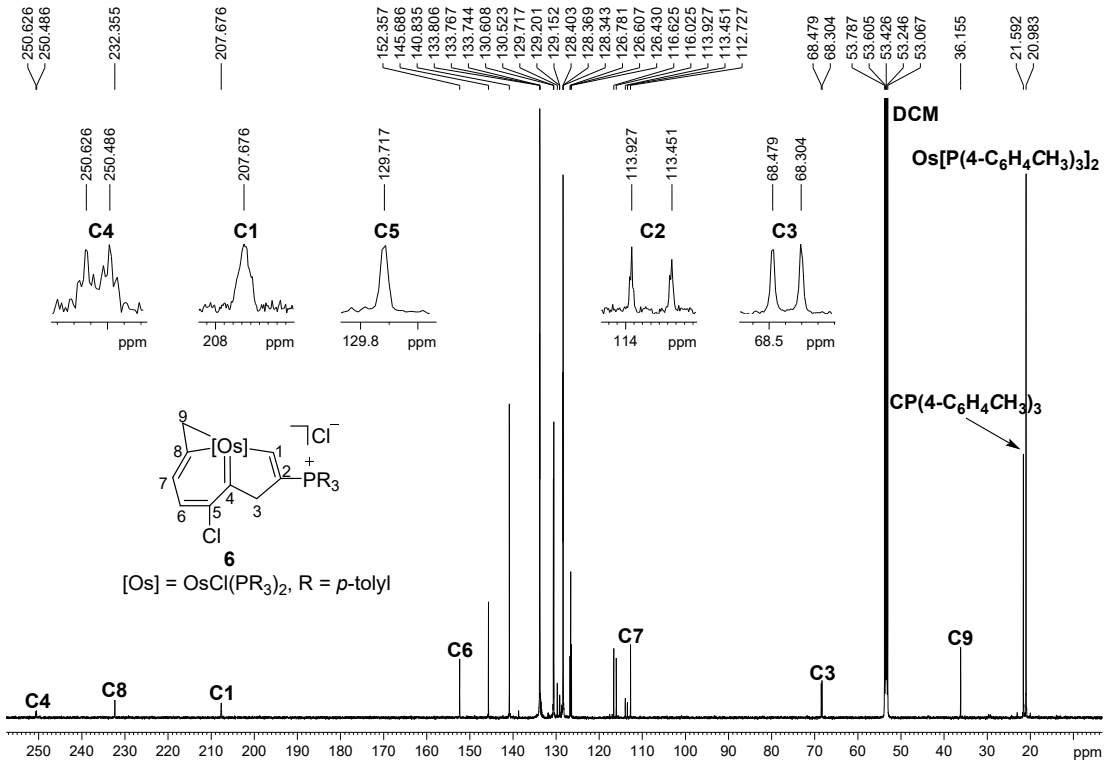


Figure S44. $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectra for complex **6**.

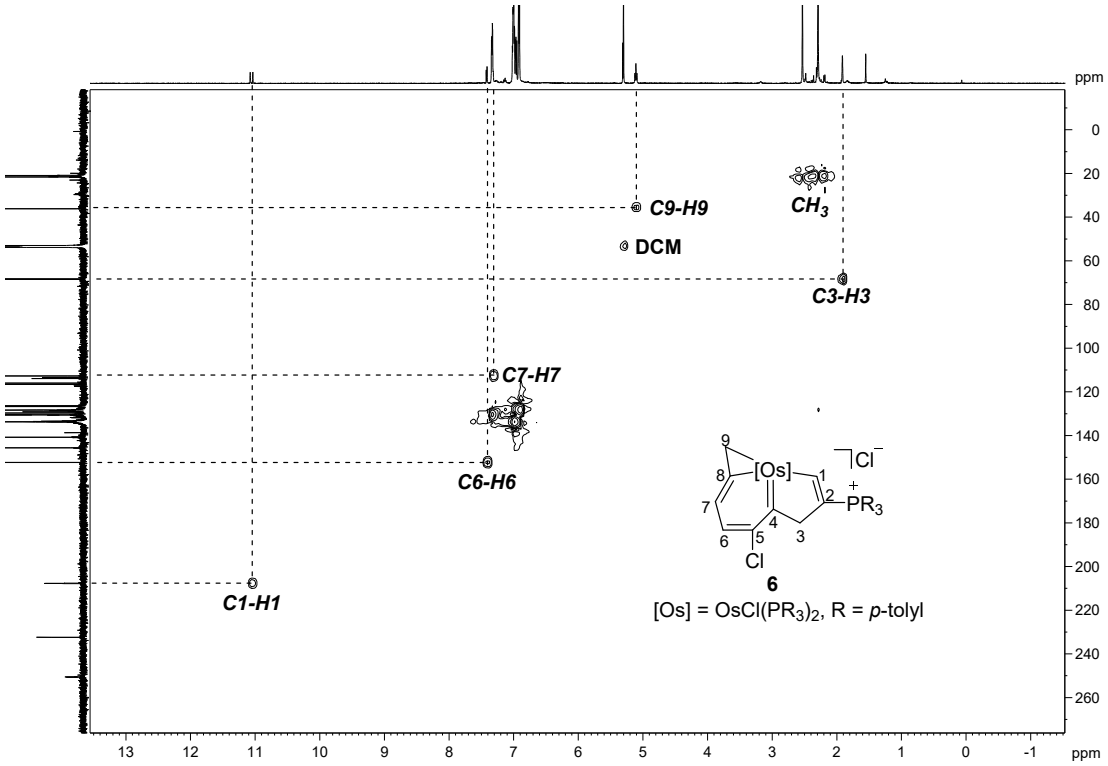


Figure S45. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectra for complex **6**.

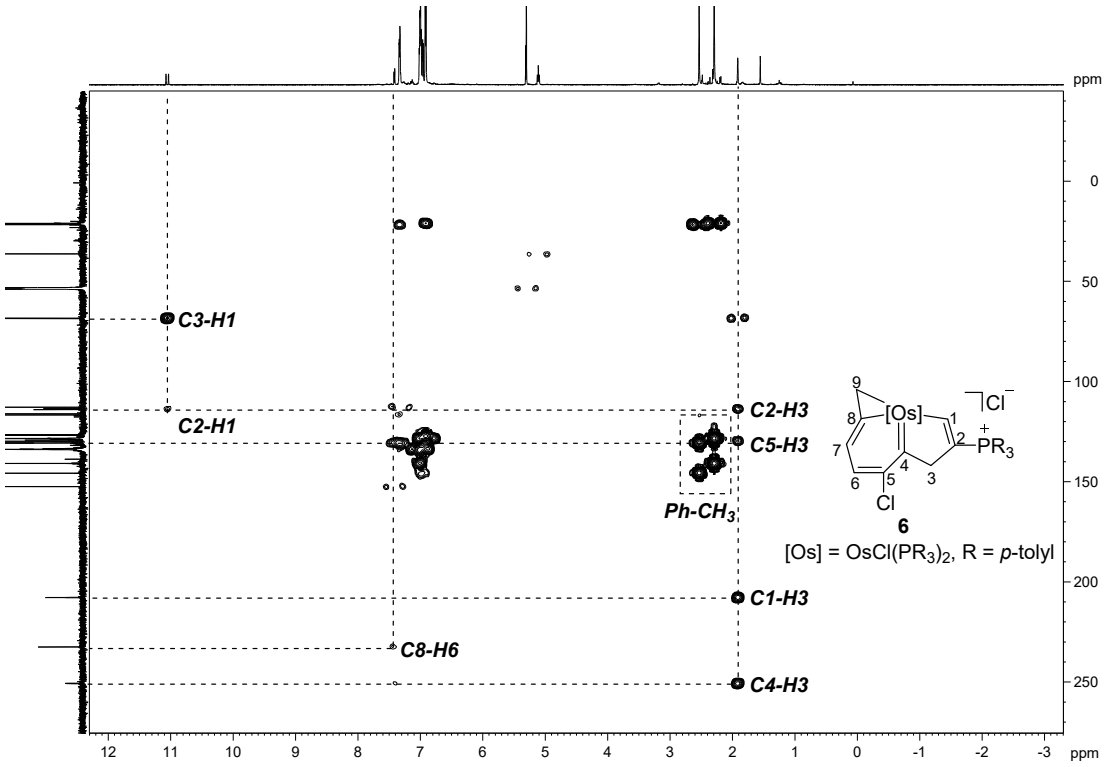


Figure S46. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectra for complex **6**.

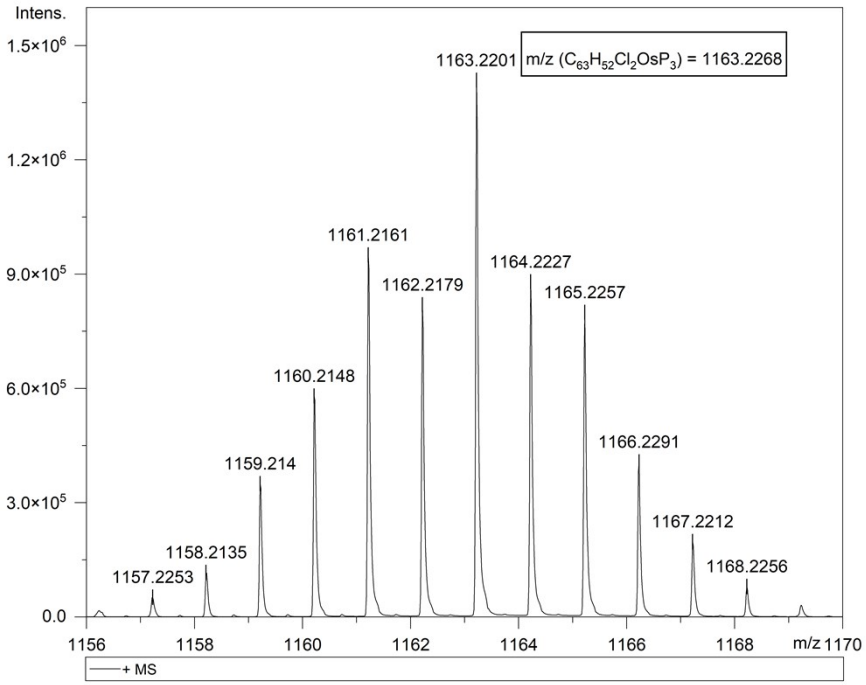


Figure S47. Positive-ion ESI-MS spectra of [**4**]$^+$ ($[C_{63}H_{52}Cl_2OsP_3]^+$) measured in methanol.

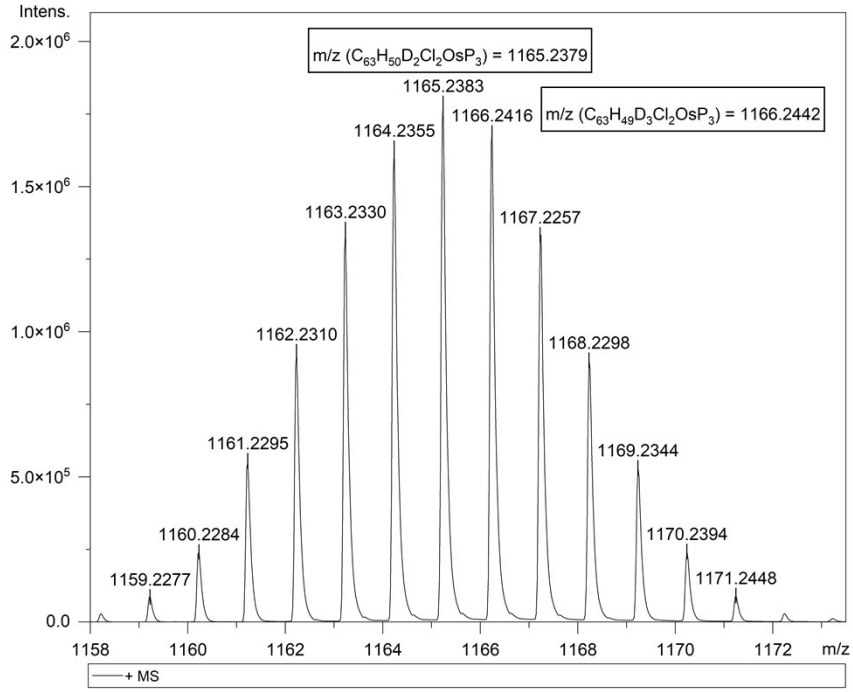


Figure S48. Positive-ion ESI-MS spectra of [**4a**]$^+$ ($[C_{63}H_{50}D_2Cl_2OsP_3]^+$ and $[C_{63}H_{49}D_3Cl_2OsP_3]^+$) measured in methanol.

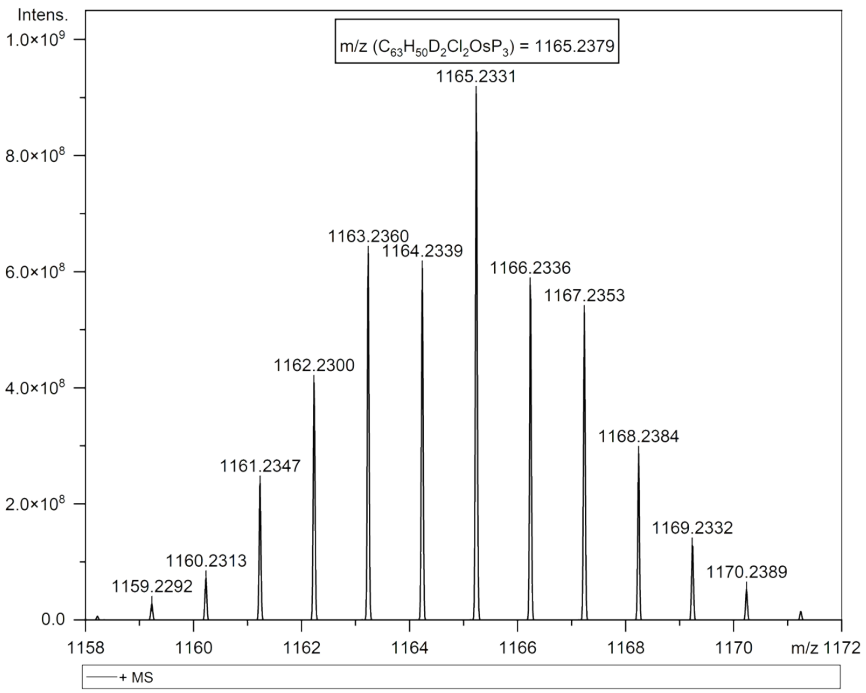


Figure S49. Positive-ion ESI-MS spectra of [**4b**]$^+$ ([$C_{63}H_{50}D_2Cl_2OsP_3$]$^+$) measured in methanol.

4. X-ray Crystallographic Analysis

Single-crystal X-ray diffraction data were recorded on a Rigaku XtaLAB Synergy, Dualflex, HyPix diffractometer with mirror-monochromated Cu Kα radiation (λ = 1.54184 Å) for **1** and **4** or Mo Kα radiation (λ = 0.71073 Å) for **3**. The structures were solved with Olex 2 (Dolomanov *et al.*, 2009) by ShelXT[2] structure solution program by intrinsic phasing method, and all of them were refined with the ShelXL[3] refinement package using least-squares minimization. All non-hydrogen atoms were refined anisotropically except for otherwise stated. The hydrogen atoms were placed at their idealized positions and assumed the riding model unless otherwise stated. Single crystals suitable for X-ray diffraction were from a solution of dichloromethane (**1**, **3**, and **4**) with layered hexane. The disordered solvents were removed from the dataset using the SOLVENT MASK routine of Olex 2. X-ray crystal structure information is available at the Cambridge Crystallographic Data Centre (CCDC) under deposition numbers CCDC 2190320 (**1**), CCDC 2190338 (**3**), CCDC 2190323 (**4**). Further details on the crystal data, data collection, and refinements are provided in **Table S3**.

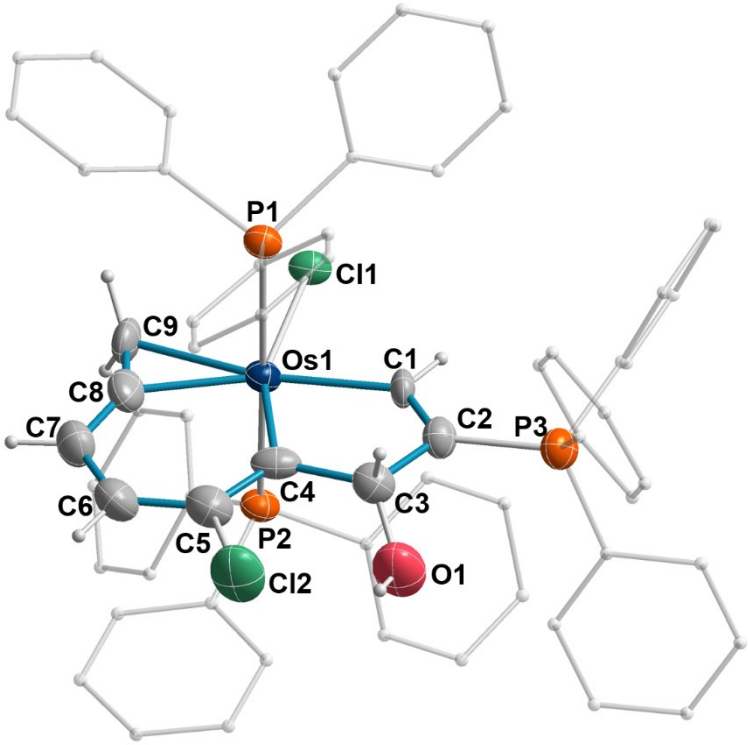


Figure S50. Single-crystal X-ray structure for cationic complex **1** with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms in PPh_3 have been omitted for clarity. Selected bond distances (Å) and angles (°): Os1–C1 2.076(5), Os1–C4 2.044(6), Os1–C8 2.064(7), Os1–C9 2.209(6), C1–C2 1.343(9), C2–C3 1.484(9), C3–C4 1.552(10), C4–C5 1.384(10), C5–C6 1.380(11), C6–C7 1.378(11), C7–C8 1.362(10), C8–C9 1.338(11), C3–O1 1.460(20), C5–Cl2 1.775(8); Os1–C1–C2 121.3(4), C1–C2–C3 115.2(5), C2–C3–C4 108.8(5), C3–C4–Os1 117.3(4), C4–Os1–C1 77.2(3), Os1–C4–C5 129.2(6), C4–C5–C6 126.9(7), C5–C6–C7 124.4(7), C6–C7–C8 120.9(7), C7–C8–Os1 134.7(6), C8–Os1–C4 83.5(3), C9–C8–Os1 77.8(4), C8–C9–Os1 66.0(4), C8–Os1–C9 36.3(3).

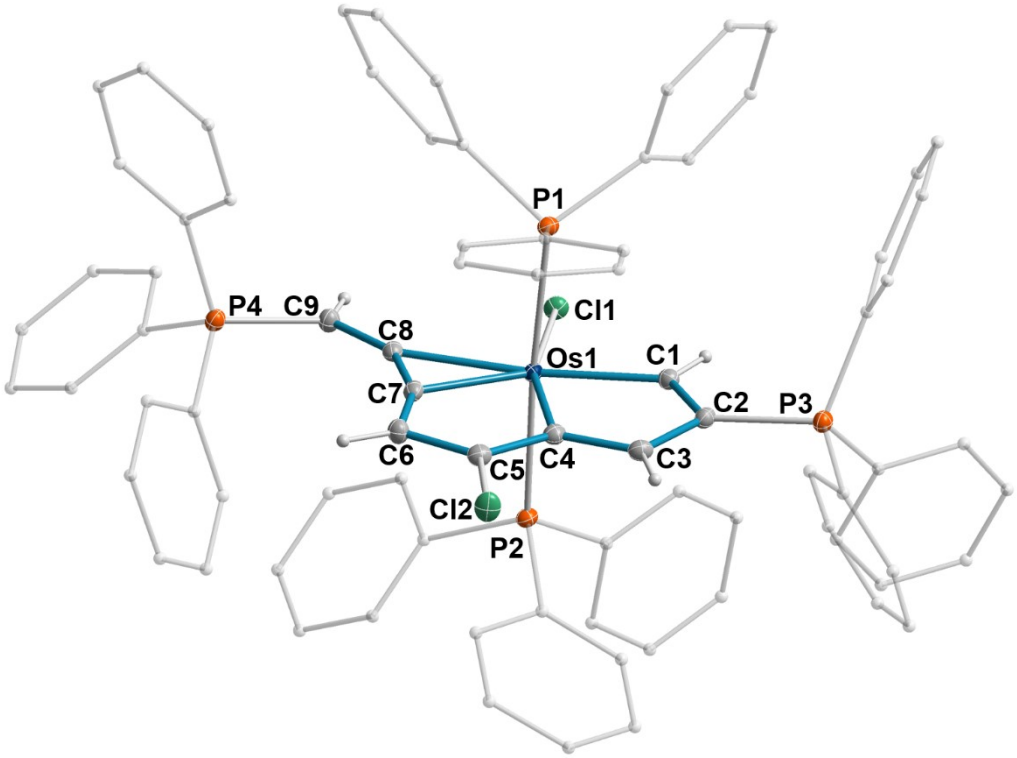


Figure S51. Single-crystal X-ray structure for cationic complex **3** with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms in PPh_3 have been omitted for clarity. Selected bond distances (Å) and angles (°): Os1–C1 2.054(2), Os1–C4 2.077(2), Os1–C7 2.009(2), Os1–C8 2.156(2), C1–C2 1.393(3), C2–C3 1.412(3), C3–C4 1.381(3), C4–C5 1.417(3), C5–C6 1.388(3), C6–C7 1.385(3), C7–C8 1.352(3), C8–C9 1.340(3), C5–Cl2 1.720(2); Os1–C1–C2 119.09(15), C1–C2–C3 113.65(19), C2–C3–C4 113.21(19), Os1–C4–C3 118.96(15), C1–Os1–C4 75.04(8), Os1–C4–C5 118.10(15), C4–C5–C6 114.73(19), C5–C6–C7 108.79(19), C6–C7–Os1 125.49(15), C7–Os1–C4 72.88(8), Os1–C7–C8 77.09(13), Os1–C8–C7 65.22(12), C7–Os1–C8 37.69(8), Os1–C8–C9 147.67(16).

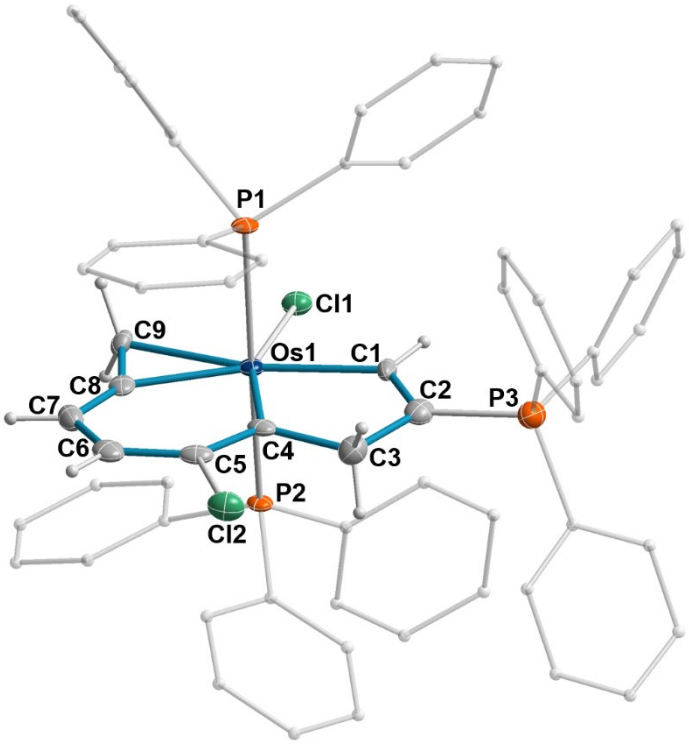


Figure S52. Single-crystal X-ray structure for cationic complex **4** with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms in PPh_3 have been omitted for clarity. Selected bond distances (Å) and angles (°): Os1–C1 2.098(4), Os1–C4 2.041(4), Os1–C8 2.046(4), Os1–C9 2.198(4), C1–C2 1.332(7), C2–C3 1.493(6), C3–C4 1.510(6), C4–C5 1.420(6), C5–C6 1.370(7), C6–C7 1.406(7), C7–C8 1.362(7), C8–C9 1.363(7), C5–Cl2 1.765(5); Os1–C1–C2 119.8(4), C1–C2–C3 114.9(4), C2–C3–C4 110.4(4), C3–C4–Os1 116.9(3), C4–Os1–C1 77.42(18), Os1–C4–C5 129.5(3), C4–C5–C6 127.1(4), C5–C6–C7 123.0(4), C6–C7–C8 120.4(4), C7–C8–Os1 137.2(4), C8–Os1–C4 82.57(18), C9–C8–Os1 77.4(3), C8–C9–Os1 65.3(3), C8–Os1–C9 37.24(17).

Table S3. Crystal data and structure refinement for **1**, **3**, and **4**.

Compound	**1**·CH_2Cl_2	**3**·$2CH_2Cl_2$·$2H_2O$	**4**·CH_2Cl_2
CCDC Number	2190320	2190338	2190323
Empirical formula	$C_{64}H_{54}BCl_4F_4OOsP_3$	$C_{83}H_{72}Cl_8O_2OsP_4$	$C_{64}H_{54}BCl_4F_4OsP_3$
Formula weight	1350.79	1699.08	1334.79
Temperature/K	100.00(12)	100(1)	99.98(13)
Crystal system	triclinic	triclinic	triclinic
Space group	P−1	P−1	P−1
a/Å	10.15200(10)	12.70740(10)	10.1361(2)
b/Å	12.5705(2)	15.86420(10)	12.2229(2)
c/Å	23.1569(3)	19.70260(10)	22.8285(4)
α/°	102.3440(10)	108.2270(10)	93.9940(10)
β/°	99.8500(10)	96.2310(10)	94.966(2)
γ/°	97.6070(10)	98.1170(10)	95.826(2)
Volume/Å^3	2800.15(7)	3685.24(5)	2794.32(9)
Z	2	2	2
ρ_{calc} g/cm^3	1.602	1.531	1.586
μ/mm^{-1}	7.337	2.156	7.331
F(000)	1352.0	1716.0	1336.0
Crystal size/mm^3	0.494 × 0.247 × 0.047	0.15 × 0.12 × 0.08	0.149 × 0.139 × 0.074
Radiation	Cu Kα (λ = 1.54184)	Mo Kα (λ = 0.71073)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.312 ≤ 2Θ ≤ 124.99	3.87 ≤ 2Θ ≤ 62.434	7.292 ≤ 2Θ ≤ 149.188
Index ranges	−11 ≤ h ≤ 11, −14 ≤ k ≤ 14, −26 ≤ l ≤ 26	−17 ≤ h ≤ 18, −23 ≤ k ≤ 22, −28 ≤ l ≤ 28	−12 ≤ h ≤ 12, −12 ≤ k ≤ 15, −28 ≤ l ≤ 28
Reflections collected	67098	116361	35168
Independent reflections	8941	21032	11065
Data/restraints/parameters	8941/99/703	21032/0/889	11065/0/703
Goodness-of-fit on F^2	1.060	1.064	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0550, ωR_2 = 0.1463	R_1 = 0.0267, ωR_2 = 0.0629	R_1 = 0.0434, ωR_2 = 0.1082
Final R indexes [all data]	R_1 = 0.0596, ωR_2 = 0.1489	R_1 = 0.0315, ωR_2 = 0.0642	R_1 = 0.0462, ωR_2 = 0.1097
Largest diff. peak/hole / e Å^{-3}	1.89/−1.32	1.60/−1.51	3.08/−2.04

5. Theoretical Calculations

Computational Details

All structures were optimized at the B3LYP level of density functional theory.[4] Frequency calculations were performed to confirm the characteristics of all the calculated structures as minima. Compounds **1**, **3**, and **4** are simplified through the way that the PH_3 groups were used to replace the PPh_3 ligands, which are named simplified model compounds **1'**, **3'**, and **4'**. All these structures evaluated were optimized by B3LYP-D3BJ/6-31G*;[5] the nucleus-independent chemical shifts (NICS)[6] and anisotropy of the induced current density (ACID)[7] calculations were performed at the B3LYP/6-31G* level. The effective core potentials (ECPs) of Hay and Wadt with a double-ζ valence basis set LanL2DZ[8] for all structures were used to describe Os, P, and Cl atoms. Polarization functions were added for Os (ζ(f) = 0.886), P (ζ(d) = 0.340), and Cl (ζ(d) = 0.514).[9] The single-point energy calculations were performed on the mechanism using the B3LYP-D3BJ/Def2-TZVP method with the SMD solvation method in DCM.[10] All the orbital isosurfaces and $NICS(1)_{zz}$ grids were visualized by Multiwfn.[11] Whereas the UV-Vis spectrum was used TD-DFT calculations[12] at the B3LYP-D3BJ/Def2-TZVP level of DFT with an SMD solvation model in DCM. All calculations were performed with the Gaussian 16 software package.[13]

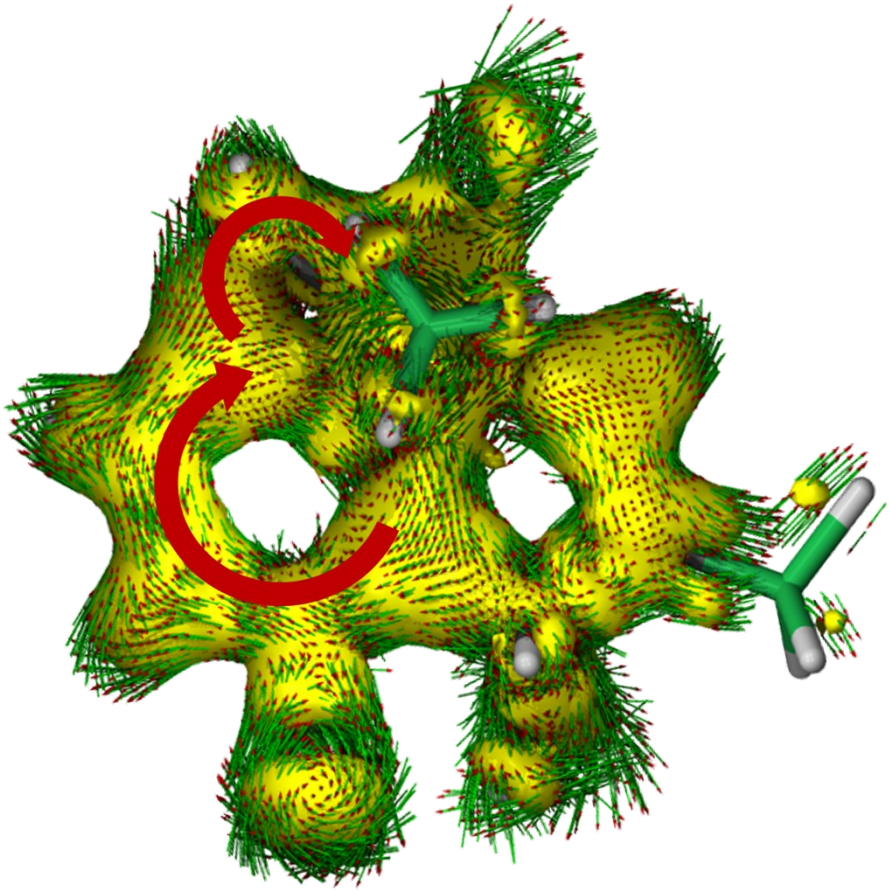


Figure S53. ACID isosurfaces of **1'** (Current density vectors are plotted onto the ACID isosurface of 0.030 a.u. to indicate diatropic ring currents).

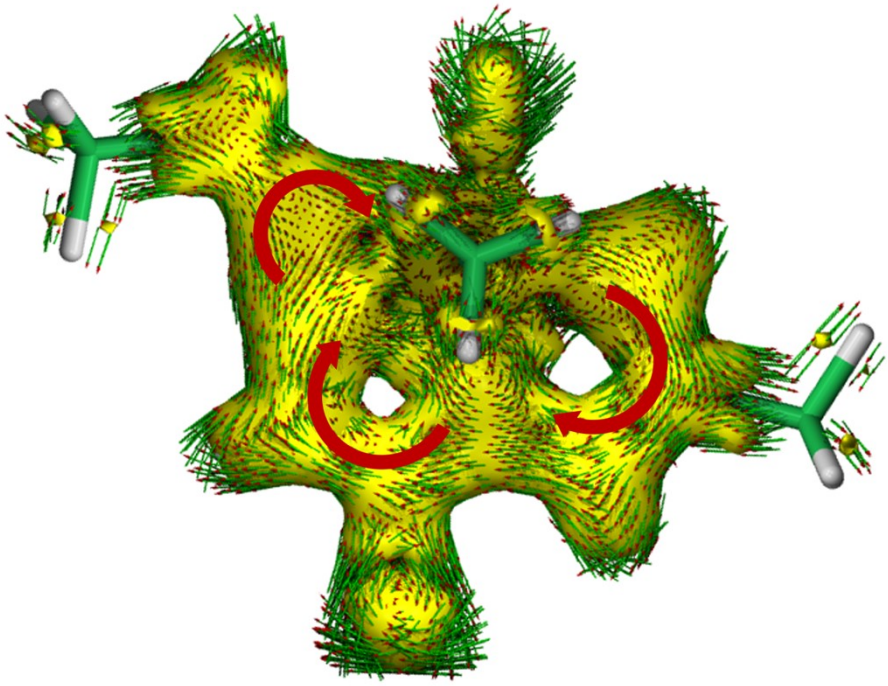


Figure S54. ACID isosurfaces of **3'** (Current density vectors are plotted onto the ACID isosurface of 0.030 a.u. to indicate diatropic ring currents).

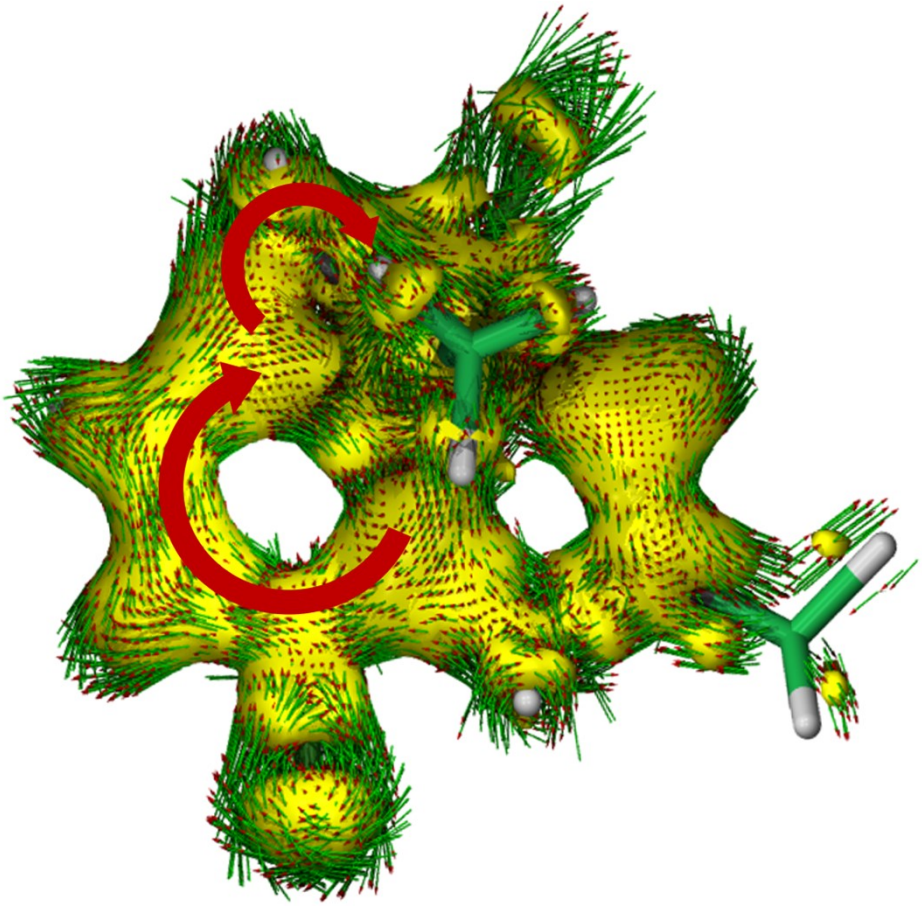
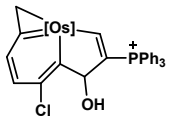


Figure S55. ACID isosurfaces of **4'** (Current density vectors are plotted onto the ACID isosurface of 0.030 a.u. to indicate diatropic ring currents).

Cartesian Coordinates



1

[Os] = $OsCl(PPh_3)_2$

E = -4542.979179 a.u.

Os	-1.42759100	-0.19896700	-0.12882500
Cl	-1.74899000	-0.07625400	-2.62998700
P	-1.05408400	-2.61892100	-0.25426300
P	-1.75818600	2.23186900	-0.24435200
P	3.24274500	0.42494100	-0.11876600
Cl	-0.06233600	0.01883300	4.45989900
C	-2.26733300	-3.71556600	-1.12233200
C	0.55054900	0.08457500	-0.68490300
H	0.83251700	0.05979600	-1.73228000
C	0.50267400	-3.15168100	-1.09871400
C	-3.53966900	2.71528900	-0.33052400
C	-1.08349000	3.23884500	-1.64128300
C	-4.23913600	3.31504300	0.72077800
H	-3.73666600	3.55998000	1.64858900
C	-3.92278900	-5.46001900	-2.56050700
H	-4.56869800	-6.13500900	-3.11414000
C	1.49152500	0.27768200	0.25498700
C	-2.99212100	-3.24915500	-2.22716900
H	-2.89058000	-2.21851000	-2.54666600
C	-1.60403200	4.53436200	-1.80719400
H	-2.40315700	4.88488700	-1.16306300
C	-0.05269400	2.80646900	-2.47872200
H	0.34793700	1.81143600	-2.38115800
C	-0.48456500	-0.10745500	1.69097700
C	-1.07431500	3.11341500	1.22773100
C	4.18225600	-1.14285000	-0.19658700
C	1.30684400	-4.19017400	-0.61644600
H	1.06953500	-4.67764100	0.32179200
C	1.90267600	-3.01002700	-3.07166700
H	2.10979700	-2.57285500	-4.04492500
C	-3.08123400	-0.49922200	1.01229100
C	-5.59121900	3.63384100	0.56965600
H	-6.12403800	4.10636900	1.38954500
C	-3.60761500	-0.56800600	-0.26224700
H	-4.14647200	0.27315300	-0.68672800
H	-3.86580500	-1.53380600	-0.68842700
C	-4.20406800	2.44541800	-1.54036300
H	-3.66275800	1.98300200	-2.36056100
C	0.79417200	-2.57658800	-2.34541600
H	0.13946700	-1.81331600	-2.75435300
C	-1.54526400	2.78117500	2.50704800
H	-2.32558100	2.03855400	2.61551600
C	-2.35394200	-5.07007800	-0.76195900
H	-1.77585800	-5.45271100	0.07192800
C	-1.10002900	5.37639500	-2.79493600
H	-1.51296000	6.37380500	-2.91241700
C	-6.25001900	3.35842700	-0.62784600
H	-7.30023500	3.60953100	-0.74208300
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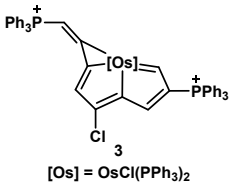

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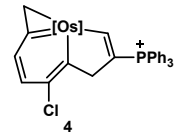

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C	-2.29980800	-4.93668000	0.26524500
H	-1.46167600	-5.59260400	0.05854000
C	-4.55280700	-4.58928800	1.08386100
H	-5.46668300	-4.98142100	1.51909000
C	-3.91444800	-0.50581400	-4.73544700
H	-4.10648800	-0.39308500	-5.79807900
C	-4.36342300	-0.20996800	2.13719400
H	-3.64150300	-0.85696800	2.62424000
C	-3.47265200	-5.43879500	0.83414200
H	-3.54686600	-6.49391900	1.07954300
C	-6.24935900	1.29486500	2.28769500
H	-6.98558200	1.82043300	2.88815100
C	-5.30609000	0.46894500	2.90483700
H	-5.30374800	0.35221900	3.98398300
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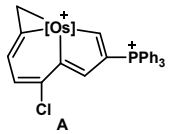

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P	0.93482300	2.62844600	-0.14146100
Cl	-0.48542400	-0.02728800	4.39588700
P	-3.23448400	-0.50649900	-0.23287300
C	2.92574500	0.52700100	1.33264500
C	2.44284300	5.02465200	0.05226100
H	1.77399500	5.32316200	0.85102000
C	0.31070800	0.05989100	1.73675400
C	1.05531700	-2.94035400	-1.74899400
C	2.31181000	3.77068200	-0.56302900
C	3.05725400	0.64036700	2.70098300
H	4.03521300	0.85308700	3.12616800
C	5.48664500	-4.01664500	0.58207900
H	5.88635200	-4.72034300	1.30555500
C	4.13913100	-3.65857700	0.64470100
H	3.50872600	-4.09315300	1.41118400
C	5.78965200	-2.58688100	-1.34186000

H	6.42579900	-2.17232400	-2.11771400
C	1.81735600	-3.40114500	-2.82709000
H	2.89786300	-3.41171800	-2.77265300
C	3.62618100	0.61649400	0.15103500
C	6.31299300	-3.48386500	-0.40772600
H	7.35940300	-3.76858400	-0.45418600
C	3.60981500	-2.75656800	-0.28845000
C	0.28054500	3.13951600	1.49731500
C	-1.09117100	3.02512900	1.77826500
H	-1.79339700	2.77671700	0.99088400
C	-1.09159900	-0.15930300	1.49608000
H	-1.80102600	-0.21526600	2.31385100
C	-0.38127600	-0.17767400	-0.72678400
H	-0.56064900	-0.30818300	-1.78957100
C	1.96847700	0.50228900	3.55059700
H	2.11376300	0.60860900	4.62007700
C	-0.36119800	3.15278100	-1.35048400
C	4.44645700	-2.21747800	-1.28490400
H	4.04573800	-1.51960200	-2.01277400
C	0.37287200	-4.42241500	0.91858500
H	0.18806200	-4.76468200	-0.09221700
C	1.11858200	-3.25822000	1.14851100
C	-0.34571800	-2.97113600	-1.84017900
H	-0.95540300	-2.67046100	-0.99548700
C	4.28636500	5.55522800	-1.42360400
H	5.05533100	6.24675300	-1.75339500
C	-1.56103200	3.24727300	3.07208500
H	-2.62370200	3.16535600	3.27301600
C	3.43296900	5.90824700	-0.37666200
H	3.53147800	6.87615900	0.10493200
C	-0.49989700	2.49780100	-2.58093800
H	0.11502600	1.63451500	-2.80883100
C	-1.08214100	4.33311800	-1.11094300
H	-0.95473500	4.87537000	-0.18069400
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H	2.01255400	-2.00014500	2.65064300
C	0.89398800	-3.60180900	3.54147300
H	1.10958700	-3.28685000	4.55753900
C	3.15381300	3.42670300	-1.63362200
H	3.02453800	2.47839200	-2.14549200
C	0.68056900	0.20191100	3.08569900
C	1.16697900	3.46038900	2.53292400
H	2.23153100	3.52923900	2.33793000
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H	-2.05256400	-3.44998500	-3.05063900
C	-1.37879200	3.00090900	-3.54393600
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C	4.13970100	4.31862200	-2.05476600
H	4.78836200	4.04741300	-2.88189900
C	-3.46545000	-0.96312400	-1.97097600
C	-1.46679700	-0.28914600	0.17488300
C	1.18835800	-3.85460200	-3.98821800
H	1.79277900	-4.20424700	-4.81914900
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C	0.68852300	3.69109300	3.82517400
H	1.38386500	3.95681700	4.61552700
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C	0.12651500	-4.74642500	3.30752500
H	-0.25633100	-5.32384900	4.14347100
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H	-4.74856500	-2.64363000	-1.49497000
C	-0.12271000	-5.15895700	1.99782800
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C	-4.95600900	2.56872300	1.83170400
H	-5.27922900	2.75540700	2.85109800
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C	-3.58202300	-3.83573300	2.11618400
H	-2.92189500	-4.59537000	2.52022500
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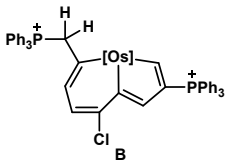

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P 0.07475100 2.38297000 -0.45152500
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C 3.32536400 -4.56860500 0.56728800
H 3.76593300 -5.07494200 1.42156700
C 2.05511500 -3.99635400 0.68476100
H 1.52633900 -4.06344000 1.62842500
C 3.42676900 -3.88473800 -1.74657600
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H	-4.23226300	4.16440800	-3.80090000
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H	-4.08099200	5.02841500	-1.47485000
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C	-4.93730800	-2.16816100	1.82270400
H	-3.96280700	-2.48453400	1.46814400
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H	-7.22307600	0.35477900	1.47545200
C	-6.56874500	3.63721200	-0.34786400
H	-7.29136300	4.08371600	-1.02342600
C	-6.07467200	4.36763300	0.73396900
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C	-5.62071400	-2.94514300	2.75565400
H	-5.16633000	-3.85946100	3.12112700
C	-5.61684800	-1.45518400	-4.13167100
H	-5.84322900	-1.80323300	-5.13484900
C	-6.87467400	-2.54317800	3.22176600
H	-7.40124400	-3.15121000	3.95075900
C	-5.00972500	-0.20937000	-3.94769800
H	-4.76182400	0.41135900	-4.80295400
C	-4.72638000	2.47907000	1.40629300
H	-4.03077100	2.02314400	2.10321800
C	-5.93707100	-2.25191000	-3.03095500
H	-6.40800600	-3.21870100	-3.17566300
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H	2.87523100	-0.40636100	-1.15739800
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C	7.26250000	-2.72060100	-1.79879700
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C	5.89185500	-1.60202900	-3.45449800
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C	5.41389800	-2.29972600	3.57433300
H	4.20376500	-2.45476400	1.80640100
C	6.35873700	-1.54120600	4.27206100
H	7.56104500	0.24907000	4.28080400
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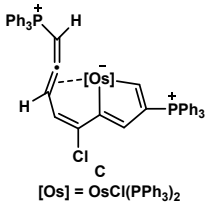

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P	-0.28712100	2.09572000	-0.76612800
C	-6.27161700	-0.02898200	-0.84532500
C	5.45041200	-0.55597600	1.35786600
C	-2.95434600	-4.42624000	-1.86704500
H	-3.71370800	-4.15687000	-2.59623700
C	-1.72806600	-1.10822200	0.96889900
C	-6.26614300	0.66870800	-2.06217600
H	-5.39365000	1.23230800	-2.37303000
C	-1.49607600	-0.68627000	2.36961100
H	-2.22722000	-0.89848400	3.14382300
C	-2.90147100	3.10873400	-1.12409500
H	-2.93089800	3.16125100	-0.04503300
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H	4.90983600	0.51145900	3.15971000
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C	1.16823700	2.73554700	-1.74879500
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H	2.87002800	-2.65108100	-4.76586600
C	-4.83722100	-1.40493400	1.34542800
C	3.19922100	-3.22725000	2.62587600
H	4.27605300	-3.15570300	2.73003300
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C	-0.97625100	-5.12281300	-0.02577900
H	-0.20657200	-5.40380500	0.68482000
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H	6.18458800	-1.80696900	-0.24566300
C	2.01541800	0.07870400	1.64610000
H	2.52529900	0.19266500	2.59798700
C	-7.39817300	0.64214200	-2.87431200
H	-7.39313500	1.17782300	-3.81861300
C	1.22955900	-3.15691700	1.20859600
C	1.01233300	-3.55963100	3.59193100
H	0.38088500	-3.74444200	4.45580500
C	2.61875900	-3.06686900	1.36950200
H	3.24991000	-2.85830900	0.51434800
C	4.65919900	2.20754800	0.97790500
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C	-0.25932200	-0.22709900	2.62288800
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H	4.26621400	-1.54613900	-1.75179400
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H	5.13728500	-1.69881400	-4.04120300
C	-4.97095600	3.89996000	2.74117900
H	-4.98978700	4.82499300	3.30963400
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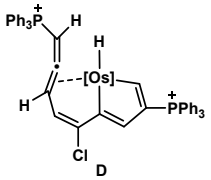

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P	0.29134900	-2.28110900	-0.35219000
P	0.17493500	2.56224000	-0.55604500
C	-5.78604400	-0.70258900	-1.43095700
C	5.28627300	-1.62338500	1.18008800
C	-3.17554400	-3.14743400	-2.42688200
H	-3.78706800	-2.66046300	-3.17820400
C	-1.78630400	0.38786200	1.18661700

C	-5.29574600	-0.06209200	-2.57755800	C	5.56548000	1.30864200	1.02394500
H	-4.69905500	0.83921000	-2.49314500	C	5.47028800	-2.71506500	3.33342600
C	-1.21759500	0.59349500	2.50272400	H	5.44104600	-2.66447700	4.41753900
H	-1.85516600	0.87377600	3.33126900	C	0.12470100	0.45881700	2.63853100
C	-2.06469400	2.54393800	-2.32125600	C	3.02492100	0.05169500	0.29855000
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H	-4.17613500	2.05522300	-0.46536900	H	-6.91037400	-2.38345100	-0.65362600
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C	-3.02433800	3.16088000	-3.12690300	C	-4.46418200	-2.42466600	1.01411300
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C	5.36128000	-0.24361400	-1.49271400	C	-0.71357300	-2.91998300	2.18202300
C	2.57615000	-3.64942900	-3.47085800	H	-1.68891300	-2.84665200	1.71698100
H	2.64333300	-3.42917100	-4.53223300	C	2.34323000	-4.24101200	-0.75230700
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H	2.13953700	1.88174000	-2.59799600	H	4.16303200	-1.99216700	-1.96313500
C	-1.56867900	-4.40721700	-0.52328200	C	5.82374600	-3.97791000	1.30010200
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C	-4.20574600	-3.42072000	1.95467900
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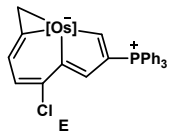

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C	-4.26545200	0.13748700	0.58666500
C	3.88112500	-2.01034300	1.90648300
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C	3.37720200	1.31030100	-0.50658200
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C	1.62155000	-2.77278300	2.28254100
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H	6.09113500	-4.63025400	-1.38069200
C	3.69534000	-2.20728900	-1.25973600
C	1.93138700	-3.03599100	3.61485600
H	1.15859300	-3.40834800	4.28013600
C	3.21496700	-2.78314100	4.09907400
H	3.45253600	-2.97639500	5.14148300
C	0.47484400	3.92064100	4.28663600
H	0.51905300	4.15876900	5.34567500
C	1.98771400	3.92198100	-2.23081300
H	2.15176600	2.90872200	-2.58051300
C	1.50992500	4.30952500	3.43610300
H	2.36700200	4.84889600	3.82971000
C	-3.94713100	0.89596600	1.72419100
H	-3.01952400	0.71314700	2.25566100
C	-3.67687100	-0.83993900	-4.01034600
H	-3.63714300	-0.05564100	-4.76024200
C	-3.75457100	3.39737600	-2.16598600
H	-4.70873700	3.56105500	-2.65947100
C	0.36728600	3.29501400	1.55124900
C	2.31504100	0.78348700	3.12743700
H	2.61985700	0.88146900	4.16311700
C	-0.60819200	3.20700800	3.77351200
H	-1.40012700	2.86610900	4.43336000
C	4.18732300	-2.26679500	3.24236300
H	5.18570500	-2.05309500	3.61391500
C	0.15685600	-5.33520300	-0.94449400
H	0.11492300	-6.32549600	-0.49829000
C	-3.50653700	-4.96068400	2.50975900
H	-3.59176100	-5.87276300	3.09356700
C	5.89443300	-3.01739400	-2.80244800
H	6.74936200	-3.32827400	-3.39697100
C	-3.97079400	-2.15508100	-4.37894700
H	-4.16368700	-2.39644300	-5.42023400
C	1.47182200	6.53694100	-1.39345300
H	1.26133000	7.55202800	-1.06745200
C	-4.01922500	-3.15905400	-3.40995900
H	-4.24901000	-4.18170000	-3.69406600
C	-3.58069000	3.76657400	-0.83405100
H	-4.40010100	4.21387700	-0.27951700
C	0.98733200	-4.36050100	-0.38630800
H	1.58229700	-4.60161000	0.48730600
C	5.15472600	-1.89413700	-3.16912000
H	5.42573100	-1.32631300	-4.05499900
C	2.25495800	6.31137800	-2.52858600
H	2.66029600	7.15141400	-3.08625800
C	4.05717300	-1.48881800	-2.40546800
H	3.46537000	-0.63313100	-2.71091800
C	-0.52485400	-3.77462500	-2.65527700
H	-1.10530700	-3.53982700	-3.54185300
C	-0.61240700	-5.04006200	-2.07131000
H	-1.26445500	-5.79640700	-2.50016300
C	1.09061600	0.28479800	2.85904000

C -4.81591100 1.89447600 2.15655800
H -4.56137700 2.48384000 3.03242500
C -6.00087500 2.14415600 1.45929000
H -6.67379300 2.92768700 1.79567200

$OPPh_3$

E = -1111.763554 a.u.

C 1.56620200 0.62798700 0.23026300
C 2.02663800 0.27005400 -1.04268300
C 2.31424100 1.50890400 1.02098900
C 3.21558900 0.81285700 -1.53134300
H 1.47109000 -0.44423400 -1.64301100
C 3.50363800 2.04670400 0.53049500
H 1.95983800 1.75015600 2.01846400
C 3.95185800 1.70345400 -0.74714400
H 3.57210800 0.53287800 -2.51864400
H 4.08342500 2.72876200 1.14593100
H 4.87949400 2.12175600 -1.12776500
C -1.32686400 1.04242500 0.23051600
C -1.24713500 1.62071900 -1.04215500
C -2.46402100 1.24885400 1.02112600
C -2.31203900 2.37852400 -1.53074000
H -0.35049500 1.49754600 -1.64220800
C -3.52477400 2.00966600 0.53077100
H -2.49563500 0.82082200 2.01839800
C -3.45169200 2.56995700 -0.74665600
H -2.24791000 2.82766700 -2.51786400
H -4.40552700 2.17010000 1.14612100
H -4.27803400 3.16384300 -1.12720600
C -0.23922000 -1.67006400 0.23036000
C -0.78049400 -1.89003800 -1.04211200
C 0.15082900 -2.75819300 1.02071500
C -0.90475900 -3.19115900 -1.53064700
H -1.12233600 -1.05192900 -1.64208500
C 0.02197800 -4.05720000 0.53033800
H 0.53770900 -2.57173700 2.01787200
C -0.50044500 -4.27393300 -0.74682400
H -1.32630600 -3.36012400 -2.51756400
H 0.32359400 -4.90021700 1.14553600
H -0.60193700 -5.28647600 -1.12736800
P 0.00013000 0.00019200 0.95198200
O 0.00022400 0.00014900 2.47250600

PPh_3

E = -1036.459997 a.u.

P -0.00016700 -0.00018400 -1.29677300
C -1.61586000 -0.36742900 -0.45037900
C -1.73796600 -1.16436700 0.69568000
C -2.77199900 0.19844000 -1.00927700
C -2.99011400 -1.38425900 1.27276300
H -0.85379100 -1.61138300 1.13775300
C -4.02089300 -0.01201200 -0.42608100
H -2.68999900 0.80822700 -1.90578400
C -4.13279400 -0.80704000 0.71670300
H -3.07128200 -2.00540200 2.16082700
H -4.90649100 0.43689300 -0.86752200
H -5.10599100 -0.97918000 1.16798000
C 0.48974200 1.58283800 -0.45065400
C -0.14237200 2.08994700 0.69246300
C 1.56105000 2.29844000 -1.00699700
C 0.29346200 3.28440800 1.26921200
H -0.97407900 1.55000800 1.13262800
C 2.00339800 3.48529100 -0.42408100
H 2.05058000 1.92028900 -1.90123300
C 1.36784300 3.98260100 0.71581000
H -0.20623600 3.66749400 2.15499700
H 2.83748100 4.02558400 -0.86346800
H 1.70553100 4.91153500 1.16685500
C 1.12587300 -1.21558400 -0.45024200
C 1.87780000 -0.92245700 0.69525700
C 1.21326500 -2.50009200 -1.00850100
C 2.69442700 -1.89679400 1.27237800
H 1.82339900 0.06699800 1.13688200
C 2.02010400 -3.47630300 -0.42527800
H 0.64359600 -2.73431700 -1.90454900
C 2.76529600 -3.17528200 0.71693000
H 3.27348700 -1.65618100 2.15999400
H 2.07366500 -4.46794600 -0.86623700
H 3.40105500 -3.93193700 1.16823700

Et_2OH^+

E = -234.073423 a.u.

H -0.44762700 1.46752100 -0.22551700
C 1.39026800 0.61104000 0.24013800
H 1.78782400 1.50574500 -0.24026700
O -0.04721600 0.57460200 -0.26574600
C -1.00354900 -0.43584800 0.34238700
H -0.88328700 -0.35635100 1.42551700
H -0.62454200 -1.38874600 -0.02119600
H 1.32692600 0.74767300 1.32227700
C -2.39232400 -0.11719300 -0.14971300

H -3.07544100 -0.86943000 0.25929900
H -2.74120900 0.86040100 0.20234300
H -2.45277400 -0.16377600 -1.24031700
C 2.09961800 -0.64761700 -0.18408900
H 2.04800900 -0.78751500 -1.26709500
H 3.15410900 -0.53738800 0.09245400
H 1.72166400 -1.53723700 0.32613300

H_2O+Et_2O

E = -310.132753 a.u.

O -2.21371200 1.65897800 -0.09554700
H -2.17335500 1.77902300 0.86451600
H -1.37764800 1.19624600 -0.30101400
C 1.31169700 0.76601100 0.21172300
H 1.25877600 1.77381900 -0.21162700
O 0.16176100 0.08962200 -0.29246800
C -0.18597400 -1.10258900 0.41142400
H -0.31719900 -0.87004100 1.48141500
H 0.62497200 -1.83986700 0.33245800
H 1.23832100 0.85800000 1.30745100
C -1.47149300 -1.64726400 -0.18684200
H -1.78870000 -2.54654300 0.35189500
H -2.26188600 -0.89350200 -0.12607900
H -1.32210300 -1.90704200 -1.23961600
C 2.62226300 0.09506600 -0.18529800
H 2.67751000 -0.01156600 -1.27329800
H 3.47114000 0.70293000 0.14761700
H 2.72682000 -0.89759600 0.26435300

Et_2O

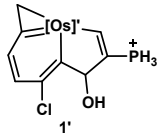
E = -233.66985 a.u.

O 0.00000000 0.00000000 0.83605600
C 0.00000000 1.19634600 0.06889800
H -0.42817600 1.96681800 0.71934200
H -0.66411600 1.10363200 -0.80410800
C 1.40445200 1.60361700 -0.37126900
H 1.85154500 0.85241600 -1.03180200
H 1.37735200 2.55537800 -0.91517200
H 2.05488600 1.71876700 0.50173800
C 0.00000000 -1.19634600 0.06889800
H 0.66411600 -1.10363200 -0.80410800
H 0.42817600 -1.96681800 0.71934200
C -1.40445200 -1.60361700 -0.37126900
H -1.37735200 -2.55537800 -0.91517200
H -2.05488600 -1.71876700 0.50173800
H -1.85154500 -0.85241600 -1.03180200

H_2

E = -1.181141952 a.u.

H 0.00000000 0.00000000 0.37142100
H 0.00000000 0.00000000 -0.37142100

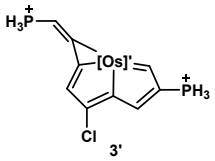


1'

[Os]' = $OsCl(PH_3)_2$

E = -567.990903109 a.u.

Os 0.000000000 0.000000000 0.000000000
Cl -1.808161049 1.760560400 0.071748511
Cl 3.963014961 -2.689705179 0.166566724
C 1.202480191 1.687505884 -0.094983940
H 0.757110955 2.669696034 -0.213589525
C 2.539251666 1.564264739 -0.031952195
C 1.881015342 -0.819227127 0.000000000
C -0.586501015 -1.944414746 0.045845569
C -1.801332789 -1.288949237 0.017490061
H -2.389230947 -1.169561177 0.922046138
H -2.375735737 -1.256034516 -0.904485526
C 3.071616874 0.169753076 0.094953870
H 3.536371752 -0.001981993 1.077923807
C 0.000000000 -3.176884473 0.000000000
H -0.605899384 -4.078943284 -0.015564197
C 1.389388283 -3.277525285 -0.041912581
H 1.846382762 -4.260969805 -0.072002883
C 2.231921692 -2.168039002 -0.008048249
O 4.075152087 0.028946047 -0.912972652
H 4.580625076 -0.779683420 -0.724415411
P 3.681483778 2.969275124 -0.215395970
H 4.514818836 3.013264358 0.845790926
H 4.401749958 2.818854022 -1.347248486
H 2.975142223 4.117884610 -0.280801232
P -0.056207844 0.236585409 2.443861740
H 0.193421975 1.520664833 2.777515725
H -1.275216484 -0.118693764 2.902440688
H 0.882274132 -0.562166310 2.994994446
P -0.061293660 -0.021720413 -2.450957482
H -1.294705924 -0.379519369 -2.867099394
H 0.231976984 1.209980368 -2.919364917
H 0.845099036 -0.907581782 -2.915932676

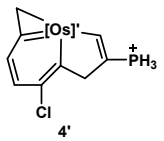


3'

[Os]' = $OsCl(PH_3)_2$

E = -498.916647910 a.u.

Os	0.000000000	0.000000000	0.000000000
Cl	-2.355515037	0.887057016	0.004408018
Cl	4.399060341	-1.628115797	-0.136242320
C	1.637841012	1.148675924	0.036344628
C	2.938282682	0.682098339	0.000000000
H	3.829207098	1.297264064	0.017370488
C	-0.843828695	-1.853663270	0.037780576
H	-1.914843009	-2.018918069	0.106363762
C	0.189867945	3.297747556	0.000138315
H	-0.867058719	3.541511994	-0.044776401
C	1.381565617	-2.653772224	-0.058795240
H	2.171645712	-3.398415385	-0.078041034
C	2.925254297	-0.713323164	-0.063272784
C	0.000000000	-2.962582444	0.000000000
C	1.635956843	-1.292657245	-0.061488309
C	0.610406780	2.028385320	0.005234569
P	-0.574516119	-4.689525158	-0.000337511
H	-0.131831106	-5.310827195	-1.114121055
H	-0.093788239	-5.323914002	1.090053012
H	-1.924080937	-4.714807698	0.022805147
P	1.349698052	4.690682255	0.164232899
H	1.225969645	5.507456861	-0.903507955
H	1.070232211	5.378520675	1.291742171
H	2.613205518	4.219289570	0.226182942
P	-0.007665773	0.033353275	-2.466752613
H	-0.874642926	-0.893662520	-2.926635573
H	-0.384400854	1.255501578	-2.899099946
H	1.231851615	-0.243527478	-2.924391875
P	-0.054268998	-0.143976293	2.457417806
H	-0.190908583	1.094171066	2.977822213
H	-1.097351054	-0.910688863	2.840342942
H	1.095697911	-0.694350880	2.901449235

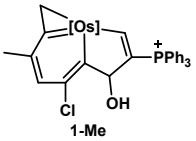


4'

[Os]' = $OsCl(PH_3)_2$

E = -492.779461868 a.u.

Os	0.000000000	0.000000000	0.000000000
Cl	-1.864761897	1.715635850	-0.002095017
Cl	3.969482756	-2.625983931	0.173431483
C	-0.586701705	-1.959626219	-0.046371942
C	-1.796048695	-1.296487136	-0.066082697
H	-2.405785220	-1.247712590	0.832037765
H	-2.344310651	-1.178856070	-0.995564011
C	1.858566118	-0.836653033	0.050601242
C	1.219810010	1.700245798	-0.002473583
H	0.814006597	2.707988998	-0.010706141
C	3.046210767	0.113064718	0.000000000
H	3.709875531	-0.088315570	0.852653850
H	3.640671467	-0.128238148	-0.891482627
C	0.000000000	-3.187631468	0.000000000
H	-0.605753236	-4.089793794	-0.025169371
C	2.230445216	-2.186116892	0.119797351
C	2.555598655	1.525795766	-0.015629571
C	1.392431218	-3.291203984	0.105243988
H	1.846511456	-4.275062269	0.162646667
P	-0.088127336	0.008273584	2.445638719
H	1.063094846	-0.495376334	2.939120497
H	-0.250713032	1.274105731	2.885791952
H	-1.125378569	-0.749344634	2.861119788
P	0.058685927	0.222487382	-2.433867543
H	-0.079328903	1.522574728	-2.770356485
H	1.238287034	-0.240137647	-2.899720857
H	-0.950493429	-0.492115149	-2.975531887
P	3.776344096	2.873858047	0.054432257
H	4.415038824	2.841232296	1.243341246
H	4.673469714	2.720821513	-0.942686324
H	3.146021316	4.059456273	-0.085389263



1-Me

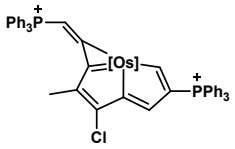
[Os] = $OsCl(PPh_3)_2$

E = -4583.18826886 a.u.

Os	-1.33425500	0.03750100	-0.23923200
Cl	-1.46463800	0.20391400	-2.74976300
P	-1.41634200	-2.40118200	-0.37028300
P	-1.25710900	2.49259700	-0.35141300
P	3.37485700	-0.10199000	0.02497600
Cl	-0.17911200	0.00457200	4.40524500
C	-2.63156900	-3.26797500	-1.47052900
C	0.69314400	-0.00933300	-0.68468200
H	1.02141100	-0.04396600	-1.71843800

C	0.13581000	-3.21874300	-0.94608200
C	-2.95290500	3.21776900	-0.46410200
C	-0.41631500	3.37419600	-1.74134700
C	-3.62205900	3.80533600	0.61331400
H	-3.12584400	3.93186000	1.56765900
C	-4.32595500	-4.72456900	-3.16191200
H	-4.98562000	-5.28796400	-3.81523100
C	1.60318100	-0.01055800	0.30548800
C	-3.26825500	-2.63456300	-2.54345100
H	-3.07801000	-1.58861400	-2.74655800
C	-0.77594700	4.71288800	-1.97459700
H	-1.56298800	5.17391200	-1.38822600
C	0.60904500	2.80230100	-2.49894300
H	0.89602900	1.77569200	-2.34173500
C	-0.48206000	-0.04210100	1.62574200
C	-0.47293900	3.28155200	1.12558800
C	4.12932300	-1.76713300	-0.01443600
C	0.69785100	-4.33336100	-0.31633500
H	0.27465800	-4.71351500	0.60625600
C	1.77149100	-3.41392100	-2.72293200
H	2.16714800	-3.07389500	-3.67630600
C	-3.05173300	0.03409900	0.82618300
C	-4.93271900	4.26422500	0.45786600
H	-5.44067000	4.72683000	1.29896900
C	-3.53294600	0.02902700	-0.47085100
H	-3.91311800	0.93575100	-0.93024500
H	-3.94338700	-0.88858600	-0.88517700
C	-3.60691700	3.09934400	-1.70334900
H	-3.09341100	2.63708700	-2.54108800
C	0.66960400	-2.76865100	-2.16414200
H	0.20113200	-1.93720600	-2.68302800
C	-0.98067900	3.00801800	2.40461900
H	-1.83864200	2.35845100	2.51321900
C	-2.82966200	-4.64442000	-1.26558300
H	-2.32439600	-5.15289000	-0.45099800
C	-0.12580400	5.45796400	-2.95536100
H	-0.41622100	6.49028000	-3.12600400
C	-5.58053200	4.14225600	-0.77098400
H	-6.59803900	4.50261300	-0.88875900
C	-3.67530100	-5.36528800	-2.10355000
H	-3.82402000	-6.42736600	-1.93262700
C	-4.11554700	-3.36475600	-3.38120500
H	-4.60441900	-2.86277300	-4.21088500
C	1.25321300	3.54985500	-3.48569100
H	2.03455700	3.08478900	-4.07509300
C	-4.91253900	3.56258200	-1.85281200
H	-5.40777200	3.46873900	-2.81462300
C	-1.81876700	-3.07994700	1.29676000
C	1.06179600	0.00238700	1.70002400
H	1.33445700	0.92128000	2.23875500
C	-1.18038700	-3.53735300	3.59004200
H	-0.41086800	-3.58685100	4.35452300
C	-3.47412200	-0.06196500	2.12955800
C	3.70306600	-2.76570500	0.87024200
H	2.86037300	-2.57737400	1.52185600
C	-0.83797000	-3.15194500	2.29414000
H	0.18337100	-2.86246400	2.07736000
C	2.34953800	-4.50999800	-2.07774200
H	3.21325600	-5.00537300	-2.50995600
C	5.37471400	0.36993100	1.94059100
H	5.79055300	-0.58715800	1.64580900
C	-2.49615500	-0.12964500	3.12001400
H	-2.80719700	-0.20240800	4.15737500
C	0.64213900	4.12116500	1.00128700
H	1.04542300	4.35058300	0.02221500
C	-3.49130600	-3.74226900	2.92398000
H	-4.52675000	-3.96499000	3.16411600
C	4.21012100	0.85042400	1.33049600
C	-0.38531400	3.55982200	3.53712700
H	-0.78636200	3.33074500	4.51916100
C	0.88863300	4.87511100	-3.71770200
H	1.38844500	5.45176300	-4.49062100
C	-3.15082600	-3.37043200	1.62344900
H	-3.92371000	-3.30755100	0.86516600
C	-2.50634700	-3.83217600	3.90921100
H	-2.77180200	-4.12731900	4.92001400
C	1.80371900	-4.97178000	-0.88186500
H	2.23659200	-5.83352500	-0.38349900
C	-1.12595800	-0.08782800	2.85532800
C	3.75636100	0.65290100	-1.59151700
C	3.40352100	-0.03726900	-2.76244300
H	2.92739800	-1.00974000	-2.69903800
C	3.69731700	0.51628300	-4.00673700
H	3.42401100	-0.01815700	-4.91124200
C	4.35354200	1.74766900	-4.08785800
H	4.59405000	2.16996600	-5.05896500
C	4.70174000	2.43384300	-2.92351400
H	5.21067100	3.39057000	-2.98549700

C	4.40303600	1.89133700	-1.67334400
H	4.68379600	2.42331200	-0.77128800
C	5.22307700	-1.99938600	-0.86499200
H	5.56369300	-1.22927600	-1.54745400
O	1.65276900	-1.11089100	2.38355200
H	1.50685600	-0.98219600	3.33663400
C	0.72531300	4.39673300	3.40690000
H	1.18637700	4.83059200	4.28920100
C	3.66434400	2.08419000	1.71695500
H	2.75937900	2.45810900	1.24866200
C	5.99128800	1.12503800	2.93804700
H	6.89294700	0.75267300	3.41418300
C	5.45991700	-4.22086500	0.05893400
H	5.97817500	-5.17469200	0.08986700
C	4.37631300	-3.98571600	0.90547800
H	4.04567400	-4.75740700	1.59390400
C	4.28608300	2.82960500	2.71595500
H	3.85432200	3.77652500	3.02188500
C	5.87947700	-3.22825400	-0.82932600
H	6.72267100	-3.40543700	-1.48984200
C	1.23217700	4.67877900	2.13827300
H	2.08584500	5.34129300	2.02518000
C	5.44810000	2.35113900	3.32640400
H	5.92842800	2.93280800	4.10736400
C	-4.94537200	-0.13169600	2.46464000
H	-5.11707700	-0.01351100	3.53891400
H	-5.50237900	0.64788800	1.93585800
H	-5.36365800	-1.09946200	2.16281300



3-Me

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P	4.71459200	-0.12310300	-0.06611500
P	0.11094600	-2.39710300	-0.26847600
P	0.07280700	2.53182700	-0.38440000
C	-5.89342000	-0.87628000	-1.39769600
C	5.29753000	-1.62786900	0.77984200
C	-3.39865700	-3.45333500	-2.13312600
H	-4.01304600	-3.04835900	-2.93131100
C	-1.41379000	0.10277700	1.05739100
C	-6.00101200	-0.28032900	-2.66458900
H	-5.54410500	0.68661800	-2.85826400
C	-1.20211300	0.18352400	2.42746300
C	-2.07491900	2.89705900	-2.18925100
H	-1.83260000	1.90390600	-2.54206800
C	0.12830000	3.16853000	1.34523600
C	1.97816200	-0.03795400	-0.84517100
H	2.32031400	-0.14958100	-1.86864000
C	-3.37704100	4.92977300	-2.37789100
H	-4.16629900	5.50029500	-2.85780700
C	5.37100000	-1.62973000	2.18306900
H	5.18490100	-0.72134900	2.74667800
C	-1.44072600	-3.29538400	-0.71294600
C	1.53581800	3.28098100	-1.22862500
C	-3.21898200	0.06416800	-0.83241400
H	-3.17495500	0.05960500	-1.91771600
C	-2.22844100	-2.79178100	-1.75777700
H	-1.91811900	-1.89364400	-2.27723600
C	-1.34165700	3.45658600	-1.13546100
C	1.34349500	-3.26543200	-1.34167700
C	-3.09078700	3.63260000	-2.80172200
H	-3.64978900	3.19184500	-3.62224700
C	5.09212700	-0.15682500	-1.83717000
C	2.24488900	-3.60401600	-3.56693200
H	2.28944200	-3.31022100	-4.61163900
C	-4.88087200	-1.00389100	1.38396100
C	2.06360600	-3.24131600	3.27205100
H	3.09032100	-3.33594000	3.60854100
C	2.08865800	2.63560200	-2.34342600
H	1.64164900	1.72077400	-2.71264700
C	-1.80557200	-4.49746200	-0.08784100
H	-1.18379300	-4.91969000	0.69368700
C	5.55754600	-2.80266500	0.06121200
H	5.51757400	-2.81075300	-1.02105100
C	2.37610900	0.10980900	1.48318100
H	2.97214100	0.14582800	2.39036200
C	-6.70596500	-0.93220300	-3.67315600
H	-6.79053500	-0.47640500	-4.65445700
C	0.48724500	-2.89809500	1.46093100
C	-0.30315400	-3.21236600	3.73671100
H	-1.12980400	-3.27915800	4.43790800
C	1.80820500	-3.00774400	1.92149400

H	2.64029400	-2.90413800	1.23525600
C	5.48059900	1.34139200	0.67533500
C	5.70876600	-2.80163900	2.85639800
H	5.78561300	-2.79596100	3.93928700
C	0.18581900	0.19675300	2.65133900
C	2.91977700	-0.00191200	0.18134400
C	-5.56149000	1.61009600	0.15600700
C	1.01102900	-3.35114600	4.18240700
H	1.21489000	-3.53389300	5.23277000
C	1.44277400	-2.87722300	-2.68656500
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H	-4.69665400	-5.13429500	-1.76862500
C	3.18620700	3.19093400	-3.00253900
H	3.61486700	2.67411400	-3.85544800
C	-6.50147700	-2.10979300	-1.13817700
H	-6.41613000	-2.57008700	-0.16043100
C	6.63855300	3.67162600	1.66287600
H	7.08941400	4.57898800	2.05260900
C	4.82335700	2.57059700	0.50675400
H	3.87787500	2.61978500	-0.02204400
C	-4.18624800	-2.22295600	1.40836200
H	-3.62558700	-2.54994300	0.54168300
C	-0.56224200	-2.97914500	2.38683200
H	-1.58502300	-2.84883800	2.05817400
C	2.04767600	-4.39520700	-0.89906300
H	1.94620000	-4.74457600	0.12091600
C	-7.30945900	-2.16798300	-3.41781700
H	-7.86124100	-2.67167700	-4.20531400
C	4.51493800	-1.13387300	-2.66540000
H	3.84797900	-1.88619900	-2.26182000
C	5.87818900	-3.97457600	0.74640500
H	6.07953900	-4.88241200	0.18696100
C	5.40695800	3.73271500	1.00441400
H	4.90081800	4.68265800	0.86949300
C	2.87561400	-5.09530700	-1.77791700
H	3.42078000	-5.96389900	-1.42063700
C	-5.61349500	-0.57985100	2.50000500
H	-6.15011800	0.36255700	2.47918500
C	-2.09380100	0.09130300	-0.11022600
C	-1.04428700	3.71455600	3.40115900
H	-1.97949400	3.86220200	3.93284600
C	-1.06696600	3.35174500	2.05395400
H	-2.02095900	3.21689700	1.55728100
C	5.95415300	-3.97651200	2.13988400
H	6.21460600	-4.88831900	2.66805000
C	-4.70168600	2.70455400	0.31039500
H	-3.63483900	2.58357400	0.16508200
C	-4.23193500	-3.01505700	2.55373500
H	-3.70861200	-3.96608000	2.56502300
C	2.97664400	-4.70372700	-3.11399400
H	3.60383400	-5.26433700	-3.80056100
C	-2.97605000	-5.15482300	-0.46828700
H	-3.25402700	-6.08331600	0.02138700
C	-2.63343200	5.49996800	-1.34141600
H	-2.83631000	6.51705400	-1.01915000
C	-1.61972900	4.77055100	-0.72242800
H	-1.04910500	5.22652500	0.07891800
C	5.93883900	0.82049300	-2.37913300
H	6.37981600	1.57975000	-1.74387600
C	-7.21289400	-2.75068100	-2.15313600
H	-7.69180400	-3.70424600	-1.95421400
C	3.72229600	4.40569700	-2.57280800
H	4.57558800	4.83828000	-3.08628500
C	2.05118200	4.52242500	-0.82517400
H	1.61215800	5.05263800	0.01247000
C	3.14038100	5.07921200	-1.49595700
H	3.53095400	6.04192500	-1.17948700
C	1.34673800	3.32470500	2.02152700
H	2.28270900	3.15535600	1.50395800
C	6.72570800	1.27876900	1.31590200
H	7.24143600	0.33088500	1.42717800
C	-5.64383200	-1.37623000	3.64527500
H	-6.20829000	-1.04936000	4.51266600
C	1.36805200	3.69108600	3.36549800
H	2.32031700	3.81594100	3.87186900
C	6.20721400	0.81606700	-3.74753500
H	6.86583200	1.56971700	-4.16722700
C	0.17292700	3.89035400	4.05924500
H	0.19106600	4.17548900	5.10639600
C	7.29798500	2.44936300	1.81395100
H	8.25904500	2.40644700	2.31616600
C	-4.95610000	-2.59150500	3.67244200
H	-4.99166600	-3.21272900	4.56218200
C	-6.95127000	1.76895700	0.27399200
H	-7.61526800	0.92225400	0.12660100
C	5.63347500	-0.15330100	-4.57239300

H	5.84492600	-0.15243900	-5.63712000
C	-5.23505000	3.95821900	0.60680000
H	-4.57065300	4.80875900	0.71154900
C	4.78967100	-1.12636100	-4.03031600
H	4.34140400	-1.88127300	-4.66685900
C	-6.61552400	4.11713700	0.74255100
H	-7.02801300	5.09531000	0.96976300
C	-7.47333200	3.02590700	0.57190900
H	-8.54689200	3.15628500	0.66342400
C	-2.26291700	0.24132800	3.47930200
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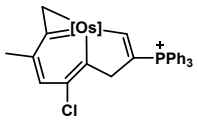

4-Me

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P	-3.27756100	-0.65956800	-0.09006300
C	2.97769200	0.62446500	0.95943700
C	2.40258500	4.70310300	0.89587000
H	1.79048500	4.70371400	1.78937000
C	2.09384000	3.86335000	-0.17820400
C	3.48357800	0.81291200	-0.31192900
H	4.09264300	0.04177900	-0.77604400
H	3.65154600	1.81406900	-0.69680000
C	-0.30190600	3.44413400	-1.57849600
C	3.49078600	-2.60266800	-1.14613400
C	0.44783600	-0.01082000	1.59604700
C	2.87358500	3.91738000	-1.34707800
H	2.62597900	3.27898900	-2.19132800
C	3.95645900	4.79009200	-1.42589100
H	4.55232200	4.82561300	-2.33299400
C	-0.65258600	-0.04389000	-0.77440800
H	-0.97112800	-0.04446400	-1.81310700
C	1.91700800	-2.78419000	1.29724300
C	4.12314900	-3.77498400	-0.70248900
H	3.72417700	-4.32979400	0.13872200
C	4.27059100	5.61799800	-0.34479800
H	5.11429900	6.29864100	-0.40760900
C	5.27327800	-4.23739500	-1.33974700
H	5.75554600	-5.14303200	-0.98370400
C	3.08472500	-2.69191600	2.06419000
H	3.99585400	-2.30440600	1.62205400
C	5.80004300	-3.54289600	-2.43037500
H	6.69731000	-3.90426200	-2.92398600
C	-1.05385200	-0.25476100	1.60294900
H	-1.26850700	-1.19623500	2.12834200
H	-1.52755500	0.52833600	2.21035900
C	3.49032400	5.57603800	0.80993700
H	3.71929100	6.22895500	1.64706000
C	-0.60650000	4.80955900	-1.42887700
H	-0.28881800	5.34008000	-0.53679700
C	4.00981900	-1.92140700	-2.25652600
H	3.50314100	-1.04167600	-2.63607800
C	-1.37936100	3.47691000	-3.74542500
H	-1.64107400	2.96004200	-4.66377400
C	3.33449100	0.56854300	2.27588000
C	0.18431100	2.94795600	2.54895300
H	1.24539200	2.76741900	2.67240400
C	-0.36828100	3.01747000	1.26111800
C	0.70743300	-3.12255700	-1.35253600
C	-0.63105500	3.06872400	3.67226200
H	-0.19240100	3.00602300	4.66280200
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H	5.55648900	-1.85131500	-3.74514200
C	-0.69928500	2.78016500	-2.74089200
H	-0.43022900	1.74566100	-2.89276500
C	1.02408300	-0.03807500	2.87136700
C	-1.75124700	3.18773500	1.11919200
H	-2.19554300	3.23292300	0.13214900
C	0.02064800	-2.58864900	-2.45041100
H	0.18740400	-1.55807500	-2.73705300
C	-1.69096000	4.82526900	-3.58718100
H	-2.21591000	5.36195600	-4.37203600
C	0.74427700	-3.26529500	1.89628900
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H	3.99570300	-3.01506900	3.98494900
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H	2.61932100	0.15017000	4.25672400
C	-1.30626400	5.49108500	-2.41942200

H	-1.53648700	6.54412800	-2.28832100
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C	1.91323300	-3.57267800	3.98972800
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C	-0.84243500	-3.39287200	-3.19688900
H	-1.38139300	-2.96225800	-4.03557000
C	0.74399800	-3.65938300	3.23221000
H	-0.17322200	-4.02616600	3.68271900
C	-3.67480800	-0.49589500	-1.85181700
C	-1.00414600	-4.74019100	-2.87323100
H	-1.67399500	-5.36616500	-3.45538800
C	-4.15821400	-1.59815500	-2.56855800
H	-4.30245400	-2.55160500	-2.07347700
C	-4.38257800	0.39411000	0.91329600
C	-2.00911300	3.24212700	3.52280500
H	-2.64503200	3.32517400	4.39912700
C	-0.28118900	-5.28932600	-1.81109600
H	-0.37711200	-6.34518900	-1.57414900
C	-3.47235700	0.73495200	-2.49624800
H	-3.06797500	1.58318700	-1.95432500
C	-2.61493200	-3.33847500	0.16955600
H	-1.69001200	-3.05073700	-0.31727400
C	-4.81352800	-2.74587600	1.02624100
H	-5.57947700	-2.00234900	1.21758600
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H	-3.63649100	3.42250000	2.11996500
C	-3.77540700	0.85991000	-3.84990300
H	-3.62632600	1.81430700	-4.34209700
C	-4.44562000	-1.46522400	-3.92685400
H	-4.81857100	-2.31950300	-4.48314300
C	-5.25900000	1.31163200	0.32169800
H	-5.31652900	1.39858100	-0.75736800
C	-2.83576800	-4.66512100	0.53493500
H	-2.06856100	-5.40498900	0.33622600
C	-5.02598400	-4.07629300	1.38571700
H	-5.96182000	-4.36417700	1.85444600
C	-4.26011200	-0.23791900	-4.56533000
H	-4.49109000	-0.13606300	-5.62128300
C	-4.33171500	0.27397900	2.31203900
H	-3.66438800	-0.44272300	2.77899300
C	-4.03669400	-5.03289100	1.14618900
H	-4.20392600	-6.06666600	1.43320200
C	-6.02768200	1.98449400	2.51591000
H	-6.67106800	2.59940300	3.13780700
C	-5.15471200	1.06732900	3.10706700
H	-5.11421500	0.96849900	4.18725400
C	-6.07669800	2.10712500	1.12627400
H	-6.75921700	2.81361200	0.66427100
C	4.75909700	0.81477600	2.72177500
H	4.79391300	1.28992800	3.70797200
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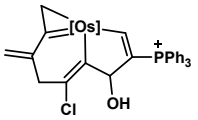
H	5.28220500	1.45757300	2.00971700



1-Me'

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P	-1.51280000	2.33456800	-0.37036800
P	3.34589600	0.19887100	-0.00818700
Cl	-0.13842700	0.16583000	4.43554500
C	-2.28858500	-3.56772700	-1.36182300
C	0.65976000	0.00526600	-0.68352400
H	0.98147700	-0.05497000	-1.71782100
C	0.45552400	-3.19031500	-0.89257300
C	-3.27086100	2.88152400	-0.52614300
C	-0.74271300	3.26636800	-1.76765400
C	-3.99589900	3.48773500	0.50432900
H	-3.51840300	3.72699400	1.44651500
C	-3.81421700	-5.22998100	-3.02267100
H	-4.40867800	-5.87368900	-3.66430600
C	1.56586300	0.14675100	0.29514400
C	-2.99416300	-3.02565200	-2.44191400
H	-2.91956900	-1.96827800	-2.66184400
C	-1.23224800	4.55453700	-2.04268600
H	-2.07343700	4.94725900	-1.48220100
C	0.34865500	2.78181600	-2.49312600
H	0.73479600	1.79412700	-2.30184400
C	-0.46531700	-0.02132800	1.69674000
C	-0.83709700	3.22534600	1.09957500
C	4.23696500	-1.39872800	0.01641800
C	1.18509600	-4.17617500	-0.22316700
H	0.85191800	-4.54732100	0.73901900
C	2.03334800	-3.28556400	-2.72855700

H	2.34357500	-2.95953200	-3.71783900
C	-3.01208600	-0.22783600	0.80677500
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C	-3.56206000	-0.37586100	-0.46711400
H	-4.08950600	0.44760600	-0.94065900
H	-3.88904800	-1.36196800	-0.78761600
C	-3.90176000	2.62145200	-1.75605600
H	-3.34335700	2.14593100	-2.55709300
C	0.87735200	-2.75479700	-2.15963600
H	0.28557300	-2.02332000	-2.70338800
C	-1.35403900	2.96221500	2.37734600
H	-2.17163700	2.26395700	2.49354700
C	-2.33002700	-4.95418500	-1.13516000
H	-1.76506300	-5.38996200	-0.31748800
C	-0.64229300	5.33657300	-3.03270000
H	-1.03254900	6.32917100	-3.23668300
C	-5.96335000	3.56120300	-0.90604300
H	-7.00560500	3.82802700	-1.05323700
C	-3.09310800	-5.77779800	-1.95770400
H	-3.12133000	-6.84723000	-1.77090900
C	-3.75668900	-3.85889700	-3.26477700
H	-4.29985800	-3.42827300	-4.10080200
C	0.93370300	3.56598100	-3.48816600
H	1.76951900	3.16829800	-4.05155400
C	-5.23979000	2.96279800	-1.94143100
H	-5.71687000	2.76081800	-2.89581000
C	-1.45132000	-3.22009800	1.39176400
C	1.05878000	0.19761500	1.70236200
H	1.25059300	1.17892700	2.15906200
C	-0.72301700	-3.50649100	3.68593200
H	0.05140900	-3.40926700	4.44062200
C	-3.47998100	-0.12961500	2.14796400
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C	-0.45912400	-3.10752900	2.37602600
H	0.50330900	-2.67199300	2.13694800
C	2.77837900	-4.25040600	-2.04467600
H	3.68291000	-4.65667100	-2.48613000
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H	5.80442800	-0.01536800	1.60189500
C	0.22157800	4.13498900	0.96975300
H	0.62782900	4.36005800	-0.00927300
C	-2.98094900	-4.09451200	3.06080100
H	-3.96444400	-4.47378400	3.32183700
C	4.11195600	1.27656000	1.24042800
C	-0.82414500	3.59303300	3.50087800
H	-1.22995800	3.37052700	4.48238300
C	0.44114200	4.84118000	-3.76134000
H	0.89529100	5.44648100	-4.54052900
C	-2.71997900	-3.70144300	1.74777300
H	-3.50168100	-3.78187900	1.00043100
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H	-2.18378300	-4.31281300	5.05304500
C	2.34499400	-4.69960000	-0.79954800
H	2.90826300	-5.46104100	-0.27003300
C	-1.07468300	-0.06332600	2.88323900
C	3.64944100	0.91725200	-1.65827300
C	3.31605000	0.17011700	-2.79980900
H	2.89635900	-0.82448500	-2.69746700
C	3.56021000	0.69552100	-4.06671600
H	3.30077800	0.11656600	-4.94758500
C	4.14887200	1.95607400	-4.20090100
H	4.35042900	2.35720400	-5.18965900
C	4.47965900	2.69814800	-3.06618700
H	4.93688600	3.67727600	-3.16850100
C	4.22937600	2.18406100	-1.79349000
H	4.49626500	2.76090200	-0.91533700
C	5.28763500	-1.61042000	-0.89112600
H	5.51369200	-0.87561300	-1.65456600
O	1.81325600	-0.78401800	2.43012400
H	1.63257200	-0.63823700	3.37513000
C	0.23100900	4.49740100	3.36415400
H	0.64182400	4.99048800	4.24006100
C	3.47575600	2.48207800	1.57308700
H	2.53921300	2.76062900	1.10086000
C	5.88324700	1.76896100	2.80619100
H	6.81647900	1.49205500	3.28654000
C	5.78854500	-3.71560400	0.18757700
H	6.39347400	-4.61482300	0.25703700
C	4.74737800	-3.50086700	1.09129000
H	4.53654300	-4.23446600	1.86360700
C	4.04712600	3.32183600	2.52615100
H	3.54565400	4.24594500	2.79303600
C	6.05361500	-2.77202800	-0.80654800
H	6.86346300	-2.93215700	-1.51164900
C	0.74626500	4.77083300	2.09706400
H	1.55133700	5.49048700	1.97727500

C 5.24926500 2.96633000 3.14274000
H 5.69017000 3.62157000 3.88784000
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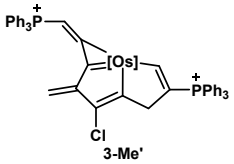

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P 4.67153200 -0.08872900 -0.03570400
P 0.12694900 -2.41288400 -0.24919000
P 0.06980900 2.49679800 -0.48336000
C -5.98839600 -1.06424100 -1.19088800
C 5.46060800 -1.30169000 1.07528800
C -3.57017000 -3.66091700 -1.47736600
H -4.23828700 -3.41332000 -2.29610600
C -1.49197300 0.16155600 1.08533100
C -6.06605000 -0.69570500 -2.54345200
H -5.57850400 0.20825800 -2.89826900
C -1.30201200 0.34247400 2.50039000
C -2.21433700 2.82464500 -2.10289600
H -1.97096000 1.84058900 -2.48041900
C 0.41228500 3.23306300 1.16582000
C 1.97203000 -0.08325300 -0.75284400
H 2.31054700 -0.19316500 -1.77872400
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H -4.37898700 5.39696000 -2.64156800
C 5.42559300 -1.07988800 2.46273700
H 4.94366500 -0.19679700 2.86825800
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C 1.37750500 3.16208200 -1.60193200
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H -2.06821300 -2.22975000 -2.06788000
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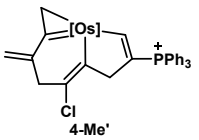

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P	0.76380400	2.63606600	-0.21109000	C	0.60861700	-3.14908600	-1.33915500
P	-3.26624600	-0.55907900	-0.10715400	C	-0.67666200	3.13205400	3.61943500
C	2.94771500	0.54584100	0.92385900	H	-0.27796600	3.07040900	4.62661200
C	2.53646100	4.60039500	0.93629400	C	5.08928100	-2.63713900	-2.77629800
H	1.89931000	4.63465900	1.81142500	H	5.50400000	-2.13610400	-3.64602000
C	2.21774100	3.77244900	-0.14413000	C	-0.54232600	2.78144000	-2.78095700
C	3.55738000	0.67455900	-0.32421400	H	-0.31359700	1.73522000	-2.91790600
H	4.16520800	-0.13802700	-0.71470600	C	0.98449300	0.01639100	2.90506700
H	3.81413200	1.65828300	-0.70708900	C	-1.69498900	3.24062900	1.02461800
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C	3.39717100	-2.75413800	-1.04454600	C	-0.03439900	-2.59050900	-2.45100600
C	0.44376300	-0.00204600	1.68305400	H	0.16861600	-1.56414600	-2.72858900
C	3.02963200	3.78696000	-1.29209900	C	-1.42117300	4.85972800	-3.67024100
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H	4.77266900	4.61583200	-2.23564300	H	-0.36272100	-3.34837600	1.29796300
C	-0.61989500	-0.02852400	-0.75941600	C	2.82299700	-3.21692600	3.48873100
H	-0.93693400	-0.01791400	-1.79809500	H	3.71862700	-3.17870100	4.10226200
C	1.73779500	-2.85622100	1.34991900	C	-1.53038500	-0.22350200	0.21061500
C	3.99661600	-3.92567600	-0.55674900	C	-1.04162100	5.51847900	-2.49665800
H	3.57499300	-4.44477800	0.29604600	H	-1.23072300	6.58132900	-2.37962600
C	4.47672700	5.42505600	-0.25625300	C	-3.66037500	-2.26584500	0.39305200
H	5.35141600	6.06711200	-0.29863000	C	0.42904100	-4.51172600	-1.05383500
C	5.14141200	-4.43549800	-1.16766000	H	0.94927800	-4.96729000	-0.21843500
H	5.59799000	-5.34092800	-0.77865300	C	1.62196300	-3.67796600	4.02958800
C	2.87982700	-2.79783000	2.15976900	H	1.57651400	-3.99298600	5.06738500
H	3.81538900	-2.42628000	1.75486600	C	-0.89748500	-3.36763900	-3.22601900
C	5.69458700	-3.78953400	-2.27473700	H	-1.40199400	-2.91738100	-4.07571700
H	6.58710100	-4.18826000	-2.74784000	C	0.47830300	-3.72357900	3.23190600
C	-1.06239700	-0.23157400	1.62984500	H	-0.46407300	-4.06861800	3.64640500
H	-1.31760600	-1.17790600	2.12750800	C	-3.62790500	-0.37405000	-1.87489800
H	-1.56245300	0.55144900	2.21332700	C	-1.10191900	-4.71248900	-2.91745900
C	3.66530300	5.42223500	0.87759100	H	-1.77119500	-5.31724500	-3.52228700
H	3.90047000	6.06834500	1.71834500	C	-4.13215200	-1.45607200	-2.60782600
C	-0.40005800	4.81628000	-1.48164100	H	-4.31252100	-2.40847900	-2.12287100
H	-0.08689100	5.33987300	-0.58392400	C	-4.35474700	0.52910600	0.87584300
C	3.94289000	-2.12064800	-2.17092600	C	-2.04138400	3.34484700	3.41417900
H	3.46104200	-1.24028100	-2.58132200	H	-2.70721600	3.46218600	4.26396400
C	-1.16364100	3.49803900	-3.80950500	C	-0.42095500	-5.28739800	-1.84110100
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C	3.35534200	0.60616500	2.28816400	C	-3.37936000	0.85500400	-2.50667200
C	0.17536300	2.96575100	2.52981400	H	-2.95918300	1.68712900	-1.95187700

C	-2.72626900	-3.27054500	0.10475100
H	-1.79625900	-3.02182300	-0.39312500
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H	-5.26198500	1.52046200	-0.81743200
C	-3.00569000	-4.59032000	0.45423200
H	-2.27851700	-5.36300100	0.23162400
C	-5.14972500	-3.90925600	1.35126500
H	-6.09081000	-4.15818600	1.83161500
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H	-4.37436000	0.03806600	-5.65363700
C	-4.32224900	0.42363100	2.27638800
H	-3.66562100	-0.29130300	2.76022300
C	-4.21270800	-4.90893700	1.08093300
H	-4.42536100	-5.93773900	1.35544600
C	-6.00817500	2.14875300	2.43973800
H	-6.65417100	2.77561200	3.04682400
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C	-6.03986500	2.25562400	1.04837800
H	-6.71147300	2.96159900	0.56990700
C	2.36955000	0.31093000	3.38759200
H	2.73182500	-0.53356600	3.98519500
H	2.33067600	1.16345400	4.08103600
C	4.63897800	0.94841600	2.54437900
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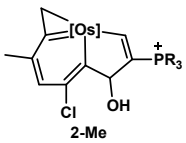
H	5.01432900	1.03889300	3.56111300



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P	1.02245500	-2.61041700	-0.31413600
P	-3.24865000	0.44309900	-0.02588200
Cl	0.17529500	0.04318200	4.45168200
C	3.29858900	2.90875400	-1.07037700
C	-0.58802400	0.05642800	-0.66126600
H	-0.90876700	0.09343600	-1.69747600
C	0.47778200	3.25339600	-1.06129800
C	2.61371200	-3.54555700	-0.33628500
C	0.15959900	-3.37911300	-1.75399100
C	3.20368900	-4.11169400	0.79628000
H	2.68189000	-4.12076500	1.74506700
C	5.46919600	4.07414800	-2.46001300
C	-1.51145200	0.15114400	0.31131100
C	3.79329300	2.31882500	-2.24162400
H	3.32938500	1.42028700	-2.63226600
C	0.26544500	-4.77507500	-1.89774200
H	0.86764900	-5.34722100	-1.19964100
C	-0.62037100	-2.67001500	-2.66850100
H	-0.69886300	-1.59763300	-2.60464600
C	0.53569400	-0.00569800	1.67820900
C	0.05611200	-3.27758000	1.11248900
C	-3.71053300	2.19473000	-0.20044600
C	0.22552200	4.57419200	-0.67145400
H	0.74457400	5.00257300	0.17907200
C	-1.07476100	3.53937100	-2.89882600
H	-1.55277800	3.13968000	-3.79060100
C	3.09041700	-0.44958800	0.93026500
C	4.46831500	-4.69778500	0.71279100
H	4.90794000	-5.14064900	1.60283700
C	3.59620800	-0.47753300	-0.35628400
H	3.84173200	-1.41601400	-0.84254200
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H	2.87511200	-3.13184600	-2.44171100
C	-0.16377700	2.75033600	-2.20211200
H	0.08946100	1.76271600	-2.56971900
C	0.51794500	-3.07604200	2.42272100
H	1.45212200	-2.55838800	2.58929900
C	3.88197600	4.10143700	-0.61526400
H	3.50267600	4.59307800	0.27349300
C	-0.39390400	-5.43326800	-2.92881800
H	-0.29689300	-6.51203600	-3.02141100
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C	4.95173200	4.66899200	-1.30143100
H	5.39039200	5.59281900	-0.93269100
C	4.86593800	2.89727200	-2.91834100

H	5.23552600	2.42464500	-3.82480900
C	-1.26366900	-3.33808500	-3.71054800
H	-1.83891500	-2.76095400	-4.42576900
C	4.57159100	-4.16973300	-1.62723200
H	5.09782500	-4.18584300	-2.57825300
C	1.92843000	2.86101900	1.48166600
C	-1.00692400	0.12310300	1.71840700
H	-1.38213500	-0.75217200	2.26959400
C	0.89745700	3.54880500	3.56476100
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H	-1.54635200	-4.11419900	-0.06782500
C	3.23653400	3.01594600	3.51827700
H	4.19381200	2.91265700	4.02271000
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C	-0.22074700	-3.51801600	3.51459100
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C	-1.16926300	-4.72361400	-3.85843600
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C	-4.21356800	-1.56267600	-4.09205900
C	-4.57947400	-2.18206000	-2.88955900
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C	-4.31441800	-1.58465300	-1.66089000
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C	-4.83500500	2.54160900	-0.96455600
H	-5.40456200	1.77779300	-1.48382200
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H	-1.32808400	1.22864200	3.30414900
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C	-3.89935600	-1.57626800	1.76365000
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C	-4.64222800	-2.16536000	2.78188300
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C	-1.88667900	-5.44101100	-4.97407400
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C	-6.54670200	-2.15380000	4.44805000
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H	-3.87565500	-1.83621700	-6.21126700
H	-4.41461900	-3.29858100	-5.36244400
H	-5.56299700	-2.00566300	-5.71580500
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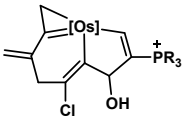

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Cl 0.12226000 -0.18781700 4.47954500
C 2.85615200 3.27776000 -1.20107600
C -0.55411600 0.07975200 -0.65163500
H -0.85559800 0.17842700 -1.68934800
C 0.07227000 3.26398800 -0.79929200
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C -2.04857900 4.68851900 -2.00455000
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H -5.63175300 0.64697100 1.67168300
C -0.65181700 -4.12184700 0.88317600

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C	-4.13336000	-0.84347700	1.22862600
C	0.28316200	-3.67630300	3.46518300
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C	-0.81731600	-4.66673600	-3.89192400
C	3.21346400	3.30041400	1.92381200
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H	-1.94609700	5.94713400	-0.26524100
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C	-3.48502700	-0.26501800	-4.07321400
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H	-2.76564100	-2.51376400	1.04370300
C	-5.89289600	-1.12778600	2.85829400
H	-6.76179600	-0.73259700	3.37738700
C	-5.26613800	4.32601500	0.12816200
C	-4.14202000	4.05220600	0.91550700
H	-3.76100900	4.81876100	1.58452900
C	-4.29279700	-2.89062800	2.50280000
H	-3.90306700	-3.87453500	2.74332200
C	-5.73863600	3.31850300	-0.72629800
H	-6.61475700	3.50519700	-1.34160900
C	-1.30202700	-4.69252600	1.97762700
H	-2.16716400	-5.32865000	1.80661600
C	-5.42319700	-2.40901300	3.17787600
C	2.54964200	-0.02070100	3.36289200
H	2.71892500	-0.70454400	4.20202300
H	2.75900500	0.98657200	3.74966000
C	4.75057700	-0.83093100	2.46526100
H	5.42683500	-1.00994100	1.63643800
H	5.09195500	-1.10222400	3.46110500
C	5.62009200	5.55560600	-3.64344900
H	6.57370100	5.68550900	-3.11565700
H	5.83321700	5.05357200	-4.59175400
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C	-3.20071700	5.42401900	-2.63911600
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H	2.46116300	5.09058900	5.83876000
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C	-1.49075200	-5.38515900	-5.03381000
H	-2.48636800	-4.97462400	-5.23215000
H	-0.90582800	-5.28717300	-5.95745900
H	-1.59650500	-6.45551600	-4.82930700
C	7.03218800	-4.75556100	-0.89797000
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H	7.04611800	-5.62017000	-1.57322400
H	7.69999800	-4.00104500	-1.32871900
C	-1.61276800	-5.01932800	4.46931100
H	-2.30882000	-4.27055500	4.87095400
H	-2.19829400	-5.90268900	4.19520100
H	-0.93463200	-5.29802300	5.28204600
C	-4.40481100	-2.02350100	-5.64339000
H	-3.52083900	-2.54910800	-6.02865300
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H	-5.43648500	-3.96761300	4.67604000
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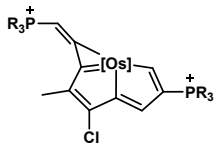

5-Me

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P	4.70977100	-0.15986900	-0.07678600
P	0.09133200	-2.38400400	-0.22581800
P	0.09708900	2.54490400	-0.44187900
C	-5.90636200	-0.82879200	-1.39025900
C	5.26101800	-1.63395400	0.83393200
C	-3.43140700	-3.46442800	-2.05704400
H	-4.05138800	-3.06320000	-2.85401700
C	-1.41342600	0.14856100	1.05762600
C	-5.93598300	-0.31277500	-2.69626400
H	-5.39282600	0.59611200	-2.94171000
C	-1.19650200	0.24868800	2.42565500
C	-2.12118200	2.87469400	-2.16383200
H	-1.86720500	1.89224500	-2.53831100
C	0.21663500	3.20662700	1.27324700
C	1.97088800	-0.05469900	-0.85074000
H	2.30842300	-0.20160300	-1.87130400
C	-3.53454800	4.85606400	-2.25783800
C	5.35168300	-1.57752200	2.23501000
H	5.21593800	-0.63665000	2.75864300
C	-1.45989100	-3.28251800	-0.65787300
C	1.55546000	3.24427900	-1.32899100
C	-3.21927200	0.08119700	-0.83160700
H	-3.16893100	0.05790600	-1.91613500
C	-2.26114600	-2.79456100	-1.69737900
H	-1.96283900	-1.90011200	-2.22975700
C	-1.34531900	3.45120900	-1.15043600
C	1.32918600	-3.25222300	-1.28892500
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H	-3.79560800	3.10746200	-3.48537500
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H	2.15465400	-3.40182700	-4.58759500
C	-4.89426900	-0.94334400	1.38611700
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H	1.64668700	1.63579700	-2.75987400
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H	-1.19375000	-4.90207300	0.75304600
C	5.45228400	-2.85743000	0.17920200
H	5.39278900	-2.92381100	-0.90015100
C	2.37929900	0.14372200	1.47152700
H	2.97922100	0.19348400	2.37543800
C	-6.66763200	-0.96684500	-3.68023700
H	-6.68100400	-0.56834900	-4.69080500
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C	4.88119300	2.55388900	0.37661100
H	3.92634900	2.60335600	-0.13469300
C	-4.22447100	-2.17531500	1.42635900
H	-3.68305400	-2.53269300	0.55928800
C	-0.60452000	-2.92217200	2.42971500
H	-1.62597600	-2.82316700	2.08648700
C	2.13246500	-4.30306500	-0.82706200
H	2.09668400	-4.61352600	0.20948300
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C	4.47748700	-1.26596600	-2.63803800
H	3.79376700	-1.98820200	-2.20888300
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H	5.85613400	-4.95068100	0.40243400
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H	3.60228700	-5.78564800	-1.32438500
C	-5.59745000	-0.49139800	2.50987100
H	-6.11760800	0.46054700	2.48488800
C	-2.09656800	0.11636100	-0.10679600
C	-0.87020300	3.74106200	3.37931600
H	-1.78733700	3.88673000	3.94397400
C	-0.94622000	3.39276900	2.03158600
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C	-4.66426500	2.72970500	0.38935500
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C	-4.26013000	-2.93909200	2.58852700
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H	-1.03948100	5.23927500	0.03235400
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C	-7.36670000	-2.62400600	-2.07694500
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C	2.10277800	4.48597300	-0.97012000
H	1.66166000	5.06823400	-0.16847800
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H	4.26034900	-2.07110700	-4.60680000
C	-6.56303600	4.22187900	0.68929200
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H	-8.49897000	3.30669400	0.43066000
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C	-4.99614700	-3.33991900	4.97721700
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H	-4.13207300	-4.00813600	5.04297800
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H	6.23364700	0.51007500	-6.47520000
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H	5.01320800	-0.76650400	-6.65179000
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H	1.28800600	4.89026400	5.70497400
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H	5.32229800	4.21366100	-4.23200000
H	5.10387700	5.79829200	-3.46761000
C	-4.75298700	5.56866700	-2.78276000
H	-4.96567400	5.29328100	-3.82023000
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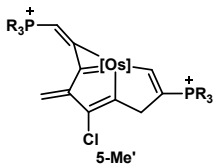

5-Me'

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P	0.13510500	-2.44954600	-0.23249800
P	-0.01320700	2.46090200	-0.49038200
C	-6.08136500	-0.93402800	-1.14579300
C	5.47675800	-1.24547500	1.00113800
C	-3.60306300	-3.71157400	-1.32171700
H	-4.29419000	-3.47037100	-2.12458500
C	-1.49970300	0.10684000	1.11946700
C	-6.10983100	-0.55711200	-2.49901100
H	-5.52801500	0.29192900	-2.84773400
C	-1.29618000	0.28299300	2.53456900
C	-2.38192000	2.71729300	-2.01217800
H	-2.14794800	1.72738700	-2.37837400
C	0.32930800	3.20300800	1.15326500
C	1.94076700	-0.08551000	-0.76161200
H	2.26957500	-0.19039400	-1.79088300
C	-3.77126900	4.71556300	-2.10852400
C	5.46842100	-1.02302900	2.38930200
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C	-1.48163600	-3.33361700	-0.20910300
C	1.28995300	3.13001200	-1.60662700
C	-3.34013000	-0.12580200	-0.71911600
H	-3.30824300	-0.22814600	-1.80016600
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C	-1.54338000	3.32052800	-1.06405900
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C	-3.48085600	3.40708500	-2.51542100
H	-4.11739100	2.92578900	-3.25441100
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C	1.83606200	-3.56641600	-3.85656500
H	2.07665500	-3.10087500	-4.80835300
C	-5.00336800	-0.84027200	1.62064600
C	3.11840400	-3.60655900	2.35142200
H	4.15493400	-3.91486900	2.26943700
C	1.78757200	2.37724400	-2.67648300
H	1.37470800	1.39965400	-2.88589300
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H	-1.12143600	-4.58177200	1.52012800
C	6.12970300	-2.37288100	0.49032100
H	6.16301800	-2.55228100	-0.57831500
C	-6.88927900	-1.27543700	-3.39812600
H	-6.90459200	-0.98349100	-4.44436400
C	1.04715000	-2.96843600	1.26689000
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H	0.72707900	-2.91708300	4.65576200
C	2.38720300	-3.36529500	1.19019900
H	2.86382400	-3.49485200	0.22573300
C	5.33936700	1.59004400	0.27900200
C	6.10404800	-1.91756900	3.24142400
H	6.09411700	-1.73238100	4.31171300
C	0.14703600	0.29451800	2.72717100
C	2.86641700	-0.03546100	0.21848900
C	-5.49633100	1.66947600	0.17389500
C	2.54121600	-3.44603300	3.61563400
C	1.32914900	-2.77082200	-2.82590700
H	1.17044800	-1.71654100	-2.99653900

C	0.89048700	0.15592000	1.61223700
C	-3.95736500	-4.68284300	-0.37630700
C	2.79091300	2.89697200	-3.49396100
H	3.18307900	2.28788700	-4.30382400
C	-6.84153200	-2.02445100	-0.70910000
H	-6.81638100	-2.32751900	0.33201900
C	6.41398300	4.15528800	0.71163900
C	4.67425700	2.72326600	-0.21152100
H	3.75406300	2.61693200	-0.77474500
C	-4.20782800	-1.96955700	1.85465800
H	-3.56568200	-2.35603800	1.07592600
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H	-0.57199500	-2.48191400	2.61711400
C	1.14692400	-4.73710500	-1.43735400
H	0.86079900	-5.21230400	-0.50443600
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H	4.68691000	4.85623200	-0.37551200
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H	1.81000200	-6.57962900	-2.30605200
C	-5.82490500	-0.33524200	2.63981100
H	-6.43763300	0.54338900	2.46588600
C	-2.20200900	-0.01265800	-0.02755400
C	-0.46332300	3.80620100	3.36459500
H	-1.29284000	3.95902300	4.04991700
C	-0.72239800	3.41263300	2.05544400
H	-1.74793000	3.26794600	1.73492700
C	6.75877400	-3.05560500	2.74334800
C	-4.62268800	2.54821000	0.83476000
H	-3.66285900	2.19494600	1.19683500
C	-4.23120400	-2.57979100	3.10428100
H	-3.60606100	-3.45090400	3.27668300
C	2.02679500	-4.94064800	-3.69518600
C	-3.03708300	-4.98502800	0.63804600
H	-3.27922400	-5.75513700	1.36610600
C	-2.91442200	5.31779200	-1.17909300
H	-3.10407300	6.33980500	-0.86134000
C	-1.81516800	4.63629300	-0.66047700
H	-1.17240200	5.13620000	0.05547900
C	5.71435200	0.45871700	-2.62163200
H	6.07371400	1.39257600	-2.20536000
C	-7.62151100	-2.73115700	-1.62218800
H	-8.20939000	-3.57685100	-1.27757800
C	3.29911800	4.18480700	-3.29085700
C	1.75594400	4.44214200	-1.42487700
H	1.36101900	5.05770700	-0.62391100
C	2.74003500	4.95863300	-2.26199300
H	3.08660600	5.97806500	-2.11135400
C	1.64208800	3.39999200	1.59784300
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C	6.55313900	1.73784500	0.96456500
H	7.08876100	0.86830600	1.32823000
C	-5.83363900	-0.95664400	3.88538400
H	-6.46389800	-0.55860500	4.67557800
C	1.89298700	3.79260900	2.90915200
H	2.92047600	3.94151300	3.23104900
C	5.97839900	0.14798200	-3.95282800
H	6.54292900	0.84925900	-4.56082100
C	0.84805000	3.99115600	3.82036900
C	7.07653000	3.01034300	1.17714000
H	8.01761100	3.11638800	1.70939200
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C	-6.72504000	2.13191500	-0.30549300
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C	5.53863000	-1.05685100	-4.51783700
C	-4.98481300	3.87437200	1.01231900
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H	4.43917600	-2.87158400	-4.13032500
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C	-7.07202400	3.47181800	-0.12481300
H	-8.02628700	3.83015800	-0.49993800
C	2.39116000	0.09011100	1.63976700
H	2.79948900	0.98245000	2.13550900
H	2.70895400	-0.76578100	2.25006900
C	-2.28713800	0.42063600	3.44413800
H	-3.32804900	0.38484300	3.15402800
H	-2.05243400	0.57522100	4.49206100
C	7.46332100	-4.00578800	3.67617800
H	6.88840900	-4.16318500	4.59479200
H	7.63540900	-4.97776000	3.20585200
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H	6.67276900	5.88614800	1.96726500

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H 6.60948000 6.25627100 0.24077600
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H 5.37627000 4.67081900 -3.58535100
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H 2.07513800 4.87423900 5.36773700
H 0.33187600 4.96667400 5.68132800
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H -5.19007400 -2.03660000 6.29512500
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H -5.80721100 6.46029100 0.27814800
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H -8.78566400 -4.11815900 -3.57714400
H -9.45063300 -2.58429600 -4.14972700
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H 1.83984200 -6.54805900 -5.12343000
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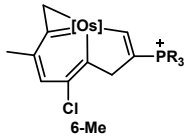

6-Me

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Cl 0.06164200 -0.39173500 -4.33448900
P -1.95827400 -2.09505100 0.32294100
P -0.87770400 2.66667900 0.12792100
P 3.17607800 -0.55002900 0.18357200
C -3.06768100 0.54944000 -1.10568200
C -2.60986400 4.66005000 -1.02313600
H -1.97145200 4.68221200 -1.89804400
C -2.31365800 3.82126600 0.05323000
C -3.62730600 0.73476900 0.14409900
H -4.23387600 -0.04871500 0.59076000
H -3.83475300 1.73450000 0.51347800
C 0.05680700 3.46772800 1.51190500
C -3.57882300 -2.67030900 1.00552400
C -0.50265300 -0.02687200 -1.64569100
C -3.13613400 3.85903900 1.19386800
H -2.90519900 3.22610600 2.04701500
C -4.23699000 4.70675900 1.23675300
H -4.86071700 4.72528800 2.12694800
C 0.51145400 -0.00131900 0.76120400
H 0.79372900 0.02874400 1.80975600
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C -4.16700000 -3.85945500 0.54772900
H -3.72076600 -4.41330500 -0.27038800
C -4.55315500 5.54178700 0.15352600
C -5.32949500 -4.34486200 1.14040700
H -5.76985700 -5.26733200 0.77034800
C -3.02538400 -2.76917400 -2.18942900
H -3.97177300 -2.41846300 -1.79262400
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H 1.25697900 -1.17994300 -2.10060200
H 1.48181800 0.54925900 -2.19590400
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H 0.08526500 5.34666800 0.43855400
C -4.16569700 -2.00153800 2.08932100

H	-3.70003300	-1.10829800	2.48967200
C	1.03939700	3.56076500	3.72157300
H	1.26352300	3.06167600	4.66042800
C	-3.37557300	0.47502100	-2.43429200
C	-0.32852200	2.93144700	-2.62200800
H	-1.38529800	2.74071800	-2.76687500
C	0.19405200	3.02533400	-1.32261700
C	-0.77646100	-3.10554800	1.32246500
C	0.50746200	3.03701400	-3.72749200
H	0.08567500	2.95089900	-4.72481300
C	-5.33013200	-2.49781900	2.67248000
H	-5.76940300	-1.96465400	3.51178000
C	0.40640800	2.83722400	2.70582100
H	0.13965200	1.80423600	2.87287300
C	-1.03181000	-0.07634700	-2.93981900
C	1.57095000	3.21440900	-1.16398600
H	2.00161800	3.28290200	-0.17209200
C	-0.11021500	-2.53845000	2.41467900
H	-0.32195900	-1.51588800	2.69918700
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C	-0.68758200	-3.27702100	-1.91371300
H	0.20335800	-3.32944400	-1.30044500
C	-2.93918800	-3.13730700	-3.53228300
H	-3.82600100	-3.07766700	-4.15805200
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H	1.33046400	-2.82600200	3.97885100
C	-0.61038400	-3.64134000	-3.25288700
H	0.34091700	-3.97338400	-3.66031700
C	3.50361300	-0.34145800	1.95225600
C	1.05029900	-4.63451100	2.84327800
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H	3.28859300	1.99698500	4.40458800
C	4.21530200	-1.25153400	4.07539800
H	4.59132200	-2.08925700	4.65605800
C	5.07451500	1.50450500	-0.22023200
H	5.08355700	1.63634100	0.85601300
C	2.91916800	-4.58247200	-0.37131000
H	2.16536800	-5.34417900	-0.20178900
C	5.13067900	-3.93722000	-1.07494000
H	6.11214900	-4.19930500	-1.46053600
C	3.97085900	-0.02746700	4.70994500
C	4.30035800	0.34746300	-2.20070200
H	3.69821200	-0.42297200	-2.67124000
C	4.17260800	-4.94382400	-0.88453400
C	5.91664200	2.15318900	-2.41190900
C	5.11626300	1.15328500	-2.98563200
H	5.13243300	1.00717700	-4.06190200
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C	-4.79002900	0.68026100	-2.93035400
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H	4.81266300	-0.66279000	6.59850100
H	4.68876500	1.09641500	6.40978600
H	3.24179500	0.13920300	6.73095200
C	4.47625900	-6.37577000	-1.24320800
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H	5.53278100	-6.61327400	-1.08498600
H	3.87380500	-7.07240500	-0.65253700
C	6.77024700	3.04403200	-3.27729700
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H	-1.16296500	-3.04839200	-6.09705300
C	-7.21568400	-4.18145200	2.82160100
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H	-7.29234400	-5.27018000	2.73844200
H	-7.28549100	-3.91220300	3.88017100
C	2.79160000	3.27255600	-4.78192100
H	2.40095000	3.95507700	-5.54455000
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C	2.04059300	5.68820400	4.66684400
H	2.97859900	6.13557000	4.31675500
H	1.40554500	6.51003000	5.01851500
H	2.26887100	5.05139100	5.52675500
C	-5.75957400	6.44492300	0.20643000
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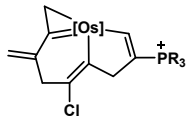

6-Me'

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P	-0.99956500	2.60980400	0.12000200
P	3.16052200	-0.40527700	0.21179000
C	-3.04388100	0.41896900	-1.09277300
C	-2.79294100	4.55304200	-1.02643100
H	-2.12876600	4.63661800	-1.87826200
C	-2.48876200	3.69363300	0.03134400
C	-3.71414200	0.52914900	0.12605300
H	-4.30016800	-0.30749900	0.49887600
H	-4.03049600	1.50373800	0.48746600
C	-0.13440700	3.44103400	1.53154400
C	-3.44399700	-2.87991900	0.87376100
C	-0.49078000	-0.02847500	-1.74139700
C	-3.34524400	3.65389100	1.14667300
H	-3.10729300	3.00558800	1.98631100
C	-4.48643500	4.44700300	1.18222400
H	-5.13603100	4.40676000	2.05307400
C	0.46821300	0.01676900	0.74345500
H	0.74247900	0.06309300	1.79314200
C	-1.64320900	-2.93290800	-1.41510400
C	-3.98128000	-4.06681900	0.35375800
H	-3.49986200	-4.57053500	-0.47659900
C	-4.81052000	5.30216000	0.11695400
C	-5.13672400	-4.61731300	0.90323600
H	-5.53714600	-5.53798200	0.48626500
C	-2.72395000	-2.90582300	-2.30523400
H	-3.70310700	-2.58603900	-1.96378800
C	-5.78705900	-4.01089800	1.98539400
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H	1.32656200	-1.14790700	-2.09308500
H	1.51555600	0.58825700	-2.19462000
C	-3.94370900	5.34394700	-0.97870100
H	-4.16222900	6.01311300	-1.80692500
C	0.13270300	4.81550800	1.38104800
H	-0.12508900	5.31819000	0.45414600
C	-4.07386600	-2.27843600	1.97368200
H	-3.64802500	-1.38559800	2.41788500
C	0.75081600	3.57201200	3.78001400
H	0.95344700	3.08195500	4.72855300
C	-3.39601400	0.45101300	-2.47437700
C	-0.40672600	2.95605100	-2.61356300
H	-1.45522400	2.74687700	-2.78810400
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C	-0.64443400	-3.13953700	1.32294700
C	0.44580300	3.12094500	-3.69841900
H	0.04805000	3.04490200	-4.70625600
C	-5.22945000	-2.83969100	2.51294100
H	-5.70219700	-2.35919800	3.36582900
C	0.18632700	2.82514700	2.74087600
H	-0.05147500	1.78372200	2.89986700
C	-0.97875500	-0.03478800	-2.98516700
C	1.44998400	3.26602400	-1.10987000
H	1.85689100	3.32875700	-0.10751900
C	-0.04212900	-2.53363100	2.43117400
H	-0.30535400	-1.51800100	2.69616600
C	1.03349600	4.93127500	3.63545300

C	-0.39199500	-3.33929300	-1.89392800
H	0.46470200	-3.35993000	-1.23304400
C	-2.55180400	-3.27704600	-3.63689800
H	-3.40454000	-3.25442100	-4.31108700
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C	0.50697900	-5.20238200	1.87129200
H	0.69500500	-6.25303500	1.66275300
C	3.11544100	1.06381600	2.58650500
H	2.67996400	1.86877400	2.00405400
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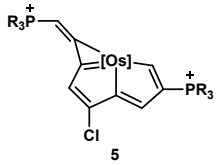

5

[Os] = OsCl(PR$_3$)$_2$, R = *p*-tolyl

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